Full wwPDB EM Validation Report ⓘ

Dec 9, 2022 – 04:01 AM JST

PDB ID	:	5Y6P
EMDB ID	:	EMD-6769
Title	:	Structure of the phycobilisome from the red alga Griffithsia pacifica
Authors	:	Zhang, J.; Ma, J.F.; Liu, D.S.; Sun, S.; Sui, S.F.
Deposited on	:	2017-08-13
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

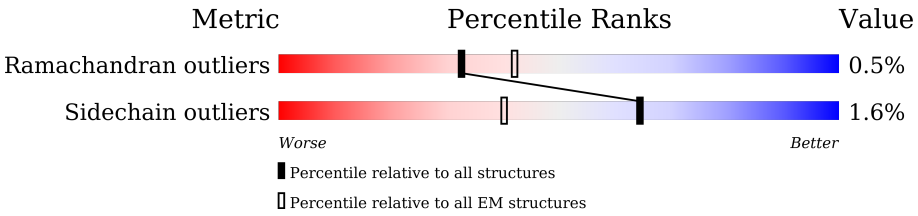
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	260	81% · 16%
1	B1	260	82% · 15%
2	C1	192	6% 74% 6% 20%
2	D1	192	6% 75% · · 20%
3	E1	307	79% 5% 16%
3	F1	307	79% 6% 16%
4	G1	161	84% 16% ·
4	I1	161	96% · ·
4	K1	161	7% 94% · ··

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Mol	Chain	Length	Quality of chain
4	N1	161	88% 11%
4	P1	161	88% 11%
4	R1	161	96%
4	T1	161	93% 6%
4	X1	161	5% 96%
4	Z1	161	9% 95%
4	b1	161	84% 15%
4	d1	161	89% 9%
4	f1	161	89% 10%
4	i1	161	95%
4	k1	161	90% 9%
4	o1	161	95%
4	q1	161	89% 10%
4	s1	161	79% 20%
4	u1	161	95%
4	w1	161	89% 9%
4	y1	161	79% 20%
5	H1	161	94% 6%
5	J1	161	94% 6%
5	L1	161	94% 6%
5	M1	161	5% 93% 7%
5	O1	161	91% 9%
5	S1	161	91% 9%
5	U1	161	92% 8%
5	W1	161	89% 11%

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Mol	Chain	Length	Quality of chain
5	Y1	161	94% 6%
5	a1	161	93% 7%
5	c1	161	95% 5%
5	e1	161	91% 9%
5	h1	161	5% 93% 7%
5	j1	161	89% 11%
5	l1	161	94% 6%
5	n1	161	91% 9%
5	p1	161	92% 8%
5	r1	161	91% 9%
5	t1	161	93% 7%
5	v1	161	91% 9%
5	x1	161	92% 8%
5	z1	161	93% 7%
6	Q1	174	91% 8%
6	g1	174	90% 9%
7	V1	161	7% 96%
7	m1	161	7% 96%
8	a2	885	7% 84% 6% 9%
8	b2	885	6% 84% 6% 9%
9	c2	93	89% 9%
9	d2	93	91% 6%
10	A3	164	7% 98%
10	A4	164	7% 96%
10	A5	164	51% 93% 7%

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Mol	Chain	Length	Quality of chain
10	A6	164	92% 7%
10	A7	164	92% 7%
10	A9	164	12% 96%
10	B8	164	13% 98%
10	C3	164	17% 96%
10	C4	164	16% 96%
10	C5	164	54% 93% 6%
10	C6	164	91% 9%
10	C7	164	87% 12%
10	C9	164	10% 97%
10	D8	164	26% 96%
10	E2	164	98%
10	E3	164	35% 96%
10	E4	164	50% 94% 5%
10	E5	164	38% 94% 5%
10	E6	164	91% 9%
10	E7	164	90% 9%
10	E9	164	18% 94% 6%
10	F8	164	100% 99%
10	G2	164	13% 98%
10	G3	164	24% 96%
10	G4	164	56% 95% 5%
10	G5	164	55% 97%
10	G6	164	87% 12%
10	G7	164	5% 91% 8%

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Mol	Chain	Length	Quality of chain
10	G9	164	13% 98%
10	H8	164	100% 99%
10	I2	164	5% 95% 5%
10	I3	164	23% 98%
10	I4	164	38% 94% 5%
10	I5	164	41% 92% 8%
10	I6	164	5% 91% 7%
10	I7	164	93% 6%
10	I9	164	27% 96%
10	J8	164	100% 98%
10	K2	164	94% 6%
10	K3	164	34% 97%
10	K4	164	55% 96%
10	K5	164	100% 97%
10	K6	164	94% 5%
10	K7	164	86% 13%
10	K9	164	99% 99%
10	L8	164	100% 99%
10	M2	164	6% 99%
10	M3	164	26% 96%
10	M4	164	42% 91% 9%
10	M5	164	100% 97%
10	M6	164	95%
10	M7	164	90% 9%
10	M9	164	100% 99%

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Mol	Chain	Length	Quality of chain
10	N8	164	100% 99%
10	O2	164	9% 98%
10	O3	164	95% 98%
10	O4	164	100% 97%
10	O5	164	100% 97%
10	O6	164	92% 7%
10	O7	164	94% 5%
10	O9	164	100% 98%
10	P8	164	100% 99%
10	Q2	164	95% 5%
10	Q3	164	92% 97%
10	Q4	164	100% 97%
10	Q5	164	100% 97%
10	Q6	164	91% 8%
10	Q7	164	91% 8%
10	Q9	164	100% 99%
10	S2	164	8% 99%
10	S3	164	88% 97%
10	S4	164	100% 97%
10	S5	164	100% 97%
10	S6	164	92% 7%
10	S7	164	93% 6%
10	S9	164	100% 99%
10	U2	164	7% 97%
10	U3	164	95% 97%

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Mol	Chain	Length	Quality of chain
10	U4	164	100% 97%
10	U5	164	100% 96%
10	U6	164	5% 93% 6%
10	U7	164	93% 7%
10	U9	164	100% 99%
10	W2	164	95% 5%
10	W3	164	90% 97%
10	W4	164	100% 97%
10	W6	164	95%
10	W7	164	88% 11%
10	Y2	164	8% 99%
10	Y3	164	95% 97%
10	Y4	164	100% 96%
10	Y6	164	5% 96%
10	Y7	164	90% 9%
10	aA	164	9% 94% 6%
10	aC	164	5% 95% 5%
10	aE	164	93% 7%
10	aG	164	8% 96%
10	aI	164	5% 95% 5%
10	aK	164	83% 95% 5%
10	aM	164	87% 98%
10	aO	164	90% 97%
10	aQ	164	86% 96%
10	aS	164	90% 96%

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Mol	Chain	Length	Quality of chain
10	aU	164	87% 96%
10	am	164	5% 97%
10	ao	164	96%
10	aq	164	95% 5%
10	as	164	93% 7%
10	au	164	96%
10	aw	164	5% 97%
10	ay	164	24% 96%
10	bA	164	9% 95% 5%
10	bC	164	92% 7%
10	bE	164	90% 9%
10	bG	164	8% 95% 5%
10	bI	164	95% 5%
10	bK	164	83% 93% 5%
10	bM	164	86% 95% 5%
10	bO	164	90% 96%
10	bQ	164	87% 96%
10	bS	164	90% 96%
10	bU	164	87% 95% 5%
10	bm	164	91% 9%
10	bt	164	91% 9%
10	bu	164	95% 5%
10	bv	164	93% 7%
10	bw	164	93% 7%
10	bx	164	96%

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Mol	Chain	Length	Quality of chain
10	by	164	95% 5%
10	cA	164	21% 96%
10	cC	164	44% 95%
10	cD	164	59% 96%
10	cG	164	35% 98%
10	cI	164	16% 97%
10	cK	164	33% 96%
10	cS	164	35% 95% 5%
10	cT	164	34% 97%
10	cU	164	16% 98%
10	cV	164	49% 97%
10	cW	164	22% 95% 5%
10	cX	164	62% 98%
10	cZ	164	82% 96%
10	cm	164	89% 10%
10	ct	164	89% 10%
10	cu	164	93% 6%
10	cv	164	92% 7%
10	cw	164	93% 7%
10	cx	164	95% 5%
10	cy	164	94% 6%
10	dA	164	87% 13%
10	dC	164	5% 98%
10	dE	164	98%
10	dG	164	96%

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Mol	Chain	Length	Quality of chain
10	dI	164	98%
10	dJ	164	92% 8%
10	dM	164	98%
10	dO	164	93% 7%
10	dQ	164	5% 97%
10	dS	164	98%
10	dU	164	5% 96%
10	dW	164	93% 7%
10	dZ	164	9% 97%
10	da	164	88% 97%
10	db	164	92% 95% 5%
10	dc	164	86% 96%
10	de	164	86% 96%
10	dg	164	91% 97%
10	dk	164	91% 96%
10	dm	164	87% 98%
10	do	164	87% 97%
10	dq	164	87% 97%
10	ds	164	91% 97%
10	du	164	85% 98%
10	e2	164	35% 96%
10	e3	164	98%
10	eA	164	11% 96%
10	eC	164	7% 95%
10	eE	164	13% 96%

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Mol	Chain	Length	Quality of chain
10	eG	164	16% 92% 8%
10	eI	164	10% 96%
10	eK	164	11% 95% 5%
10	eM	164	12% 92% 8%
10	eO	164	14% 96%
10	eQ	164	6% 95%
10	eS	164	12% 95% 5%
10	eU	164	13% 96%
10	eW	164	12% 95% 5%
10	ea	164	16% 98%
10	ed	164	15% 97%
10	ef	164	9% 95% 5%
10	eh	164	7% 98%
10	ej	164	20% 96%
10	ek	164	8% 96%
10	em	164	15% 97%
10	eo	164	10% 97%
10	eq	164	7% 98%
10	es	164	20% 98%
10	eu	164	17% 98%
10	f6	164	12% 92% 7%
10	f7	164	5% 94% 5%
10	fb	164	97% 95%
10	fe	164	99% 95%
10	fg	164	98% 94% 5%

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Mol	Chain	Length	Quality of chain
10	fh	164	96% 95%
10	fk	164	98% 95%
10	fl	164	95% 94% 5%
10	fn	164	99% 93% 7%
10	fp	164	98% 95% 5%
10	fr	164	99% 95% 5%
10	ft	164	97% 96%
10	fv	164	97% 96%
10	fx	164	96% 96%
10	g2	164	23% 96%
10	g3	164	13% 98%
10	g6	164	5% 93% 7%
10	g7	164	11% 95% 5%
10	gb	164	95% 5%
10	gc	164	96%
10	gf	164	96%
10	gh	164	93% 6%
10	gj	164	95%
10	gl	164	96%
10	gm	164	90% 10%
10	go	164	95% 5%
10	gq	164	92% 8%
10	gs	164	95% 5%
10	gu	164	97%
10	gw	164	96%

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Mol	Chain	Length	Quality of chain
10	h6	164	5% 94% 5%
10	h7	164	8% 92% 7%
10	hA	164	96% 96%
10	hC	164	97% 96%
10	hE	164	97% 97%
10	hF	164	97% 97%
10	hI	164	99% 97%
10	hK	164	96% 97%
10	hM	164	98% 97%
10	hO	164	98% 97%
10	hQ	164	98% 97%
10	hS	164	98% 96%
10	hU	164	98% 97%
10	hW	164	97% 97%
10	i2	164	23% 98%
10	i3	164	94% 6%
10	i6	164	10% 97%
10	i7	164	7% 88% 12%
10	i8	164	98% 95%
10	iA	164	91% 8%
10	iB	164	93% 7%
10	j6	164	7% 89% 10%
10	j7	164	91% 8%
10	j8	164	93% 98%
10	k2	164	33% 97%

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Mol	Chain	Length	Quality of chain
10	k3	164	94% 6%
10	k6	164	24% 93% 6%
10	k7	164	21% 91% 8%
10	k8	164	88% 95% 5%
10	l8	164	96% 96%
10	la	164	16% 87% 12%
10	lc	164	51% 96%
10	le	164	32% 95% 5%
10	lg	164	29% 95% 5%
10	li	164	47% 92% 8%
10	lk	164	30% 96%
10	lm	164	49% 97%
10	lo	164	35% 96%
10	lq	164	18% 93% 7%
10	ls	164	30% 96%
10	lu	164	32% 96%
10	lw	164	46% 94% 6%
10	m2	164	26% 97%
10	m3	164	5% 96%
10	m4	164	10% 91% 8%
10	m5	164	9% 91% 9%
10	m6	164	28% 96%
10	m7	164	24% 92% 7%
10	m8	164	96% 95%
10	m9	164	5% 97%

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Mol	Chain	Length	Quality of chain
10	o2	164	95% 98%
10	o3	164	10% 98%
10	o4	164	32% 97%
10	o5	164	33% 96%
10	o6	164	21% 91% 8%
10	o7	164	25% 94% 5%
10	o9	164	96%
10	q2	164	92% 98%
10	q3	164	95% 5%
10	q4	164	16% 91% 8%
10	q5	164	16% 91% 8%
10	q6	164	32% 96%
10	q7	164	21% 93% 6%
10	q8	164	93% 93% 5%
10	q9	164	95% 5%
10	r8	164	96% 94% 5%
10	s2	164	87% 98%
10	s3	164	9% 98%
10	s4	164	10% 91% 8%
10	s5	164	10% 92% 7%
10	s6	164	19% 93% 6%
10	s7	164	25% 92% 7%
10	s8	164	96% 95% 5%
10	s9	164	93% 7%
10	t8	164	96% 93% 7%

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Mol	Chain	Length	Quality of chain
10	u2	164	95% 98%
10	u3	164	7% 96%
10	u4	164	37% 93% 7%
10	u5	164	38% 93% 7%
10	u6	164	26% 94% 5%
10	u7	164	16% 95% 5%
10	u8	164	87% 95% 5%
10	u9	164	95% 5%
10	v8	164	13% 96%
10	w2	164	90% 98%
10	w3	164	95% 5%
10	w4	164	20% 95% 5%
10	w5	164	20% 95% 5%
10	w6	164	96% 97%
10	w7	164	92% 95% 5%
10	w9	164	97%
10	x8	164	11% 98%
10	y2	164	95% 98%
10	y3	164	6% 99%
10	y4	164	29% 92% 8%
10	y5	164	29% 91% 9%
10	y9	164	25% 96%
10	z8	164	20% 95% 5%
11	A8	177	20% 95% 5%
11	B3	177	7% 97%

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Mol	Chain	Length	Quality of chain
11	B4	177	7% 98%
11	B5	177	48% 95%
11	B6	177	94% 6%
11	B7	177	94% 6%
11	B9	177	10% 97%
11	C8	177	27% 98%
11	D3	177	24% 98%
11	D4	177	23% 97%
11	D5	177	34% 96%
11	D6	177	97%
11	D7	177	94% 6%
11	D9	177	19% 97%
11	E8	177	34% 96%
11	F2	177	7% 97%
11	F3	177	29% 98%
11	F4	177	49% 96%
11	F5	177	57% 98%
11	F6	177	92% 8%
11	F7	177	5% 97%
11	F9	177	20% 95% 5%
11	G8	177	100% 98%
11	H2	177	5% 97%
11	H3	177	16% 98%
11	H4	177	33% 95% 5%
11	H5	177	63% 97%

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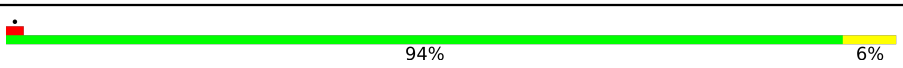
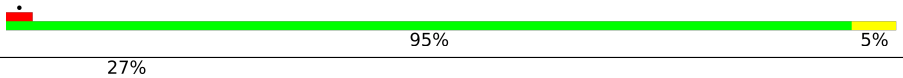
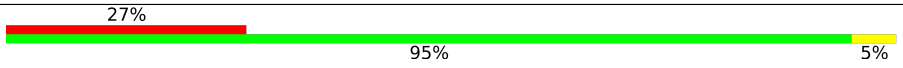
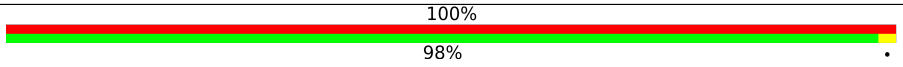
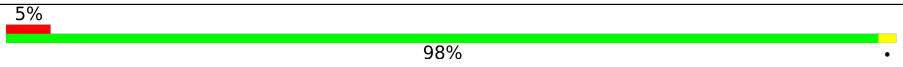
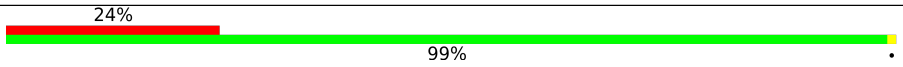
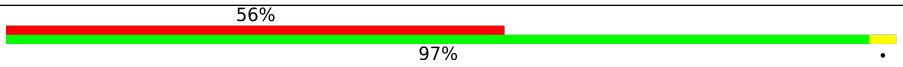
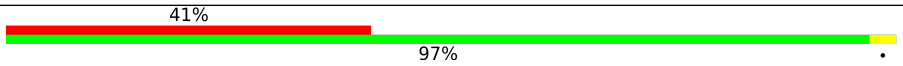
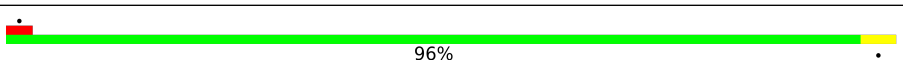
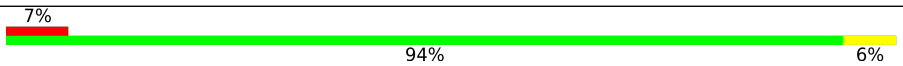
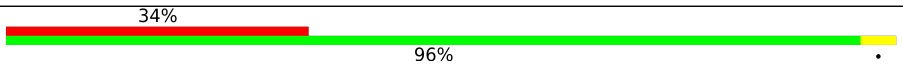
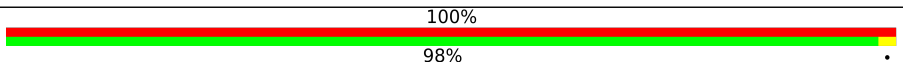
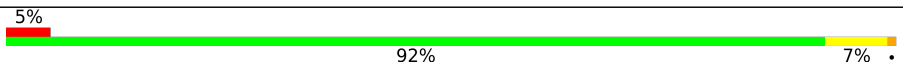
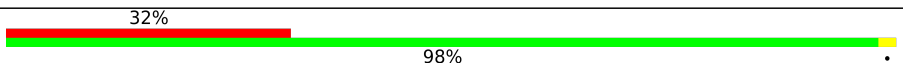
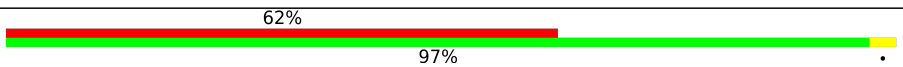
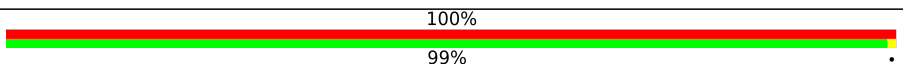
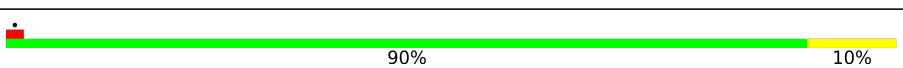
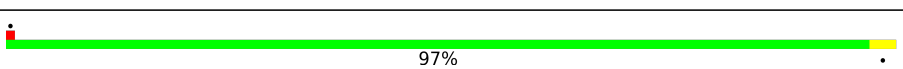
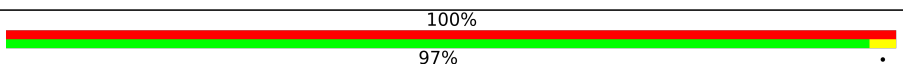
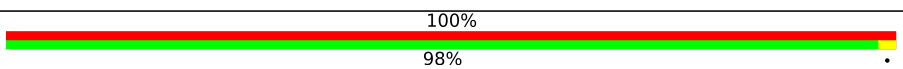
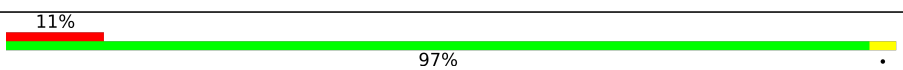
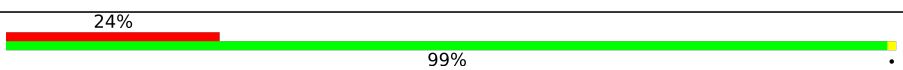
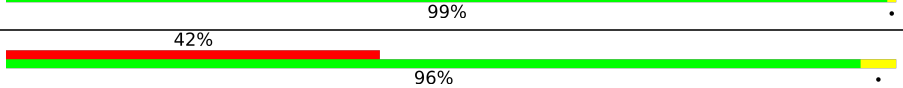
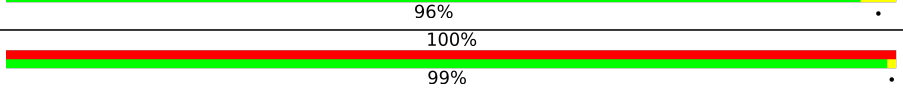
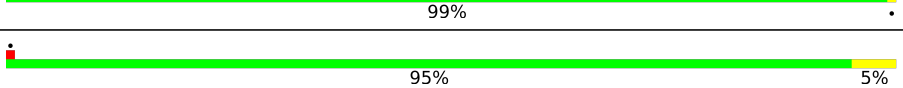
Mol	Chain	Length	Quality of chain
11	H6	177	
11	H7	177	
11	H9	177	
11	I8	177	
11	J2	177	
11	J3	177	
11	J4	177	
11	J5	177	
11	J6	177	
11	J7	177	
11	J9	177	
11	K8	177	
11	L2	177	
11	L3	177	
11	L4	177	
11	L5	177	
11	L6	177	
11	L7	177	
11	L9	177	
11	M8	177	
11	N2	177	
11	N3	177	
11	N4	177	
11	N5	177	
11	N6	177	

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Mol	Chain	Length	Quality of chain
11	N7	177	92% 8%
11	N9	177	100% 98%
11	O8	177	100% 98%
11	P2	177	11% 98%
11	P3	177	95% 99%
11	P4	177	100% 99%
11	P5	177	100% 99%
11	P6	177	93% 7%
11	P7	177	95% 5%
11	P9	177	100% 98%
11	Q8	177	100% 99%
11	R2	177	6% 99%
11	R3	177	89% 97%
11	R4	177	100% 99%
11	R5	177	100% 100%
11	R6	177	94% 6%
11	R7	177	92% 8%
11	R9	177	100% 97%
11	T2	177	5% 96%
11	T3	177	94% 98%
11	T4	177	100% 99%
11	T5	177	100% 99%
11	T6	177	93% 7%
11	T7	177	96%
11	T9	177	100% 98%

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Mol	Chain	Length	Quality of chain
11	V2	177	97%
11	V3	177	86% 99%
11	V4	177	100% 100%
11	V5	177	100% 99%
11	V6	177	97%
11	V7	177	93% 7%
11	V9	177	100% 98%
11	X2	177	5% 98%
11	X3	177	94% 99%
11	X4	177	100% 99%
11	X6	177	93% 7%
11	X7	177	90% 10%
11	Z2	177	9% 97%
11	Z3	177	95% 99%
11	Z4	177	100% 99%
11	Z6	177	10% 94% 6%
11	Z7	177	5% 94% 6%
11	a6	177	6% 94% 6%
11	a7	177	91% 9%
11	aB	177	95% 5%
11	aD	177	98%
11	aF	177	12% 98%
11	aH	177	7% 97%
11	aJ	177	8% 98%
11	aL	177	81% 99%

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Mol	Chain	Length	Quality of chain
11	aN	177	88% 99%
11	aP	177	85% 98%
11	aR	177	84% 98%
11	aT	177	86% 98%
11	aV	177	86% 99%
11	an	177	94% 6%
11	ap	177	93% 7%
11	ar	177	5% 94% 6%
11	at	177	93% 7%
11	av	177	93% 6%
11	ax	177	8% 95% 5%
11	az	177	15% 93% 7%
11	b6	177	5% 96%
11	b7	177	5% 96%
11	bB	177	94% 6%
11	bD	177	97%
11	bF	177	9% 98%
11	bH	177	7% 96%
11	bJ	177	7% 97%
11	bL	177	81% 97%
11	bN	177	89% 99%
11	bP	177	86% 98%
11	bR	177	85% 98%
11	bT	177	85% 98%
11	bV	177	86% 99%

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Mol	Chain	Length	Quality of chain
11	bn	177	97%
11	bo	177	96%
11	bp	177	98%
11	bq	177	97%
11	br	177	95% 5%
11	bs	177	95% 5%
11	bz	177	6% 98%
11	c6	177	92% 8%
11	c7	177	10% 94% 6%
11	cB	177	39% 99%
11	cE	177	41% 99%
11	cF	177	50% 98%
11	cH	177	12% 99%
11	cJ	177	23% 99%
11	cL	177	28% 97%
11	cM	177	27% 99%
11	cN	177	14% 99%
11	cO	177	40% 99%
11	cP	177	44% 99%
11	cQ	177	53% 99%
11	cR	177	28% 97%
11	cY	177	90% 99%
11	cn	177	95% 5%
11	co	177	94% 6%
11	cp	177	97%

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Mol	Chain	Length	Quality of chain
11	cq	177	95% 5%
11	cr	177	95%
11	cs	177	92% 8%
11	cz	177	97%
11	d6	177	7% 97%
11	d7	177	6% 96%
11	dB	177	98%
11	dD	177	99%
11	dF	177	8% 99%
11	dH	177	98%
11	dK	177	96%
11	dL	177	93% 6%
11	dN	177	95% 5%
11	dP	177	98%
11	dR	177	99%
11	dT	177	8% 99%
11	dV	177	97%
11	dX	177	93% 7%
11	dY	177	20% 98%
11	dd	177	88% 99%
11	df	177	90% 98%
11	dh	177	89% 99%
11	di	177	82% 99%
11	dj	177	77% 99%
11	dl	177	85% 99%

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Mol	Chain	Length	Quality of chain
11	dn	177	83% 99%
11	dp	177	90% 99%
11	dr	177	92% 99%
11	dt	177	78% 99%
11	dv	177	89% 99%
11	e6	177	8% 98%
11	e7	177	5% 98%
11	eB	177	11% 98%
11	eD	177	9% 99%
11	eF	177	15% 98%
11	eH	177	16% 98%
11	eJ	177	9% 96%
11	eL	177	17% 98%
11	eN	177	15% 99%
11	eP	177	11% 99%
11	eR	177	9% 98%
11	eT	177	10% 96%
11	eV	177	18% 98%
11	eX	177	16% 97%
11	eb	177	9% 96%
11	ec	177	15% 96%
11	ee	177	16% 94% 6%
11	eg	177	10% 99%
11	ei	177	13% 97%
11	el	177	10% 96%

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Mol	Chain	Length	Quality of chain
11	en	177	17% 97%
11	ep	177	12% 99%
11	er	177	13% 97%
11	et	177	18% 98%
11	ev	177	15% 96%
11	f2	177	30% 98%
11	f3	177	7% 97%
11	f8	177	93% 99%
11	fa	177	92% 99%
11	fc	177	99% 99%
11	ff	177	99% 99%
11	fi	177	100% 99%
11	fj	177	98% 99%
11	fm	177	97% 99%
11	fo	177	99% 99%
11	fq	177	99% 99%
11	fs	177	98% 98%
11	fu	177	97% 99%
11	fw	177	93% 99%
11	fy	177	98% 99%
11	g8	177	90% 98%
11	ga	177	97%
11	gd	177	96%
11	ge	177	99%
11	gg	177	98%

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Mol	Chain	Length	Quality of chain
11	gi	177	99%
11	gk	177	99%
11	gn	177	98%
11	gp	177	99%
11	gr	177	97%
11	gt	177	98%
11	gv	177	5% 98%
11	gx	177	5% 97%
11	h2	177	16% 97%
11	h3	177	5% 98%
11	h8	177	98% 98%
11	hB	177	96% 100%
11	hD	177	98% 100%
11	hG	177	98% 100%
11	hH	177	98% 100%
11	hJ	177	97% 100%
11	hL	177	98% 100%
11	hN	177	98% 100%
11	hP	177	98% 100%
11	hR	177	97% 100%
11	hT	177	98% 100%
11	hV	177	99% 100%
11	hX	177	96% 100%
11	iC	177	5% 95%
11	iD	177	93% 6%

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Mol	Chain	Length	Quality of chain
11	iE	177	6% 78% 5% 18%
11	iF	177	10% 80% 18%
11	iG	177	11% 80% 16%
11	iH	177	11% 81% 16%
11	j2	177	26% 98%
11	j3	177	99%
11	jI	177	20% 79% 19%
11	jJ	177	20% 79% 19%
11	jK	177	16% 80% 18%
11	jL	177	17% 81% 18%
11	jM	177	23% 81% 18%
11	jN	177	24% 81% 18%
11	jO	177	16% 77% 5% 18%
11	jP	177	18% 79% 18%
11	kQ	177	53% 79% 19%
11	kR	177	54% 79% 19%
11	kS	177	54% 80% 17%
11	kT	177	50% 79% 18%
11	kU	177	53% 80% 19%
11	kV	177	54% 80% 19%
11	kW	177	53% 81% 17%
11	kX	177	51% 81% 17%
11	l2	177	32% 99%
11	l3	177	5% 93% 7%
11	l6	177	28% 97%

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Mol	Chain	Length	Quality of chain
11	l7	177	22% 96%
11	lb	177	29% 99%
11	ld	177	51% 97%
11	lf	177	21% 98%
11	lh	177	31% 95% 5%
11	lj	177	51% 97%
11	ll	177	30% 98%
11	ln	177	52% 98%
11	lp	177	23% 99%
11	lr	177	28% 99%
11	lt	177	28% 99%
11	lv	177	33% 96%
11	lx	177	52% 98%
11	n2	177	25% 99%
11	n3	177	11% 97%
11	n4	177	15% 98%
11	n5	177	16% 98%
11	n6	177	33% 95% 5%
11	n7	177	27% 95% 5%
11	n8	177	94% 98%
11	n9	177	95% 5%
11	o8	177	96% 98%
11	p2	177	96% 99%
11	p3	177	12% 99%
11	p4	177	21% 99%

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Mol	Chain	Length	Quality of chain
11	p5	177	21% 99%
11	p6	177	23% 97%
11	p7	177	32% 95% 5%
11	p8	177	92% 99%
11	p9	177	92% 8%
11	r2	177	90% 98%
11	r3	177	6% 97%
11	r4	177	8% 97%
11	r5	177	8% 97%
11	r6	177	11% 94% 6%
11	r7	177	23% 94% 5%
11	r9	177	5% 94% 6%
11	t2	177	93% 99%
11	t3	177	7% 99%
11	t4	177	34% 96%
11	t5	177	33% 95% 5%
11	t6	177	24% 94% 6%
11	t7	177	16% 98%
11	t9	177	94% 6%
11	v2	177	87% 98%
11	v3	177	97%
11	v4	177	35% 95% 5%
11	v5	177	34% 94% 6%
11	v6	177	22% 98%
11	v7	177	11% 94% 6%

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Mol	Chain	Length	Quality of chain
11	v9	177	95% 5%
11	w8	177	12% 97%
11	x2	177	95% 98%
11	x3	177	5% 99%
11	x4	177	20% 93% 7%
11	x5	177	20% 95% 5%
11	x6	177	95% 98%
11	x7	177	94% 99%
11	x9	177	8% 95%
11	y6	177	95% 98%
11	y7	177	93% 95% 5%
11	y8	177	19% 98%
11	z2	177	93% 98%
11	z3	177	8% 97%
11	z4	177	37% 96%
11	z5	177	37% 97%
11	z6	177	92% 97%
11	z7	177	93% 98%
11	z9	177	17% 94% 6%
12	34	318	44% 79% 8% 13%
12	A2	318	79% 8% 13%
12	U8	318	14% 81% 6% 13%
12	Y5	318	44% 80% 7% 13%
12	Z9	318	15% 80% 7% 13%
12	a3	318	79% 8% 13%

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Mol	Chain	Length	Quality of chain
12	aY	318	82% 13%
12	b8	318	82% 5% 13%
12	b9	318	81% 6% 13%
12	bY	318	80% 7% 13%
12	dw	318	78% 83% 13%
12	dx	318	77% 84% 13%
12	ey	318	8% 82% 5% 13%
12	ez	318	9% 83% 13%
13	B2	477	5% 73% 5% 22%
13	b3	477	72% 7% 22%
14	44	285	86% 84% 14%
14	C2	285	19% 83% 14%
14	D2	285	77% 83% 16%
14	T8	285	86% 84% 14%
14	Y9	285	86% 84% 14%
14	Z5	285	86% 84% 14%
14	aZ	285	78% 84% 14%
14	bZ	285	78% 84% 14%
14	c3	285	19% 83% 14%
14	c8	285	82% 14%
14	c9	285	81% 5% 14%
14	d3	285	77% 83% 16%
14	d8	285	16% 80% 16%
14	d9	285	17% 80% 16%
14	e8	285	79% 81% 16%

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Mol	Chain	Length	Quality of chain
14	e9	285	79% 82% 16%
15	14	232	11% 94%
15	R8	232	7% 86% 11%
15	W5	232	9% 93% 5%
15	W9	232	7% 81% 16%
15	aW	232	91% 7%
15	bW	232	89% 9%
16	24	371	18% 83% 5% 11%
16	S8	371	82% 7% 11%
16	X5	371	15% 80% 9% 11%
16	X9	371	81% 8% 11%
16	aX	371	82% 7% 11%
16	bX	371	81% 8% 11%
17	V8	162	97%
17	X8	162	95%
17	Z8	162	98%
17	a4	162	19% 98%
17	a5	162	15% 98%
17	aa	162	97%
17	ac	162	95%
17	ae	162	98%
17	ag	162	96%
17	ai	162	98%
17	ak	162	93% 6%
17	b4	162	94% 6%

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Mol	Chain	Length	Quality of chain
17	b5	162	96%
17	ba	162	94% 5%
17	bc	162	94% 5%
17	be	162	97%
17	bg	162	97%
17	bi	162	96%
17	bk	162	96%
17	ca	162	93% 6%
17	cc	162	93% 6%
17	ce	162	96%
17	cg	162	96%
17	ci	162	94% 5%
17	ck	162	97%
17	d4	162	17% 98%
17	d5	162	17% 98%
17	f4	162	7% 96%
17	f5	162	9% 95%
17	g9	162	96%
17	i4	162	13% 98%
17	i5	162	12% 97%
17	i9	162	98%
17	k4	162	92% 7%
17	k5	162	91% 8%
17	k9	162	94% 5%
18	W8	172	96%

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Mol	Chain	Length	Quality of chain
18	Y8	172	97%
18	ab	172	95% 5%
18	ad	172	96%
18	af	172	97%
18	ah	172	95% 5%
18	aj	172	98%
18	al	172	96%
18	bb	172	93% 7%
18	bd	172	95%
18	bf	172	95%
18	bh	172	96%
18	bj	172	93% 7%
18	bl	172	96%
18	c4	172	8% 96%
18	c5	172	6% 94% 6%
18	cb	172	94% 6%
18	cd	172	96%
18	cf	172	96%
18	ch	172	94% 6%
18	cj	172	92% 8%
18	cl	172	94% 6%
18	e4	172	13% 95% 5%
18	e5	172	15% 94% 6%
18	f9	172	98%
18	g4	172	6% 94% 6%

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Mol	Chain	Length	Quality of chain
18	g5	172	5% 94% 6%
18	h4	172	19% 98%
18	h5	172	20% 99%
18	h9	172	97%
18	j4	172	8% 97%
18	j5	172	8% 95% 5%
18	j9	172	98%
18	l4	172	11% 95% 5%
18	l5	172	11% 93% 7%
18	l9	172	96%
19	a8	514	67% 30%
19	a9	514	68% 30%
20	dy	352	24% 81% 5% 14%
20	dz	352	23% 80% 5% 14%
21	ew	276	81% 16%
21	ex	276	80% 16%
21	fd	276	70% 68% 29%
21	fz	276	69% 68% 29%
22	eY	352	12% 84% 12%
22	eZ	352	13% 85% 12%
23	hY	350	63% 65% 35%
23	hZ	350	63% 65% 35%
23	ly	350	25% 70% 28%
23	lz	350	24% 69% 28%
24	gy	297	85% 12%

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Mol	Chain	Length	Quality of chain
24	gz	297	
25	ka	362	
25	kb	362	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	PVN	34	1004	X	-	-	-
29	PVN	44	303	X	-	-	-
29	PVN	A2	1004	X	-	-	-
29	PVN	C2	303	X	-	-	-
29	PVN	D2	303	X	-	-	-
29	PVN	T8	303	X	-	-	-
29	PVN	U8	1004	X	-	-	-
29	PVN	Y5	1004	X	-	-	-
29	PVN	Y9	303	X	-	-	-
29	PVN	Z5	304	X	-	-	-
29	PVN	Z9	1004	X	-	-	-
29	PVN	a3	1004	X	-	-	-
29	PVN	aY	403	X	-	-	-
29	PVN	aZ	303	X	-	-	-
29	PVN	b8	1004	X	-	-	-
29	PVN	b9	405	X	-	-	-
29	PVN	bY	1004	X	-	-	-
29	PVN	bZ	304	X	-	-	-
29	PVN	c3	303	X	-	-	-
29	PVN	c8	303	X	-	-	-
29	PVN	c9	303	X	-	-	-
29	PVN	d3	302	X	-	-	-
29	PVN	d8	303	X	-	-	-
29	PVN	d9	304	X	-	-	-
29	PVN	dw	404	X	-	-	-
29	PVN	dx	405	X	-	-	-
29	PVN	e8	303	X	-	-	-
29	PVN	e9	304	X	-	-	-
29	PVN	eY	403	X	-	-	-
29	PVN	eZ	402	X	-	-	-
29	PVN	ey	1004	X	-	-	-
29	PVN	ez	1004	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	PVN	hY	404	X	-	-	-
29	PVN	hZ	403	X	-	-	-
29	PVN	ly	404	X	-	-	-
29	PVN	lz	403	X	-	-	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 1234811 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called LRC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	219	Total	C	N	O	S	0	0
			1647	1047	276	318	6		
1	B1	220	Total	C	N	O	S	0	0
			1652	1050	277	319	6		

- Molecule 2 is a protein called LRC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	154	Total	C	N	O	S	0	0
			1171	729	207	232	3		
2	D1	153	Total	C	N	O	S	0	0
			1162	724	205	230	3		

- Molecule 3 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E1	259	Total	C	N	O	S	0	0
			2014	1272	335	401	6		
3	F1	259	Total	C	N	O	S	0	0
			2014	1272	335	401	6		

- Molecule 4 is a protein called alpha_APC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	I1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	K1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	N1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	P1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	R1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	T1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	X1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	Z1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	b1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	d1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	f1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	i1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	k1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	o1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	q1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	s1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	u1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	w1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		
4	y1	160	Total	C	N	O	S	0	0
			1221	764	207	242	8		

- Molecule 5 is a protein called beta_APC.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	J1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	L1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	M1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	O1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	S1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	U1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	W1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	Y1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	a1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	c1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	e1	160	Total	C	N	O	S	0	0
			1217	765	205	240	7		
5	h1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	j1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	l1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	n1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	p1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	r1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	t1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	v1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	x1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		
5	z1	161	Total	C	N	O	S	0	0
			1224	768	206	243	7		

- Molecule 6 is a protein called ApcF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q1	174	Total	C	N	O	S	0	0
			1398	889	232	272	5		
6	g1	174	Total	C	N	O	S	0	0
			1398	889	232	272	5		

- Molecule 7 is a protein called ApcD.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V1	160	Total	C	N	O	S	0	0
			1261	805	209	241	6		
7	m1	160	Total	C	N	O	S	0	0
			1261	805	209	241	6		

- Molecule 8 is a protein called LCM.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a2	801	Total	C	N	O	S	0	0
			6494	4160	1125	1192	17		
8	b2	801	Total	C	N	O	S	0	0
			6494	4160	1125	1192	17		

- Molecule 9 is a protein called LC.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c2	91	Total	C	N	O	S	0	0
			717	450	128	134	5		
9	d2	91	Total	C	N	O	S	0	0
			717	450	128	134	5		

- Molecule 10 is a protein called R-phycoerythrin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	g2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	i2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	k2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	o2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	y2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	E2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	I2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	K2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	W2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Y2	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	A3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	C3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	E3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	I3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	K3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	W3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Y3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	e3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	g3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	i3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	k3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	o3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	y3	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	A4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	C4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	E4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	I4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	K4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	W4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Y4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	o4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	y4	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	A5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	C5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	E5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	I5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	K5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	o5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	y5	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	i8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	j8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	k8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	l8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	A6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	C6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	E6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	I6	163	Total	C	N	O	S	0	0
			1239	770	216	247	6		
10	K6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	W6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Y6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	f6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	g6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	h6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	i6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	j6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	k6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	o6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	q6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w6	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	r8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	t8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	A7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	C7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	E7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G7	163	Total	C	N	O	S	0	0
			1239	770	216	247	6		
10	I7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	K7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	W7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	f7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	g7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	h7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	i7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	j7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	k7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	o7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w7	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	v8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	x8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	z8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	B8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	D8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	F8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	H8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	J8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	L8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	N8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	P8	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	m9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	o9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	q9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	s9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	u9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	w9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	y9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	A9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	C9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	E9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	G9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	I9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	K9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	M9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	O9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	Q9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	S9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	U9	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	am	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ao	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aq	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	as	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	au	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aw	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ay	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aC	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aE	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aG	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aI	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aK	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aM	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aO	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aQ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aS	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	aU	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bm	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bt	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bu	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	bv	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bw	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bx	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	by	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bC	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bE	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bG	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bI	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bK	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bM	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bO	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bQ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bS	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	bU	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cm	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ct	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cu	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cv	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cw	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cx	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	cy	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cC	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cD	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cG	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cI	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cK	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cS	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cT	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cU	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cV	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cW	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cX	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	cZ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	da	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	db	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dc	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	de	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dg	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dk	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dm	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	do	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dq	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ds	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	du	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dC	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dE	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dG	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dI	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dJ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dM	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dO	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dQ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dS	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dU	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dW	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	dZ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ea	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ed	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ef	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eh	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	ej	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ek	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	em	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eo	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eq	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	es	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eu	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eC	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eE	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eG	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eI	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eK	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eM	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eO	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eQ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eS	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eU	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	eW	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	la	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lc	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	le	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lg	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	li	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lk	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lm	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lo	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lq	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ls	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lu	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	lw	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fb	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fe	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fg	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fh	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fk	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fl	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fn	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fp	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fr	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	ft	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	fv	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	fx	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gb	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gc	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gf	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gh	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gj	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gl	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gm	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	go	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gq	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gs	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gu	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	gw	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hC	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hE	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hF	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hI	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hK	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hM	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hO	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	hQ	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hS	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hU	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	hW	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	iA	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		
10	iB	164	Total	C	N	O	S	0	0
			1246	773	217	250	6		

- Molecule 11 is a protein called R-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	h2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	j2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	l2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	t2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	x2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	J2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	T2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	V2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	X2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	Z2	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	B3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	D3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	J3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	T3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	V3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	X3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	f3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	h3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	j3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	l3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	t3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	x3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z3	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	B4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	D4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	J4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	T4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	V4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	X4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	Z4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	t4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	x4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z4	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	B5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	D5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	J5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	T5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	V5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	t5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	x5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z5	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	f8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	g8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	h8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	B6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	D6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	J6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	T6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	V6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	X6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	Z6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	a6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	b6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	c6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	d6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	e6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	l6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	t6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	x6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	y6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z6	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	o8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	B7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	D7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	J7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	T7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	V7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	X7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	Z7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	a7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	b7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	c7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	d7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	e7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	l7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	t7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	x7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	y7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z7	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	w8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	y8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	A8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	C8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	E8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	G8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	I8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	K8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	M8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	O8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	Q8	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	n9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	p9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	r9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	t9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	v9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	x9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	z9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	B9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	D9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	F9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	H9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	J9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	L9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	N9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	P9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	R9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	T9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	V9	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	an	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ap	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ar	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	at	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	av	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ax	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	az	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aB	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	aD	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aF	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aH	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aJ	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aL	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aN	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aP	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aR	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aT	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	aV	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bn	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bo	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bp	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bq	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	br	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bs	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bz	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bB	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bD	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bF	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bH	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	bJ	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bL	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bN	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bP	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bR	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bT	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	bV	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cn	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	co	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cp	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cq	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cr	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cs	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cz	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cB	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cE	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cF	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cH	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cJ	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cL	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cM	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	cN	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cO	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cP	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cQ	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cR	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	cY	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dd	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	df	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dh	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	di	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dj	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dl	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dn	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dp	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dr	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dt	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dv	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dB	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dD	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dF	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dH	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	dK	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dL	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dN	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dP	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dR	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dT	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dV	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dX	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	dY	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eb	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ec	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ee	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eg	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ei	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	el	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	en	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ep	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	er	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	et	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ev	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eB	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	eD	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eF	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eH	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eJ	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eL	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eN	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eP	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eR	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eT	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eV	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	eX	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lb	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ld	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lf	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lh	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lj	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ll	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ln	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lp	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lr	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lt	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	lv	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	lx	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fa	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fc	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ff	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fi	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fj	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fm	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fo	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fq	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fs	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fu	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fw	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	fy	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ga	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gd	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	ge	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gg	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gi	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gk	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gn	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	gp	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gr	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gt	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gv	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	gx	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hB	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hD	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hG	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hH	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hJ	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hL	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hN	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hP	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hR	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hT	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hV	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	hX	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	iC	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	iD	177	Total	C	N	O	S	0	0
			1286	793	223	258	12		
11	iE	146	Total	C	N	O	S	0	0
			1054	646	185	212	11		
11	iF	146	Total	C	N	O	S	0	0
			1054	646	185	212	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	iG	148	Total	C	N	O	S	0	0
			1073	661	187	214	11		
11	iH	148	Total	C	N	O	S	0	0
			1073	661	187	214	11		
11	jI	144	Total	C	N	O	S	0	0
			1040	639	183	207	11		
11	jJ	144	Total	C	N	O	S	0	0
			1040	639	183	207	11		
11	jK	145	Total	C	N	O	S	0	0
			1048	643	184	210	11		
11	jL	145	Total	C	N	O	S	0	0
			1048	643	184	210	11		
11	jM	145	Total	C	N	O	S	0	0
			1048	643	184	210	11		
11	jN	145	Total	C	N	O	S	0	0
			1048	643	184	210	11		
11	jO	145	Total	C	N	O	S	0	0
			1048	643	184	210	11		
11	jP	145	Total	C	N	O	S	0	0
			1048	643	184	210	11		
11	kQ	144	Total	C	N	O	S	0	0
			1040	639	183	207	11		
11	kR	144	Total	C	N	O	S	0	0
			1040	639	183	207	11		
11	kS	147	Total	C	N	O	S	0	0
			1062	652	186	213	11		
11	kT	146	Total	C	N	O	S	0	0
			1054	646	185	212	11		
11	kU	144	Total	C	N	O	S	0	0
			1040	639	183	207	11		
11	kV	144	Total	C	N	O	S	0	0
			1040	639	183	207	11		
11	kW	147	Total	C	N	O	S	0	0
			1062	652	186	213	11		
11	kX	147	Total	C	N	O	S	0	0
			1062	652	186	213	11		

- Molecule 12 is a protein called LR_gamma4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	a3	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	34	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	Y5	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	b8	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	b9	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	U8	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	Z9	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	aY	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	bY	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	dw	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	dx	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	ey	277	Total	C	N	O	S	0	0
			2107	1311	381	393	22		
12	ez	276	Total	C	N	O	S	0	0
			2095	1302	380	391	22		

- Molecule 13 is a protein called LRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B2	374	Total	C	N	O	S	0	0
			2934	1838	500	581	15		
13	b3	374	Total	C	N	O	S	0	0
			2934	1838	500	581	15		

- Molecule 14 is a protein called LR_gamma5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C2	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	D2	239	Total	C	N	O	S	0	0
			1830	1143	328	348	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
14	c3	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	d3	239	Total	C	N	O	S	0	0
			1830	1143	328	348	11		
14	44	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	Z5	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	c8	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	d8	239	Total	C	N	O	S	0	0
			1830	1143	328	348	11		
14	e8	239	Total	C	N	O	S	0	0
			1830	1143	328	348	11		
14	c9	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	d9	239	Total	C	N	O	S	0	0
			1830	1143	328	348	11		
14	e9	239	Total	C	N	O	S	0	0
			1830	1143	328	348	11		
14	T8	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	Y9	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	aZ	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		
14	bZ	245	Total	C	N	O	S	0	0
			1879	1175	337	356	11		

- Molecule 15 is a protein called LRC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	14	227	Total	C	N	O	S	0	0
			1879	1205	324	343	7		
15	W5	227	Total	C	N	O	S	0	0
			1879	1205	324	343	7		
15	R8	226	Total	C	N	O	S	0	0
			1870	1199	323	341	7		
15	W9	226	Total	C	N	O	S	0	0
			1870	1199	323	341	7		
15	aW	228	Total	C	N	O	S	0	0
			1887	1209	325	346	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
15	bW	228	Total	C	N	O	S	0	0
			1887	1209	325	346	7		

- Molecule 16 is a protein called LR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	24	331	Total	C	N	O	S	0	0
			2575	1628	449	485	13		
16	X5	331	Total	C	N	O	S	0	0
			2581	1631	452	485	13		
16	S8	331	Total	C	N	O	S	0	0
			2581	1631	452	485	13		
16	X9	331	Total	C	N	O	S	0	0
			2581	1631	452	485	13		
16	aX	331	Total	C	N	O	S	0	0
			2581	1631	452	485	13		
16	bX	331	Total	C	N	O	S	0	0
			2581	1631	452	485	13		

- Molecule 17 is a protein called alpha_PC.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a4	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	b4	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	d4	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	f4	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	i4	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	k4	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	a5	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	b5	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	d5	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	f5	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	i5	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	k5	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	V8	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	X8	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	Z8	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	g9	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	i9	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	k9	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	aa	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ac	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ae	162	Total	C	N	O	S	1	0
			1230	772	208	244	6		
17	ag	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ai	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ak	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ba	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	bc	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	be	162	Total	C	N	O	S	1	0
			1230	772	208	244	6		
17	bg	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	bi	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	bk	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ca	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	cc	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ce	162	Total	C	N	O	S	1	0
			1230	772	208	244	6		
17	cg	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ci	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		
17	ck	162	Total	C	N	O	S	0	0
			1226	770	208	242	6		

- Molecule 18 is a protein called beta_PC.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c4	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	e4	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	g4	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	h4	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	j4	172	Total	C	N	O	S	1	0
			1282	791	227	255	9		
18	l4	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	c5	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	e5	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	g5	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	h5	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	j5	172	Total	C	N	O	S	1	0
			1282	791	227	255	9		
18	l5	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	W8	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	Y8	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	f9	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	h9	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	j9	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	l9	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	ab	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	ad	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	af	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	ah	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	aj	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	al	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	bb	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	bd	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	bf	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	bh	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	bj	172	Total	C	N	O	S	1	0
			1282	791	227	255	9		
18	bl	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	cb	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	cd	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	cf	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	ch	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		
18	cj	172	Total	C	N	O	S	1	0
			1282	791	227	255	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	cl	172	Total	C	N	O	S	0	0
			1281	791	227	254	9		

- Molecule 19 is a protein called LRC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a8	362	Total	C	N	O	S	0	0
			2916	1855	508	541	12		
19	a9	362	Total	C	N	O	S	0	0
			2916	1855	508	541	12		

- Molecule 20 is a protein called LR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	dy	303	Total	C	N	O	S	0	0
			2377	1495	400	467	15		
20	dz	303	Total	C	N	O	S	0	0
			2377	1495	400	467	15		

- Molecule 21 is a protein called LR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	ew	233	Total	C	N	O	S	0	0
			1821	1153	314	344	10		
21	ex	233	Total	C	N	O	S	0	0
			1821	1153	314	344	10		
21	fd	196	Total	C	N	O	S	0	0
			1550	985	262	294	9		
21	fz	196	Total	C	N	O	S	0	0
			1550	985	262	294	9		

- Molecule 22 is a protein called LR_gamma7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	eY	309	Total	C	N	O	S	0	0
			2327	1441	427	440	19		
22	eZ	309	Total	C	N	O	S	0	0
			2327	1441	427	440	19		

- Molecule 23 is a protein called LR_gamma8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	ly	251	Total	C	N	O	S	0	0
			1928	1199	343	366	20		
23	lz	251	Total	C	N	O	S	0	0
			1928	1199	343	366	20		
23	hY	229	Total	C	N	O	S	0	0
			1748	1081	311	337	19		
23	hZ	229	Total	C	N	O	S	0	0
			1748	1081	311	337	19		

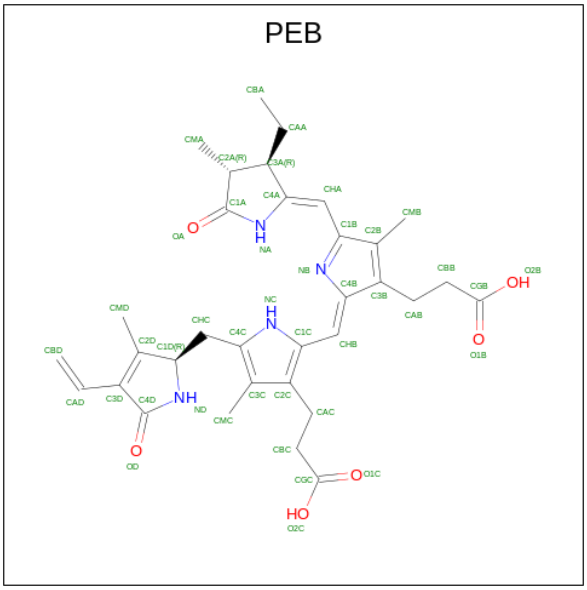
- Molecule 24 is a protein called LR_gamma6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	gy	260	Total	C	N	O	S	0	0
			2006	1264	356	371	15		
24	gz	260	Total	C	N	O	S	0	0
			2006	1264	356	371	15		

- Molecule 25 is a protein called LR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	ka	273	Total	C	N	O	S	0	0
			2038	1293	342	394	9		
25	kb	273	Total	C	N	O	S	0	0
			2038	1293	342	394	9		

- Molecule 26 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
26	A1	1	Total	C	N	O	0
			43	33	4	6	
26	B1	1	Total	C	N	O	0
			43	33	4	6	
26	e2	1	Total	C	N	O	0
			86	66	8	12	
26	e2	1	Total	C	N	O	0
			86	66	8	12	
26	f2	1	Total	C	N	O	0
			86	66	8	12	
26	f2	1	Total	C	N	O	0
			86	66	8	12	
26	g2	1	Total	C	N	O	0
			86	66	8	12	
26	g2	1	Total	C	N	O	0
			86	66	8	12	
26	h2	1	Total	C	N	O	0
			86	66	8	12	
26	h2	1	Total	C	N	O	0
			86	66	8	12	
26	i2	1	Total	C	N	O	0
			86	66	8	12	
26	i2	1	Total	C	N	O	0
			86	66	8	12	
26	j2	1	Total	C	N	O	0
			86	66	8	12	
26	j2	1	Total	C	N	O	0
			86	66	8	12	
26	k2	1	Total	C	N	O	0
			86	66	8	12	
26	k2	1	Total	C	N	O	0
			86	66	8	12	
26	l2	1	Total	C	N	O	0
			86	66	8	12	
26	l2	1	Total	C	N	O	0
			86	66	8	12	
26	m2	1	Total	C	N	O	0
			86	66	8	12	
26	m2	1	Total	C	N	O	0
			86	66	8	12	
26	n2	1	Total	C	N	O	0
			86	66	8	12	
26	n2	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	o2	1	Total	C	N	O	0
			86	66	8	12	
26	o2	1	Total	C	N	O	0
			86	66	8	12	
26	p2	1	Total	C	N	O	0
			86	66	8	12	
26	p2	1	Total	C	N	O	0
			86	66	8	12	
26	q2	1	Total	C	N	O	0
			86	66	8	12	
26	q2	1	Total	C	N	O	0
			86	66	8	12	
26	r2	1	Total	C	N	O	0
			86	66	8	12	
26	r2	1	Total	C	N	O	0
			86	66	8	12	
26	s2	1	Total	C	N	O	0
			86	66	8	12	
26	s2	1	Total	C	N	O	0
			86	66	8	12	
26	t2	1	Total	C	N	O	0
			86	66	8	12	
26	t2	1	Total	C	N	O	0
			86	66	8	12	
26	u2	1	Total	C	N	O	0
			86	66	8	12	
26	u2	1	Total	C	N	O	0
			86	66	8	12	
26	v2	1	Total	C	N	O	0
			86	66	8	12	
26	v2	1	Total	C	N	O	0
			86	66	8	12	
26	w2	1	Total	C	N	O	0
			129	99	12	18	
26	w2	1	Total	C	N	O	0
			129	99	12	18	
26	w2	1	Total	C	N	O	0
			129	99	12	18	
26	x2	1	Total	C	N	O	0
			43	33	4	6	
26	y2	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	y2	1	Total	C	N	O	0
			86	66	8	12	
26	z2	1	Total	C	N	O	0
			86	66	8	12	
26	z2	1	Total	C	N	O	0
			86	66	8	12	
26	A2	1	Total	C	N	O	0
			129	99	12	18	
26	A2	1	Total	C	N	O	0
			129	99	12	18	
26	A2	1	Total	C	N	O	0
			129	99	12	18	
26	B2	1	Total	C	N	O	0
			86	66	8	12	
26	B2	1	Total	C	N	O	0
			86	66	8	12	
26	C2	1	Total	C	N	O	0
			86	66	8	12	
26	C2	1	Total	C	N	O	0
			86	66	8	12	
26	D2	1	Total	C	N	O	0
			86	66	8	12	
26	D2	1	Total	C	N	O	0
			86	66	8	12	
26	E2	1	Total	C	N	O	0
			86	66	8	12	
26	E2	1	Total	C	N	O	0
			86	66	8	12	
26	F2	1	Total	C	N	O	0
			86	66	8	12	
26	F2	1	Total	C	N	O	0
			86	66	8	12	
26	G2	1	Total	C	N	O	0
			86	66	8	12	
26	G2	1	Total	C	N	O	0
			86	66	8	12	
26	H2	1	Total	C	N	O	0
			43	33	4	6	
26	I2	1	Total	C	N	O	0
			86	66	8	12	
26	I2	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	J2	1	Total	C	N	O	0
			43	33	4	6	
26	K2	1	Total	C	N	O	0
			86	66	8	12	
26	K2	1	Total	C	N	O	0
			86	66	8	12	
26	L2	1	Total	C	N	O	0
			86	66	8	12	
26	L2	1	Total	C	N	O	0
			86	66	8	12	
26	M2	1	Total	C	N	O	0
			86	66	8	12	
26	M2	1	Total	C	N	O	0
			86	66	8	12	
26	N2	1	Total	C	N	O	0
			86	66	8	12	
26	N2	1	Total	C	N	O	0
			86	66	8	12	
26	O2	1	Total	C	N	O	0
			86	66	8	12	
26	O2	1	Total	C	N	O	0
			86	66	8	12	
26	P2	1	Total	C	N	O	0
			86	66	8	12	
26	P2	1	Total	C	N	O	0
			86	66	8	12	
26	Q2	1	Total	C	N	O	0
			43	33	4	6	
26	R2	1	Total	C	N	O	0
			86	66	8	12	
26	R2	1	Total	C	N	O	0
			86	66	8	12	
26	S2	1	Total	C	N	O	0
			86	66	8	12	
26	S2	1	Total	C	N	O	0
			86	66	8	12	
26	T2	1	Total	C	N	O	0
			86	66	8	12	
26	T2	1	Total	C	N	O	0
			86	66	8	12	
26	U2	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	U2	1	Total	C	N	O	0
			86	66	8	12	
26	V2	1	Total	C	N	O	0
			86	66	8	12	
26	V2	1	Total	C	N	O	0
			86	66	8	12	
26	W2	1	Total	C	N	O	0
			86	66	8	12	
26	W2	1	Total	C	N	O	0
			86	66	8	12	
26	X2	1	Total	C	N	O	0
			86	66	8	12	
26	X2	1	Total	C	N	O	0
			86	66	8	12	
26	Y2	1	Total	C	N	O	0
			86	66	8	12	
26	Y2	1	Total	C	N	O	0
			86	66	8	12	
26	Z2	1	Total	C	N	O	0
			86	66	8	12	
26	Z2	1	Total	C	N	O	0
			86	66	8	12	
26	A3	1	Total	C	N	O	0
			86	66	8	12	
26	A3	1	Total	C	N	O	0
			86	66	8	12	
26	B3	1	Total	C	N	O	0
			86	66	8	12	
26	B3	1	Total	C	N	O	0
			86	66	8	12	
26	C3	1	Total	C	N	O	0
			86	66	8	12	
26	C3	1	Total	C	N	O	0
			86	66	8	12	
26	D3	1	Total	C	N	O	0
			86	66	8	12	
26	D3	1	Total	C	N	O	0
			86	66	8	12	
26	E3	1	Total	C	N	O	0
			86	66	8	12	
26	E3	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	F3	1	Total	C	N	O	0
			86	66	8	12	
26	F3	1	Total	C	N	O	0
			86	66	8	12	
26	G3	1	Total	C	N	O	0
			86	66	8	12	
26	G3	1	Total	C	N	O	0
			86	66	8	12	
26	H3	1	Total	C	N	O	0
			86	66	8	12	
26	H3	1	Total	C	N	O	0
			86	66	8	12	
26	I3	1	Total	C	N	O	0
			86	66	8	12	
26	I3	1	Total	C	N	O	0
			86	66	8	12	
26	J3	1	Total	C	N	O	0
			86	66	8	12	
26	J3	1	Total	C	N	O	0
			86	66	8	12	
26	K3	1	Total	C	N	O	0
			86	66	8	12	
26	K3	1	Total	C	N	O	0
			86	66	8	12	
26	L3	1	Total	C	N	O	0
			86	66	8	12	
26	L3	1	Total	C	N	O	0
			86	66	8	12	
26	M3	1	Total	C	N	O	0
			86	66	8	12	
26	M3	1	Total	C	N	O	0
			86	66	8	12	
26	N3	1	Total	C	N	O	0
			86	66	8	12	
26	N3	1	Total	C	N	O	0
			86	66	8	12	
26	O3	1	Total	C	N	O	0
			86	66	8	12	
26	O3	1	Total	C	N	O	0
			86	66	8	12	
26	P3	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	P3	1	Total	C	N	O	0
			86	66	8	12	
26	Q3	1	Total	C	N	O	0
			86	66	8	12	
26	Q3	1	Total	C	N	O	0
			86	66	8	12	
26	R3	1	Total	C	N	O	0
			86	66	8	12	
26	R3	1	Total	C	N	O	0
			86	66	8	12	
26	S3	1	Total	C	N	O	0
			129	99	12	18	
26	S3	1	Total	C	N	O	0
			129	99	12	18	
26	S3	1	Total	C	N	O	0
			129	99	12	18	
26	T3	1	Total	C	N	O	0
			86	66	8	12	
26	T3	1	Total	C	N	O	0
			86	66	8	12	
26	U3	1	Total	C	N	O	0
			86	66	8	12	
26	U3	1	Total	C	N	O	0
			86	66	8	12	
26	V3	1	Total	C	N	O	0
			86	66	8	12	
26	V3	1	Total	C	N	O	0
			86	66	8	12	
26	W3	1	Total	C	N	O	0
			129	99	12	18	
26	W3	1	Total	C	N	O	0
			129	99	12	18	
26	W3	1	Total	C	N	O	0
			129	99	12	18	
26	X3	1	Total	C	N	O	0
			43	33	4	6	
26	Y3	1	Total	C	N	O	0
			86	66	8	12	
26	Y3	1	Total	C	N	O	0
			86	66	8	12	
26	Z3	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	Z3	1	Total	C	N	O	0
			86	66	8	12	
26	a3	1	Total	C	N	O	0
			129	99	12	18	
26	a3	1	Total	C	N	O	0
			129	99	12	18	
26	a3	1	Total	C	N	O	0
			129	99	12	18	
26	b3	1	Total	C	N	O	0
			86	66	8	12	
26	b3	1	Total	C	N	O	0
			86	66	8	12	
26	c3	1	Total	C	N	O	0
			86	66	8	12	
26	c3	1	Total	C	N	O	0
			86	66	8	12	
26	d3	1	Total	C	N	O	0
			43	33	4	6	
26	e3	1	Total	C	N	O	0
			86	66	8	12	
26	e3	1	Total	C	N	O	0
			86	66	8	12	
26	f3	1	Total	C	N	O	0
			86	66	8	12	
26	f3	1	Total	C	N	O	0
			86	66	8	12	
26	g3	1	Total	C	N	O	0
			86	66	8	12	
26	g3	1	Total	C	N	O	0
			86	66	8	12	
26	h3	1	Total	C	N	O	0
			43	33	4	6	
26	i3	1	Total	C	N	O	0
			129	99	12	18	
26	i3	1	Total	C	N	O	0
			129	99	12	18	
26	i3	1	Total	C	N	O	0
			129	99	12	18	
26	j3	1	Total	C	N	O	0
			43	33	4	6	
26	k3	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	k3	1	Total	C	N	O	0
			86	66	8	12	
26	l3	1	Total	C	N	O	0
			43	33	4	6	
26	m3	1	Total	C	N	O	0
			86	66	8	12	
26	m3	1	Total	C	N	O	0
			86	66	8	12	
26	n3	1	Total	C	N	O	0
			86	66	8	12	
26	n3	1	Total	C	N	O	0
			86	66	8	12	
26	o3	1	Total	C	N	O	0
			86	66	8	12	
26	o3	1	Total	C	N	O	0
			86	66	8	12	
26	p3	1	Total	C	N	O	0
			86	66	8	12	
26	p3	1	Total	C	N	O	0
			86	66	8	12	
26	q3	1	Total	C	N	O	0
			43	33	4	6	
26	r3	1	Total	C	N	O	0
			86	66	8	12	
26	r3	1	Total	C	N	O	0
			86	66	8	12	
26	s3	1	Total	C	N	O	0
			86	66	8	12	
26	s3	1	Total	C	N	O	0
			86	66	8	12	
26	t3	1	Total	C	N	O	0
			86	66	8	12	
26	t3	1	Total	C	N	O	0
			86	66	8	12	
26	u3	1	Total	C	N	O	0
			86	66	8	12	
26	u3	1	Total	C	N	O	0
			86	66	8	12	
26	v3	1	Total	C	N	O	0
			86	66	8	12	
26	v3	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	w3	1	Total	C	N	O	0
			86	66	8	12	
26	w3	1	Total	C	N	O	0
			86	66	8	12	
26	x3	1	Total	C	N	O	0
			86	66	8	12	
26	x3	1	Total	C	N	O	0
			86	66	8	12	
26	y3	1	Total	C	N	O	0
			86	66	8	12	
26	y3	1	Total	C	N	O	0
			86	66	8	12	
26	z3	1	Total	C	N	O	0
			86	66	8	12	
26	z3	1	Total	C	N	O	0
			86	66	8	12	
26	A4	1	Total	C	N	O	0
			86	66	8	12	
26	A4	1	Total	C	N	O	0
			86	66	8	12	
26	B4	1	Total	C	N	O	0
			86	66	8	12	
26	B4	1	Total	C	N	O	0
			86	66	8	12	
26	C4	1	Total	C	N	O	0
			86	66	8	12	
26	C4	1	Total	C	N	O	0
			86	66	8	12	
26	D4	1	Total	C	N	O	0
			86	66	8	12	
26	D4	1	Total	C	N	O	0
			86	66	8	12	
26	E4	1	Total	C	N	O	0
			86	66	8	12	
26	E4	1	Total	C	N	O	0
			86	66	8	12	
26	F4	1	Total	C	N	O	0
			86	66	8	12	
26	F4	1	Total	C	N	O	0
			86	66	8	12	
26	G4	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	G4	1	Total	C	N	O	0
			86	66	8	12	
26	H4	1	Total	C	N	O	0
			86	66	8	12	
26	H4	1	Total	C	N	O	0
			86	66	8	12	
26	I4	1	Total	C	N	O	0
			86	66	8	12	
26	I4	1	Total	C	N	O	0
			86	66	8	12	
26	J4	1	Total	C	N	O	0
			86	66	8	12	
26	J4	1	Total	C	N	O	0
			86	66	8	12	
26	K4	1	Total	C	N	O	0
			86	66	8	12	
26	K4	1	Total	C	N	O	0
			86	66	8	12	
26	L4	1	Total	C	N	O	0
			86	66	8	12	
26	L4	1	Total	C	N	O	0
			86	66	8	12	
26	M4	1	Total	C	N	O	0
			86	66	8	12	
26	M4	1	Total	C	N	O	0
			86	66	8	12	
26	N4	1	Total	C	N	O	0
			86	66	8	12	
26	N4	1	Total	C	N	O	0
			86	66	8	12	
26	O4	1	Total	C	N	O	0
			86	66	8	12	
26	O4	1	Total	C	N	O	0
			86	66	8	12	
26	P4	1	Total	C	N	O	0
			86	66	8	12	
26	P4	1	Total	C	N	O	0
			86	66	8	12	
26	Q4	1	Total	C	N	O	0
			129	99	12	18	
26	Q4	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	Q4	1	Total	C	N	O	0
			129	99	12	18	
26	R4	1	Total	C	N	O	0
			86	66	8	12	
26	R4	1	Total	C	N	O	0
			86	66	8	12	
26	S4	1	Total	C	N	O	0
			86	66	8	12	
26	S4	1	Total	C	N	O	0
			86	66	8	12	
26	T4	1	Total	C	N	O	0
			43	33	4	6	
26	U4	1	Total	C	N	O	0
			86	66	8	12	
26	U4	1	Total	C	N	O	0
			86	66	8	12	
26	V4	1	Total	C	N	O	0
			86	66	8	12	
26	V4	1	Total	C	N	O	0
			86	66	8	12	
26	W4	1	Total	C	N	O	0
			86	66	8	12	
26	W4	1	Total	C	N	O	0
			86	66	8	12	
26	X4	1	Total	C	N	O	0
			86	66	8	12	
26	X4	1	Total	C	N	O	0
			86	66	8	12	
26	Y4	1	Total	C	N	O	0
			86	66	8	12	
26	Y4	1	Total	C	N	O	0
			86	66	8	12	
26	Z4	1	Total	C	N	O	0
			86	66	8	12	
26	Z4	1	Total	C	N	O	0
			86	66	8	12	
26	24	1	Total	C	N	O	0
			43	33	4	6	
26	34	1	Total	C	N	O	0
			172	132	16	24	
26	34	1	Total	C	N	O	0
			172	132	16	24	

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Mol	Chain	Residues	Atoms				AltConf
26	34	1	Total	C	N	O	0
			172	132	16	24	
26	34	1	Total	C	N	O	0
			172	132	16	24	
26	44	1	Total	C	N	O	0
			86	66	8	12	
26	44	1	Total	C	N	O	0
			86	66	8	12	
26	a4	1	Total	C	N	O	0
			43	33	4	6	
26	b4	1	Total	C	N	O	0
			43	33	4	6	
26	c4	1	Total	C	N	O	0
			86	66	8	12	
26	c4	1	Total	C	N	O	0
			86	66	8	12	
26	d4	1	Total	C	N	O	0
			43	33	4	6	
26	e4	1	Total	C	N	O	0
			86	66	8	12	
26	e4	1	Total	C	N	O	0
			86	66	8	12	
26	f4	1	Total	C	N	O	0
			43	33	4	6	
26	g4	1	Total	C	N	O	0
			86	66	8	12	
26	g4	1	Total	C	N	O	0
			86	66	8	12	
26	h4	1	Total	C	N	O	0
			86	66	8	12	
26	h4	1	Total	C	N	O	0
			86	66	8	12	
26	i4	1	Total	C	N	O	0
			43	33	4	6	
26	j4	1	Total	C	N	O	0
			86	66	8	12	
26	j4	1	Total	C	N	O	0
			86	66	8	12	
26	k4	1	Total	C	N	O	0
			43	33	4	6	
26	l4	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	l4	1	Total	C	N	O	0
			86	66	8	12	
26	m4	1	Total	C	N	O	0
			43	33	4	6	
26	n4	1	Total	C	N	O	0
			86	66	8	12	
26	n4	1	Total	C	N	O	0
			86	66	8	12	
26	o4	1	Total	C	N	O	0
			86	66	8	12	
26	o4	1	Total	C	N	O	0
			86	66	8	12	
26	p4	1	Total	C	N	O	0
			86	66	8	12	
26	p4	1	Total	C	N	O	0
			86	66	8	12	
26	q4	1	Total	C	N	O	0
			86	66	8	12	
26	q4	1	Total	C	N	O	0
			86	66	8	12	
26	r4	1	Total	C	N	O	0
			43	33	4	6	
26	s4	1	Total	C	N	O	0
			86	66	8	12	
26	s4	1	Total	C	N	O	0
			86	66	8	12	
26	t4	1	Total	C	N	O	0
			86	66	8	12	
26	t4	1	Total	C	N	O	0
			86	66	8	12	
26	u4	1	Total	C	N	O	0
			86	66	8	12	
26	u4	1	Total	C	N	O	0
			86	66	8	12	
26	v4	1	Total	C	N	O	0
			86	66	8	12	
26	v4	1	Total	C	N	O	0
			86	66	8	12	
26	w4	1	Total	C	N	O	0
			86	66	8	12	
26	w4	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	x4	1	Total	C	N	O	0
			43	33	4	6	
26	y4	1	Total	C	N	O	0
			86	66	8	12	
26	y4	1	Total	C	N	O	0
			86	66	8	12	
26	z4	1	Total	C	N	O	0
			86	66	8	12	
26	z4	1	Total	C	N	O	0
			86	66	8	12	
26	A5	1	Total	C	N	O	0
			129	99	12	18	
26	A5	1	Total	C	N	O	0
			129	99	12	18	
26	A5	1	Total	C	N	O	0
			129	99	12	18	
26	B5	1	Total	C	N	O	0
			86	66	8	12	
26	B5	1	Total	C	N	O	0
			86	66	8	12	
26	C5	1	Total	C	N	O	0
			86	66	8	12	
26	C5	1	Total	C	N	O	0
			86	66	8	12	
26	D5	1	Total	C	N	O	0
			86	66	8	12	
26	D5	1	Total	C	N	O	0
			86	66	8	12	
26	E5	1	Total	C	N	O	0
			86	66	8	12	
26	E5	1	Total	C	N	O	0
			86	66	8	12	
26	F5	1	Total	C	N	O	0
			86	66	8	12	
26	F5	1	Total	C	N	O	0
			86	66	8	12	
26	G5	1	Total	C	N	O	0
			86	66	8	12	
26	G5	1	Total	C	N	O	0
			86	66	8	12	
26	H5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
26	I5	1	Total	C	N	O	0
			86	66	8	12	
26	I5	1	Total	C	N	O	0
			86	66	8	12	
26	J5	1	Total	C	N	O	0
			86	66	8	12	
26	J5	1	Total	C	N	O	0
			86	66	8	12	
26	K5	1	Total	C	N	O	0
			86	66	8	12	
26	K5	1	Total	C	N	O	0
			86	66	8	12	
26	L5	1	Total	C	N	O	0
			86	66	8	12	
26	L5	1	Total	C	N	O	0
			86	66	8	12	
26	M5	1	Total	C	N	O	0
			86	66	8	12	
26	M5	1	Total	C	N	O	0
			86	66	8	12	
26	N5	1	Total	C	N	O	0
			86	66	8	12	
26	N5	1	Total	C	N	O	0
			86	66	8	12	
26	O5	1	Total	C	N	O	0
			86	66	8	12	
26	O5	1	Total	C	N	O	0
			86	66	8	12	
26	P5	1	Total	C	N	O	0
			43	33	4	6	
26	Q5	1	Total	C	N	O	0
			86	66	8	12	
26	Q5	1	Total	C	N	O	0
			86	66	8	12	
26	R5	1	Total	C	N	O	0
			86	66	8	12	
26	R5	1	Total	C	N	O	0
			86	66	8	12	
26	S5	1	Total	C	N	O	0
			129	99	12	18	
26	S5	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	S5	1	Total	C	N	O	0
			129	99	12	18	
26	T5	1	Total	C	N	O	0
			43	33	4	6	
26	U5	1	Total	C	N	O	0
			86	66	8	12	
26	U5	1	Total	C	N	O	0
			86	66	8	12	
26	V5	1	Total	C	N	O	0
			86	66	8	12	
26	V5	1	Total	C	N	O	0
			86	66	8	12	
26	W5	1	Total	C	N	O	0
			43	33	4	6	
26	X5	1	Total	C	N	O	0
			43	33	4	6	
26	Y5	1	Total	C	N	O	0
			129	99	12	18	
26	Y5	1	Total	C	N	O	0
			129	99	12	18	
26	Y5	1	Total	C	N	O	0
			129	99	12	18	
26	Z5	1	Total	C	N	O	0
			129	99	12	18	
26	Z5	1	Total	C	N	O	0
			129	99	12	18	
26	Z5	1	Total	C	N	O	0
			129	99	12	18	
26	a5	1	Total	C	N	O	0
			43	33	4	6	
26	b5	1	Total	C	N	O	0
			43	33	4	6	
26	c5	1	Total	C	N	O	0
			86	66	8	12	
26	c5	1	Total	C	N	O	0
			86	66	8	12	
26	d5	1	Total	C	N	O	0
			43	33	4	6	
26	e5	1	Total	C	N	O	0
			43	33	4	6	
26	f5	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
26	g5	1	Total	C	N	O	0
			86	66	8	12	
26	g5	1	Total	C	N	O	0
			86	66	8	12	
26	h5	1	Total	C	N	O	0
			86	66	8	12	
26	h5	1	Total	C	N	O	0
			86	66	8	12	
26	i5	1	Total	C	N	O	0
			43	33	4	6	
26	j5	1	Total	C	N	O	0
			86	66	8	12	
26	j5	1	Total	C	N	O	0
			86	66	8	12	
26	k5	1	Total	C	N	O	0
			43	33	4	6	
26	l5	1	Total	C	N	O	0
			86	66	8	12	
26	l5	1	Total	C	N	O	0
			86	66	8	12	
26	m5	1	Total	C	N	O	0
			129	99	12	18	
26	m5	1	Total	C	N	O	0
			129	99	12	18	
26	m5	1	Total	C	N	O	0
			129	99	12	18	
26	n5	1	Total	C	N	O	0
			86	66	8	12	
26	n5	1	Total	C	N	O	0
			86	66	8	12	
26	o5	1	Total	C	N	O	0
			86	66	8	12	
26	o5	1	Total	C	N	O	0
			86	66	8	12	
26	p5	1	Total	C	N	O	0
			43	33	4	6	
26	q5	1	Total	C	N	O	0
			86	66	8	12	
26	q5	1	Total	C	N	O	0
			86	66	8	12	
26	r5	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	r5	1	Total	C	N	O	0
			86	66	8	12	
26	s5	1	Total	C	N	O	0
			86	66	8	12	
26	s5	1	Total	C	N	O	0
			86	66	8	12	
26	t5	1	Total	C	N	O	0
			86	66	8	12	
26	t5	1	Total	C	N	O	0
			86	66	8	12	
26	u5	1	Total	C	N	O	0
			86	66	8	12	
26	u5	1	Total	C	N	O	0
			86	66	8	12	
26	v5	1	Total	C	N	O	0
			86	66	8	12	
26	v5	1	Total	C	N	O	0
			86	66	8	12	
26	w5	1	Total	C	N	O	0
			86	66	8	12	
26	w5	1	Total	C	N	O	0
			86	66	8	12	
26	x5	1	Total	C	N	O	0
			43	33	4	6	
26	y5	1	Total	C	N	O	0
			86	66	8	12	
26	y5	1	Total	C	N	O	0
			86	66	8	12	
26	z5	1	Total	C	N	O	0
			86	66	8	12	
26	z5	1	Total	C	N	O	0
			86	66	8	12	
26	f8	1	Total	C	N	O	0
			86	66	8	12	
26	f8	1	Total	C	N	O	0
			86	66	8	12	
26	g8	1	Total	C	N	O	0
			43	33	4	6	
26	h8	1	Total	C	N	O	0
			86	66	8	12	
26	h8	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	i8	1	Total	C	N	O	0
			43	33	4	6	
26	j8	1	Total	C	N	O	0
			86	66	8	12	
26	j8	1	Total	C	N	O	0
			86	66	8	12	
26	k8	1	Total	C	N	O	0
			129	99	12	18	
26	k8	1	Total	C	N	O	0
			129	99	12	18	
26	k8	1	Total	C	N	O	0
			129	99	12	18	
26	l8	1	Total	C	N	O	0
			86	66	8	12	
26	l8	1	Total	C	N	O	0
			86	66	8	12	
26	m8	1	Total	C	N	O	0
			86	66	8	12	
26	m8	1	Total	C	N	O	0
			86	66	8	12	
26	A6	1	Total	C	N	O	0
			86	66	8	12	
26	A6	1	Total	C	N	O	0
			86	66	8	12	
26	B6	1	Total	C	N	O	0
			86	66	8	12	
26	B6	1	Total	C	N	O	0
			86	66	8	12	
26	C6	1	Total	C	N	O	0
			86	66	8	12	
26	C6	1	Total	C	N	O	0
			86	66	8	12	
26	D6	1	Total	C	N	O	0
			43	33	4	6	
26	E6	1	Total	C	N	O	0
			86	66	8	12	
26	E6	1	Total	C	N	O	0
			86	66	8	12	
26	F6	1	Total	C	N	O	0
			86	66	8	12	
26	F6	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	G6	1	Total	C	N	O	0
			86	66	8	12	
26	G6	1	Total	C	N	O	0
			86	66	8	12	
26	H6	1	Total	C	N	O	0
			86	66	8	12	
26	H6	1	Total	C	N	O	0
			86	66	8	12	
26	I6	1	Total	C	N	O	0
			86	66	8	12	
26	I6	1	Total	C	N	O	0
			86	66	8	12	
26	J6	1	Total	C	N	O	0
			86	66	8	12	
26	J6	1	Total	C	N	O	0
			86	66	8	12	
26	K6	1	Total	C	N	O	0
			86	66	8	12	
26	K6	1	Total	C	N	O	0
			86	66	8	12	
26	L6	1	Total	C	N	O	0
			43	33	4	6	
26	M6	1	Total	C	N	O	0
			86	66	8	12	
26	M6	1	Total	C	N	O	0
			86	66	8	12	
26	N6	1	Total	C	N	O	0
			86	66	8	12	
26	N6	1	Total	C	N	O	0
			86	66	8	12	
26	O6	1	Total	C	N	O	0
			86	66	8	12	
26	O6	1	Total	C	N	O	0
			86	66	8	12	
26	P6	1	Total	C	N	O	0
			86	66	8	12	
26	P6	1	Total	C	N	O	0
			86	66	8	12	
26	Q6	1	Total	C	N	O	0
			86	66	8	12	
26	Q6	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	R6	1	Total	C	N	O	0
			86	66	8	12	
26	R6	1	Total	C	N	O	0
			86	66	8	12	
26	S6	1	Total	C	N	O	0
			86	66	8	12	
26	S6	1	Total	C	N	O	0
			86	66	8	12	
26	T6	1	Total	C	N	O	0
			86	66	8	12	
26	T6	1	Total	C	N	O	0
			86	66	8	12	
26	U6	1	Total	C	N	O	0
			86	66	8	12	
26	U6	1	Total	C	N	O	0
			86	66	8	12	
26	V6	1	Total	C	N	O	0
			86	66	8	12	
26	V6	1	Total	C	N	O	0
			86	66	8	12	
26	W6	1	Total	C	N	O	0
			86	66	8	12	
26	W6	1	Total	C	N	O	0
			86	66	8	12	
26	X6	1	Total	C	N	O	0
			86	66	8	12	
26	X6	1	Total	C	N	O	0
			86	66	8	12	
26	Y6	1	Total	C	N	O	0
			43	33	4	6	
26	Z6	1	Total	C	N	O	0
			86	66	8	12	
26	Z6	1	Total	C	N	O	0
			86	66	8	12	
26	a6	1	Total	C	N	O	0
			86	66	8	12	
26	a6	1	Total	C	N	O	0
			86	66	8	12	
26	b6	1	Total	C	N	O	0
			86	66	8	12	
26	b6	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	c6	1	Total	C	N	O	0
			129	99	12	18	
26	c6	1	Total	C	N	O	0
			129	99	12	18	
26	c6	1	Total	C	N	O	0
			129	99	12	18	
26	d6	1	Total	C	N	O	0
			86	66	8	12	
26	d6	1	Total	C	N	O	0
			86	66	8	12	
26	e6	1	Total	C	N	O	0
			86	66	8	12	
26	e6	1	Total	C	N	O	0
			86	66	8	12	
26	f6	1	Total	C	N	O	0
			86	66	8	12	
26	f6	1	Total	C	N	O	0
			86	66	8	12	
26	g6	1	Total	C	N	O	0
			86	66	8	12	
26	g6	1	Total	C	N	O	0
			86	66	8	12	
26	h6	1	Total	C	N	O	0
			86	66	8	12	
26	h6	1	Total	C	N	O	0
			86	66	8	12	
26	i6	1	Total	C	N	O	0
			86	66	8	12	
26	i6	1	Total	C	N	O	0
			86	66	8	12	
26	j6	1	Total	C	N	O	0
			86	66	8	12	
26	j6	1	Total	C	N	O	0
			86	66	8	12	
26	k6	1	Total	C	N	O	0
			86	66	8	12	
26	k6	1	Total	C	N	O	0
			86	66	8	12	
26	l6	1	Total	C	N	O	0
			86	66	8	12	
26	l6	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	m6	1	Total	C	N	O	0
			86	66	8	12	
26	m6	1	Total	C	N	O	0
			86	66	8	12	
26	n6	1	Total	C	N	O	0
			86	66	8	12	
26	n6	1	Total	C	N	O	0
			86	66	8	12	
26	o6	1	Total	C	N	O	0
			86	66	8	12	
26	o6	1	Total	C	N	O	0
			86	66	8	12	
26	p6	1	Total	C	N	O	0
			86	66	8	12	
26	p6	1	Total	C	N	O	0
			86	66	8	12	
26	q6	1	Total	C	N	O	0
			86	66	8	12	
26	q6	1	Total	C	N	O	0
			86	66	8	12	
26	r6	1	Total	C	N	O	0
			86	66	8	12	
26	r6	1	Total	C	N	O	0
			86	66	8	12	
26	s6	1	Total	C	N	O	0
			86	66	8	12	
26	s6	1	Total	C	N	O	0
			86	66	8	12	
26	t6	1	Total	C	N	O	0
			86	66	8	12	
26	t6	1	Total	C	N	O	0
			86	66	8	12	
26	u6	1	Total	C	N	O	0
			86	66	8	12	
26	u6	1	Total	C	N	O	0
			86	66	8	12	
26	v6	1	Total	C	N	O	0
			86	66	8	12	
26	v6	1	Total	C	N	O	0
			86	66	8	12	
26	w6	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	w6	1	Total	C	N	O	0
			86	66	8	12	
26	x6	1	Total	C	N	O	0
			86	66	8	12	
26	x6	1	Total	C	N	O	0
			86	66	8	12	
26	y6	1	Total	C	N	O	0
			129	99	12	18	
26	y6	1	Total	C	N	O	0
			129	99	12	18	
26	y6	1	Total	C	N	O	0
			129	99	12	18	
26	z6	1	Total	C	N	O	0
			86	66	8	12	
26	z6	1	Total	C	N	O	0
			86	66	8	12	
26	n8	1	Total	C	N	O	0
			43	33	4	6	
26	o8	1	Total	C	N	O	0
			86	66	8	12	
26	o8	1	Total	C	N	O	0
			86	66	8	12	
26	p8	1	Total	C	N	O	0
			86	66	8	12	
26	p8	1	Total	C	N	O	0
			86	66	8	12	
26	q8	1	Total	C	N	O	0
			86	66	8	12	
26	q8	1	Total	C	N	O	0
			86	66	8	12	
26	r8	1	Total	C	N	O	0
			86	66	8	12	
26	r8	1	Total	C	N	O	0
			86	66	8	12	
26	s8	1	Total	C	N	O	0
			86	66	8	12	
26	s8	1	Total	C	N	O	0
			86	66	8	12	
26	t8	1	Total	C	N	O	0
			86	66	8	12	
26	t8	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	u8	1	Total	C	N	O	0
			86	66	8	12	
26	u8	1	Total	C	N	O	0
			86	66	8	12	
26	A7	1	Total	C	N	O	0
			43	33	4	6	
26	B7	1	Total	C	N	O	0
			43	33	4	6	
26	C7	1	Total	C	N	O	0
			86	66	8	12	
26	C7	1	Total	C	N	O	0
			86	66	8	12	
26	D7	1	Total	C	N	O	0
			86	66	8	12	
26	D7	1	Total	C	N	O	0
			86	66	8	12	
26	E7	1	Total	C	N	O	0
			86	66	8	12	
26	E7	1	Total	C	N	O	0
			86	66	8	12	
26	F7	1	Total	C	N	O	0
			43	33	4	6	
26	G7	1	Total	C	N	O	0
			86	66	8	12	
26	G7	1	Total	C	N	O	0
			86	66	8	12	
26	H7	1	Total	C	N	O	0
			86	66	8	12	
26	H7	1	Total	C	N	O	0
			86	66	8	12	
26	I7	1	Total	C	N	O	0
			86	66	8	12	
26	I7	1	Total	C	N	O	0
			86	66	8	12	
26	J7	1	Total	C	N	O	0
			43	33	4	6	
26	K7	1	Total	C	N	O	0
			86	66	8	12	
26	K7	1	Total	C	N	O	0
			86	66	8	12	
26	L7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
26	M7	1	Total	C	N	O	0
			129	99	12	18	
26	M7	1	Total	C	N	O	0
			129	99	12	18	
26	M7	1	Total	C	N	O	0
			129	99	12	18	
26	N7	1	Total	C	N	O	0
			86	66	8	12	
26	N7	1	Total	C	N	O	0
			86	66	8	12	
26	O7	1	Total	C	N	O	0
			86	66	8	12	
26	O7	1	Total	C	N	O	0
			86	66	8	12	
26	P7	1	Total	C	N	O	0
			86	66	8	12	
26	P7	1	Total	C	N	O	0
			86	66	8	12	
26	Q7	1	Total	C	N	O	0
			86	66	8	12	
26	Q7	1	Total	C	N	O	0
			86	66	8	12	
26	R7	1	Total	C	N	O	0
			86	66	8	12	
26	R7	1	Total	C	N	O	0
			86	66	8	12	
26	S7	1	Total	C	N	O	0
			86	66	8	12	
26	S7	1	Total	C	N	O	0
			86	66	8	12	
26	T7	1	Total	C	N	O	0
			86	66	8	12	
26	T7	1	Total	C	N	O	0
			86	66	8	12	
26	U7	1	Total	C	N	O	0
			86	66	8	12	
26	U7	1	Total	C	N	O	0
			86	66	8	12	
26	V7	1	Total	C	N	O	0
			86	66	8	12	
26	V7	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	W7	1	Total	C	N	O	0
			86	66	8	12	
26	W7	1	Total	C	N	O	0
			86	66	8	12	
26	X7	1	Total	C	N	O	0
			86	66	8	12	
26	X7	1	Total	C	N	O	0
			86	66	8	12	
26	Y7	1	Total	C	N	O	0
			129	99	12	18	
26	Y7	1	Total	C	N	O	0
			129	99	12	18	
26	Y7	1	Total	C	N	O	0
			129	99	12	18	
26	Z7	1	Total	C	N	O	0
			86	66	8	12	
26	Z7	1	Total	C	N	O	0
			86	66	8	12	
26	a7	1	Total	C	N	O	0
			86	66	8	12	
26	a7	1	Total	C	N	O	0
			86	66	8	12	
26	b7	1	Total	C	N	O	0
			43	33	4	6	
26	c7	1	Total	C	N	O	0
			86	66	8	12	
26	c7	1	Total	C	N	O	0
			86	66	8	12	
26	d7	1	Total	C	N	O	0
			86	66	8	12	
26	d7	1	Total	C	N	O	0
			86	66	8	12	
26	e7	1	Total	C	N	O	0
			86	66	8	12	
26	e7	1	Total	C	N	O	0
			86	66	8	12	
26	f7	1	Total	C	N	O	0
			86	66	8	12	
26	f7	1	Total	C	N	O	0
			86	66	8	12	
26	g7	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	g7	1	Total	C	N	O	0
			86	66	8	12	
26	h7	1	Total	C	N	O	0
			86	66	8	12	
26	h7	1	Total	C	N	O	0
			86	66	8	12	
26	i7	1	Total	C	N	O	0
			86	66	8	12	
26	i7	1	Total	C	N	O	0
			86	66	8	12	
26	j7	1	Total	C	N	O	0
			86	66	8	12	
26	j7	1	Total	C	N	O	0
			86	66	8	12	
26	k7	1	Total	C	N	O	0
			86	66	8	12	
26	k7	1	Total	C	N	O	0
			86	66	8	12	
26	l7	1	Total	C	N	O	0
			86	66	8	12	
26	l7	1	Total	C	N	O	0
			86	66	8	12	
26	m7	1	Total	C	N	O	0
			86	66	8	12	
26	m7	1	Total	C	N	O	0
			86	66	8	12	
26	n7	1	Total	C	N	O	0
			86	66	8	12	
26	n7	1	Total	C	N	O	0
			86	66	8	12	
26	o7	1	Total	C	N	O	0
			86	66	8	12	
26	o7	1	Total	C	N	O	0
			86	66	8	12	
26	p7	1	Total	C	N	O	0
			43	33	4	6	
26	q7	1	Total	C	N	O	0
			86	66	8	12	
26	q7	1	Total	C	N	O	0
			86	66	8	12	
26	r7	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	r7	1	Total	C	N	O	0
			86	66	8	12	
26	s7	1	Total	C	N	O	0
			86	66	8	12	
26	s7	1	Total	C	N	O	0
			86	66	8	12	
26	t7	1	Total	C	N	O	0
			86	66	8	12	
26	t7	1	Total	C	N	O	0
			86	66	8	12	
26	u7	1	Total	C	N	O	0
			86	66	8	12	
26	u7	1	Total	C	N	O	0
			86	66	8	12	
26	v7	1	Total	C	N	O	0
			86	66	8	12	
26	v7	1	Total	C	N	O	0
			86	66	8	12	
26	w7	1	Total	C	N	O	0
			86	66	8	12	
26	w7	1	Total	C	N	O	0
			86	66	8	12	
26	x7	1	Total	C	N	O	0
			86	66	8	12	
26	x7	1	Total	C	N	O	0
			86	66	8	12	
26	y7	1	Total	C	N	O	0
			86	66	8	12	
26	y7	1	Total	C	N	O	0
			86	66	8	12	
26	z7	1	Total	C	N	O	0
			86	66	8	12	
26	z7	1	Total	C	N	O	0
			86	66	8	12	
26	a8	1	Total	C	N	O	0
			86	66	8	12	
26	a8	1	Total	C	N	O	0
			86	66	8	12	
26	b8	1	Total	C	N	O	0
			129	99	12	18	
26	b8	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	b8	1	Total	C	N	O	0
			129	99	12	18	
26	c8	1	Total	C	N	O	0
			86	66	8	12	
26	c8	1	Total	C	N	O	0
			86	66	8	12	
26	d8	1	Total	C	N	O	0
			86	66	8	12	
26	d8	1	Total	C	N	O	0
			86	66	8	12	
26	e8	1	Total	C	N	O	0
			86	66	8	12	
26	e8	1	Total	C	N	O	0
			86	66	8	12	
26	a9	1	Total	C	N	O	0
			129	99	12	18	
26	a9	1	Total	C	N	O	0
			129	99	12	18	
26	a9	1	Total	C	N	O	0
			129	99	12	18	
26	b9	1	Total	C	N	O	0
			172	132	16	24	
26	b9	1	Total	C	N	O	0
			172	132	16	24	
26	b9	1	Total	C	N	O	0
			172	132	16	24	
26	b9	1	Total	C	N	O	0
			172	132	16	24	
26	c9	1	Total	C	N	O	0
			86	66	8	12	
26	c9	1	Total	C	N	O	0
			86	66	8	12	
26	d9	1	Total	C	N	O	0
			129	99	12	18	
26	d9	1	Total	C	N	O	0
			129	99	12	18	
26	d9	1	Total	C	N	O	0
			129	99	12	18	
26	e9	1	Total	C	N	O	0
			129	99	12	18	
26	e9	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	e9	1	Total	C	N	O	0
			129	99	12	18	
26	v8	1	Total	C	N	O	0
			86	66	8	12	
26	v8	1	Total	C	N	O	0
			86	66	8	12	
26	w8	1	Total	C	N	O	0
			86	66	8	12	
26	w8	1	Total	C	N	O	0
			86	66	8	12	
26	x8	1	Total	C	N	O	0
			86	66	8	12	
26	x8	1	Total	C	N	O	0
			86	66	8	12	
26	y8	1	Total	C	N	O	0
			86	66	8	12	
26	y8	1	Total	C	N	O	0
			86	66	8	12	
26	z8	1	Total	C	N	O	0
			86	66	8	12	
26	z8	1	Total	C	N	O	0
			86	66	8	12	
26	A8	1	Total	C	N	O	0
			86	66	8	12	
26	A8	1	Total	C	N	O	0
			86	66	8	12	
26	B8	1	Total	C	N	O	0
			86	66	8	12	
26	B8	1	Total	C	N	O	0
			86	66	8	12	
26	C8	1	Total	C	N	O	0
			86	66	8	12	
26	C8	1	Total	C	N	O	0
			86	66	8	12	
26	D8	1	Total	C	N	O	0
			86	66	8	12	
26	D8	1	Total	C	N	O	0
			86	66	8	12	
26	E8	1	Total	C	N	O	0
			86	66	8	12	
26	E8	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	F8	1	Total	C	N	O	0
			86	66	8	12	
26	F8	1	Total	C	N	O	0
			86	66	8	12	
26	G8	1	Total	C	N	O	0
			86	66	8	12	
26	G8	1	Total	C	N	O	0
			86	66	8	12	
26	H8	1	Total	C	N	O	0
			86	66	8	12	
26	H8	1	Total	C	N	O	0
			86	66	8	12	
26	I8	1	Total	C	N	O	0
			86	66	8	12	
26	I8	1	Total	C	N	O	0
			86	66	8	12	
26	J8	1	Total	C	N	O	0
			86	66	8	12	
26	J8	1	Total	C	N	O	0
			86	66	8	12	
26	K8	1	Total	C	N	O	0
			86	66	8	12	
26	K8	1	Total	C	N	O	0
			86	66	8	12	
26	L8	1	Total	C	N	O	0
			86	66	8	12	
26	L8	1	Total	C	N	O	0
			86	66	8	12	
26	M8	1	Total	C	N	O	0
			86	66	8	12	
26	M8	1	Total	C	N	O	0
			86	66	8	12	
26	N8	1	Total	C	N	O	0
			86	66	8	12	
26	N8	1	Total	C	N	O	0
			86	66	8	12	
26	O8	1	Total	C	N	O	0
			86	66	8	12	
26	O8	1	Total	C	N	O	0
			86	66	8	12	
26	P8	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	P8	1	Total	C	N	O	0
			86	66	8	12	
26	Q8	1	Total	C	N	O	0
			86	66	8	12	
26	Q8	1	Total	C	N	O	0
			86	66	8	12	
26	S8	1	Total	C	N	O	0
			43	33	4	6	
26	T8	1	Total	C	N	O	0
			86	66	8	12	
26	T8	1	Total	C	N	O	0
			86	66	8	12	
26	U8	1	Total	C	N	O	0
			129	99	12	18	
26	U8	1	Total	C	N	O	0
			129	99	12	18	
26	U8	1	Total	C	N	O	0
			129	99	12	18	
26	V8	1	Total	C	N	O	0
			43	33	4	6	
26	W8	1	Total	C	N	O	0
			86	66	8	12	
26	W8	1	Total	C	N	O	0
			86	66	8	12	
26	X8	1	Total	C	N	O	0
			43	33	4	6	
26	Y8	1	Total	C	N	O	0
			86	66	8	12	
26	Y8	1	Total	C	N	O	0
			86	66	8	12	
26	Z8	1	Total	C	N	O	0
			43	33	4	6	
26	f9	1	Total	C	N	O	0
			86	66	8	12	
26	f9	1	Total	C	N	O	0
			86	66	8	12	
26	g9	1	Total	C	N	O	0
			43	33	4	6	
26	h9	1	Total	C	N	O	0
			86	66	8	12	
26	h9	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	i9	1	Total	C	N	O	0
			43	33	4	6	
26	j9	1	Total	C	N	O	0
			86	66	8	12	
26	j9	1	Total	C	N	O	0
			86	66	8	12	
26	k9	1	Total	C	N	O	0
			43	33	4	6	
26	l9	1	Total	C	N	O	0
			86	66	8	12	
26	l9	1	Total	C	N	O	0
			86	66	8	12	
26	m9	1	Total	C	N	O	0
			43	33	4	6	
26	n9	1	Total	C	N	O	0
			43	33	4	6	
26	o9	1	Total	C	N	O	0
			43	33	4	6	
26	p9	1	Total	C	N	O	0
			86	66	8	12	
26	p9	1	Total	C	N	O	0
			86	66	8	12	
26	q9	1	Total	C	N	O	0
			86	66	8	12	
26	q9	1	Total	C	N	O	0
			86	66	8	12	
26	r9	1	Total	C	N	O	0
			86	66	8	12	
26	r9	1	Total	C	N	O	0
			86	66	8	12	
26	s9	1	Total	C	N	O	0
			86	66	8	12	
26	s9	1	Total	C	N	O	0
			86	66	8	12	
26	t9	1	Total	C	N	O	0
			86	66	8	12	
26	t9	1	Total	C	N	O	0
			86	66	8	12	
26	u9	1	Total	C	N	O	0
			86	66	8	12	
26	u9	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	v9	1	Total	C	N	O	0
			86	66	8	12	
26	v9	1	Total	C	N	O	0
			86	66	8	12	
26	w9	1	Total	C	N	O	0
			86	66	8	12	
26	w9	1	Total	C	N	O	0
			86	66	8	12	
26	x9	1	Total	C	N	O	0
			86	66	8	12	
26	x9	1	Total	C	N	O	0
			86	66	8	12	
26	y9	1	Total	C	N	O	0
			86	66	8	12	
26	y9	1	Total	C	N	O	0
			86	66	8	12	
26	z9	1	Total	C	N	O	0
			86	66	8	12	
26	z9	1	Total	C	N	O	0
			86	66	8	12	
26	A9	1	Total	C	N	O	0
			86	66	8	12	
26	A9	1	Total	C	N	O	0
			86	66	8	12	
26	B9	1	Total	C	N	O	0
			86	66	8	12	
26	B9	1	Total	C	N	O	0
			86	66	8	12	
26	C9	1	Total	C	N	O	0
			86	66	8	12	
26	C9	1	Total	C	N	O	0
			86	66	8	12	
26	D9	1	Total	C	N	O	0
			86	66	8	12	
26	D9	1	Total	C	N	O	0
			86	66	8	12	
26	E9	1	Total	C	N	O	0
			86	66	8	12	
26	E9	1	Total	C	N	O	0
			86	66	8	12	
26	F9	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	F9	1	Total	C	N	O	0
			86	66	8	12	
26	G9	1	Total	C	N	O	0
			86	66	8	12	
26	G9	1	Total	C	N	O	0
			86	66	8	12	
26	H9	1	Total	C	N	O	0
			86	66	8	12	
26	H9	1	Total	C	N	O	0
			86	66	8	12	
26	I9	1	Total	C	N	O	0
			86	66	8	12	
26	I9	1	Total	C	N	O	0
			86	66	8	12	
26	J9	1	Total	C	N	O	0
			86	66	8	12	
26	J9	1	Total	C	N	O	0
			86	66	8	12	
26	K9	1	Total	C	N	O	0
			86	66	8	12	
26	K9	1	Total	C	N	O	0
			86	66	8	12	
26	L9	1	Total	C	N	O	0
			86	66	8	12	
26	L9	1	Total	C	N	O	0
			86	66	8	12	
26	M9	1	Total	C	N	O	0
			86	66	8	12	
26	M9	1	Total	C	N	O	0
			86	66	8	12	
26	N9	1	Total	C	N	O	0
			86	66	8	12	
26	N9	1	Total	C	N	O	0
			86	66	8	12	
26	O9	1	Total	C	N	O	0
			86	66	8	12	
26	O9	1	Total	C	N	O	0
			86	66	8	12	
26	P9	1	Total	C	N	O	0
			86	66	8	12	
26	P9	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	Q9	1	Total	C	N	O	0
			86	66	8	12	
26	Q9	1	Total	C	N	O	0
			86	66	8	12	
26	R9	1	Total	C	N	O	0
			86	66	8	12	
26	R9	1	Total	C	N	O	0
			86	66	8	12	
26	S9	1	Total	C	N	O	0
			86	66	8	12	
26	S9	1	Total	C	N	O	0
			86	66	8	12	
26	T9	1	Total	C	N	O	0
			86	66	8	12	
26	T9	1	Total	C	N	O	0
			86	66	8	12	
26	U9	1	Total	C	N	O	0
			86	66	8	12	
26	U9	1	Total	C	N	O	0
			86	66	8	12	
26	V9	1	Total	C	N	O	0
			86	66	8	12	
26	V9	1	Total	C	N	O	0
			86	66	8	12	
26	X9	1	Total	C	N	O	0
			43	33	4	6	
26	Y9	1	Total	C	N	O	0
			86	66	8	12	
26	Y9	1	Total	C	N	O	0
			86	66	8	12	
26	Z9	1	Total	C	N	O	0
			172	132	16	24	
26	Z9	1	Total	C	N	O	0
			172	132	16	24	
26	Z9	1	Total	C	N	O	0
			172	132	16	24	
26	Z9	1	Total	C	N	O	0
			172	132	16	24	
26	aa	1	Total	C	N	O	0
			43	33	4	6	
26	ab	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	ab	1	Total	C	N	O	0
			86	66	8	12	
26	ac	1	Total	C	N	O	0
			43	33	4	6	
26	ad	1	Total	C	N	O	0
			86	66	8	12	
26	ad	1	Total	C	N	O	0
			86	66	8	12	
26	ae	1	Total	C	N	O	0
			43	33	4	6	
26	af	1	Total	C	N	O	0
			86	66	8	12	
26	af	1	Total	C	N	O	0
			86	66	8	12	
26	ag	1	Total	C	N	O	0
			43	33	4	6	
26	ah	1	Total	C	N	O	0
			86	66	8	12	
26	ah	1	Total	C	N	O	0
			86	66	8	12	
26	ai	1	Total	C	N	O	0
			43	33	4	6	
26	aj	1	Total	C	N	O	0
			86	66	8	12	
26	aj	1	Total	C	N	O	0
			86	66	8	12	
26	ak	1	Total	C	N	O	0
			43	33	4	6	
26	al	1	Total	C	N	O	0
			86	66	8	12	
26	al	1	Total	C	N	O	0
			86	66	8	12	
26	am	1	Total	C	N	O	0
			43	33	4	6	
26	an	1	Total	C	N	O	0
			43	33	4	6	
26	ao	1	Total	C	N	O	0
			86	66	8	12	
26	ao	1	Total	C	N	O	0
			86	66	8	12	
26	ap	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	ap	1	Total	C	N	O	0
			86	66	8	12	
26	aq	1	Total	C	N	O	0
			86	66	8	12	
26	aq	1	Total	C	N	O	0
			86	66	8	12	
26	ar	1	Total	C	N	O	0
			86	66	8	12	
26	ar	1	Total	C	N	O	0
			86	66	8	12	
26	as	1	Total	C	N	O	0
			86	66	8	12	
26	as	1	Total	C	N	O	0
			86	66	8	12	
26	at	1	Total	C	N	O	0
			86	66	8	12	
26	at	1	Total	C	N	O	0
			86	66	8	12	
26	au	1	Total	C	N	O	0
			86	66	8	12	
26	au	1	Total	C	N	O	0
			86	66	8	12	
26	av	1	Total	C	N	O	0
			86	66	8	12	
26	av	1	Total	C	N	O	0
			86	66	8	12	
26	aw	1	Total	C	N	O	0
			86	66	8	12	
26	aw	1	Total	C	N	O	0
			86	66	8	12	
26	ax	1	Total	C	N	O	0
			43	33	4	6	
26	ay	1	Total	C	N	O	0
			86	66	8	12	
26	ay	1	Total	C	N	O	0
			86	66	8	12	
26	az	1	Total	C	N	O	0
			86	66	8	12	
26	az	1	Total	C	N	O	0
			86	66	8	12	
26	aA	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	aA	1	Total	C	N	O	0
			86	66	8	12	
26	aB	1	Total	C	N	O	0
			86	66	8	12	
26	aB	1	Total	C	N	O	0
			86	66	8	12	
26	aC	1	Total	C	N	O	0
			86	66	8	12	
26	aC	1	Total	C	N	O	0
			86	66	8	12	
26	aD	1	Total	C	N	O	0
			86	66	8	12	
26	aD	1	Total	C	N	O	0
			86	66	8	12	
26	aE	1	Total	C	N	O	0
			86	66	8	12	
26	aE	1	Total	C	N	O	0
			86	66	8	12	
26	aF	1	Total	C	N	O	0
			129	99	12	18	
26	aF	1	Total	C	N	O	0
			129	99	12	18	
26	aF	1	Total	C	N	O	0
			129	99	12	18	
26	aG	1	Total	C	N	O	0
			43	33	4	6	
26	aH	1	Total	C	N	O	0
			86	66	8	12	
26	aH	1	Total	C	N	O	0
			86	66	8	12	
26	aI	1	Total	C	N	O	0
			86	66	8	12	
26	aI	1	Total	C	N	O	0
			86	66	8	12	
26	aJ	1	Total	C	N	O	0
			86	66	8	12	
26	aJ	1	Total	C	N	O	0
			86	66	8	12	
26	aK	1	Total	C	N	O	0
			86	66	8	12	
26	aK	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	aL	1	Total	C	N	O	0
			86	66	8	12	
26	aL	1	Total	C	N	O	0
			86	66	8	12	
26	aM	1	Total	C	N	O	0
			86	66	8	12	
26	aM	1	Total	C	N	O	0
			86	66	8	12	
26	aN	1	Total	C	N	O	0
			129	99	12	18	
26	aN	1	Total	C	N	O	0
			129	99	12	18	
26	aN	1	Total	C	N	O	0
			129	99	12	18	
26	aO	1	Total	C	N	O	0
			43	33	4	6	
26	aP	1	Total	C	N	O	0
			86	66	8	12	
26	aP	1	Total	C	N	O	0
			86	66	8	12	
26	aQ	1	Total	C	N	O	0
			86	66	8	12	
26	aQ	1	Total	C	N	O	0
			86	66	8	12	
26	aR	1	Total	C	N	O	0
			86	66	8	12	
26	aR	1	Total	C	N	O	0
			86	66	8	12	
26	aS	1	Total	C	N	O	0
			86	66	8	12	
26	aS	1	Total	C	N	O	0
			86	66	8	12	
26	aT	1	Total	C	N	O	0
			86	66	8	12	
26	aT	1	Total	C	N	O	0
			86	66	8	12	
26	aU	1	Total	C	N	O	0
			86	66	8	12	
26	aU	1	Total	C	N	O	0
			86	66	8	12	
26	aV	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	aV	1	Total	C	N	O	0
			86	66	8	12	
26	aW	1	Total	C	N	O	0
			86	66	8	12	
26	aW	1	Total	C	N	O	0
			86	66	8	12	
26	aX	1	Total	C	N	O	0
			86	66	8	12	
26	aX	1	Total	C	N	O	0
			86	66	8	12	
26	aY	1	Total	C	N	O	0
			129	99	12	18	
26	aY	1	Total	C	N	O	0
			129	99	12	18	
26	aY	1	Total	C	N	O	0
			129	99	12	18	
26	aZ	1	Total	C	N	O	0
			86	66	8	12	
26	aZ	1	Total	C	N	O	0
			86	66	8	12	
26	ba	1	Total	C	N	O	0
			43	33	4	6	
26	bb	1	Total	C	N	O	0
			43	33	4	6	
26	bc	1	Total	C	N	O	0
			43	33	4	6	
26	bd	1	Total	C	N	O	0
			86	66	8	12	
26	bd	1	Total	C	N	O	0
			86	66	8	12	
26	be	1	Total	C	N	O	0
			43	33	4	6	
26	bf	1	Total	C	N	O	0
			43	33	4	6	
26	bg	1	Total	C	N	O	0
			43	33	4	6	
26	bh	1	Total	C	N	O	0
			86	66	8	12	
26	bh	1	Total	C	N	O	0
			86	66	8	12	
26	bi	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
26	bj	1	Total	C	N	O	0
			86	66	8	12	
26	bj	1	Total	C	N	O	0
			86	66	8	12	
26	bk	1	Total	C	N	O	0
			43	33	4	6	
26	bl	1	Total	C	N	O	0
			86	66	8	12	
26	bl	1	Total	C	N	O	0
			86	66	8	12	
26	bm	1	Total	C	N	O	0
			86	66	8	12	
26	bm	1	Total	C	N	O	0
			86	66	8	12	
26	bn	1	Total	C	N	O	0
			43	33	4	6	
26	bo	1	Total	C	N	O	0
			43	33	4	6	
26	bp	1	Total	C	N	O	0
			43	33	4	6	
26	bq	1	Total	C	N	O	0
			86	66	8	12	
26	bq	1	Total	C	N	O	0
			86	66	8	12	
26	br	1	Total	C	N	O	0
			86	66	8	12	
26	br	1	Total	C	N	O	0
			86	66	8	12	
26	bs	1	Total	C	N	O	0
			129	99	12	18	
26	bs	1	Total	C	N	O	0
			129	99	12	18	
26	bs	1	Total	C	N	O	0
			129	99	12	18	
26	bt	1	Total	C	N	O	0
			86	66	8	12	
26	bt	1	Total	C	N	O	0
			86	66	8	12	
26	bu	1	Total	C	N	O	0
			86	66	8	12	
26	bu	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	bv	1	Total	C	N	O	0
			86	66	8	12	
26	bv	1	Total	C	N	O	0
			86	66	8	12	
26	bw	1	Total	C	N	O	0
			86	66	8	12	
26	bw	1	Total	C	N	O	0
			86	66	8	12	
26	bx	1	Total	C	N	O	0
			86	66	8	12	
26	bx	1	Total	C	N	O	0
			86	66	8	12	
26	by	1	Total	C	N	O	0
			86	66	8	12	
26	by	1	Total	C	N	O	0
			86	66	8	12	
26	bz	1	Total	C	N	O	0
			86	66	8	12	
26	bz	1	Total	C	N	O	0
			86	66	8	12	
26	bA	1	Total	C	N	O	0
			86	66	8	12	
26	bA	1	Total	C	N	O	0
			86	66	8	12	
26	bB	1	Total	C	N	O	0
			86	66	8	12	
26	bB	1	Total	C	N	O	0
			86	66	8	12	
26	bC	1	Total	C	N	O	0
			86	66	8	12	
26	bC	1	Total	C	N	O	0
			86	66	8	12	
26	bD	1	Total	C	N	O	0
			86	66	8	12	
26	bD	1	Total	C	N	O	0
			86	66	8	12	
26	bE	1	Total	C	N	O	0
			86	66	8	12	
26	bE	1	Total	C	N	O	0
			86	66	8	12	
26	bF	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	bF	1	Total	C	N	O	0
			86	66	8	12	
26	bG	1	Total	C	N	O	0
			86	66	8	12	
26	bG	1	Total	C	N	O	0
			86	66	8	12	
26	bH	1	Total	C	N	O	0
			86	66	8	12	
26	bH	1	Total	C	N	O	0
			86	66	8	12	
26	bI	1	Total	C	N	O	0
			86	66	8	12	
26	bI	1	Total	C	N	O	0
			86	66	8	12	
26	bJ	1	Total	C	N	O	0
			86	66	8	12	
26	bJ	1	Total	C	N	O	0
			86	66	8	12	
26	bK	1	Total	C	N	O	0
			86	66	8	12	
26	bK	1	Total	C	N	O	0
			86	66	8	12	
26	bL	1	Total	C	N	O	0
			86	66	8	12	
26	bL	1	Total	C	N	O	0
			86	66	8	12	
26	bM	1	Total	C	N	O	0
			86	66	8	12	
26	bM	1	Total	C	N	O	0
			86	66	8	12	
26	bN	1	Total	C	N	O	0
			86	66	8	12	
26	bN	1	Total	C	N	O	0
			86	66	8	12	
26	bO	1	Total	C	N	O	0
			86	66	8	12	
26	bO	1	Total	C	N	O	0
			86	66	8	12	
26	bP	1	Total	C	N	O	0
			86	66	8	12	
26	bP	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	bQ	1	Total	C	N	O	0
			129	99	12	18	
26	bQ	1	Total	C	N	O	0
			129	99	12	18	
26	bQ	1	Total	C	N	O	0
			129	99	12	18	
26	bR	1	Total	C	N	O	0
			43	33	4	6	
26	bS	1	Total	C	N	O	0
			86	66	8	12	
26	bS	1	Total	C	N	O	0
			86	66	8	12	
26	bT	1	Total	C	N	O	0
			43	33	4	6	
26	bU	1	Total	C	N	O	0
			86	66	8	12	
26	bU	1	Total	C	N	O	0
			86	66	8	12	
26	bV	1	Total	C	N	O	0
			86	66	8	12	
26	bV	1	Total	C	N	O	0
			86	66	8	12	
26	bW	1	Total	C	N	O	0
			43	33	4	6	
26	bX	1	Total	C	N	O	0
			86	66	8	12	
26	bX	1	Total	C	N	O	0
			86	66	8	12	
26	bY	1	Total	C	N	O	0
			129	99	12	18	
26	bY	1	Total	C	N	O	0
			129	99	12	18	
26	bY	1	Total	C	N	O	0
			129	99	12	18	
26	bZ	1	Total	C	N	O	0
			129	99	12	18	
26	bZ	1	Total	C	N	O	0
			129	99	12	18	
26	bZ	1	Total	C	N	O	0
			129	99	12	18	
26	ca	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
26	cb	1	Total	C	N	O	0
			86	66	8	12	
26	cb	1	Total	C	N	O	0
			86	66	8	12	
26	cc	1	Total	C	N	O	0
			43	33	4	6	
26	cd	1	Total	C	N	O	0
			86	66	8	12	
26	cd	1	Total	C	N	O	0
			86	66	8	12	
26	ce	1	Total	C	N	O	0
			43	33	4	6	
26	cf	1	Total	C	N	O	0
			43	33	4	6	
26	cg	1	Total	C	N	O	0
			43	33	4	6	
26	ch	1	Total	C	N	O	0
			86	66	8	12	
26	ch	1	Total	C	N	O	0
			86	66	8	12	
26	ci	1	Total	C	N	O	0
			43	33	4	6	
26	cj	1	Total	C	N	O	0
			86	66	8	12	
26	cj	1	Total	C	N	O	0
			86	66	8	12	
26	ck	1	Total	C	N	O	0
			43	33	4	6	
26	cl	1	Total	C	N	O	0
			86	66	8	12	
26	cl	1	Total	C	N	O	0
			86	66	8	12	
26	cm	1	Total	C	N	O	0
			86	66	8	12	
26	cm	1	Total	C	N	O	0
			86	66	8	12	
26	cn	1	Total	C	N	O	0
			43	33	4	6	
26	co	1	Total	C	N	O	0
			43	33	4	6	
26	cp	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	cp	1	Total	C	N	O	0
			86	66	8	12	
26	cq	1	Total	C	N	O	0
			86	66	8	12	
26	cq	1	Total	C	N	O	0
			86	66	8	12	
26	cr	1	Total	C	N	O	0
			86	66	8	12	
26	cr	1	Total	C	N	O	0
			86	66	8	12	
26	cs	1	Total	C	N	O	0
			86	66	8	12	
26	cs	1	Total	C	N	O	0
			86	66	8	12	
26	ct	1	Total	C	N	O	0
			86	66	8	12	
26	ct	1	Total	C	N	O	0
			86	66	8	12	
26	cu	1	Total	C	N	O	0
			86	66	8	12	
26	cu	1	Total	C	N	O	0
			86	66	8	12	
26	cv	1	Total	C	N	O	0
			86	66	8	12	
26	cv	1	Total	C	N	O	0
			86	66	8	12	
26	cw	1	Total	C	N	O	0
			86	66	8	12	
26	cw	1	Total	C	N	O	0
			86	66	8	12	
26	cx	1	Total	C	N	O	0
			86	66	8	12	
26	cx	1	Total	C	N	O	0
			86	66	8	12	
26	cy	1	Total	C	N	O	0
			86	66	8	12	
26	cy	1	Total	C	N	O	0
			86	66	8	12	
26	cz	1	Total	C	N	O	0
			86	66	8	12	
26	cz	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	cA	1	Total	C	N	O	0
			86	66	8	12	
26	cA	1	Total	C	N	O	0
			86	66	8	12	
26	cB	1	Total	C	N	O	0
			86	66	8	12	
26	cB	1	Total	C	N	O	0
			86	66	8	12	
26	cC	1	Total	C	N	O	0
			129	99	12	18	
26	cC	1	Total	C	N	O	0
			129	99	12	18	
26	cC	1	Total	C	N	O	0
			129	99	12	18	
26	cD	1	Total	C	N	O	0
			86	66	8	12	
26	cD	1	Total	C	N	O	0
			86	66	8	12	
26	cE	1	Total	C	N	O	0
			86	66	8	12	
26	cE	1	Total	C	N	O	0
			86	66	8	12	
26	cF	1	Total	C	N	O	0
			43	33	4	6	
26	cG	1	Total	C	N	O	0
			86	66	8	12	
26	cG	1	Total	C	N	O	0
			86	66	8	12	
26	cH	1	Total	C	N	O	0
			43	33	4	6	
26	cI	1	Total	C	N	O	0
			86	66	8	12	
26	cI	1	Total	C	N	O	0
			86	66	8	12	
26	cJ	1	Total	C	N	O	0
			86	66	8	12	
26	cJ	1	Total	C	N	O	0
			86	66	8	12	
26	cK	1	Total	C	N	O	0
			86	66	8	12	
26	cK	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	cL	1	Total	C	N	O	0
			86	66	8	12	
26	cL	1	Total	C	N	O	0
			86	66	8	12	
26	cM	1	Total	C	N	O	0
			86	66	8	12	
26	cM	1	Total	C	N	O	0
			86	66	8	12	
26	cN	1	Total	C	N	O	0
			43	33	4	6	
26	cO	1	Total	C	N	O	0
			86	66	8	12	
26	cO	1	Total	C	N	O	0
			86	66	8	12	
26	cP	1	Total	C	N	O	0
			86	66	8	12	
26	cP	1	Total	C	N	O	0
			86	66	8	12	
26	cQ	1	Total	C	N	O	0
			43	33	4	6	
26	cR	1	Total	C	N	O	0
			86	66	8	12	
26	cR	1	Total	C	N	O	0
			86	66	8	12	
26	cS	1	Total	C	N	O	0
			86	66	8	12	
26	cS	1	Total	C	N	O	0
			86	66	8	12	
26	cT	1	Total	C	N	O	0
			86	66	8	12	
26	cT	1	Total	C	N	O	0
			86	66	8	12	
26	cU	1	Total	C	N	O	0
			86	66	8	12	
26	cU	1	Total	C	N	O	0
			86	66	8	12	
26	cV	1	Total	C	N	O	0
			129	99	12	18	
26	cV	1	Total	C	N	O	0
			129	99	12	18	
26	cV	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	cW	1	Total	C	N	O	0
			86	66	8	12	
26	cW	1	Total	C	N	O	0
			86	66	8	12	
26	cX	1	Total	C	N	O	0
			86	66	8	12	
26	cX	1	Total	C	N	O	0
			86	66	8	12	
26	cY	1	Total	C	N	O	0
			86	66	8	12	
26	cY	1	Total	C	N	O	0
			86	66	8	12	
26	cZ	1	Total	C	N	O	0
			86	66	8	12	
26	cZ	1	Total	C	N	O	0
			86	66	8	12	
26	da	1	Total	C	N	O	0
			86	66	8	12	
26	da	1	Total	C	N	O	0
			86	66	8	12	
26	db	1	Total	C	N	O	0
			86	66	8	12	
26	db	1	Total	C	N	O	0
			86	66	8	12	
26	dc	1	Total	C	N	O	0
			129	99	12	18	
26	dc	1	Total	C	N	O	0
			129	99	12	18	
26	dc	1	Total	C	N	O	0
			129	99	12	18	
26	dd	1	Total	C	N	O	0
			86	66	8	12	
26	dd	1	Total	C	N	O	0
			86	66	8	12	
26	de	1	Total	C	N	O	0
			86	66	8	12	
26	de	1	Total	C	N	O	0
			86	66	8	12	
26	df	1	Total	C	N	O	0
			86	66	8	12	
26	df	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	dg	1	Total	C	N	O	0
			86	66	8	12	
26	dg	1	Total	C	N	O	0
			86	66	8	12	
26	dh	1	Total	C	N	O	0
			86	66	8	12	
26	dh	1	Total	C	N	O	0
			86	66	8	12	
26	di	1	Total	C	N	O	0
			86	66	8	12	
26	di	1	Total	C	N	O	0
			86	66	8	12	
26	dj	1	Total	C	N	O	0
			86	66	8	12	
26	dj	1	Total	C	N	O	0
			86	66	8	12	
26	dk	1	Total	C	N	O	0
			86	66	8	12	
26	dk	1	Total	C	N	O	0
			86	66	8	12	
26	dl	1	Total	C	N	O	0
			86	66	8	12	
26	dl	1	Total	C	N	O	0
			86	66	8	12	
26	dm	1	Total	C	N	O	0
			86	66	8	12	
26	dm	1	Total	C	N	O	0
			86	66	8	12	
26	dn	1	Total	C	N	O	0
			86	66	8	12	
26	dn	1	Total	C	N	O	0
			86	66	8	12	
26	do	1	Total	C	N	O	0
			86	66	8	12	
26	do	1	Total	C	N	O	0
			86	66	8	12	
26	dp	1	Total	C	N	O	0
			86	66	8	12	
26	dp	1	Total	C	N	O	0
			86	66	8	12	
26	dq	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	dq	1	Total	C	N	O	0
			86	66	8	12	
26	dr	1	Total	C	N	O	0
			86	66	8	12	
26	dr	1	Total	C	N	O	0
			86	66	8	12	
26	ds	1	Total	C	N	O	0
			86	66	8	12	
26	ds	1	Total	C	N	O	0
			86	66	8	12	
26	dt	1	Total	C	N	O	0
			86	66	8	12	
26	dt	1	Total	C	N	O	0
			86	66	8	12	
26	du	1	Total	C	N	O	0
			129	99	12	18	
26	du	1	Total	C	N	O	0
			129	99	12	18	
26	du	1	Total	C	N	O	0
			129	99	12	18	
26	dv	1	Total	C	N	O	0
			43	33	4	6	
26	dw	1	Total	C	N	O	0
			129	99	12	18	
26	dw	1	Total	C	N	O	0
			129	99	12	18	
26	dw	1	Total	C	N	O	0
			129	99	12	18	
26	dx	1	Total	C	N	O	0
			172	132	16	24	
26	dx	1	Total	C	N	O	0
			172	132	16	24	
26	dx	1	Total	C	N	O	0
			172	132	16	24	
26	dx	1	Total	C	N	O	0
			172	132	16	24	
26	dy	1	Total	C	N	O	0
			43	33	4	6	
26	dz	1	Total	C	N	O	0
			86	66	8	12	
26	dz	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	dA	1	Total	C	N	O	0
			86	66	8	12	
26	dA	1	Total	C	N	O	0
			86	66	8	12	
26	dB	1	Total	C	N	O	0
			43	33	4	6	
26	dC	1	Total	C	N	O	0
			86	66	8	12	
26	dC	1	Total	C	N	O	0
			86	66	8	12	
26	dD	1	Total	C	N	O	0
			86	66	8	12	
26	dD	1	Total	C	N	O	0
			86	66	8	12	
26	dE	1	Total	C	N	O	0
			43	33	4	6	
26	dF	1	Total	C	N	O	0
			86	66	8	12	
26	dF	1	Total	C	N	O	0
			86	66	8	12	
26	dG	1	Total	C	N	O	0
			86	66	8	12	
26	dG	1	Total	C	N	O	0
			86	66	8	12	
26	dH	1	Total	C	N	O	0
			86	66	8	12	
26	dH	1	Total	C	N	O	0
			86	66	8	12	
26	dI	1	Total	C	N	O	0
			86	66	8	12	
26	dI	1	Total	C	N	O	0
			86	66	8	12	
26	dJ	1	Total	C	N	O	0
			86	66	8	12	
26	dJ	1	Total	C	N	O	0
			86	66	8	12	
26	dK	1	Total	C	N	O	0
			86	66	8	12	
26	dK	1	Total	C	N	O	0
			86	66	8	12	
26	dL	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	dL	1	Total	C	N	O	0
			86	66	8	12	
26	dM	1	Total	C	N	O	0
			86	66	8	12	
26	dM	1	Total	C	N	O	0
			86	66	8	12	
26	dN	1	Total	C	N	O	0
			86	66	8	12	
26	dN	1	Total	C	N	O	0
			86	66	8	12	
26	dO	1	Total	C	N	O	0
			86	66	8	12	
26	dO	1	Total	C	N	O	0
			86	66	8	12	
26	dP	1	Total	C	N	O	0
			86	66	8	12	
26	dP	1	Total	C	N	O	0
			86	66	8	12	
26	dQ	1	Total	C	N	O	0
			86	66	8	12	
26	dQ	1	Total	C	N	O	0
			86	66	8	12	
26	dR	1	Total	C	N	O	0
			86	66	8	12	
26	dR	1	Total	C	N	O	0
			86	66	8	12	
26	dS	1	Total	C	N	O	0
			43	33	4	6	
26	dT	1	Total	C	N	O	0
			86	66	8	12	
26	dT	1	Total	C	N	O	0
			86	66	8	12	
26	dU	1	Total	C	N	O	0
			86	66	8	12	
26	dU	1	Total	C	N	O	0
			86	66	8	12	
26	dV	1	Total	C	N	O	0
			86	66	8	12	
26	dV	1	Total	C	N	O	0
			86	66	8	12	
26	dW	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	dW	1	Total	C	N	O	0
			86	66	8	12	
26	dX	1	Total	C	N	O	0
			86	66	8	12	
26	dX	1	Total	C	N	O	0
			86	66	8	12	
26	dY	1	Total	C	N	O	0
			86	66	8	12	
26	dY	1	Total	C	N	O	0
			86	66	8	12	
26	dZ	1	Total	C	N	O	0
			86	66	8	12	
26	dZ	1	Total	C	N	O	0
			86	66	8	12	
26	ea	1	Total	C	N	O	0
			129	99	12	18	
26	ea	1	Total	C	N	O	0
			129	99	12	18	
26	ea	1	Total	C	N	O	0
			129	99	12	18	
26	eb	1	Total	C	N	O	0
			43	33	4	6	
26	ec	1	Total	C	N	O	0
			86	66	8	12	
26	ec	1	Total	C	N	O	0
			86	66	8	12	
26	ed	1	Total	C	N	O	0
			86	66	8	12	
26	ed	1	Total	C	N	O	0
			86	66	8	12	
26	ee	1	Total	C	N	O	0
			86	66	8	12	
26	ee	1	Total	C	N	O	0
			86	66	8	12	
26	ef	1	Total	C	N	O	0
			86	66	8	12	
26	ef	1	Total	C	N	O	0
			86	66	8	12	
26	eg	1	Total	C	N	O	0
			86	66	8	12	
26	eg	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	eh	1	Total	C	N	O	0
			86	66	8	12	
26	eh	1	Total	C	N	O	0
			86	66	8	12	
26	ei	1	Total	C	N	O	0
			86	66	8	12	
26	ei	1	Total	C	N	O	0
			86	66	8	12	
26	ej	1	Total	C	N	O	0
			86	66	8	12	
26	ej	1	Total	C	N	O	0
			86	66	8	12	
26	ek	1	Total	C	N	O	0
			86	66	8	12	
26	ek	1	Total	C	N	O	0
			86	66	8	12	
26	el	1	Total	C	N	O	0
			86	66	8	12	
26	el	1	Total	C	N	O	0
			86	66	8	12	
26	em	1	Total	C	N	O	0
			86	66	8	12	
26	em	1	Total	C	N	O	0
			86	66	8	12	
26	en	1	Total	C	N	O	0
			86	66	8	12	
26	en	1	Total	C	N	O	0
			86	66	8	12	
26	eo	1	Total	C	N	O	0
			86	66	8	12	
26	eo	1	Total	C	N	O	0
			86	66	8	12	
26	ep	1	Total	C	N	O	0
			86	66	8	12	
26	ep	1	Total	C	N	O	0
			86	66	8	12	
26	eq	1	Total	C	N	O	0
			86	66	8	12	
26	eq	1	Total	C	N	O	0
			86	66	8	12	
26	er	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	er	1	Total	C	N	O	0
			86	66	8	12	
26	es	1	Total	C	N	O	0
			86	66	8	12	
26	es	1	Total	C	N	O	0
			86	66	8	12	
26	et	1	Total	C	N	O	0
			86	66	8	12	
26	et	1	Total	C	N	O	0
			86	66	8	12	
26	eu	1	Total	C	N	O	0
			86	66	8	12	
26	eu	1	Total	C	N	O	0
			86	66	8	12	
26	ev	1	Total	C	N	O	0
			86	66	8	12	
26	ev	1	Total	C	N	O	0
			86	66	8	12	
26	ew	1	Total	C	N	O	0
			43	33	4	6	
26	ey	1	Total	C	N	O	0
			129	99	12	18	
26	ey	1	Total	C	N	O	0
			129	99	12	18	
26	ey	1	Total	C	N	O	0
			129	99	12	18	
26	ez	1	Total	C	N	O	0
			129	99	12	18	
26	ez	1	Total	C	N	O	0
			129	99	12	18	
26	ez	1	Total	C	N	O	0
			129	99	12	18	
26	eA	1	Total	C	N	O	0
			86	66	8	12	
26	eA	1	Total	C	N	O	0
			86	66	8	12	
26	eB	1	Total	C	N	O	0
			129	99	12	18	
26	eB	1	Total	C	N	O	0
			129	99	12	18	
26	eB	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	eC	1	Total	C	N	O	0
			86	66	8	12	
26	eC	1	Total	C	N	O	0
			86	66	8	12	
26	eD	1	Total	C	N	O	0
			86	66	8	12	
26	eD	1	Total	C	N	O	0
			86	66	8	12	
26	eE	1	Total	C	N	O	0
			86	66	8	12	
26	eE	1	Total	C	N	O	0
			86	66	8	12	
26	eF	1	Total	C	N	O	0
			86	66	8	12	
26	eF	1	Total	C	N	O	0
			86	66	8	12	
26	eG	1	Total	C	N	O	0
			86	66	8	12	
26	eG	1	Total	C	N	O	0
			86	66	8	12	
26	eH	1	Total	C	N	O	0
			86	66	8	12	
26	eH	1	Total	C	N	O	0
			86	66	8	12	
26	eI	1	Total	C	N	O	0
			86	66	8	12	
26	eI	1	Total	C	N	O	0
			86	66	8	12	
26	eJ	1	Total	C	N	O	0
			86	66	8	12	
26	eJ	1	Total	C	N	O	0
			86	66	8	12	
26	eK	1	Total	C	N	O	0
			86	66	8	12	
26	eK	1	Total	C	N	O	0
			86	66	8	12	
26	eL	1	Total	C	N	O	0
			86	66	8	12	
26	eL	1	Total	C	N	O	0
			86	66	8	12	
26	eM	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	eM	1	Total	C	N	O	0
			86	66	8	12	
26	eN	1	Total	C	N	O	0
			86	66	8	12	
26	eN	1	Total	C	N	O	0
			86	66	8	12	
26	eO	1	Total	C	N	O	0
			86	66	8	12	
26	eO	1	Total	C	N	O	0
			86	66	8	12	
26	eP	1	Total	C	N	O	0
			129	99	12	18	
26	eP	1	Total	C	N	O	0
			129	99	12	18	
26	eP	1	Total	C	N	O	0
			129	99	12	18	
26	eQ	1	Total	C	N	O	0
			86	66	8	12	
26	eQ	1	Total	C	N	O	0
			86	66	8	12	
26	eR	1	Total	C	N	O	0
			86	66	8	12	
26	eR	1	Total	C	N	O	0
			86	66	8	12	
26	eS	1	Total	C	N	O	0
			86	66	8	12	
26	eS	1	Total	C	N	O	0
			86	66	8	12	
26	eT	1	Total	C	N	O	0
			86	66	8	12	
26	eT	1	Total	C	N	O	0
			86	66	8	12	
26	eU	1	Total	C	N	O	0
			86	66	8	12	
26	eU	1	Total	C	N	O	0
			86	66	8	12	
26	eV	1	Total	C	N	O	0
			86	66	8	12	
26	eV	1	Total	C	N	O	0
			86	66	8	12	
26	eW	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	eW	1	Total	C	N	O	0
			86	66	8	12	
26	eX	1	Total	C	N	O	0
			43	33	4	6	
26	eY	1	Total	C	N	O	0
			86	66	8	12	
26	eY	1	Total	C	N	O	0
			86	66	8	12	
26	eZ	1	Total	C	N	O	0
			43	33	4	6	
26	la	1	Total	C	N	O	0
			86	66	8	12	
26	la	1	Total	C	N	O	0
			86	66	8	12	
26	lb	1	Total	C	N	O	0
			86	66	8	12	
26	lb	1	Total	C	N	O	0
			86	66	8	12	
26	lc	1	Total	C	N	O	0
			86	66	8	12	
26	lc	1	Total	C	N	O	0
			86	66	8	12	
26	ld	1	Total	C	N	O	0
			86	66	8	12	
26	ld	1	Total	C	N	O	0
			86	66	8	12	
26	le	1	Total	C	N	O	0
			86	66	8	12	
26	le	1	Total	C	N	O	0
			86	66	8	12	
26	lf	1	Total	C	N	O	0
			86	66	8	12	
26	lf	1	Total	C	N	O	0
			86	66	8	12	
26	lg	1	Total	C	N	O	0
			86	66	8	12	
26	lg	1	Total	C	N	O	0
			86	66	8	12	
26	lh	1	Total	C	N	O	0
			86	66	8	12	
26	lh	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	li	1	Total	C	N	O	0
			129	99	12	18	
26	li	1	Total	C	N	O	0
			129	99	12	18	
26	li	1	Total	C	N	O	0
			129	99	12	18	
26	lj	1	Total	C	N	O	0
			43	33	4	6	
26	lk	1	Total	C	N	O	0
			86	66	8	12	
26	lk	1	Total	C	N	O	0
			86	66	8	12	
26	ll	1	Total	C	N	O	0
			86	66	8	12	
26	ll	1	Total	C	N	O	0
			86	66	8	12	
26	lm	1	Total	C	N	O	0
			86	66	8	12	
26	lm	1	Total	C	N	O	0
			86	66	8	12	
26	ln	1	Total	C	N	O	0
			86	66	8	12	
26	ln	1	Total	C	N	O	0
			86	66	8	12	
26	lo	1	Total	C	N	O	0
			129	99	12	18	
26	lo	1	Total	C	N	O	0
			129	99	12	18	
26	lo	1	Total	C	N	O	0
			129	99	12	18	
26	lp	1	Total	C	N	O	0
			86	66	8	12	
26	lp	1	Total	C	N	O	0
			86	66	8	12	
26	lq	1	Total	C	N	O	0
			129	99	12	18	
26	lq	1	Total	C	N	O	0
			129	99	12	18	
26	lq	1	Total	C	N	O	0
			129	99	12	18	
26	lr	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	lr	1	Total	C	N	O	0
			86	66	8	12	
26	ls	1	Total	C	N	O	0
			86	66	8	12	
26	ls	1	Total	C	N	O	0
			86	66	8	12	
26	lt	1	Total	C	N	O	0
			86	66	8	12	
26	lt	1	Total	C	N	O	0
			86	66	8	12	
26	lu	1	Total	C	N	O	0
			86	66	8	12	
26	lu	1	Total	C	N	O	0
			86	66	8	12	
26	lv	1	Total	C	N	O	0
			43	33	4	6	
26	lw	1	Total	C	N	O	0
			129	99	12	18	
26	lw	1	Total	C	N	O	0
			129	99	12	18	
26	lw	1	Total	C	N	O	0
			129	99	12	18	
26	ly	1	Total	C	N	O	0
			129	99	12	18	
26	ly	1	Total	C	N	O	0
			129	99	12	18	
26	ly	1	Total	C	N	O	0
			129	99	12	18	
26	lz	1	Total	C	N	O	0
			86	66	8	12	
26	lz	1	Total	C	N	O	0
			86	66	8	12	
26	fa	1	Total	C	N	O	0
			43	33	4	6	
26	fb	1	Total	C	N	O	0
			86	66	8	12	
26	fb	1	Total	C	N	O	0
			86	66	8	12	
26	fc	1	Total	C	N	O	0
			86	66	8	12	
26	fc	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	fd	1	Total	C	N	O	0
			129	99	12	18	
26	fd	1	Total	C	N	O	0
			129	99	12	18	
26	fd	1	Total	C	N	O	0
			129	99	12	18	
26	fe	1	Total	C	N	O	0
			86	66	8	12	
26	fe	1	Total	C	N	O	0
			86	66	8	12	
26	ff	1	Total	C	N	O	0
			129	99	12	18	
26	ff	1	Total	C	N	O	0
			129	99	12	18	
26	ff	1	Total	C	N	O	0
			129	99	12	18	
26	fg	1	Total	C	N	O	0
			86	66	8	12	
26	fg	1	Total	C	N	O	0
			86	66	8	12	
26	fh	1	Total	C	N	O	0
			86	66	8	12	
26	fh	1	Total	C	N	O	0
			86	66	8	12	
26	fi	1	Total	C	N	O	0
			86	66	8	12	
26	fi	1	Total	C	N	O	0
			86	66	8	12	
26	fj	1	Total	C	N	O	0
			86	66	8	12	
26	fj	1	Total	C	N	O	0
			86	66	8	12	
26	fk	1	Total	C	N	O	0
			86	66	8	12	
26	fk	1	Total	C	N	O	0
			86	66	8	12	
26	fl	1	Total	C	N	O	0
			86	66	8	12	
26	fl	1	Total	C	N	O	0
			86	66	8	12	
26	fm	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	fm	1	Total	C	N	O	0
			86	66	8	12	
26	fn	1	Total	C	N	O	0
			86	66	8	12	
26	fn	1	Total	C	N	O	0
			86	66	8	12	
26	fo	1	Total	C	N	O	0
			86	66	8	12	
26	fo	1	Total	C	N	O	0
			86	66	8	12	
26	fp	1	Total	C	N	O	0
			86	66	8	12	
26	fp	1	Total	C	N	O	0
			86	66	8	12	
26	fq	1	Total	C	N	O	0
			86	66	8	12	
26	fq	1	Total	C	N	O	0
			86	66	8	12	
26	fr	1	Total	C	N	O	0
			86	66	8	12	
26	fr	1	Total	C	N	O	0
			86	66	8	12	
26	fs	1	Total	C	N	O	0
			86	66	8	12	
26	fs	1	Total	C	N	O	0
			86	66	8	12	
26	ft	1	Total	C	N	O	0
			86	66	8	12	
26	ft	1	Total	C	N	O	0
			86	66	8	12	
26	fu	1	Total	C	N	O	0
			43	33	4	6	
26	fv	1	Total	C	N	O	0
			86	66	8	12	
26	fv	1	Total	C	N	O	0
			86	66	8	12	
26	fw	1	Total	C	N	O	0
			86	66	8	12	
26	fw	1	Total	C	N	O	0
			86	66	8	12	
26	fx	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	fx	1	Total	C	N	O	0
			86	66	8	12	
26	fy	1	Total	C	N	O	0
			43	33	4	6	
26	fz	1	Total	C	N	O	0
			43	33	4	6	
26	ga	1	Total	C	N	O	0
			86	66	8	12	
26	ga	1	Total	C	N	O	0
			86	66	8	12	
26	gb	1	Total	C	N	O	0
			86	66	8	12	
26	gb	1	Total	C	N	O	0
			86	66	8	12	
26	gc	1	Total	C	N	O	0
			86	66	8	12	
26	gc	1	Total	C	N	O	0
			86	66	8	12	
26	gd	1	Total	C	N	O	0
			43	33	4	6	
26	ge	1	Total	C	N	O	0
			86	66	8	12	
26	ge	1	Total	C	N	O	0
			86	66	8	12	
26	gf	1	Total	C	N	O	0
			86	66	8	12	
26	gf	1	Total	C	N	O	0
			86	66	8	12	
26	gg	1	Total	C	N	O	0
			86	66	8	12	
26	gg	1	Total	C	N	O	0
			86	66	8	12	
26	gh	1	Total	C	N	O	0
			86	66	8	12	
26	gh	1	Total	C	N	O	0
			86	66	8	12	
26	gi	1	Total	C	N	O	0
			86	66	8	12	
26	gi	1	Total	C	N	O	0
			86	66	8	12	
26	gj	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	gj	1	Total	C	N	O	0
			86	66	8	12	
26	gk	1	Total	C	N	O	0
			86	66	8	12	
26	gk	1	Total	C	N	O	0
			86	66	8	12	
26	gl	1	Total	C	N	O	0
			86	66	8	12	
26	gl	1	Total	C	N	O	0
			86	66	8	12	
26	gm	1	Total	C	N	O	0
			86	66	8	12	
26	gm	1	Total	C	N	O	0
			86	66	8	12	
26	gn	1	Total	C	N	O	0
			86	66	8	12	
26	gn	1	Total	C	N	O	0
			86	66	8	12	
26	go	1	Total	C	N	O	0
			86	66	8	12	
26	go	1	Total	C	N	O	0
			86	66	8	12	
26	gp	1	Total	C	N	O	0
			86	66	8	12	
26	gp	1	Total	C	N	O	0
			86	66	8	12	
26	gq	1	Total	C	N	O	0
			86	66	8	12	
26	gq	1	Total	C	N	O	0
			86	66	8	12	
26	gr	1	Total	C	N	O	0
			43	33	4	6	
26	gs	1	Total	C	N	O	0
			86	66	8	12	
26	gs	1	Total	C	N	O	0
			86	66	8	12	
26	gt	1	Total	C	N	O	0
			86	66	8	12	
26	gt	1	Total	C	N	O	0
			86	66	8	12	
26	gu	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	gu	1	Total	C	N	O	0
			86	66	8	12	
26	gv	1	Total	C	N	O	0
			86	66	8	12	
26	gv	1	Total	C	N	O	0
			86	66	8	12	
26	gw	1	Total	C	N	O	0
			86	66	8	12	
26	gw	1	Total	C	N	O	0
			86	66	8	12	
26	gx	1	Total	C	N	O	0
			86	66	8	12	
26	gx	1	Total	C	N	O	0
			86	66	8	12	
26	gy	1	Total	C	N	O	0
			129	99	12	18	
26	gy	1	Total	C	N	O	0
			129	99	12	18	
26	gy	1	Total	C	N	O	0
			129	99	12	18	
26	gz	1	Total	C	N	O	0
			129	99	12	18	
26	gz	1	Total	C	N	O	0
			129	99	12	18	
26	gz	1	Total	C	N	O	0
			129	99	12	18	
26	hA	1	Total	C	N	O	0
			86	66	8	12	
26	hA	1	Total	C	N	O	0
			86	66	8	12	
26	hB	1	Total	C	N	O	0
			86	66	8	12	
26	hB	1	Total	C	N	O	0
			86	66	8	12	
26	hC	1	Total	C	N	O	0
			86	66	8	12	
26	hC	1	Total	C	N	O	0
			86	66	8	12	
26	hD	1	Total	C	N	O	0
			86	66	8	12	
26	hD	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	hE	1	Total	C	N	O	0
			86	66	8	12	
26	hE	1	Total	C	N	O	0
			86	66	8	12	
26	hF	1	Total	C	N	O	0
			86	66	8	12	
26	hF	1	Total	C	N	O	0
			86	66	8	12	
26	hG	1	Total	C	N	O	0
			43	33	4	6	
26	hH	1	Total	C	N	O	0
			86	66	8	12	
26	hH	1	Total	C	N	O	0
			86	66	8	12	
26	hI	1	Total	C	N	O	0
			86	66	8	12	
26	hI	1	Total	C	N	O	0
			86	66	8	12	
26	hJ	1	Total	C	N	O	0
			86	66	8	12	
26	hJ	1	Total	C	N	O	0
			86	66	8	12	
26	hK	1	Total	C	N	O	0
			86	66	8	12	
26	hK	1	Total	C	N	O	0
			86	66	8	12	
26	hL	1	Total	C	N	O	0
			86	66	8	12	
26	hL	1	Total	C	N	O	0
			86	66	8	12	
26	hM	1	Total	C	N	O	0
			86	66	8	12	
26	hM	1	Total	C	N	O	0
			86	66	8	12	
26	hN	1	Total	C	N	O	0
			86	66	8	12	
26	hN	1	Total	C	N	O	0
			86	66	8	12	
26	hO	1	Total	C	N	O	0
			86	66	8	12	
26	hO	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	hP	1	Total	C	N	O	0
			86	66	8	12	
26	hP	1	Total	C	N	O	0
			86	66	8	12	
26	hQ	1	Total	C	N	O	0
			86	66	8	12	
26	hQ	1	Total	C	N	O	0
			86	66	8	12	
26	hR	1	Total	C	N	O	0
			86	66	8	12	
26	hR	1	Total	C	N	O	0
			86	66	8	12	
26	hS	1	Total	C	N	O	0
			86	66	8	12	
26	hS	1	Total	C	N	O	0
			86	66	8	12	
26	hT	1	Total	C	N	O	0
			129	99	12	18	
26	hT	1	Total	C	N	O	0
			129	99	12	18	
26	hT	1	Total	C	N	O	0
			129	99	12	18	
26	hU	1	Total	C	N	O	0
			43	33	4	6	
26	hV	1	Total	C	N	O	0
			86	66	8	12	
26	hV	1	Total	C	N	O	0
			86	66	8	12	
26	hW	1	Total	C	N	O	0
			86	66	8	12	
26	hW	1	Total	C	N	O	0
			86	66	8	12	
26	hX	1	Total	C	N	O	0
			86	66	8	12	
26	hX	1	Total	C	N	O	0
			86	66	8	12	
26	hY	1	Total	C	N	O	0
			129	99	12	18	
26	hY	1	Total	C	N	O	0
			129	99	12	18	
26	hY	1	Total	C	N	O	0
			129	99	12	18	

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Mol	Chain	Residues	Atoms				AltConf
26	hZ	1	Total	C	N	O	0
			86	66	8	12	
26	hZ	1	Total	C	N	O	0
			86	66	8	12	
26	iA	1	Total	C	N	O	0
			86	66	8	12	
26	iA	1	Total	C	N	O	0
			86	66	8	12	
26	iB	1	Total	C	N	O	0
			86	66	8	12	
26	iB	1	Total	C	N	O	0
			86	66	8	12	
26	iC	1	Total	C	N	O	0
			86	66	8	12	
26	iC	1	Total	C	N	O	0
			86	66	8	12	
26	iD	1	Total	C	N	O	0
			86	66	8	12	
26	iD	1	Total	C	N	O	0
			86	66	8	12	
26	iE	1	Total	C	N	O	0
			86	66	8	12	
26	iE	1	Total	C	N	O	0
			86	66	8	12	
26	iF	1	Total	C	N	O	0
			86	66	8	12	
26	iF	1	Total	C	N	O	0
			86	66	8	12	
26	iG	1	Total	C	N	O	0
			43	33	4	6	
26	iH	1	Total	C	N	O	0
			43	33	4	6	
26	jI	1	Total	C	N	O	0
			86	66	8	12	
26	jI	1	Total	C	N	O	0
			86	66	8	12	
26	jJ	1	Total	C	N	O	0
			86	66	8	12	
26	jJ	1	Total	C	N	O	0
			86	66	8	12	
26	jK	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
26	jK	1	Total	C	N	O	0
			86	66	8	12	
26	jL	1	Total	C	N	O	0
			86	66	8	12	
26	jL	1	Total	C	N	O	0
			86	66	8	12	
26	jM	1	Total	C	N	O	0
			86	66	8	12	
26	jM	1	Total	C	N	O	0
			86	66	8	12	
26	jN	1	Total	C	N	O	0
			86	66	8	12	
26	jN	1	Total	C	N	O	0
			86	66	8	12	
26	jO	1	Total	C	N	O	0
			86	66	8	12	
26	jO	1	Total	C	N	O	0
			86	66	8	12	
26	jP	1	Total	C	N	O	0
			86	66	8	12	
26	jP	1	Total	C	N	O	0
			86	66	8	12	
26	kQ	1	Total	C	N	O	0
			86	66	8	12	
26	kQ	1	Total	C	N	O	0
			86	66	8	12	
26	kR	1	Total	C	N	O	0
			86	66	8	12	
26	kR	1	Total	C	N	O	0
			86	66	8	12	
26	kS	1	Total	C	N	O	0
			86	66	8	12	
26	kS	1	Total	C	N	O	0
			86	66	8	12	
26	kT	1	Total	C	N	O	0
			86	66	8	12	
26	kT	1	Total	C	N	O	0
			86	66	8	12	
26	kU	1	Total	C	N	O	0
			86	66	8	12	
26	kU	1	Total	C	N	O	0
			86	66	8	12	

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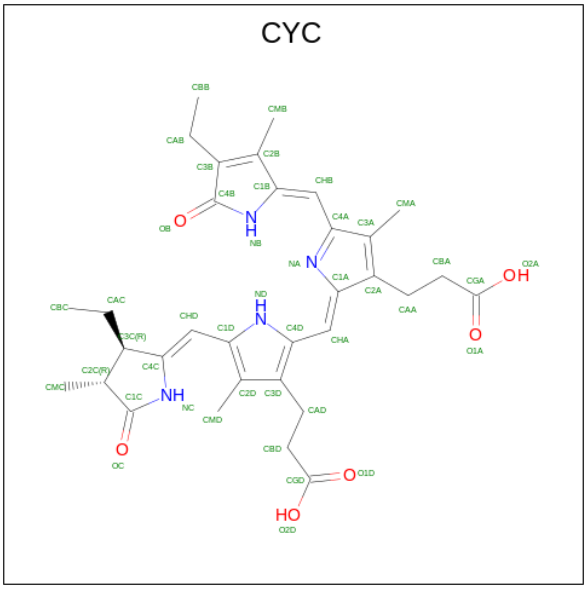
Mol	Chain	Residues	Atoms				AltConf
26	kV	1	Total	C	N	O	0
			86	66	8	12	
26	kV	1	Total	C	N	O	0
			86	66	8	12	
26	kW	1	Total	C	N	O	0
			86	66	8	12	
26	kW	1	Total	C	N	O	0
			86	66	8	12	
26	kX	1	Total	C	N	O	0
			86	66	8	12	
26	kX	1	Total	C	N	O	0
			86	66	8	12	

- Molecule 27 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
27	G1	1	Total	C	N	O	0
			43	33	4	6	
27	H1	1	Total	C	N	O	0
			43	33	4	6	
27	I1	1	Total	C	N	O	0
			43	33	4	6	
27	J1	1	Total	C	N	O	0
			43	33	4	6	
27	K1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
27	L1	1	Total	C	N	O	0
			43	33	4	6	
27	M1	1	Total	C	N	O	0
			43	33	4	6	
27	N1	1	Total	C	N	O	0
			43	33	4	6	
27	O1	1	Total	C	N	O	0
			43	33	4	6	
27	P1	1	Total	C	N	O	0
			43	33	4	6	
27	Q1	1	Total	C	N	O	0
			43	33	4	6	
27	R1	1	Total	C	N	O	0
			43	33	4	6	
27	S1	1	Total	C	N	O	0
			86	66	8	12	
27	S1	1	Total	C	N	O	0
			86	66	8	12	
27	U1	1	Total	C	N	O	0
			43	33	4	6	
27	V1	1	Total	C	N	O	0
			43	33	4	6	
27	W1	1	Total	C	N	O	0
			43	33	4	6	
27	X1	1	Total	C	N	O	0
			43	33	4	6	
27	Y1	1	Total	C	N	O	0
			43	33	4	6	
27	Z1	1	Total	C	N	O	0
			43	33	4	6	
27	a1	1	Total	C	N	O	0
			43	33	4	6	
27	b1	1	Total	C	N	O	0
			43	33	4	6	
27	c1	1	Total	C	N	O	0
			43	33	4	6	
27	d1	1	Total	C	N	O	0
			43	33	4	6	
27	e1	1	Total	C	N	O	0
			43	33	4	6	
27	f1	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
27	g1	1	Total	C	N	O	0
			43	33	4	6	
27	h1	1	Total	C	N	O	0
			43	33	4	6	
27	i1	1	Total	C	N	O	0
			43	33	4	6	
27	j1	1	Total	C	N	O	0
			43	33	4	6	
27	k1	1	Total	C	N	O	0
			43	33	4	6	
27	m1	1	Total	C	N	O	0
			43	33	4	6	
27	n1	1	Total	C	N	O	0
			43	33	4	6	
27	o1	1	Total	C	N	O	0
			43	33	4	6	
27	p1	1	Total	C	N	O	0
			43	33	4	6	
27	q1	1	Total	C	N	O	0
			43	33	4	6	
27	r1	1	Total	C	N	O	0
			43	33	4	6	
27	s1	1	Total	C	N	O	0
			43	33	4	6	
27	t1	1	Total	C	N	O	0
			43	33	4	6	
27	u1	1	Total	C	N	O	0
			43	33	4	6	
27	v1	1	Total	C	N	O	0
			43	33	4	6	
27	w1	1	Total	C	N	O	0
			43	33	4	6	
27	y1	1	Total	C	N	O	0
			43	33	4	6	
27	z1	1	Total	C	N	O	0
			43	33	4	6	
27	a2	1	Total	C	N	O	0
			86	66	8	12	
27	a2	1	Total	C	N	O	0
			86	66	8	12	
27	b2	1	Total	C	N	O	0
			43	33	4	6	

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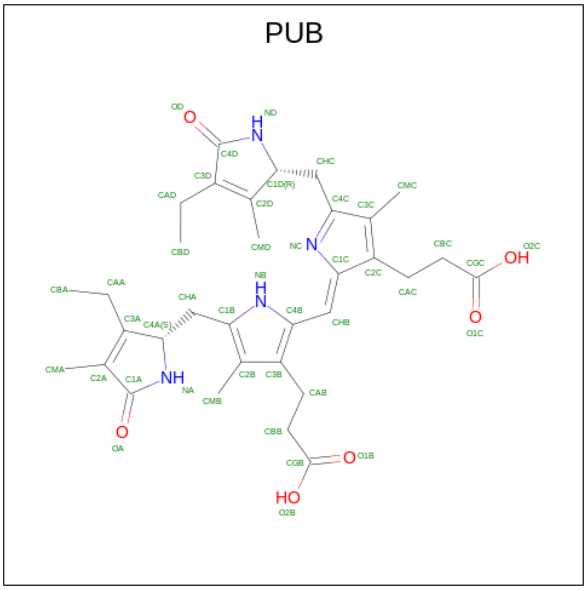
Mol	Chain	Residues	Atoms				AltConf
27	d2	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 28 is PHYCOUROBILIN (three-letter code: PUB) (formula: $C_{33}H_{42}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
28	f2	1	Total	C	N	O	0
			43	33	4	6	
28	h2	1	Total	C	N	O	0
			43	33	4	6	
28	j2	1	Total	C	N	O	0
			43	33	4	6	
28	l2	1	Total	C	N	O	0
			43	33	4	6	
28	n2	1	Total	C	N	O	0
			43	33	4	6	
28	p2	1	Total	C	N	O	0
			43	33	4	6	
28	r2	1	Total	C	N	O	0
			43	33	4	6	
28	t2	1	Total	C	N	O	0
			43	33	4	6	
28	v2	1	Total	C	N	O	0
			43	33	4	6	
28	x2	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	z2	1	Total	C	N	O	0
			43	33	4	6	
28	A2	1	Total	C	N	O	0
			86	66	8	12	
28	A2	1	Total	C	N	O	0
			86	66	8	12	
28	C2	1	Total	C	N	O	0
			86	66	8	12	
28	C2	1	Total	C	N	O	0
			86	66	8	12	
28	D2	1	Total	C	N	O	0
			86	66	8	12	
28	D2	1	Total	C	N	O	0
			86	66	8	12	
28	F2	1	Total	C	N	O	0
			43	33	4	6	
28	H2	1	Total	C	N	O	0
			43	33	4	6	
28	J2	1	Total	C	N	O	0
			43	33	4	6	
28	L2	1	Total	C	N	O	0
			43	33	4	6	
28	N2	1	Total	C	N	O	0
			43	33	4	6	
28	P2	1	Total	C	N	O	0
			43	33	4	6	
28	R2	1	Total	C	N	O	0
			43	33	4	6	
28	T2	1	Total	C	N	O	0
			43	33	4	6	
28	V2	1	Total	C	N	O	0
			43	33	4	6	
28	X2	1	Total	C	N	O	0
			43	33	4	6	
28	Z2	1	Total	C	N	O	0
			43	33	4	6	
28	B3	1	Total	C	N	O	0
			43	33	4	6	
28	D3	1	Total	C	N	O	0
			43	33	4	6	
28	F3	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	H3	1	Total	C	N	O	0
			43	33	4	6	
28	J3	1	Total	C	N	O	0
			43	33	4	6	
28	L3	1	Total	C	N	O	0
			43	33	4	6	
28	N3	1	Total	C	N	O	0
			43	33	4	6	
28	P3	1	Total	C	N	O	0
			43	33	4	6	
28	R3	1	Total	C	N	O	0
			43	33	4	6	
28	T3	1	Total	C	N	O	0
			43	33	4	6	
28	V3	1	Total	C	N	O	0
			43	33	4	6	
28	X3	1	Total	C	N	O	0
			43	33	4	6	
28	Z3	1	Total	C	N	O	0
			43	33	4	6	
28	a3	1	Total	C	N	O	0
			86	66	8	12	
28	a3	1	Total	C	N	O	0
			86	66	8	12	
28	c3	1	Total	C	N	O	0
			86	66	8	12	
28	c3	1	Total	C	N	O	0
			86	66	8	12	
28	d3	1	Total	C	N	O	0
			86	66	8	12	
28	d3	1	Total	C	N	O	0
			86	66	8	12	
28	f3	1	Total	C	N	O	0
			43	33	4	6	
28	h3	1	Total	C	N	O	0
			43	33	4	6	
28	j3	1	Total	C	N	O	0
			43	33	4	6	
28	l3	1	Total	C	N	O	0
			43	33	4	6	
28	n3	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	p3	1	Total	C	N	O	0
			43	33	4	6	
28	r3	1	Total	C	N	O	0
			43	33	4	6	
28	t3	1	Total	C	N	O	0
			43	33	4	6	
28	v3	1	Total	C	N	O	0
			43	33	4	6	
28	x3	1	Total	C	N	O	0
			43	33	4	6	
28	z3	1	Total	C	N	O	0
			43	33	4	6	
28	B4	1	Total	C	N	O	0
			43	33	4	6	
28	D4	1	Total	C	N	O	0
			43	33	4	6	
28	F4	1	Total	C	N	O	0
			43	33	4	6	
28	H4	1	Total	C	N	O	0
			43	33	4	6	
28	J4	1	Total	C	N	O	0
			43	33	4	6	
28	L4	1	Total	C	N	O	0
			43	33	4	6	
28	N4	1	Total	C	N	O	0
			43	33	4	6	
28	P4	1	Total	C	N	O	0
			43	33	4	6	
28	R4	1	Total	C	N	O	0
			43	33	4	6	
28	T4	1	Total	C	N	O	0
			43	33	4	6	
28	V4	1	Total	C	N	O	0
			43	33	4	6	
28	X4	1	Total	C	N	O	0
			43	33	4	6	
28	Z4	1	Total	C	N	O	0
			43	33	4	6	
28	34	1	Total	C	N	O	0
			86	66	8	12	
28	34	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
28	44	1	Total	C	N	O	0
			86	66	8	12	
28	44	1	Total	C	N	O	0
			86	66	8	12	
28	n4	1	Total	C	N	O	0
			43	33	4	6	
28	p4	1	Total	C	N	O	0
			43	33	4	6	
28	r4	1	Total	C	N	O	0
			43	33	4	6	
28	t4	1	Total	C	N	O	0
			43	33	4	6	
28	v4	1	Total	C	N	O	0
			43	33	4	6	
28	x4	1	Total	C	N	O	0
			43	33	4	6	
28	z4	1	Total	C	N	O	0
			43	33	4	6	
28	B5	1	Total	C	N	O	0
			43	33	4	6	
28	D5	1	Total	C	N	O	0
			43	33	4	6	
28	F5	1	Total	C	N	O	0
			43	33	4	6	
28	H5	1	Total	C	N	O	0
			43	33	4	6	
28	J5	1	Total	C	N	O	0
			43	33	4	6	
28	L5	1	Total	C	N	O	0
			43	33	4	6	
28	N5	1	Total	C	N	O	0
			43	33	4	6	
28	P5	1	Total	C	N	O	0
			43	33	4	6	
28	R5	1	Total	C	N	O	0
			43	33	4	6	
28	T5	1	Total	C	N	O	0
			43	33	4	6	
28	V5	1	Total	C	N	O	0
			43	33	4	6	
28	Y5	1	Total	C	N	O	0
			86	66	8	12	

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Mol	Chain	Residues	Atoms				AltConf
28	Y5	1	Total	C	N	O	0
			86	66	8	12	
28	Z5	1	Total	C	N	O	0
			86	66	8	12	
28	Z5	1	Total	C	N	O	0
			86	66	8	12	
28	n5	1	Total	C	N	O	0
			43	33	4	6	
28	p5	1	Total	C	N	O	0
			43	33	4	6	
28	r5	1	Total	C	N	O	0
			43	33	4	6	
28	t5	1	Total	C	N	O	0
			43	33	4	6	
28	v5	1	Total	C	N	O	0
			43	33	4	6	
28	x5	1	Total	C	N	O	0
			43	33	4	6	
28	z5	1	Total	C	N	O	0
			43	33	4	6	
28	f8	1	Total	C	N	O	0
			43	33	4	6	
28	g8	1	Total	C	N	O	0
			43	33	4	6	
28	h8	1	Total	C	N	O	0
			43	33	4	6	
28	B6	1	Total	C	N	O	0
			43	33	4	6	
28	D6	1	Total	C	N	O	0
			43	33	4	6	
28	F6	1	Total	C	N	O	0
			43	33	4	6	
28	H6	1	Total	C	N	O	0
			43	33	4	6	
28	J6	1	Total	C	N	O	0
			43	33	4	6	
28	L6	1	Total	C	N	O	0
			43	33	4	6	
28	N6	1	Total	C	N	O	0
			43	33	4	6	
28	P6	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	R6	1	Total	C	N	O	0
			43	33	4	6	
28	T6	1	Total	C	N	O	0
			43	33	4	6	
28	V6	1	Total	C	N	O	0
			43	33	4	6	
28	X6	1	Total	C	N	O	0
			43	33	4	6	
28	Z6	1	Total	C	N	O	0
			43	33	4	6	
28	a6	1	Total	C	N	O	0
			43	33	4	6	
28	b6	1	Total	C	N	O	0
			43	33	4	6	
28	c6	1	Total	C	N	O	0
			43	33	4	6	
28	d6	1	Total	C	N	O	0
			43	33	4	6	
28	e6	1	Total	C	N	O	0
			43	33	4	6	
28	l6	1	Total	C	N	O	0
			43	33	4	6	
28	n6	1	Total	C	N	O	0
			43	33	4	6	
28	p6	1	Total	C	N	O	0
			43	33	4	6	
28	r6	1	Total	C	N	O	0
			43	33	4	6	
28	t6	1	Total	C	N	O	0
			43	33	4	6	
28	u6	1	Total	C	N	O	0
			43	33	4	6	
28	v6	1	Total	C	N	O	0
			43	33	4	6	
28	x6	1	Total	C	N	O	0
			43	33	4	6	
28	y6	1	Total	C	N	O	0
			43	33	4	6	
28	z6	1	Total	C	N	O	0
			43	33	4	6	
28	n8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	o8	1	Total	C	N	O	0
			43	33	4	6	
28	p8	1	Total	C	N	O	0
			43	33	4	6	
28	B7	1	Total	C	N	O	0
			43	33	4	6	
28	D7	1	Total	C	N	O	0
			43	33	4	6	
28	F7	1	Total	C	N	O	0
			43	33	4	6	
28	H7	1	Total	C	N	O	0
			43	33	4	6	
28	J7	1	Total	C	N	O	0
			43	33	4	6	
28	L7	1	Total	C	N	O	0
			43	33	4	6	
28	N7	1	Total	C	N	O	0
			43	33	4	6	
28	P7	1	Total	C	N	O	0
			43	33	4	6	
28	R7	1	Total	C	N	O	0
			43	33	4	6	
28	T7	1	Total	C	N	O	0
			43	33	4	6	
28	V7	1	Total	C	N	O	0
			43	33	4	6	
28	X7	1	Total	C	N	O	0
			43	33	4	6	
28	Z7	1	Total	C	N	O	0
			43	33	4	6	
28	a7	1	Total	C	N	O	0
			43	33	4	6	
28	b7	1	Total	C	N	O	0
			43	33	4	6	
28	c7	1	Total	C	N	O	0
			43	33	4	6	
28	d7	1	Total	C	N	O	0
			43	33	4	6	
28	e7	1	Total	C	N	O	0
			43	33	4	6	
28	l7	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	n7	1	Total	C	N	O	0
			43	33	4	6	
28	p7	1	Total	C	N	O	0
			43	33	4	6	
28	r7	1	Total	C	N	O	0
			43	33	4	6	
28	s7	1	Total	C	N	O	0
			43	33	4	6	
28	t7	1	Total	C	N	O	0
			43	33	4	6	
28	v7	1	Total	C	N	O	0
			43	33	4	6	
28	x7	1	Total	C	N	O	0
			43	33	4	6	
28	y7	1	Total	C	N	O	0
			43	33	4	6	
28	z7	1	Total	C	N	O	0
			43	33	4	6	
28	b8	1	Total	C	N	O	0
			86	66	8	12	
28	b8	1	Total	C	N	O	0
			86	66	8	12	
28	c8	1	Total	C	N	O	0
			86	66	8	12	
28	c8	1	Total	C	N	O	0
			86	66	8	12	
28	d8	1	Total	C	N	O	0
			43	33	4	6	
28	e8	1	Total	C	N	O	0
			86	66	8	12	
28	e8	1	Total	C	N	O	0
			86	66	8	12	
28	b9	1	Total	C	N	O	0
			86	66	8	12	
28	b9	1	Total	C	N	O	0
			86	66	8	12	
28	c9	1	Total	C	N	O	0
			86	66	8	12	
28	c9	1	Total	C	N	O	0
			86	66	8	12	
28	d9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	e9	1	Total	C	N	O	0
			86	66	8	12	
28	e9	1	Total	C	N	O	0
			86	66	8	12	
28	w8	1	Total	C	N	O	0
			43	33	4	6	
28	y8	1	Total	C	N	O	0
			43	33	4	6	
28	A8	1	Total	C	N	O	0
			43	33	4	6	
28	C8	1	Total	C	N	O	0
			43	33	4	6	
28	E8	1	Total	C	N	O	0
			43	33	4	6	
28	G8	1	Total	C	N	O	0
			43	33	4	6	
28	I8	1	Total	C	N	O	0
			43	33	4	6	
28	K8	1	Total	C	N	O	0
			43	33	4	6	
28	M8	1	Total	C	N	O	0
			43	33	4	6	
28	O8	1	Total	C	N	O	0
			43	33	4	6	
28	Q8	1	Total	C	N	O	0
			43	33	4	6	
28	T8	1	Total	C	N	O	0
			86	66	8	12	
28	T8	1	Total	C	N	O	0
			86	66	8	12	
28	U8	1	Total	C	N	O	0
			86	66	8	12	
28	U8	1	Total	C	N	O	0
			86	66	8	12	
28	n9	1	Total	C	N	O	0
			43	33	4	6	
28	p9	1	Total	C	N	O	0
			43	33	4	6	
28	r9	1	Total	C	N	O	0
			43	33	4	6	
28	t9	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	v9	1	Total	C	N	O	0
			43	33	4	6	
28	x9	1	Total	C	N	O	0
			43	33	4	6	
28	z9	1	Total	C	N	O	0
			43	33	4	6	
28	B9	1	Total	C	N	O	0
			43	33	4	6	
28	D9	1	Total	C	N	O	0
			43	33	4	6	
28	F9	1	Total	C	N	O	0
			43	33	4	6	
28	H9	1	Total	C	N	O	0
			43	33	4	6	
28	J9	1	Total	C	N	O	0
			43	33	4	6	
28	L9	1	Total	C	N	O	0
			43	33	4	6	
28	N9	1	Total	C	N	O	0
			43	33	4	6	
28	P9	1	Total	C	N	O	0
			43	33	4	6	
28	R9	1	Total	C	N	O	0
			43	33	4	6	
28	T9	1	Total	C	N	O	0
			43	33	4	6	
28	V9	1	Total	C	N	O	0
			43	33	4	6	
28	Y9	1	Total	C	N	O	0
			86	66	8	12	
28	Y9	1	Total	C	N	O	0
			86	66	8	12	
28	Z9	1	Total	C	N	O	0
			86	66	8	12	
28	Z9	1	Total	C	N	O	0
			86	66	8	12	
28	an	1	Total	C	N	O	0
			43	33	4	6	
28	ap	1	Total	C	N	O	0
			43	33	4	6	
28	ar	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	at	1	Total	C	N	O	0
			43	33	4	6	
28	av	1	Total	C	N	O	0
			43	33	4	6	
28	ax	1	Total	C	N	O	0
			43	33	4	6	
28	az	1	Total	C	N	O	0
			43	33	4	6	
28	aB	1	Total	C	N	O	0
			43	33	4	6	
28	aD	1	Total	C	N	O	0
			43	33	4	6	
28	aF	1	Total	C	N	O	0
			43	33	4	6	
28	aH	1	Total	C	N	O	0
			43	33	4	6	
28	aJ	1	Total	C	N	O	0
			43	33	4	6	
28	aL	1	Total	C	N	O	0
			43	33	4	6	
28	aN	1	Total	C	N	O	0
			43	33	4	6	
28	aP	1	Total	C	N	O	0
			43	33	4	6	
28	aR	1	Total	C	N	O	0
			43	33	4	6	
28	aT	1	Total	C	N	O	0
			43	33	4	6	
28	aV	1	Total	C	N	O	0
			43	33	4	6	
28	aY	1	Total	C	N	O	0
			86	66	8	12	
28	aY	1	Total	C	N	O	0
			86	66	8	12	
28	aZ	1	Total	C	N	O	0
			86	66	8	12	
28	aZ	1	Total	C	N	O	0
			86	66	8	12	
28	bn	1	Total	C	N	O	0
			43	33	4	6	
28	bo	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	bp	1	Total	C	N	O	0
			43	33	4	6	
28	bq	1	Total	C	N	O	0
			43	33	4	6	
28	br	1	Total	C	N	O	0
			43	33	4	6	
28	bs	1	Total	C	N	O	0
			43	33	4	6	
28	bz	1	Total	C	N	O	0
			43	33	4	6	
28	bB	1	Total	C	N	O	0
			43	33	4	6	
28	bD	1	Total	C	N	O	0
			43	33	4	6	
28	bF	1	Total	C	N	O	0
			43	33	4	6	
28	bH	1	Total	C	N	O	0
			43	33	4	6	
28	bJ	1	Total	C	N	O	0
			43	33	4	6	
28	bL	1	Total	C	N	O	0
			43	33	4	6	
28	bN	1	Total	C	N	O	0
			43	33	4	6	
28	bP	1	Total	C	N	O	0
			43	33	4	6	
28	bR	1	Total	C	N	O	0
			43	33	4	6	
28	bT	1	Total	C	N	O	0
			43	33	4	6	
28	bV	1	Total	C	N	O	0
			43	33	4	6	
28	bY	1	Total	C	N	O	0
			86	66	8	12	
28	bY	1	Total	C	N	O	0
			86	66	8	12	
28	bZ	1	Total	C	N	O	0
			86	66	8	12	
28	bZ	1	Total	C	N	O	0
			86	66	8	12	
28	cn	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	co	1	Total	C	N	O	0
			43	33	4	6	
28	cp	1	Total	C	N	O	0
			43	33	4	6	
28	cq	1	Total	C	N	O	0
			43	33	4	6	
28	cr	1	Total	C	N	O	0
			43	33	4	6	
28	cs	1	Total	C	N	O	0
			43	33	4	6	
28	cz	1	Total	C	N	O	0
			43	33	4	6	
28	cB	1	Total	C	N	O	0
			43	33	4	6	
28	cE	1	Total	C	N	O	0
			43	33	4	6	
28	cF	1	Total	C	N	O	0
			43	33	4	6	
28	cH	1	Total	C	N	O	0
			43	33	4	6	
28	cJ	1	Total	C	N	O	0
			43	33	4	6	
28	cL	1	Total	C	N	O	0
			43	33	4	6	
28	cM	1	Total	C	N	O	0
			43	33	4	6	
28	cN	1	Total	C	N	O	0
			43	33	4	6	
28	cO	1	Total	C	N	O	0
			43	33	4	6	
28	cP	1	Total	C	N	O	0
			43	33	4	6	
28	cQ	1	Total	C	N	O	0
			43	33	4	6	
28	cR	1	Total	C	N	O	0
			43	33	4	6	
28	cY	1	Total	C	N	O	0
			43	33	4	6	
28	dd	1	Total	C	N	O	0
			43	33	4	6	
28	df	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	dh	1	Total	C	N	O	0
			43	33	4	6	
28	di	1	Total	C	N	O	0
			43	33	4	6	
28	dj	1	Total	C	N	O	0
			43	33	4	6	
28	dl	1	Total	C	N	O	0
			43	33	4	6	
28	dn	1	Total	C	N	O	0
			43	33	4	6	
28	dp	1	Total	C	N	O	0
			43	33	4	6	
28	dr	1	Total	C	N	O	0
			43	33	4	6	
28	dt	1	Total	C	N	O	0
			43	33	4	6	
28	dv	1	Total	C	N	O	0
			43	33	4	6	
28	dw	1	Total	C	N	O	0
			86	66	8	12	
28	dw	1	Total	C	N	O	0
			86	66	8	12	
28	dx	1	Total	C	N	O	0
			86	66	8	12	
28	dx	1	Total	C	N	O	0
			86	66	8	12	
28	dB	1	Total	C	N	O	0
			43	33	4	6	
28	dD	1	Total	C	N	O	0
			43	33	4	6	
28	dF	1	Total	C	N	O	0
			43	33	4	6	
28	dH	1	Total	C	N	O	0
			43	33	4	6	
28	dK	1	Total	C	N	O	0
			43	33	4	6	
28	dL	1	Total	C	N	O	0
			43	33	4	6	
28	dN	1	Total	C	N	O	0
			43	33	4	6	
28	dP	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	dR	1	Total	C	N	O	0
			43	33	4	6	
28	dT	1	Total	C	N	O	0
			43	33	4	6	
28	dV	1	Total	C	N	O	0
			43	33	4	6	
28	dX	1	Total	C	N	O	0
			43	33	4	6	
28	dY	1	Total	C	N	O	0
			43	33	4	6	
28	eb	1	Total	C	N	O	0
			43	33	4	6	
28	ec	1	Total	C	N	O	0
			43	33	4	6	
28	ee	1	Total	C	N	O	0
			43	33	4	6	
28	eg	1	Total	C	N	O	0
			43	33	4	6	
28	ei	1	Total	C	N	O	0
			43	33	4	6	
28	el	1	Total	C	N	O	0
			43	33	4	6	
28	en	1	Total	C	N	O	0
			43	33	4	6	
28	ep	1	Total	C	N	O	0
			43	33	4	6	
28	er	1	Total	C	N	O	0
			43	33	4	6	
28	et	1	Total	C	N	O	0
			43	33	4	6	
28	ev	1	Total	C	N	O	0
			43	33	4	6	
28	ey	1	Total	C	N	O	0
			86	66	8	12	
28	ey	1	Total	C	N	O	0
			86	66	8	12	
28	ez	1	Total	C	N	O	0
			86	66	8	12	
28	ez	1	Total	C	N	O	0
			86	66	8	12	
28	eB	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	eD	1	Total	C	N	O	0
			43	33	4	6	
28	eF	1	Total	C	N	O	0
			43	33	4	6	
28	eH	1	Total	C	N	O	0
			43	33	4	6	
28	eJ	1	Total	C	N	O	0
			43	33	4	6	
28	eL	1	Total	C	N	O	0
			43	33	4	6	
28	eN	1	Total	C	N	O	0
			43	33	4	6	
28	eP	1	Total	C	N	O	0
			43	33	4	6	
28	eR	1	Total	C	N	O	0
			43	33	4	6	
28	eT	1	Total	C	N	O	0
			43	33	4	6	
28	eV	1	Total	C	N	O	0
			43	33	4	6	
28	eX	1	Total	C	N	O	0
			43	33	4	6	
28	eY	1	Total	C	N	O	0
			86	66	8	12	
28	eY	1	Total	C	N	O	0
			86	66	8	12	
28	eZ	1	Total	C	N	O	0
			86	66	8	12	
28	eZ	1	Total	C	N	O	0
			86	66	8	12	
28	lb	1	Total	C	N	O	0
			43	33	4	6	
28	ld	1	Total	C	N	O	0
			43	33	4	6	
28	lf	1	Total	C	N	O	0
			43	33	4	6	
28	lh	1	Total	C	N	O	0
			43	33	4	6	
28	lj	1	Total	C	N	O	0
			43	33	4	6	
28	ll	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	ln	1	Total	C	N	O	0
			43	33	4	6	
28	lp	1	Total	C	N	O	0
			43	33	4	6	
28	lr	1	Total	C	N	O	0
			43	33	4	6	
28	lt	1	Total	C	N	O	0
			43	33	4	6	
28	lv	1	Total	C	N	O	0
			43	33	4	6	
28	lx	1	Total	C	N	O	0
			43	33	4	6	
28	ly	1	Total	C	N	O	0
			86	66	8	12	
28	ly	1	Total	C	N	O	0
			86	66	8	12	
28	lz	1	Total	C	N	O	0
			86	66	8	12	
28	lz	1	Total	C	N	O	0
			86	66	8	12	
28	fa	1	Total	C	N	O	0
			43	33	4	6	
28	fc	1	Total	C	N	O	0
			43	33	4	6	
28	ff	1	Total	C	N	O	0
			43	33	4	6	
28	fi	1	Total	C	N	O	0
			43	33	4	6	
28	fj	1	Total	C	N	O	0
			43	33	4	6	
28	fm	1	Total	C	N	O	0
			43	33	4	6	
28	fo	1	Total	C	N	O	0
			43	33	4	6	
28	fq	1	Total	C	N	O	0
			43	33	4	6	
28	fs	1	Total	C	N	O	0
			43	33	4	6	
28	fu	1	Total	C	N	O	0
			43	33	4	6	
28	fw	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	fy	1	Total	C	N	O	0
			43	33	4	6	
28	ga	1	Total	C	N	O	0
			43	33	4	6	
28	gd	1	Total	C	N	O	0
			43	33	4	6	
28	ge	1	Total	C	N	O	0
			43	33	4	6	
28	gg	1	Total	C	N	O	0
			43	33	4	6	
28	gi	1	Total	C	N	O	0
			43	33	4	6	
28	gk	1	Total	C	N	O	0
			43	33	4	6	
28	gn	1	Total	C	N	O	0
			43	33	4	6	
28	gp	1	Total	C	N	O	0
			43	33	4	6	
28	gr	1	Total	C	N	O	0
			43	33	4	6	
28	gt	1	Total	C	N	O	0
			43	33	4	6	
28	gv	1	Total	C	N	O	0
			43	33	4	6	
28	gx	1	Total	C	N	O	0
			43	33	4	6	
28	gy	1	Total	C	N	O	0
			86	66	8	12	
28	gy	1	Total	C	N	O	0
			86	66	8	12	
28	gz	1	Total	C	N	O	0
			86	66	8	12	
28	gz	1	Total	C	N	O	0
			86	66	8	12	
28	hB	1	Total	C	N	O	0
			43	33	4	6	
28	hD	1	Total	C	N	O	0
			43	33	4	6	
28	hG	1	Total	C	N	O	0
			43	33	4	6	
28	hH	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
28	hJ	1	Total	C	N	O	0
			43	33	4	6	
28	hL	1	Total	C	N	O	0
			43	33	4	6	
28	hN	1	Total	C	N	O	0
			43	33	4	6	
28	hP	1	Total	C	N	O	0
			43	33	4	6	
28	hR	1	Total	C	N	O	0
			43	33	4	6	
28	hT	1	Total	C	N	O	0
			43	33	4	6	
28	hV	1	Total	C	N	O	0
			43	33	4	6	
28	hX	1	Total	C	N	O	0
			43	33	4	6	
28	hY	1	Total	C	N	O	0
			86	66	8	12	
28	hY	1	Total	C	N	O	0
			86	66	8	12	
28	hZ	1	Total	C	N	O	0
			86	66	8	12	
28	hZ	1	Total	C	N	O	0
			86	66	8	12	
28	iC	1	Total	C	N	O	0
			43	33	4	6	
28	iD	1	Total	C	N	O	0
			43	33	4	6	
28	iE	1	Total	C	N	O	0
			43	33	4	6	
28	iF	1	Total	C	N	O	0
			43	33	4	6	
28	iG	1	Total	C	N	O	0
			43	33	4	6	
28	iH	1	Total	C	N	O	0
			43	33	4	6	
28	jI	1	Total	C	N	O	0
			43	33	4	6	
28	jJ	1	Total	C	N	O	0
			43	33	4	6	
28	jK	1	Total	C	N	O	0
			43	33	4	6	

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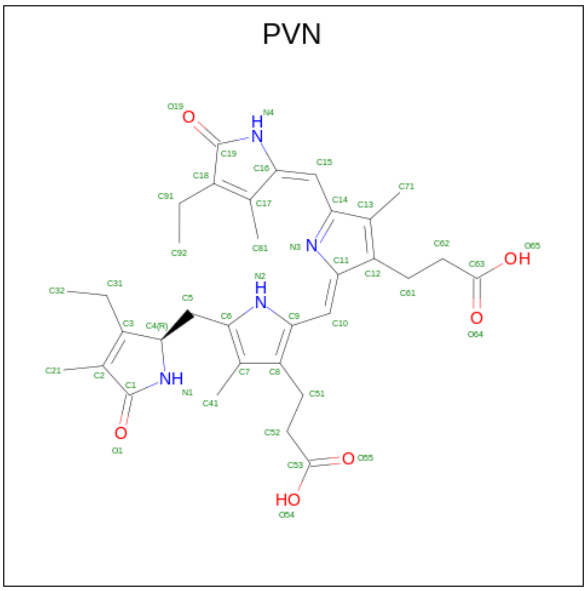
Mol	Chain	Residues	Atoms				AltConf
28	jL	1	Total	C	N	O	0
			43	33	4	6	
28	jM	1	Total	C	N	O	0
			43	33	4	6	
28	jN	1	Total	C	N	O	0
			43	33	4	6	
28	jO	1	Total	C	N	O	0
			43	33	4	6	
28	jP	1	Total	C	N	O	0
			43	33	4	6	
28	kQ	1	Total	C	N	O	0
			43	33	4	6	
28	kR	1	Total	C	N	O	0
			43	33	4	6	
28	kS	1	Total	C	N	O	0
			43	33	4	6	
28	kT	1	Total	C	N	O	0
			43	33	4	6	
28	kU	1	Total	C	N	O	0
			43	33	4	6	
28	kV	1	Total	C	N	O	0
			43	33	4	6	
28	kW	1	Total	C	N	O	0
			43	33	4	6	
28	kX	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 29 is PHYCOVIOLOBILIN (three-letter code: PVN) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
29	A2	1	Total	C	N	O	0
			43	33	4	6	
29	C2	1	Total	C	N	O	0
			43	33	4	6	
29	D2	1	Total	C	N	O	0
			43	33	4	6	
29	a3	1	Total	C	N	O	0
			43	33	4	6	
29	c3	1	Total	C	N	O	0
			43	33	4	6	
29	d3	1	Total	C	N	O	0
			43	33	4	6	
29	34	1	Total	C	N	O	0
			43	33	4	6	
29	44	1	Total	C	N	O	0
			43	33	4	6	
29	Y5	1	Total	C	N	O	0
			43	33	4	6	
29	Z5	1	Total	C	N	O	0
			43	33	4	6	
29	b8	1	Total	C	N	O	0
			43	33	4	6	
29	c8	1	Total	C	N	O	0
			43	33	4	6	
29	d8	1	Total	C	N	O	0
			43	33	4	6	
29	e8	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
29	b9	1	Total	C	N	O	0
			43	33	4	6	
29	c9	1	Total	C	N	O	0
			43	33	4	6	
29	d9	1	Total	C	N	O	0
			43	33	4	6	
29	e9	1	Total	C	N	O	0
			43	33	4	6	
29	T8	1	Total	C	N	O	0
			43	33	4	6	
29	U8	1	Total	C	N	O	0
			43	33	4	6	
29	Y9	1	Total	C	N	O	0
			43	33	4	6	
29	Z9	1	Total	C	N	O	0
			43	33	4	6	
29	aY	1	Total	C	N	O	0
			43	33	4	6	
29	aZ	1	Total	C	N	O	0
			43	33	4	6	
29	bY	1	Total	C	N	O	0
			43	33	4	6	
29	bZ	1	Total	C	N	O	0
			43	33	4	6	
29	dw	1	Total	C	N	O	0
			43	33	4	6	
29	dx	1	Total	C	N	O	0
			43	33	4	6	
29	ey	1	Total	C	N	O	0
			43	33	4	6	
29	ez	1	Total	C	N	O	0
			43	33	4	6	
29	eY	1	Total	C	N	O	0
			43	33	4	6	
29	eZ	1	Total	C	N	O	0
			43	33	4	6	
29	ly	1	Total	C	N	O	0
			43	33	4	6	
29	lz	1	Total	C	N	O	0
			43	33	4	6	
29	gy	1	Total	C	N	O	0
			43	33	4	6	

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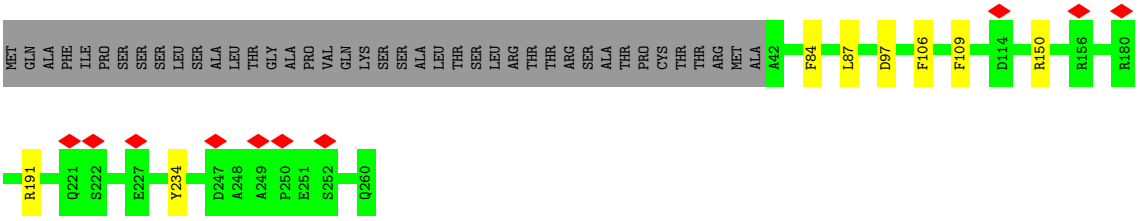
Mol	Chain	Residues	Atoms				AltConf
29	gz	1	Total	C	N	O	0
			43	33	4	6	
29	hY	1	Total	C	N	O	0
			43	33	4	6	
29	hZ	1	Total	C	N	O	0
			43	33	4	6	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

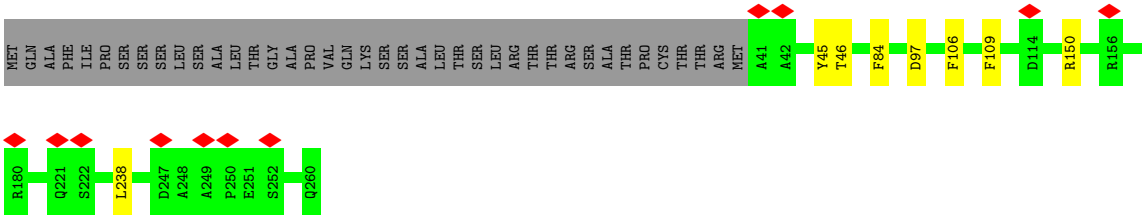
• Molecule 1: LRC6

Chain A1:



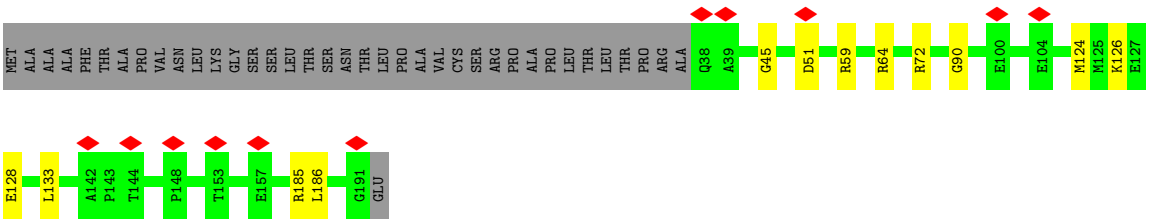
• Molecule 1: LRC6

Chain B1:



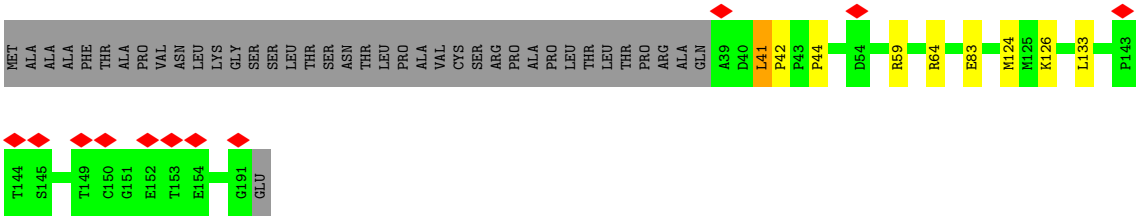
• Molecule 2: LRC4

Chain C1:

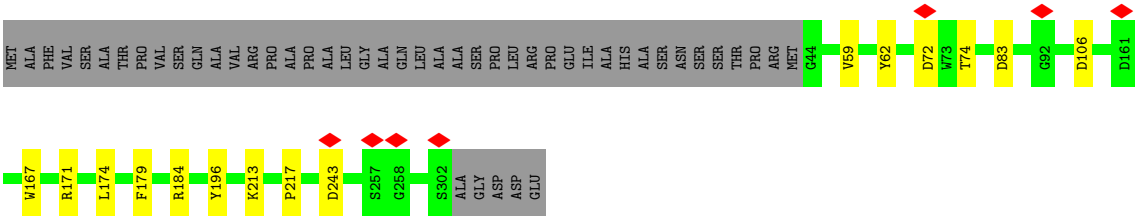


• Molecule 2: LRC4

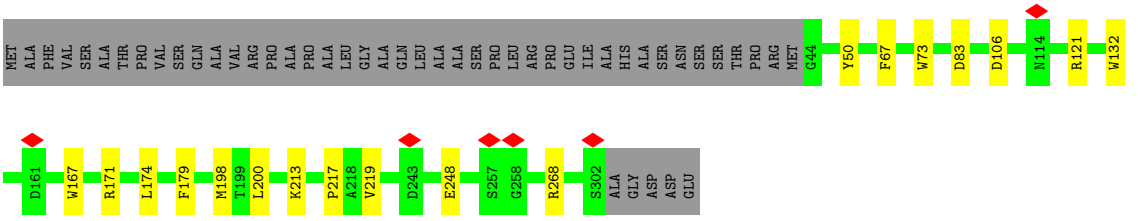
Chain D1:



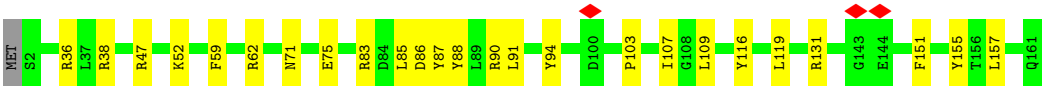
• Molecule 3: LRC5



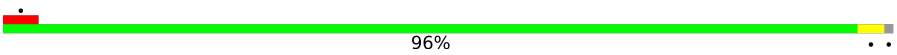
• Molecule 3: LRC5



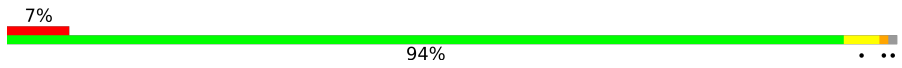
• Molecule 4: alpha_APC

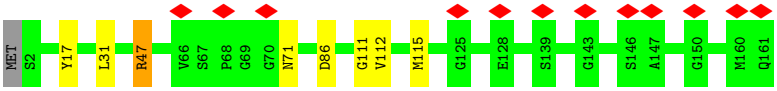


• Molecule 4: alpha_APC



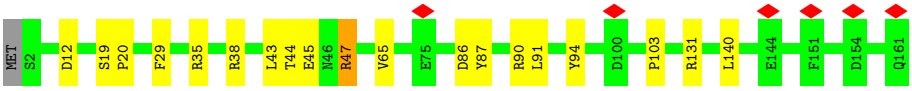
• Molecule 4: alpha_APC





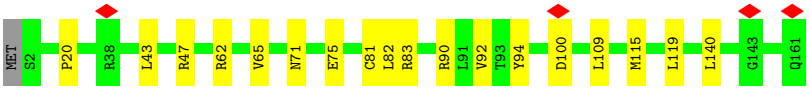
• Molecule 4: alpha_APC

Chain N1:



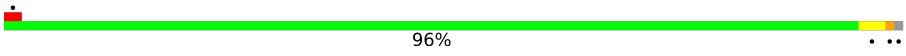
• Molecule 4: alpha_APC

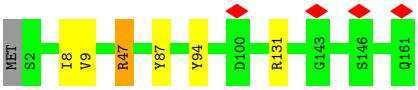
Chain P1:



• Molecule 4: alpha_APC

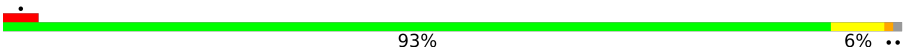
Chain R1:

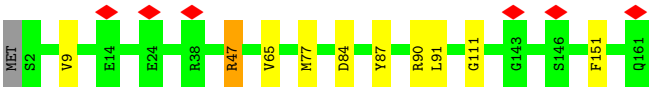




• Molecule 4: alpha_APC

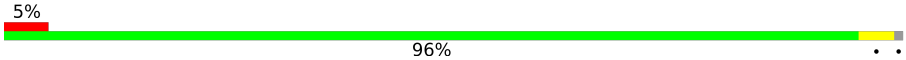
Chain T1:

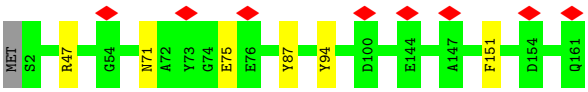




• Molecule 4: alpha_APC

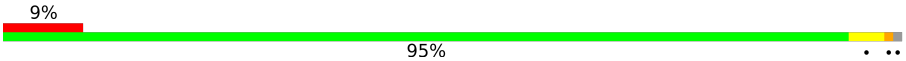
Chain X1:

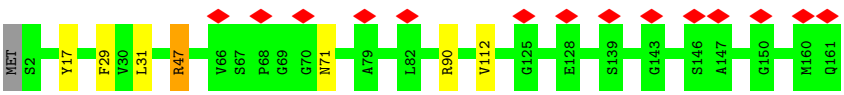




• Molecule 4: alpha_APC

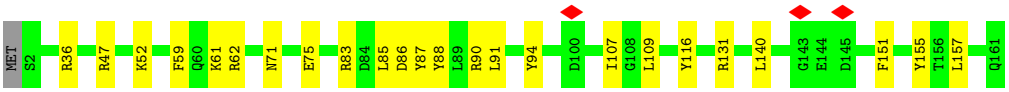
Chain Z1:





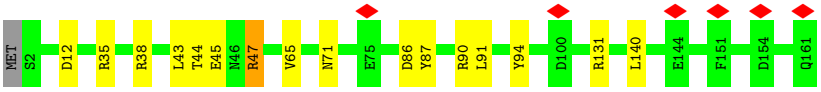
• Molecule 4: alpha_APC

Chain b1:



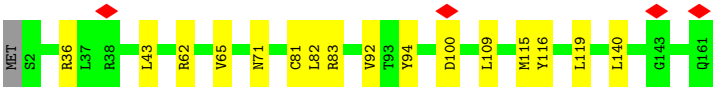
• Molecule 4: alpha_APC

Chain d1:



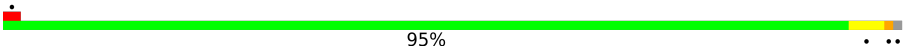
• Molecule 4: alpha_APC

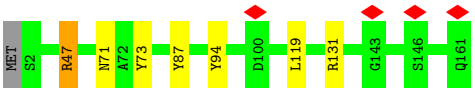
Chain f1:



• Molecule 4: alpha_APC

Chain i1:



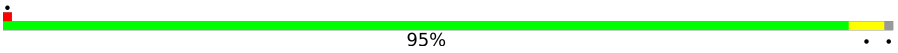


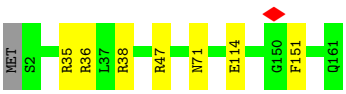
• Molecule 4: alpha_APC

Chain k1:

• Molecule 4: alpha_APC

Chain o1:



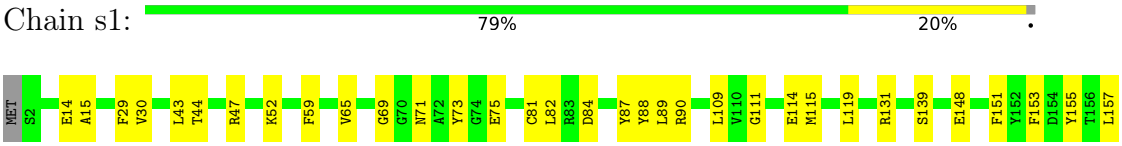


• Molecule 4: alpha_APC

Chain q1:

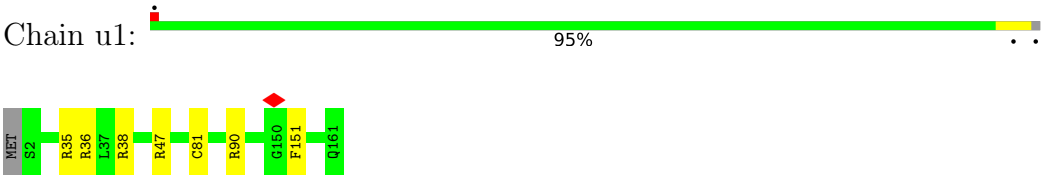
• Molecule 4: alpha_APC

Chain s1:



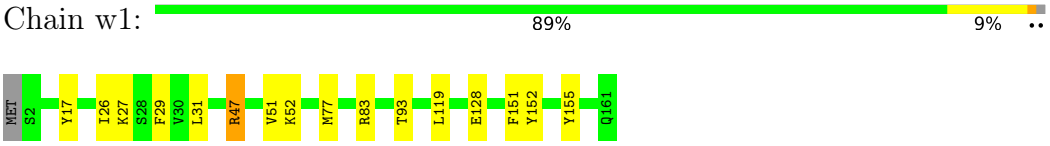
• Molecule 4: alpha_APC

Chain u1:



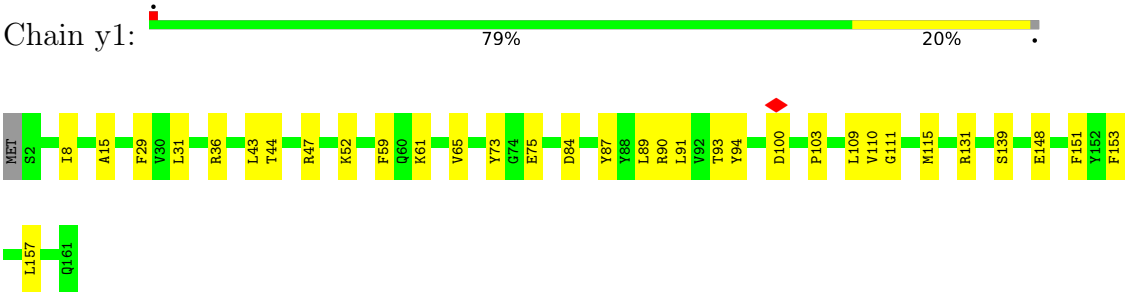
• Molecule 4: alpha_APC

Chain w1:



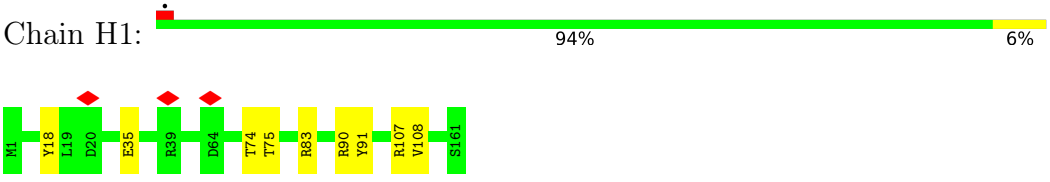
• Molecule 4: alpha_APC

Chain y1:



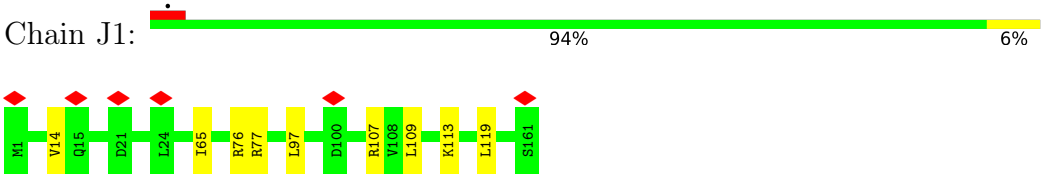
• Molecule 5: beta_APC

Chain H1:



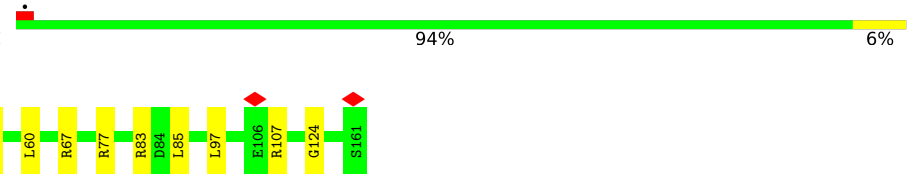
• Molecule 5: beta_APC

Chain J1:



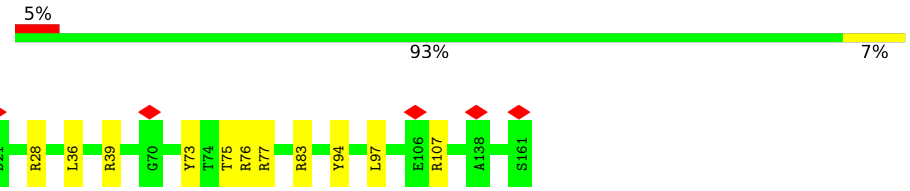
• Molecule 5: beta_APC

Chain L1:



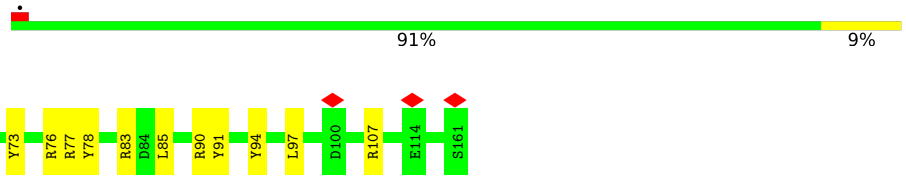
• Molecule 5: beta_APC

Chain M1:



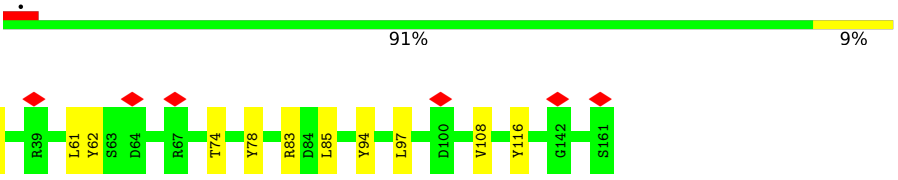
• Molecule 5: beta_APC

Chain O1:



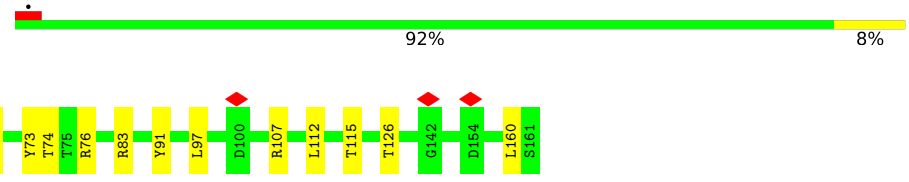
• Molecule 5: beta_APC

Chain S1:



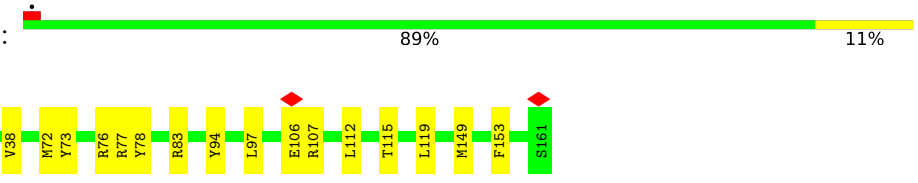
• Molecule 5: beta_APC

Chain U1:



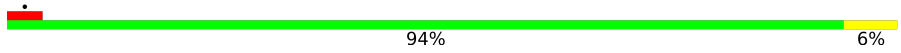
• Molecule 5: beta_APC

Chain W1:



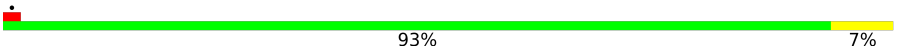
• Molecule 5: beta_APC

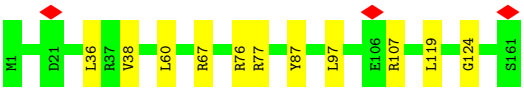
Chain Y1:



• Molecule 5: beta_APC

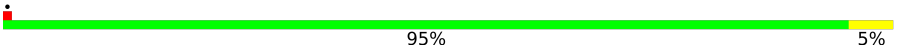
Chain a1:

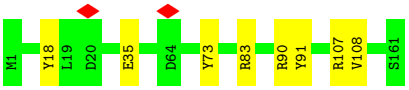




• Molecule 5: beta_APC

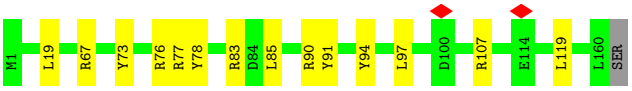
Chain c1:





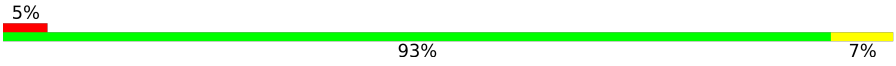
• Molecule 5: beta_APC

Chain e1:



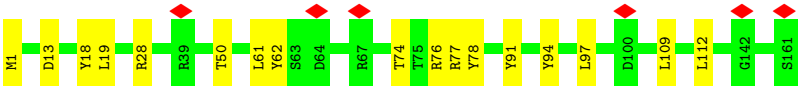
• Molecule 5: beta_APC

Chain h1:



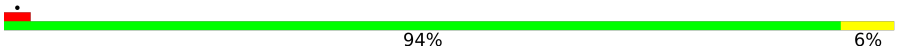
• Molecule 5: beta_APC

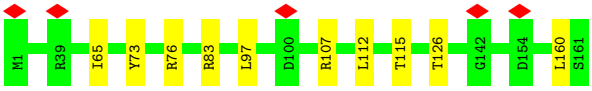
Chain j1:



• Molecule 5: beta_APC

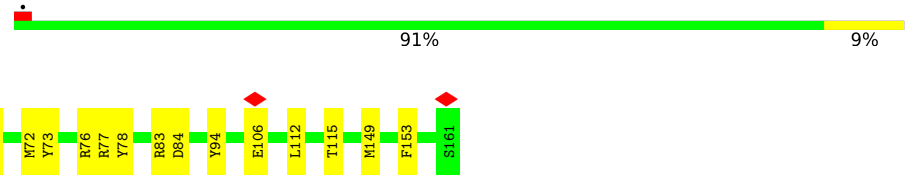
Chain l1:





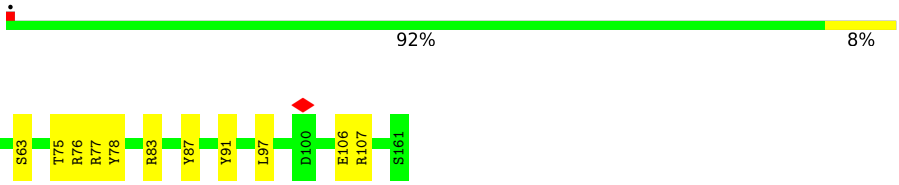
• Molecule 5: beta_APC

Chain n1:



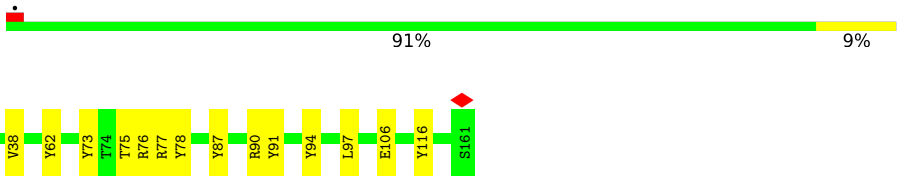
• Molecule 5: beta_APC

Chain p1:



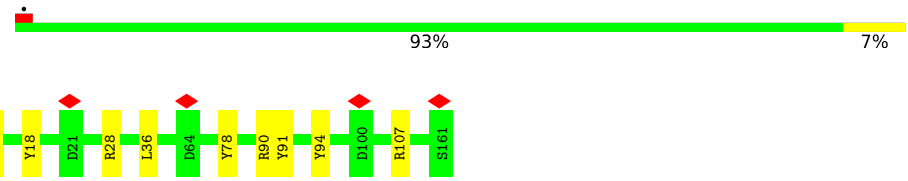
• Molecule 5: beta_APC

Chain r1:



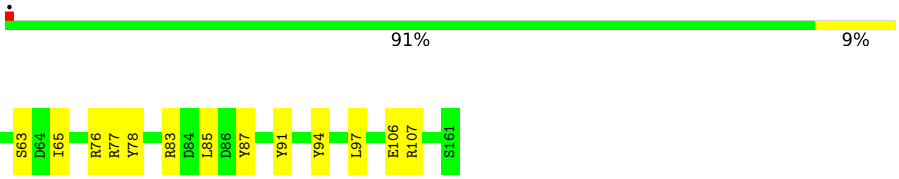
• Molecule 5: beta_APC

Chain t1:



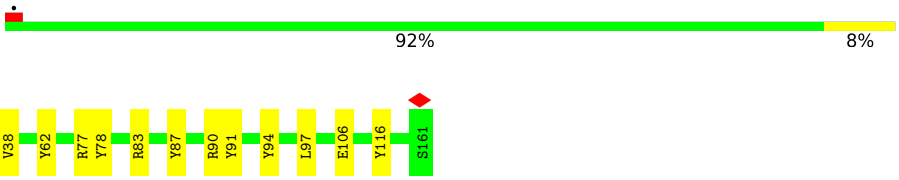
• Molecule 5: beta_APC

Chain v1:



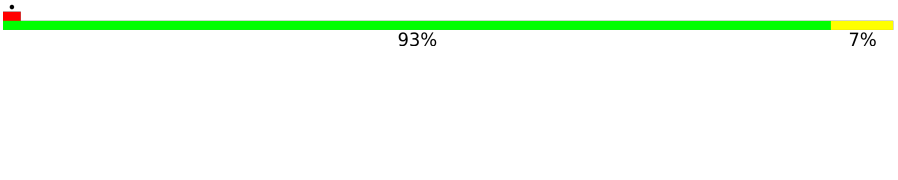
• Molecule 5: beta_APC

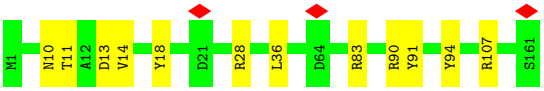
Chain x1:



• Molecule 5: beta_APC

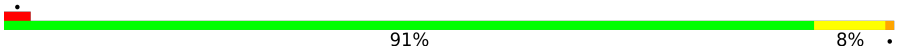
Chain z1:

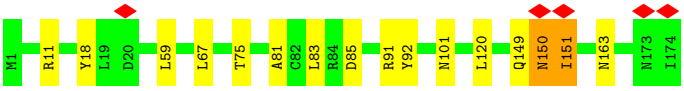




• Molecule 6: ApcF

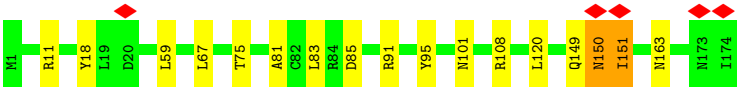
Chain Q1:





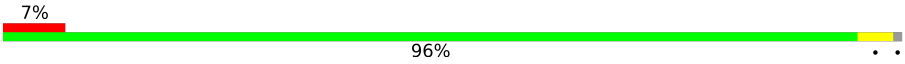
• Molecule 6: ApcF

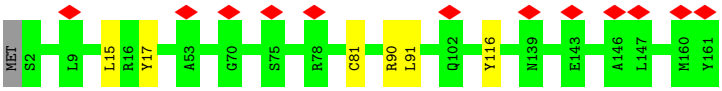
Chain g1:



• Molecule 7: ApcD

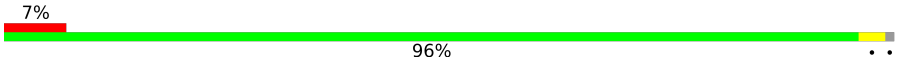
Chain V1:

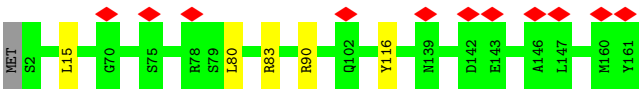




• Molecule 7: ApcD

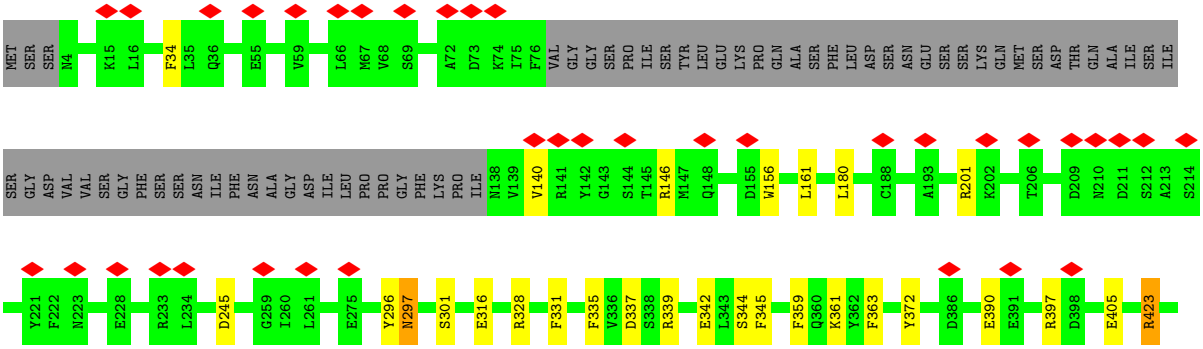
Chain m1:

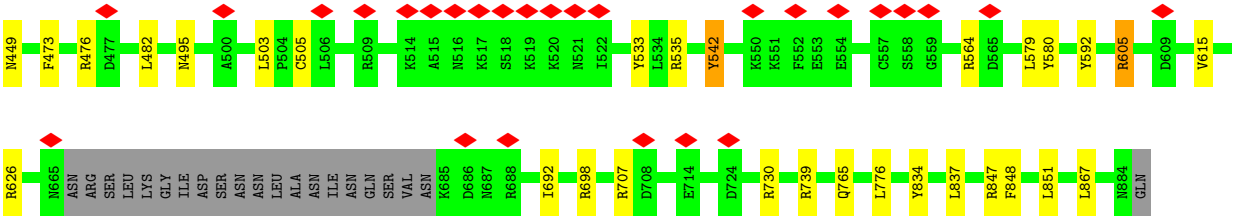




• Molecule 8: LCM

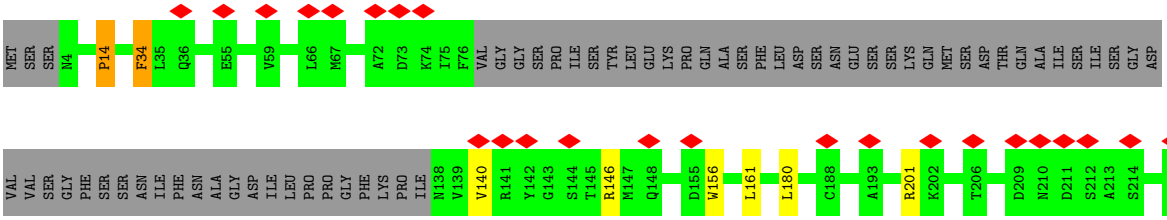
Chain a2:





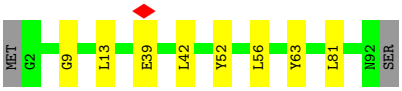
• Molecule 8: LCM

Chain b2:



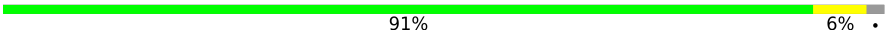
• Molecule 9: LC

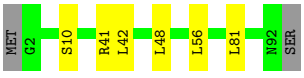
Chain c2:



• Molecule 9: LC

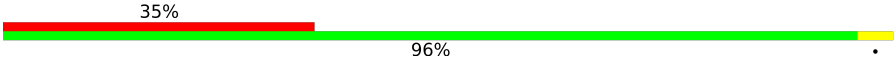
Chain d2:

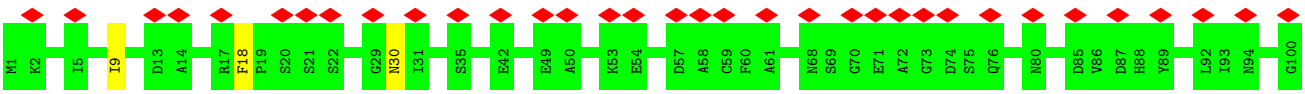


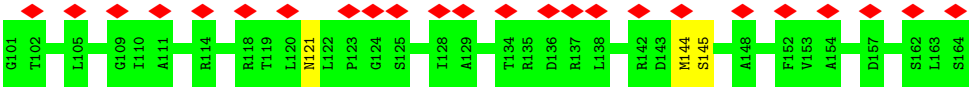


• Molecule 10: R-phycoerythrin alpha chain

Chain e2:

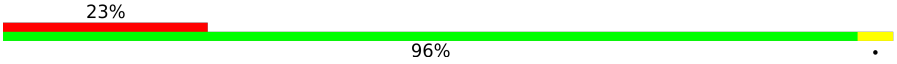


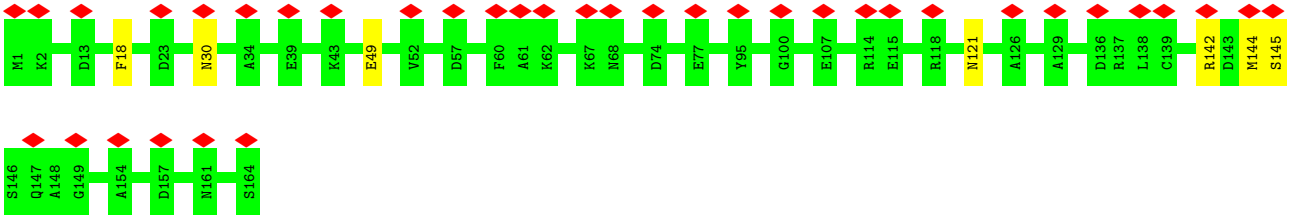




• Molecule 10: R-phycoerythrin alpha chain

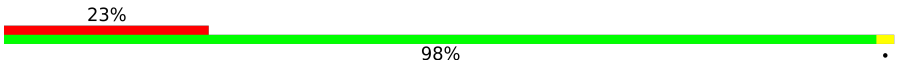
Chain g2:

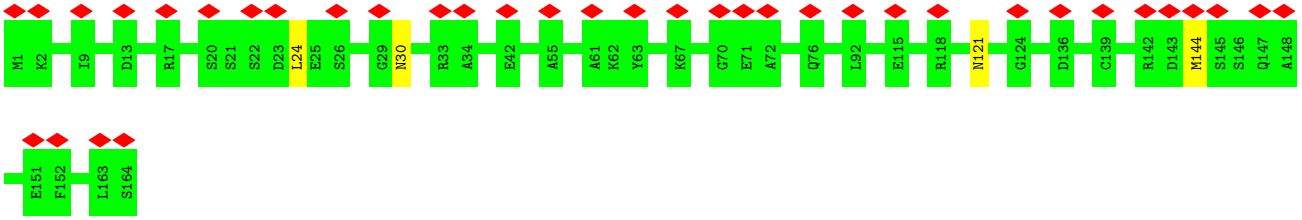




• Molecule 10: R-phycoerythrin alpha chain

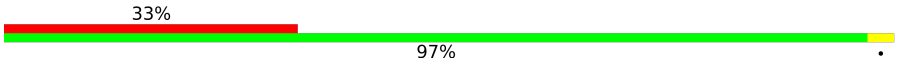
Chain i2:

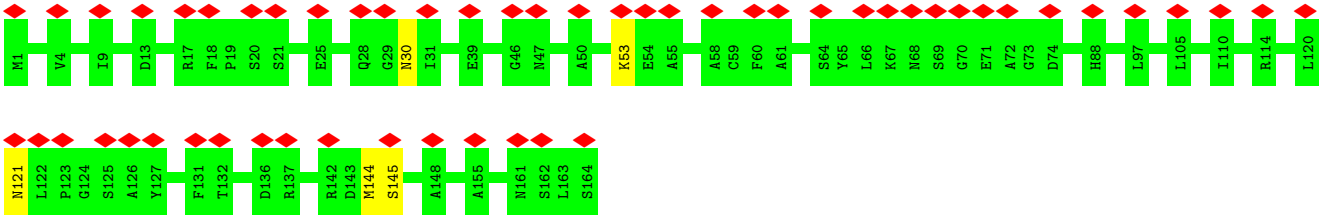




• Molecule 10: R-phycoerythrin alpha chain

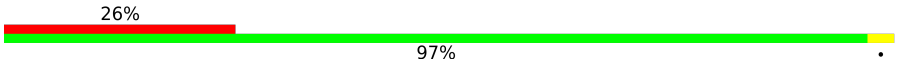
Chain k2:

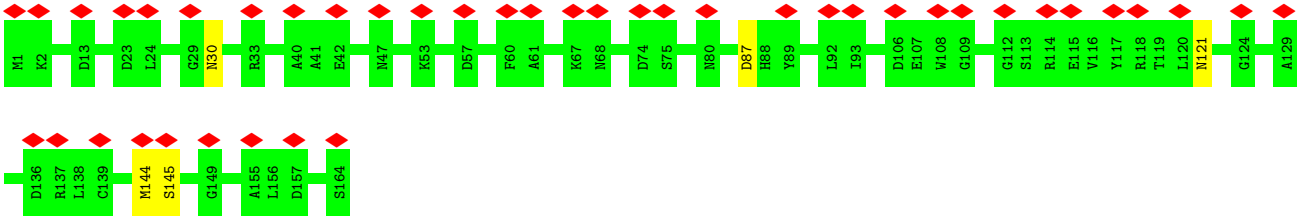




• Molecule 10: R-phycoerythrin alpha chain

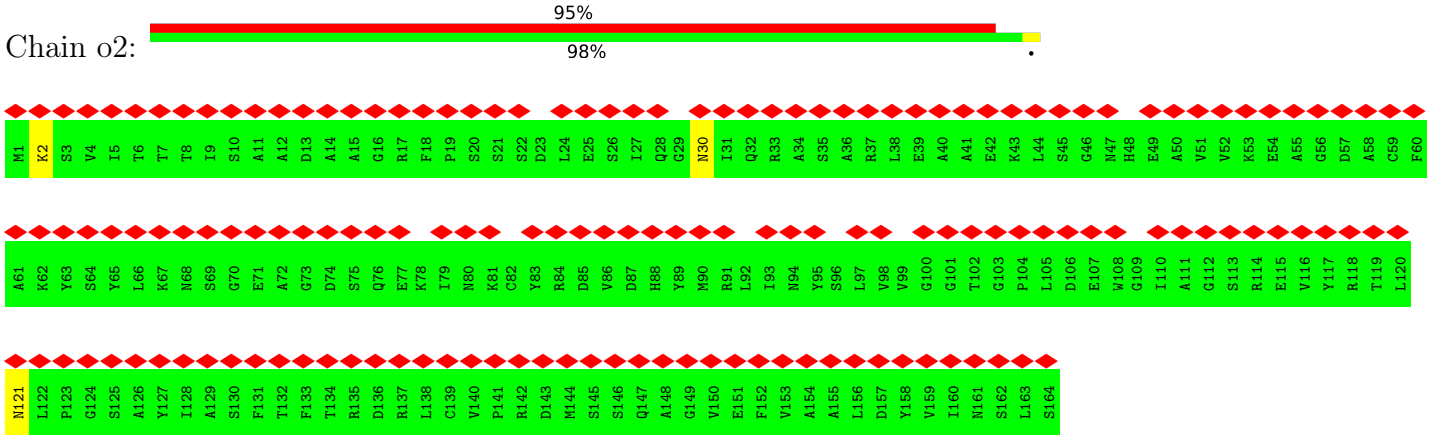
Chain m2:





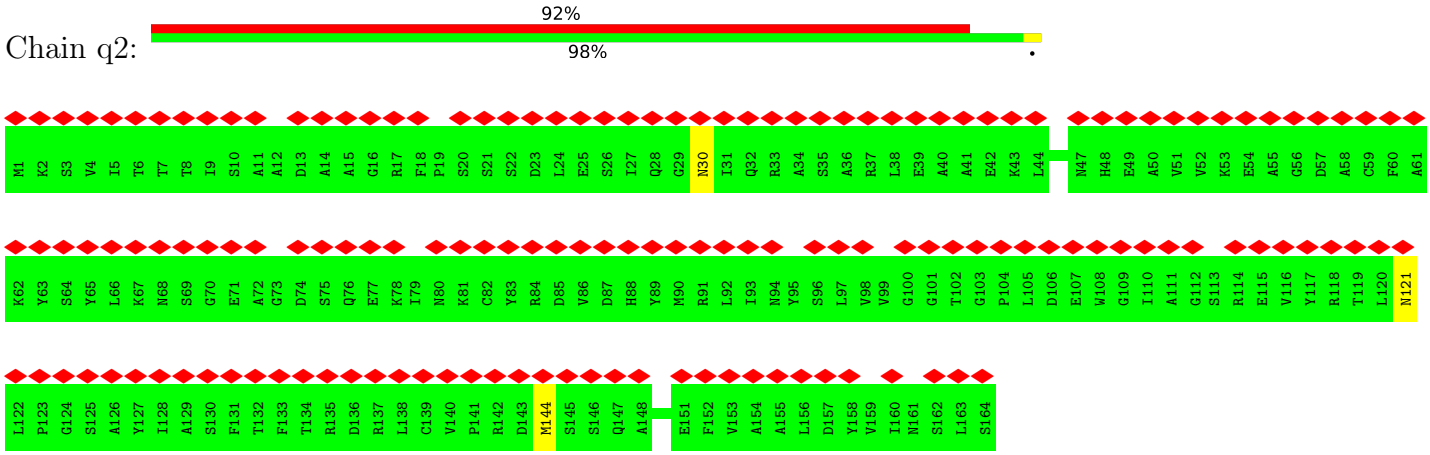
• Molecule 10: R-phycoerythrin alpha chain

Chain o2:



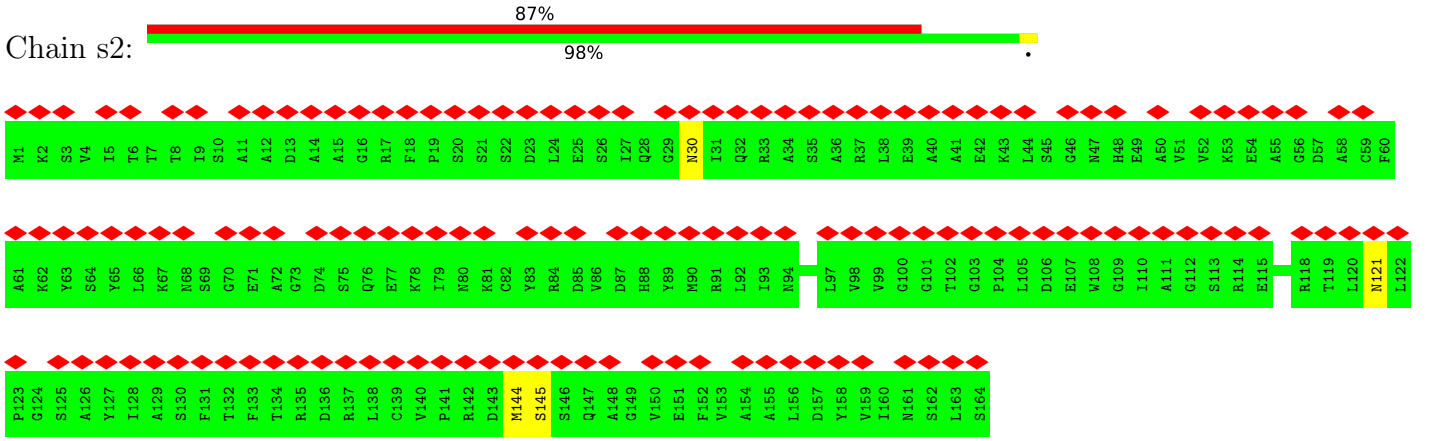
• Molecule 10: R-phycoerythrin alpha chain

Chain q2:



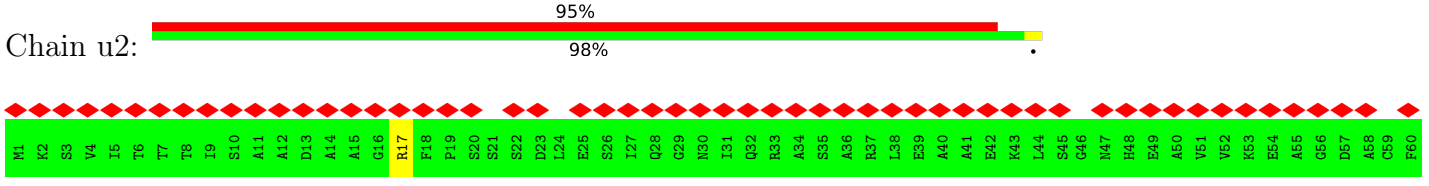
• Molecule 10: R-phycoerythrin alpha chain

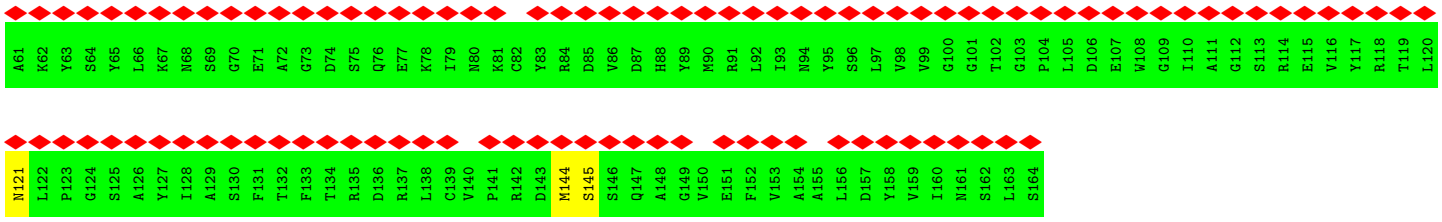
Chain s2:



• Molecule 10: R-phycoerythrin alpha chain

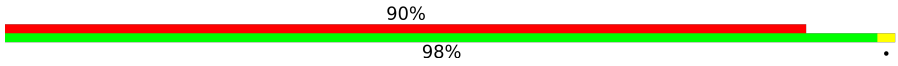
Chain u2:

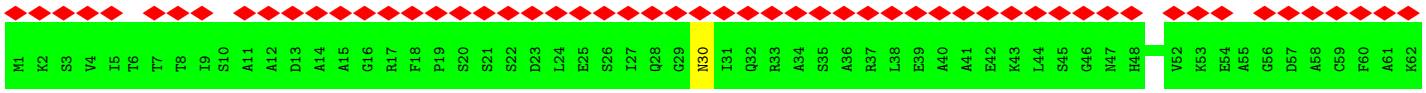


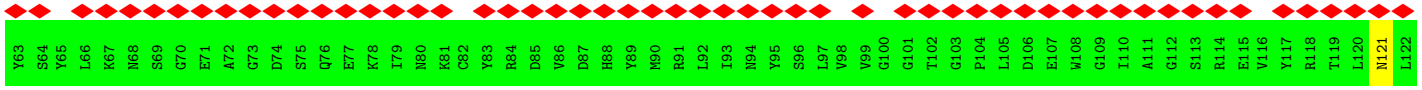


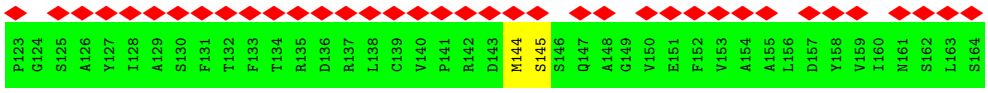
• Molecule 10: R-phycoerythrin alpha chain

Chain w2:



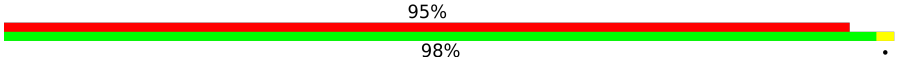


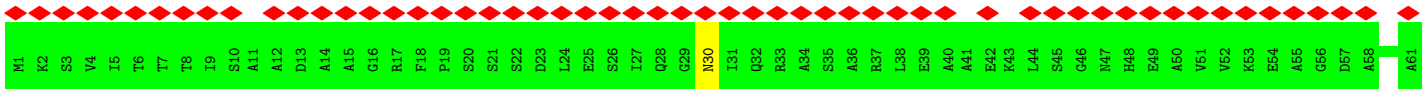


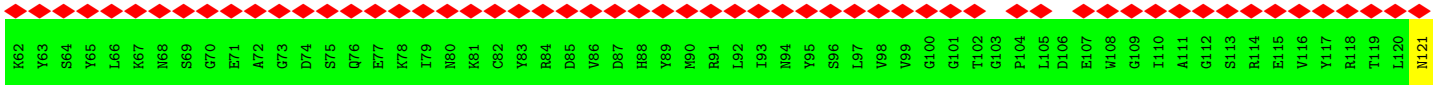


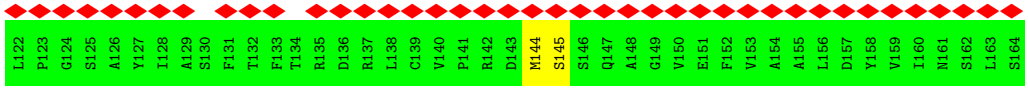
• Molecule 10: R-phycoerythrin alpha chain

Chain y2:



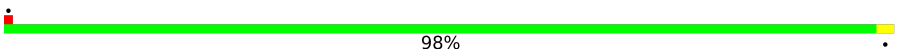






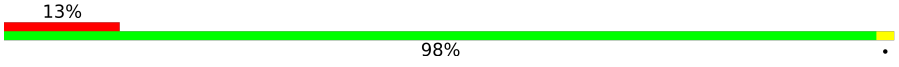
• Molecule 10: R-phycoerythrin alpha chain

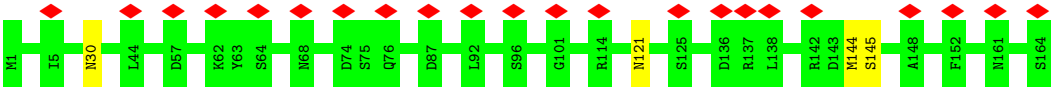
Chain E2:



• Molecule 10: R-phycoerythrin alpha chain

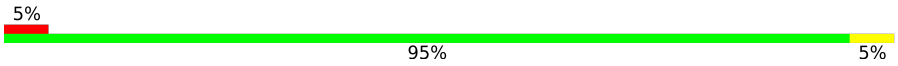
Chain G2:

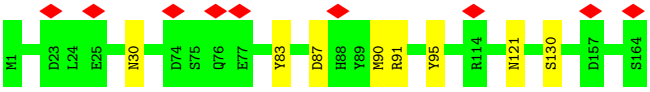




• Molecule 10: R-phycoerythrin alpha chain

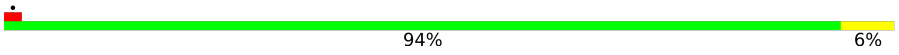
Chain I2:

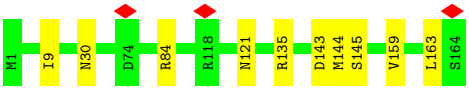




• Molecule 10: R-phycoerythrin alpha chain

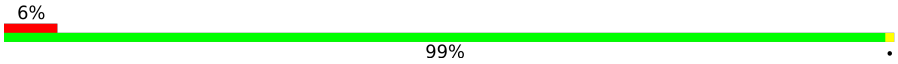
Chain K2:

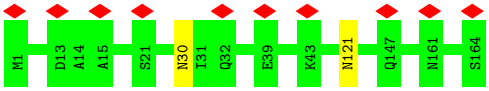




• Molecule 10: R-phycoerythrin alpha chain

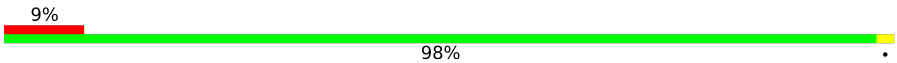
Chain M2:

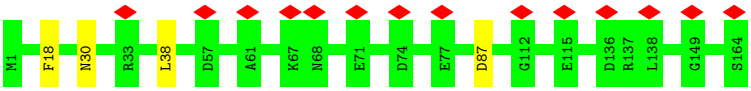




• Molecule 10: R-phycoerythrin alpha chain

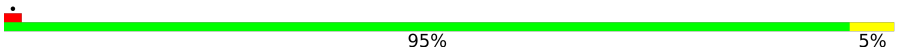
Chain O2:

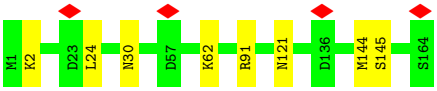




• Molecule 10: R-phycoerythrin alpha chain

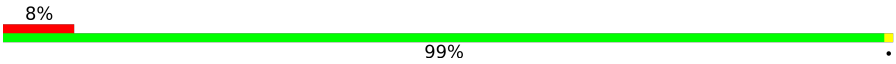
Chain Q2:

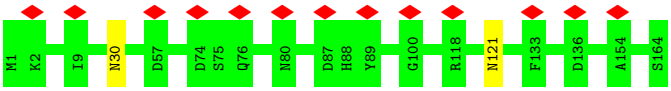




• Molecule 10: R-phycoerythrin alpha chain

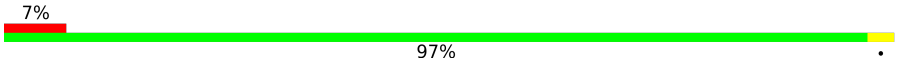
Chain S2:

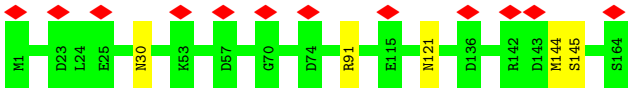




• Molecule 10: R-phycoerythrin alpha chain

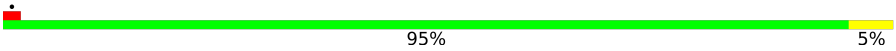
Chain U2:

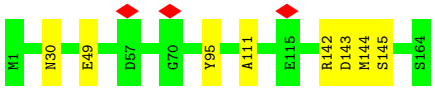




• Molecule 10: R-phycoerythrin alpha chain

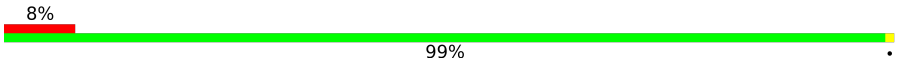
Chain W2:

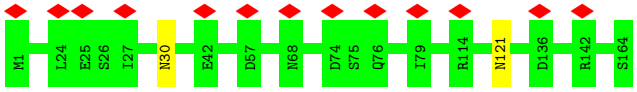




• Molecule 10: R-phycoerythrin alpha chain

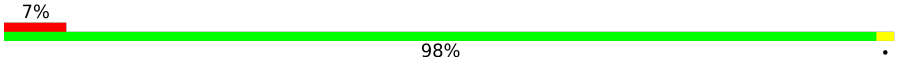
Chain Y2:

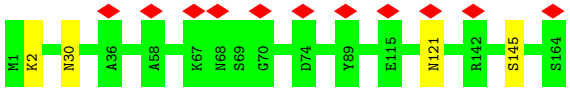




• Molecule 10: R-phycoerythrin alpha chain

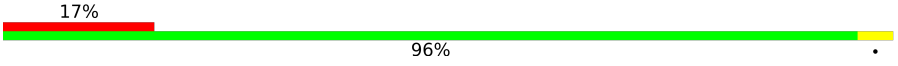
Chain A3:

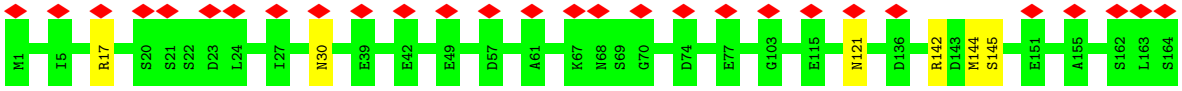




• Molecule 10: R-phycoerythrin alpha chain

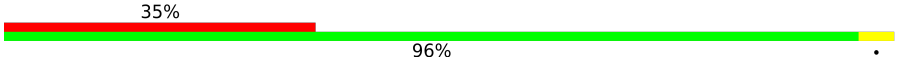
Chain C3:

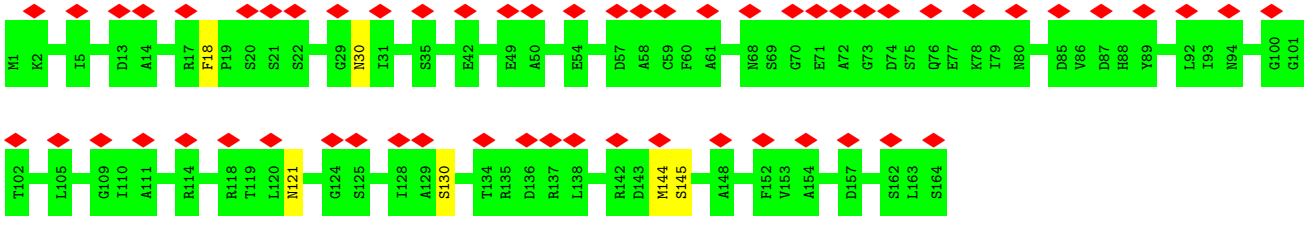




• Molecule 10: R-phycoerythrin alpha chain

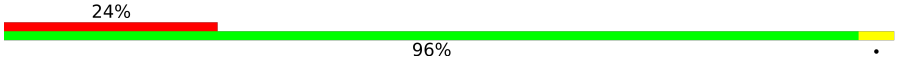
Chain E3:

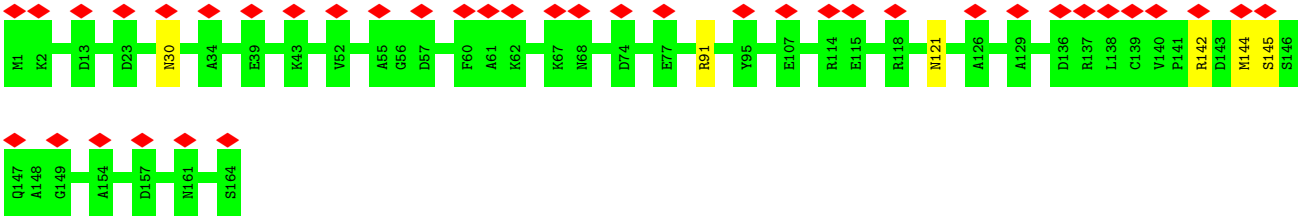




• Molecule 10: R-phycoerythrin alpha chain

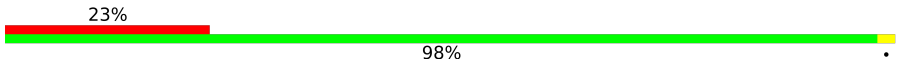
Chain G3:

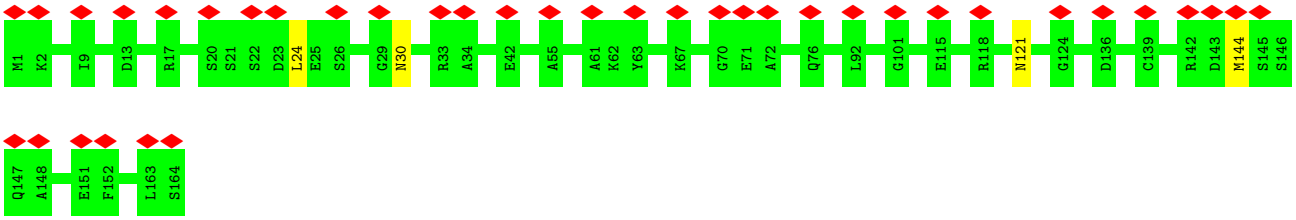




• Molecule 10: R-phycoerythrin alpha chain

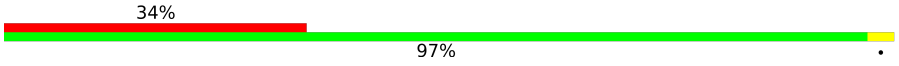
Chain I3:

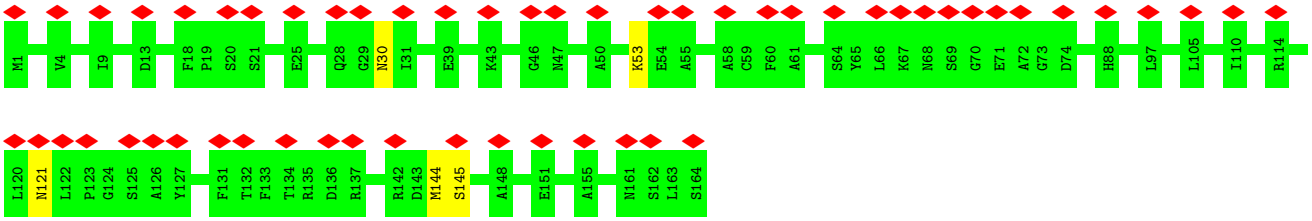




• Molecule 10: R-phycoerythrin alpha chain

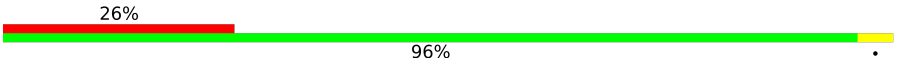
Chain K3:

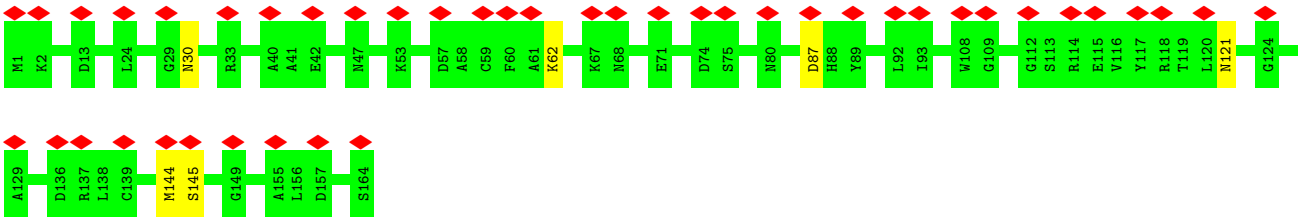




• Molecule 10: R-phycoerythrin alpha chain

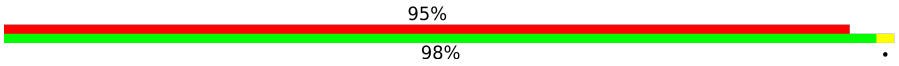
Chain M3:

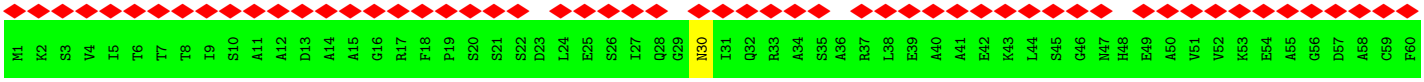


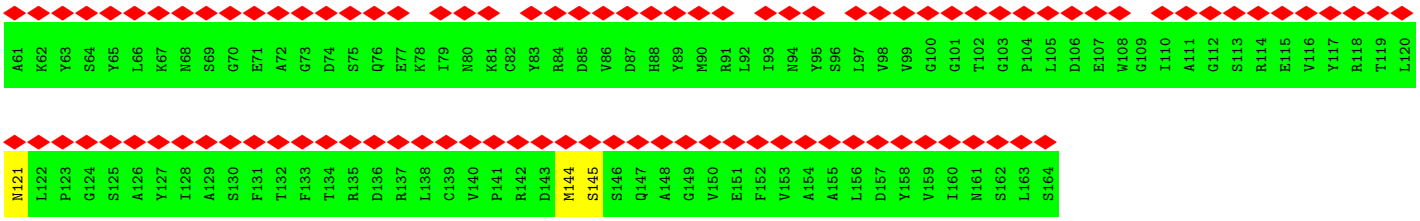


• Molecule 10: R-phycoerythrin alpha chain

Chain O3:

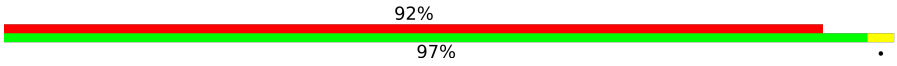


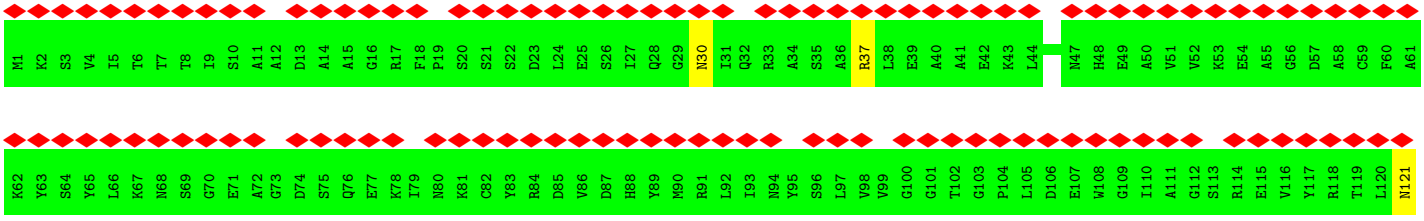




• Molecule 10: R-phycoerythrin alpha chain

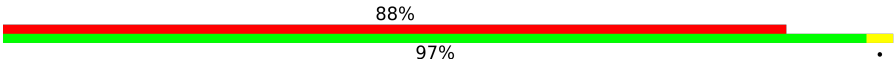
Chain Q3:

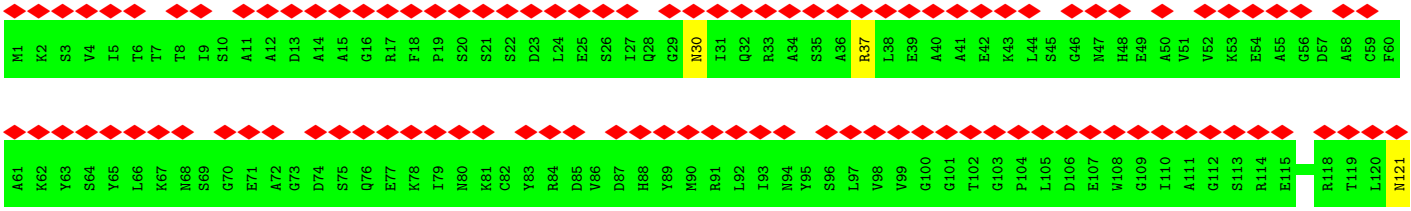




• Molecule 10: R-phycoerythrin alpha chain

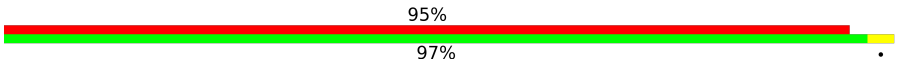
Chain S3:

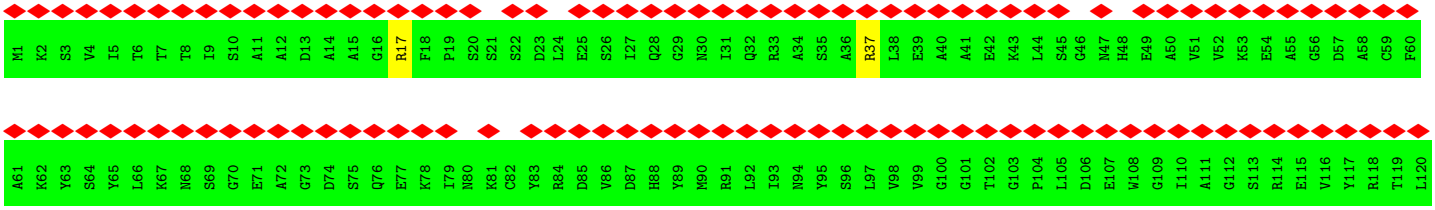


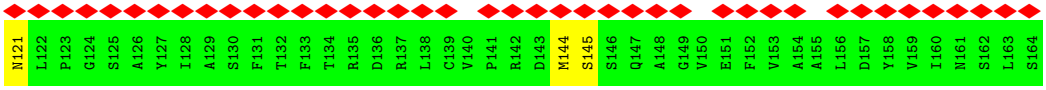


• Molecule 10: R-phycoerythrin alpha chain

Chain U3:

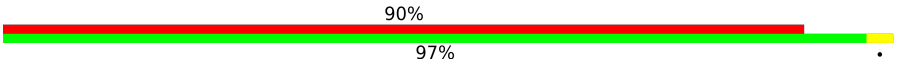


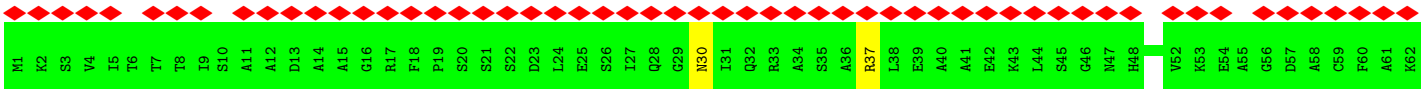


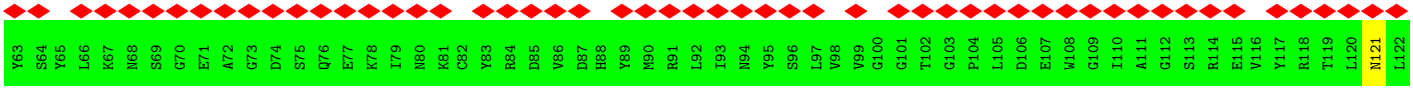


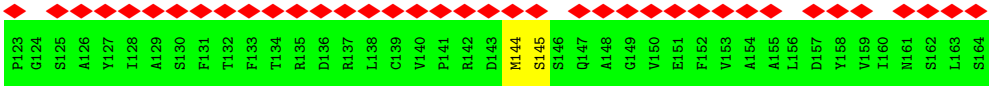
• Molecule 10: R-phycoerythrin alpha chain

Chain W3:



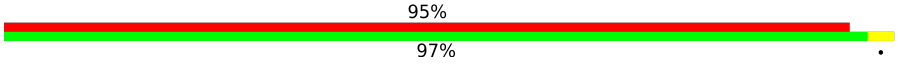


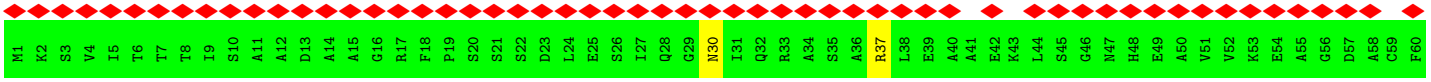


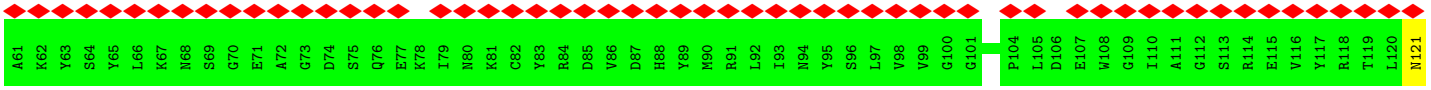


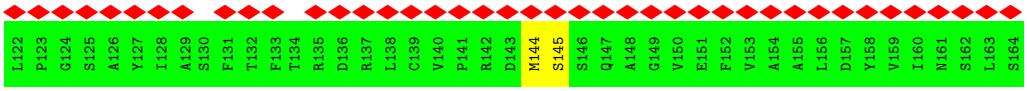
• Molecule 10: R-phycoerythrin alpha chain

Chain Y3:



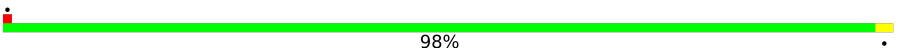






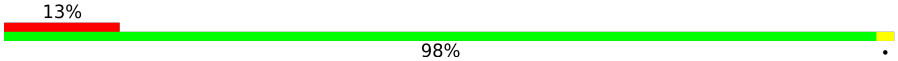
• Molecule 10: R-phycoerythrin alpha chain

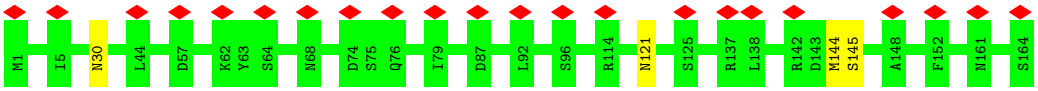
Chain e3:



• Molecule 10: R-phycoerythrin alpha chain

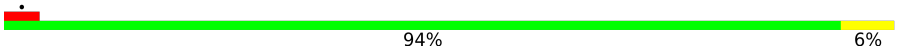
Chain g3:





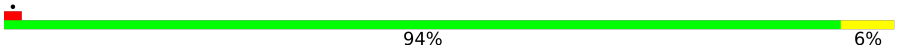
• Molecule 10: R-phycoerythrin alpha chain

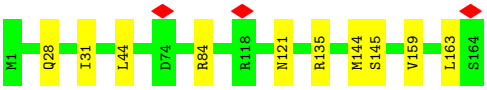
Chain i3:



• Molecule 10: R-phycoerythrin alpha chain

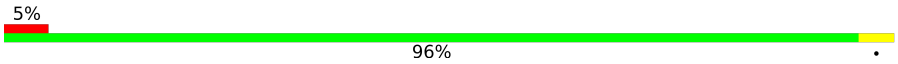
Chain k3:

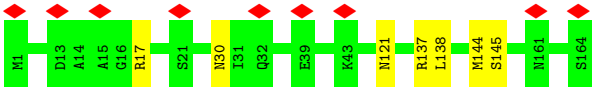




• Molecule 10: R-phycoerythrin alpha chain

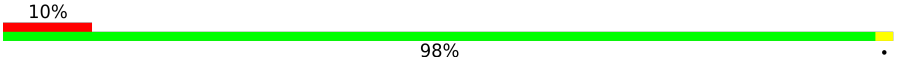
Chain m3:

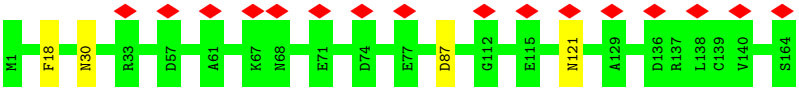




• Molecule 10: R-phycoerythrin alpha chain

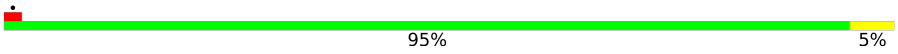
Chain o3:

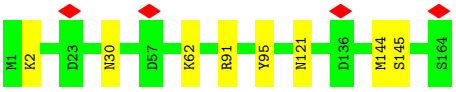




• Molecule 10: R-phycoerythrin alpha chain

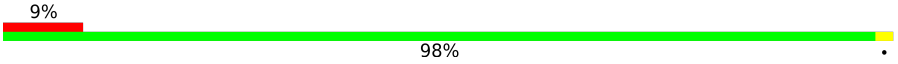
Chain q3:

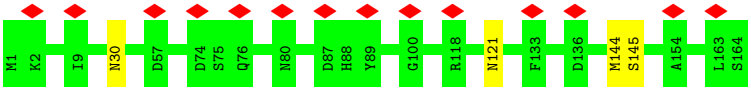




• Molecule 10: R-phycoerythrin alpha chain

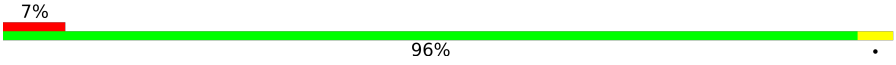
Chain s3:

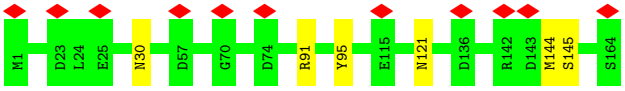




• Molecule 10: R-phycoerythrin alpha chain

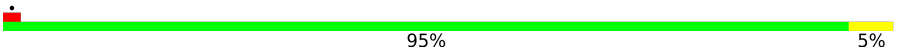
Chain u3:





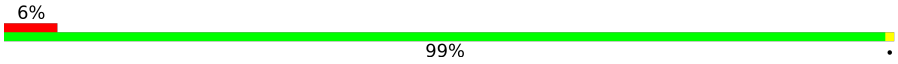
• Molecule 10: R-phycoerythrin alpha chain

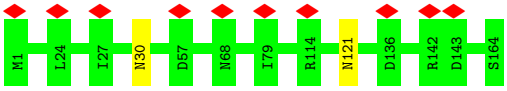
Chain w3:



• Molecule 10: R-phycoerythrin alpha chain

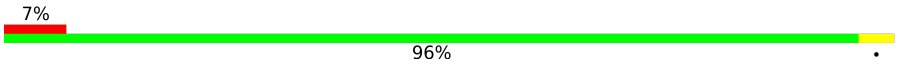
Chain y3:

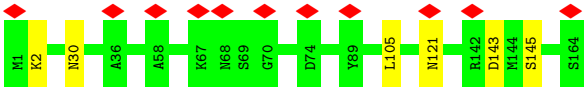




• Molecule 10: R-phycoerythrin alpha chain

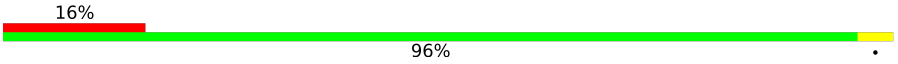
Chain A4:

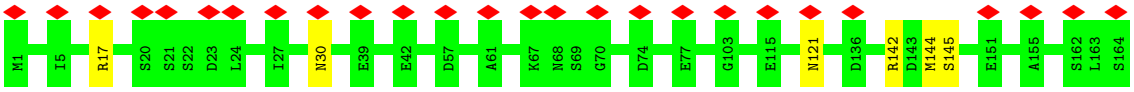




• Molecule 10: R-phycoerythrin alpha chain

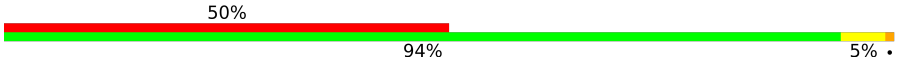
Chain C4:

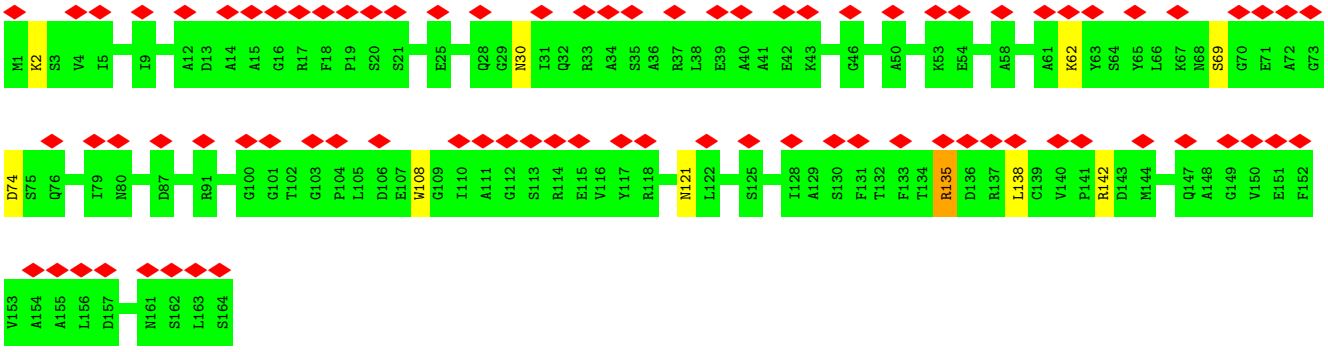




• Molecule 10: R-phycoerythrin alpha chain

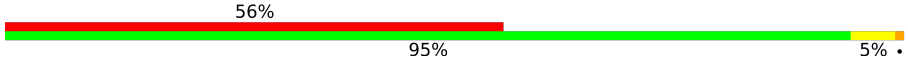
Chain E4:

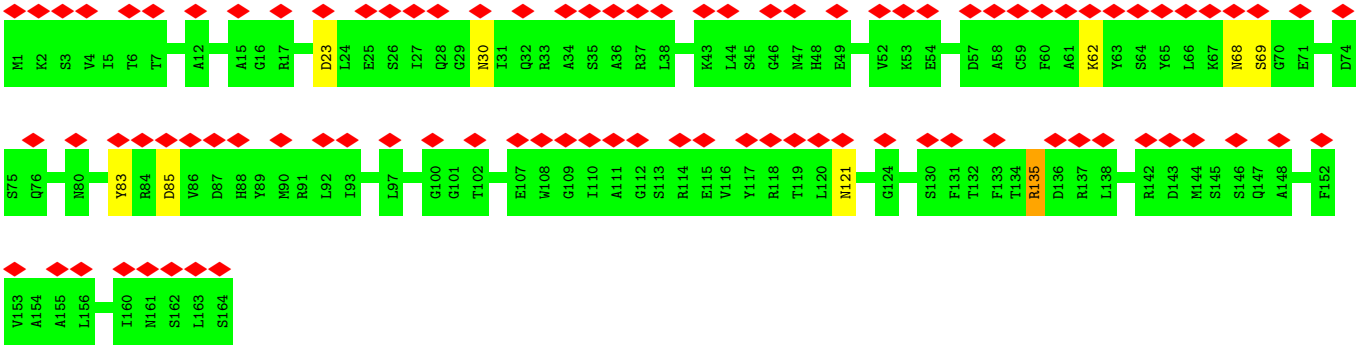




• Molecule 10: R-phycoerythrin alpha chain

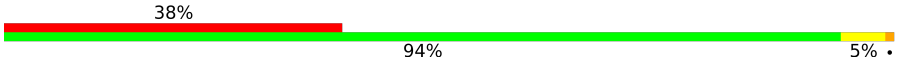
Chain G4:

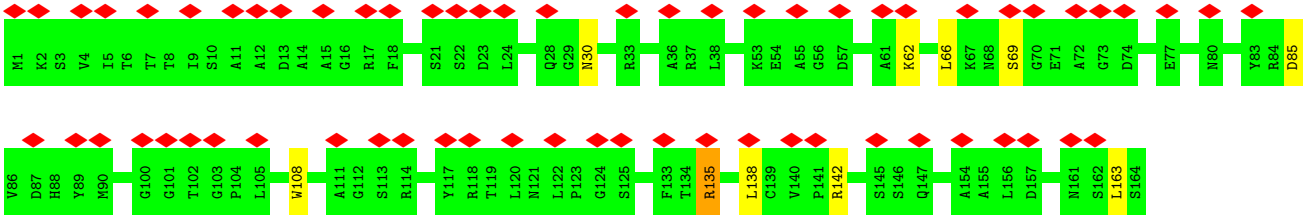




• Molecule 10: R-phycoerythrin alpha chain

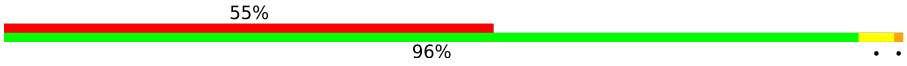
Chain I4:

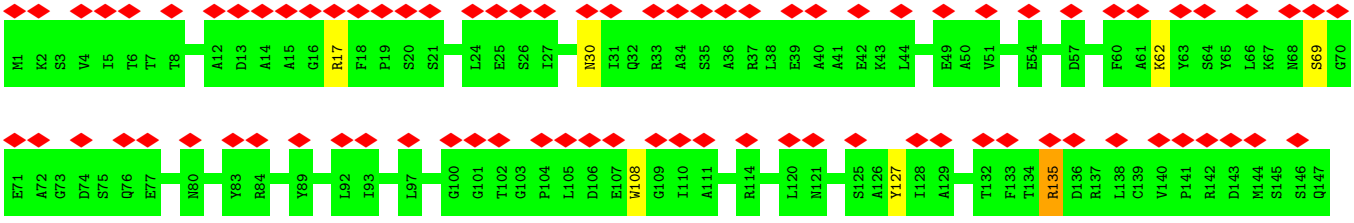




• Molecule 10: R-phycoerythrin alpha chain

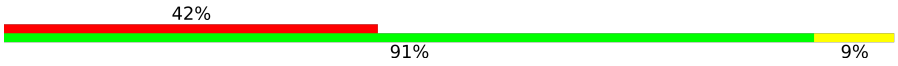
Chain K4:

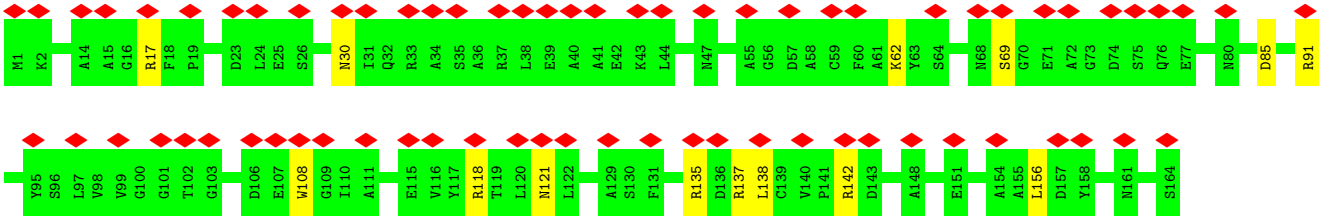




• Molecule 10: R-phycoerythrin alpha chain

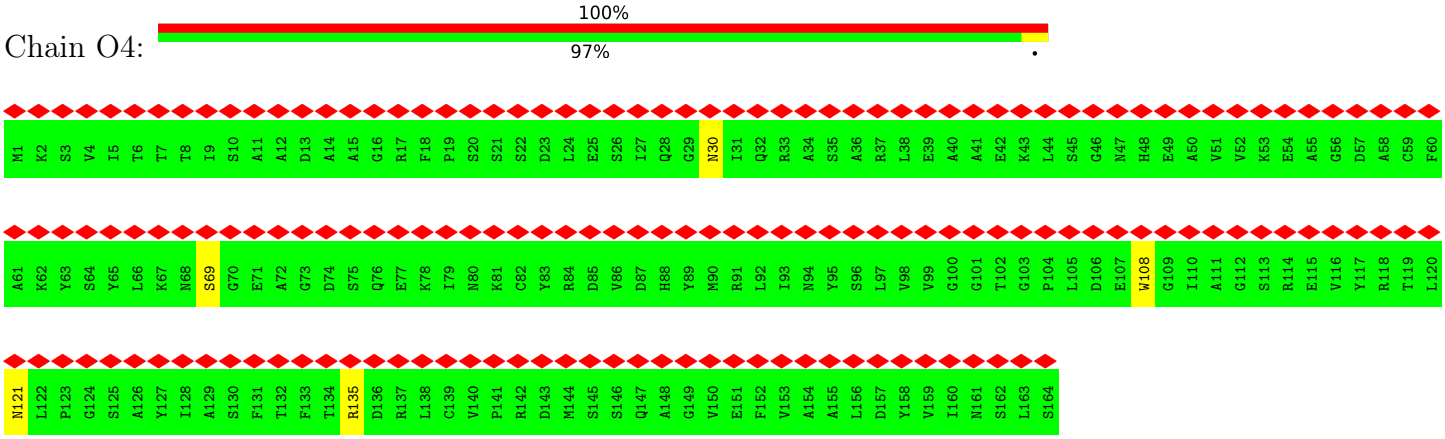
Chain M4:





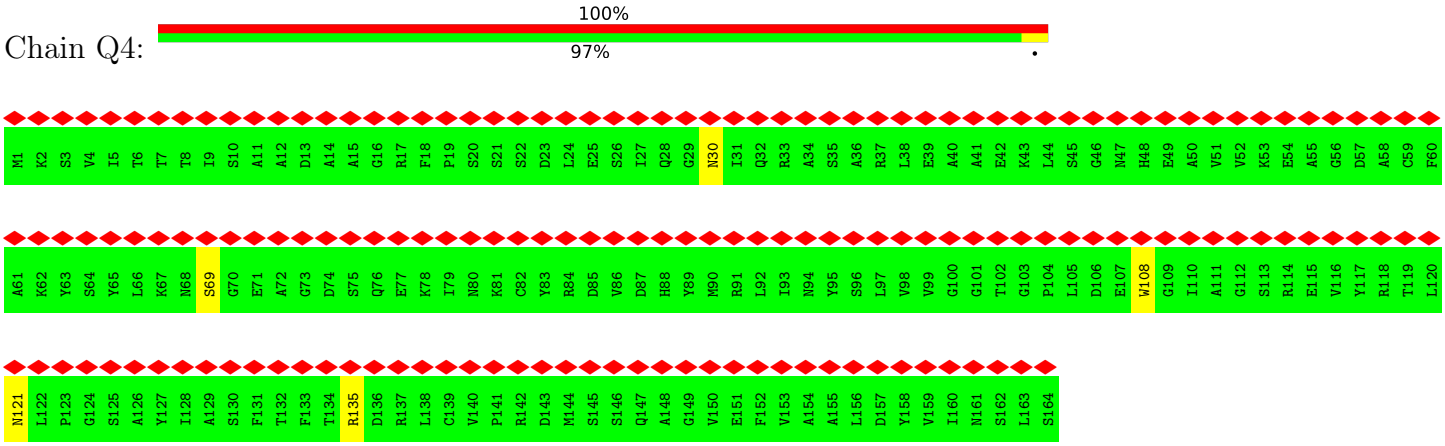
• Molecule 10: R-phycoerythrin alpha chain

Chain O4:



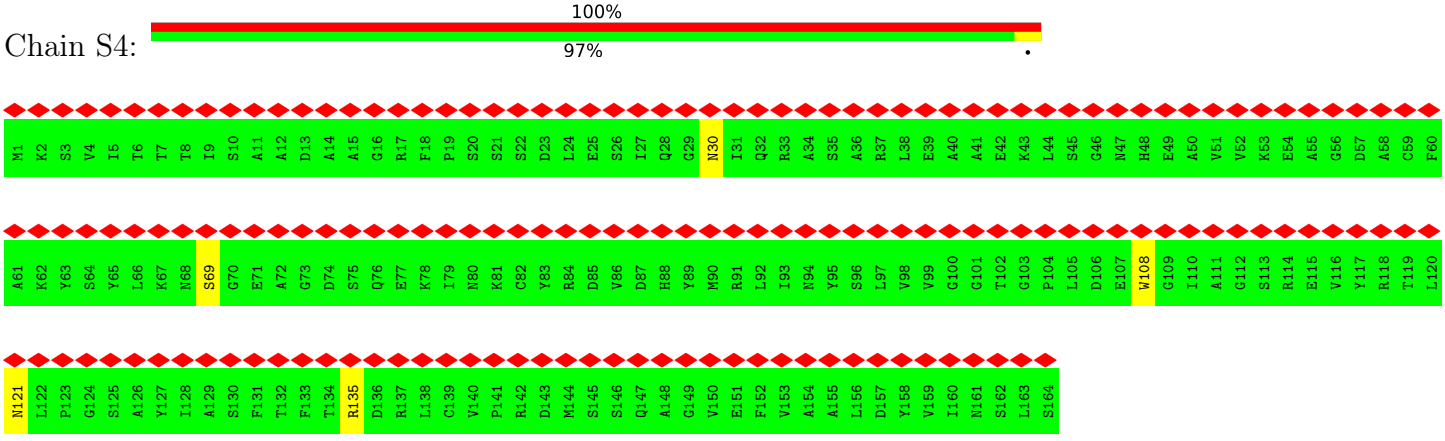
• Molecule 10: R-phycoerythrin alpha chain

Chain Q4:



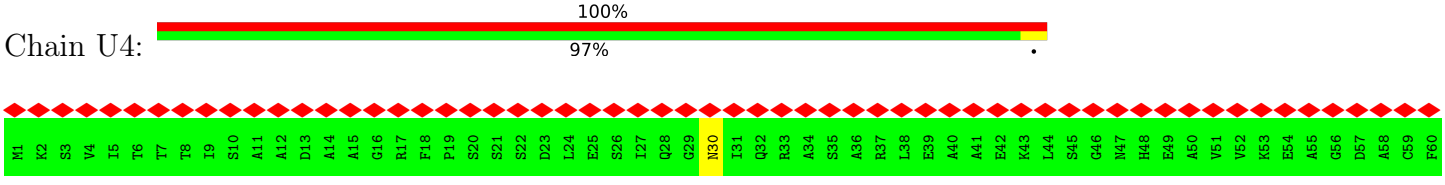
• Molecule 10: R-phycoerythrin alpha chain

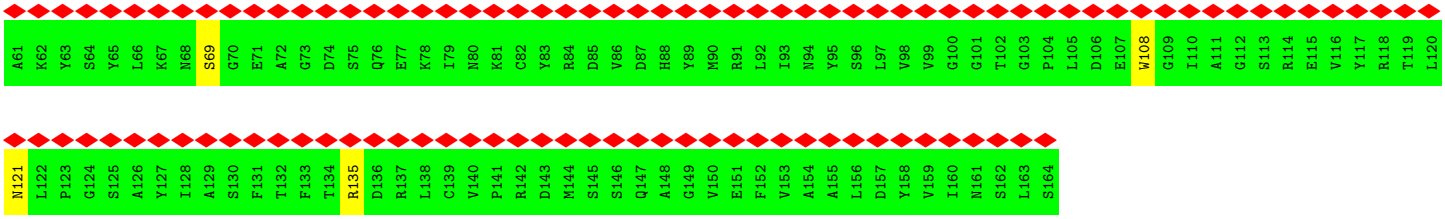
Chain S4:



• Molecule 10: R-phycoerythrin alpha chain

Chain U4:



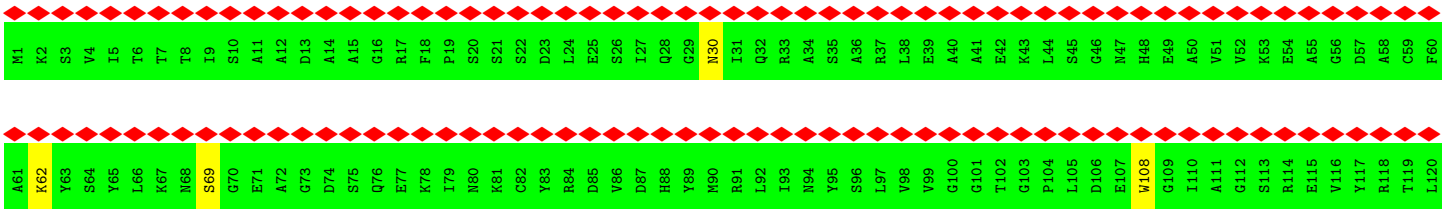


• Molecule 10: R-phycoerythrin alpha chain

Chain W4:

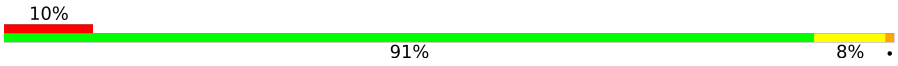
• Molecule 10: R-phycoerythrin alpha chain

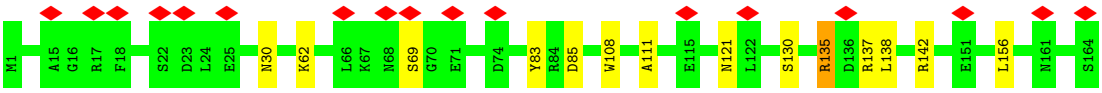
Chain Y4:



• Molecule 10: R-phycoerythrin alpha chain

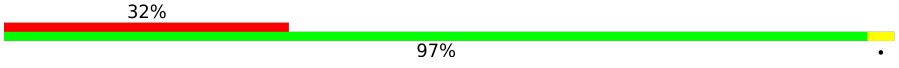
Chain m4:

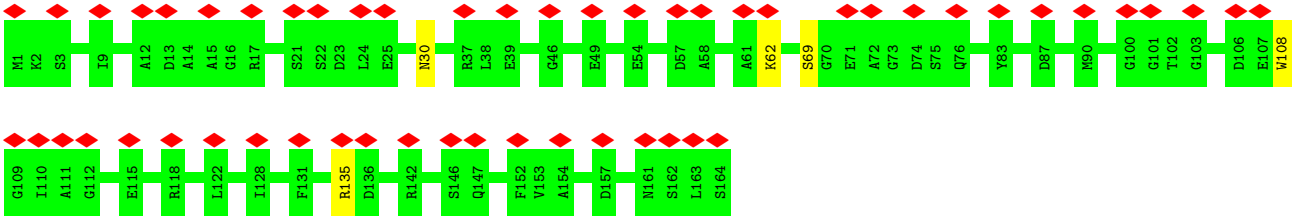




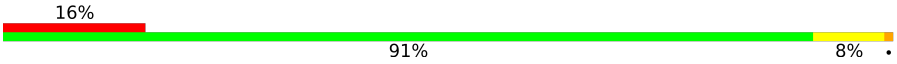
• Molecule 10: R-phycoerythrin alpha chain

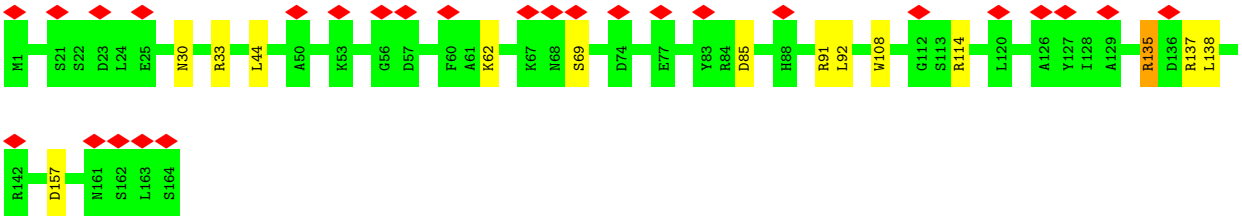
Chain o4:



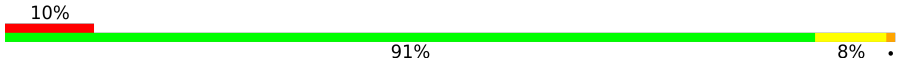


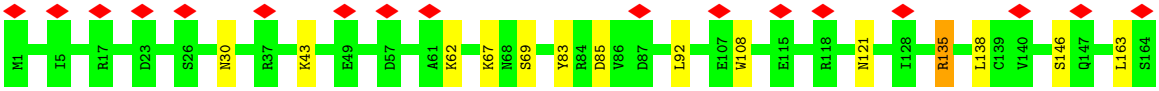
• Molecule 10: R-phycoerythrin alpha chain



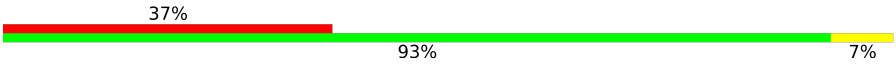


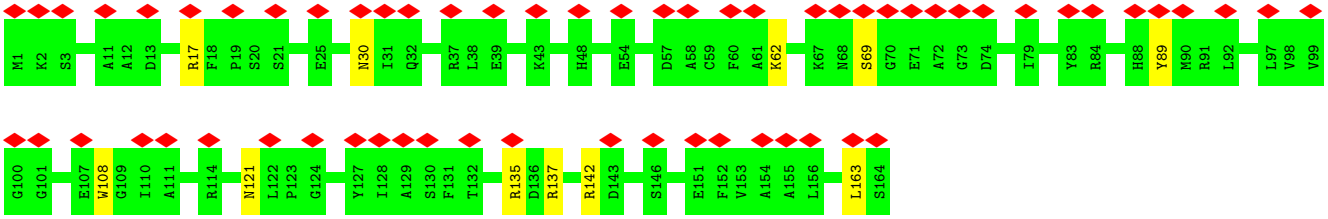
• Molecule 10: R-phycoerythrin alpha chain



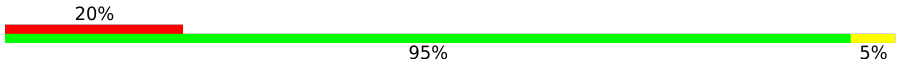


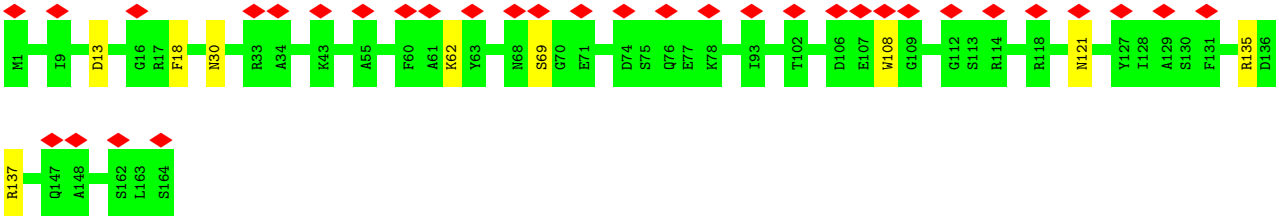
• Molecule 10: R-phycoerythrin alpha chain





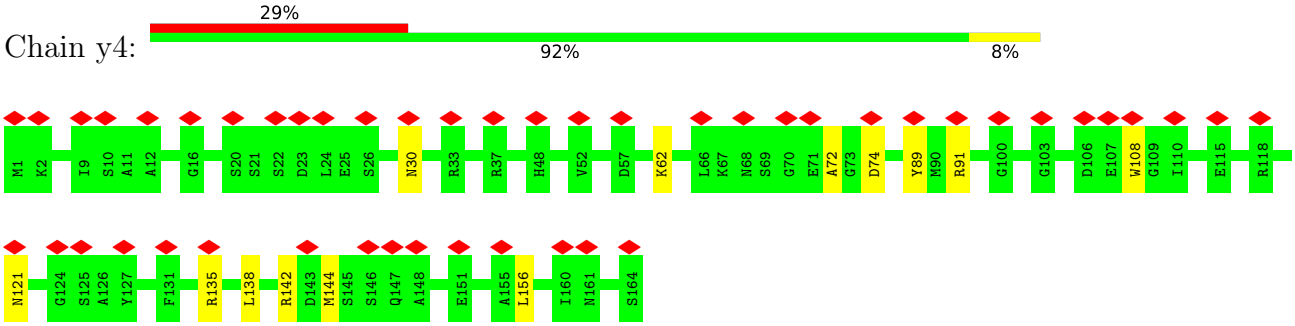
• Molecule 10: R-phycoerythrin alpha chain





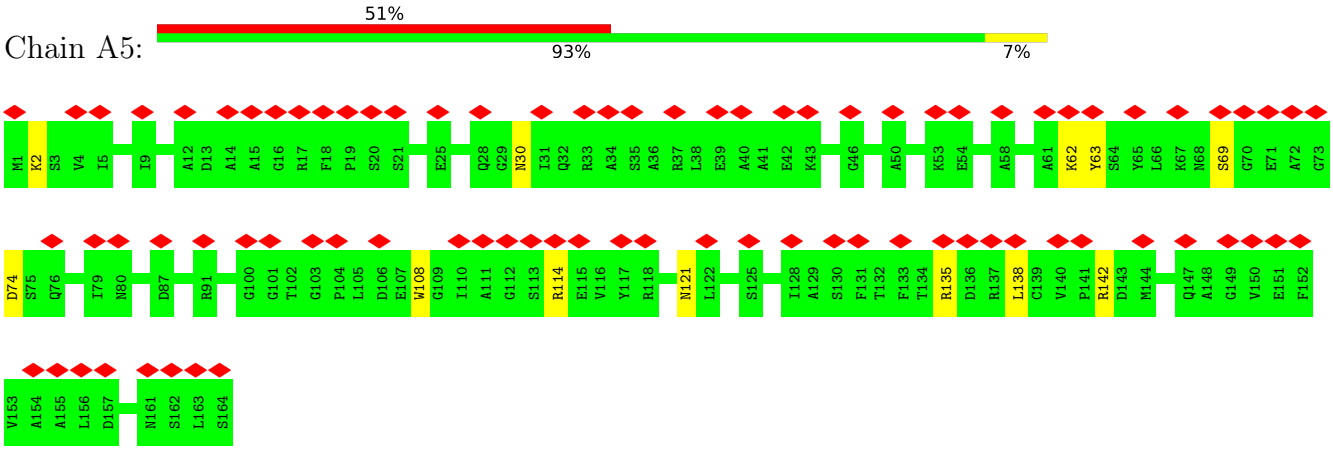
• Molecule 10: R-phycoerythrin alpha chain

Chain y4:



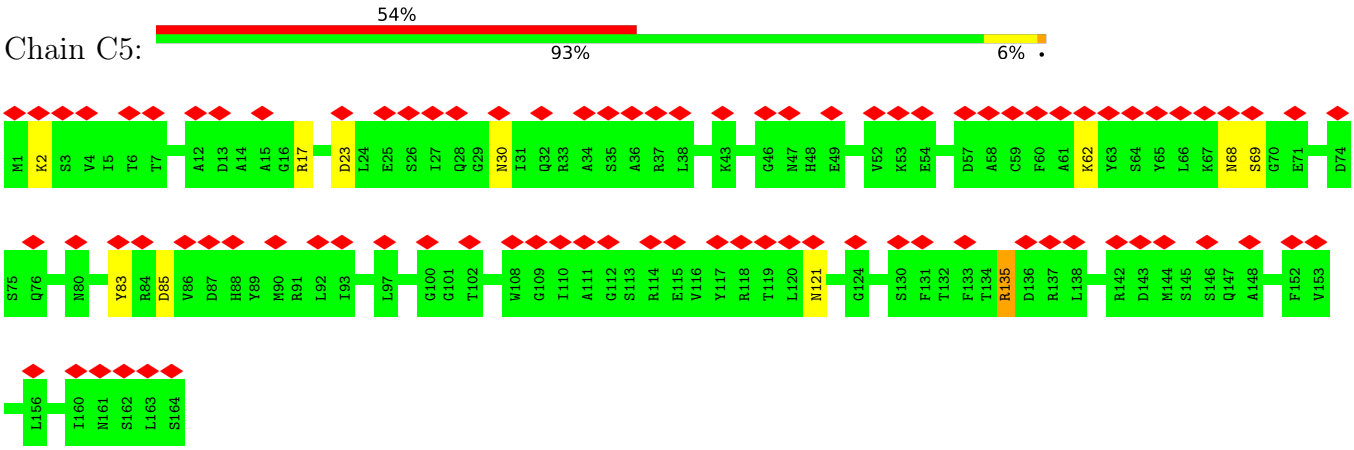
• Molecule 10: R-phycoerythrin alpha chain

Chain A5:



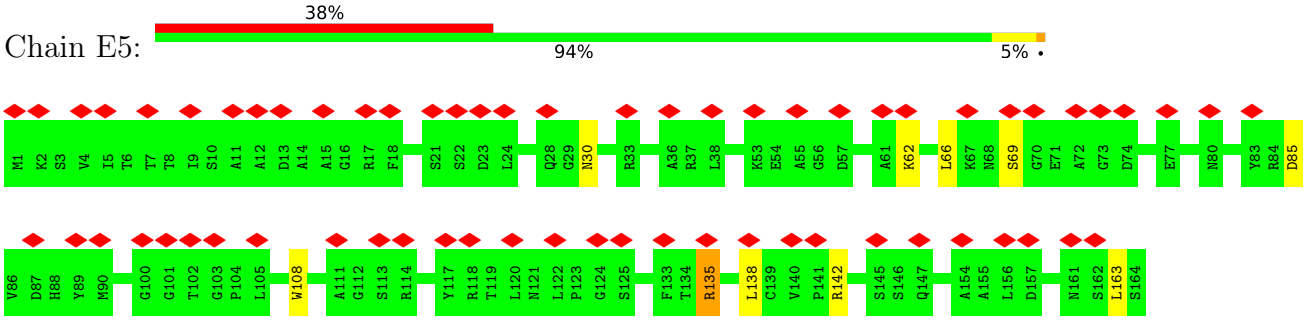
• Molecule 10: R-phycoerythrin alpha chain

Chain C5:



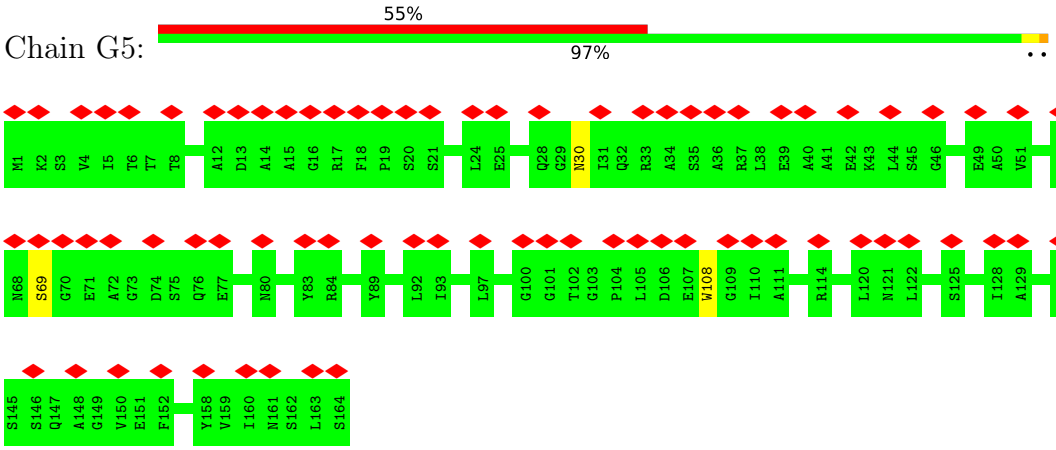
• Molecule 10: R-phycoerythrin alpha chain

Chain E5:



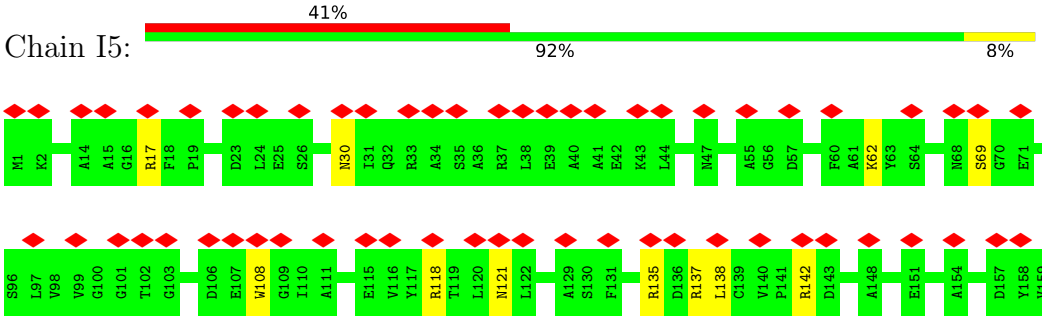
• Molecule 10: R-phycoerythrin alpha chain

Chain G5:



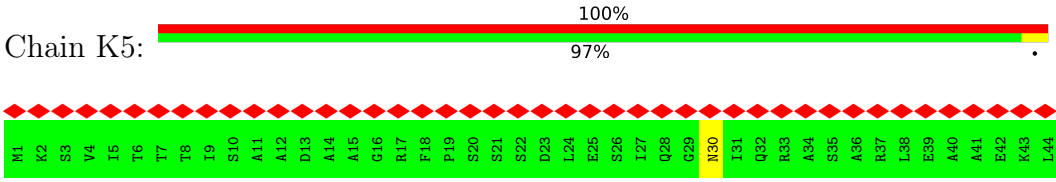
• Molecule 10: R-phycoerythrin alpha chain

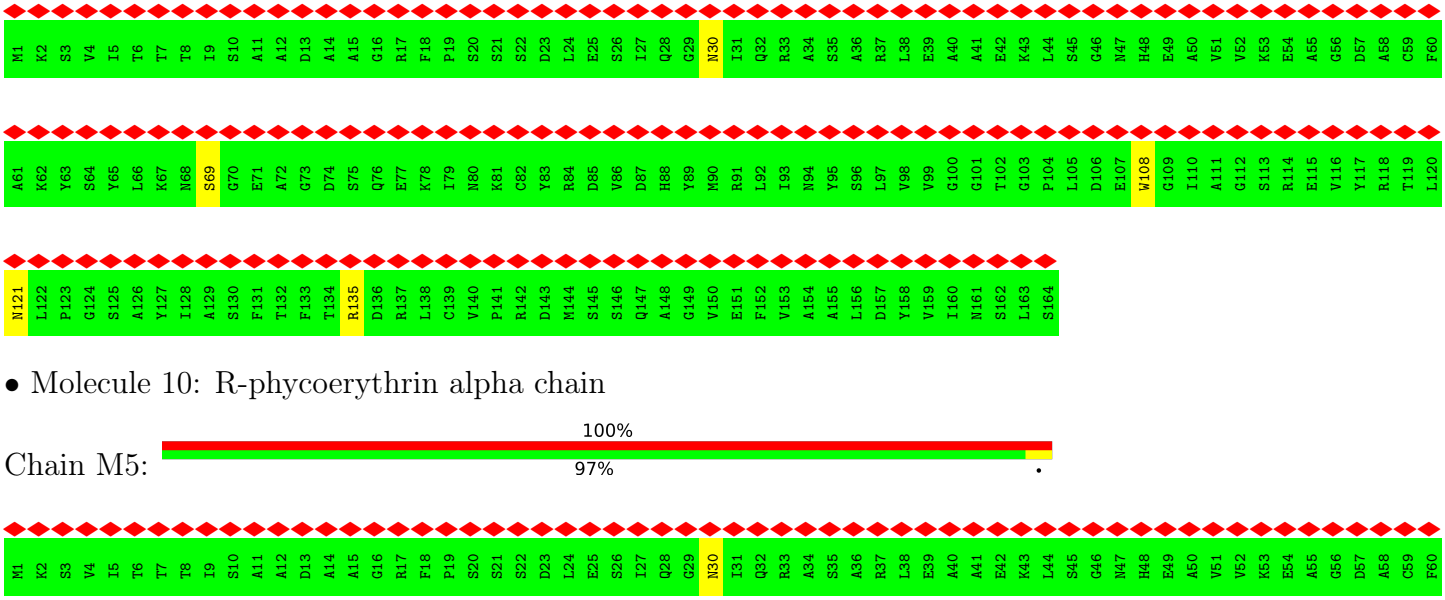
Chain I5:



• Molecule 10: R-phycoerythrin alpha chain

Chain K5:





• Molecule 10: R-phycoerythrin alpha chain

Chain M5:

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain O5:

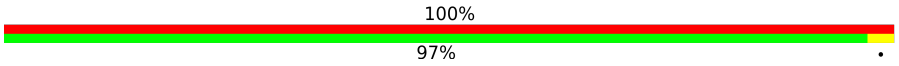
M1 K2 S3 V4 I5 T6 T7 T8 I9 S10 A11 A12 D13 A14 A15 G16 R17 F18 P19 S20 S21 S22 D23 L24 E25 S26 I27 Q28 G29 N30 I31 Q32 R33 A34 S35 A36 R37 L38 E39 A40 A41 E42 K43 L44 S45 G46 N47 H48 E49 A50 V51 V52 K53 E54 A55 G56 D57 A58 C59 F60

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain Q5:



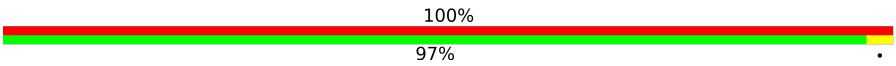
M1 K2 S3 V4 I5 T6 T7 T8 I9 S10 A11 A12 D13 A14 A15 G16 R17 F18 P19 S20 S21 S22 D23 L24 E25 S26 I27 Q28 G29 N30 I31 Q32 R33 A34 S35 A36 R37 L38 E39 A40 A41 E42 K43 L44 S45 G46 N47 H48 E49 A50 V51 V52 K53 E54 A55 G56 D57 A58 C59 F60

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain S5:



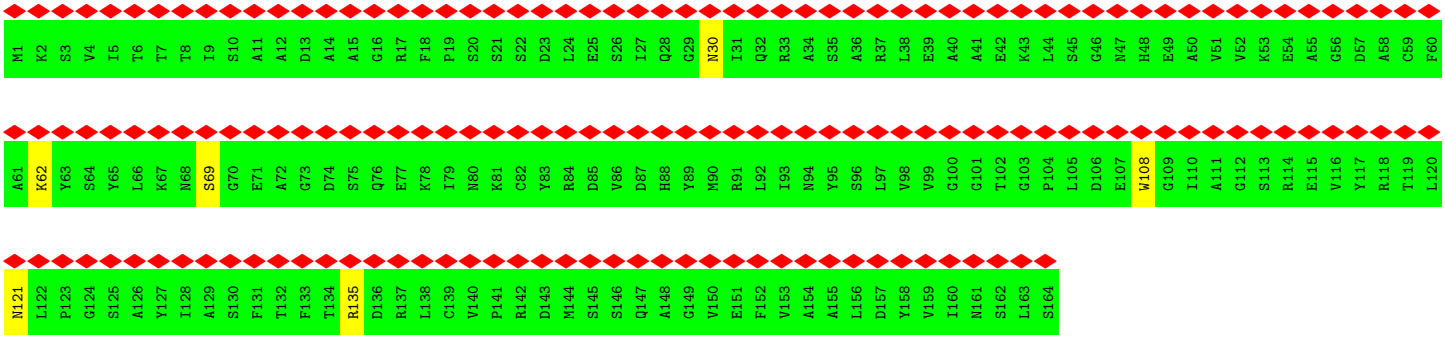
M1 K2 S3 V4 I5 T6 T7 T8 I9 S10 A11 A12 D13 A14 A15 G16 R17 F18 P19 S20 S21 S22 D23 L24 E25 S26 I27 Q28 G29 N30 I31 Q32 R33 A34 S35 A36 R37 L38 E39 A40 A41 E42 K43 L44 S45 G46 N47 H48 E49 A50 V51 V52 K53 E54 A55 G56 D57 A58 C59 F60

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

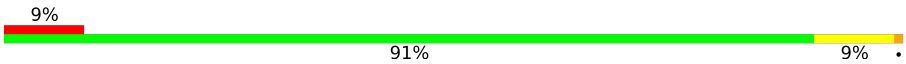
• Molecule 10: R-phycoerythrin alpha chain

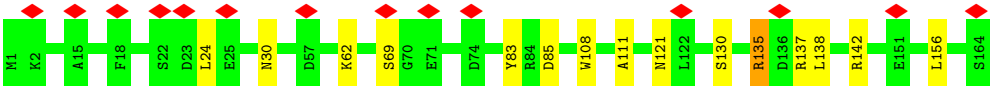
Chain U5:



• Molecule 10: R-phycoerythrin alpha chain

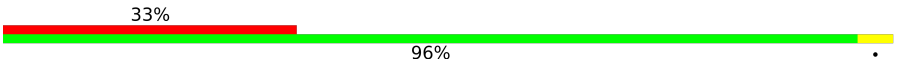
Chain m5:

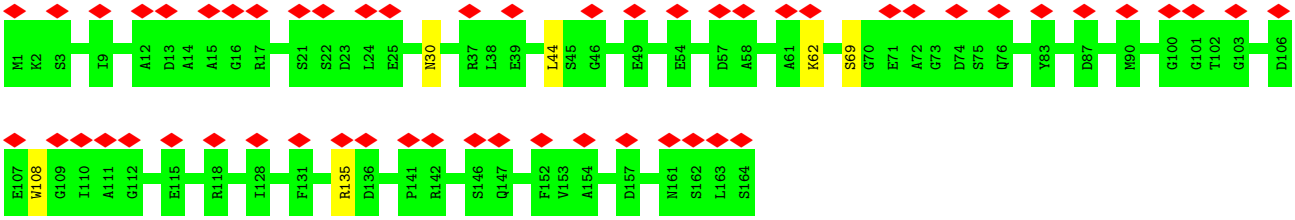




• Molecule 10: R-phycoerythrin alpha chain

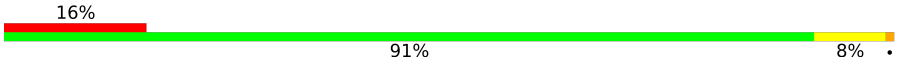
Chain o5:

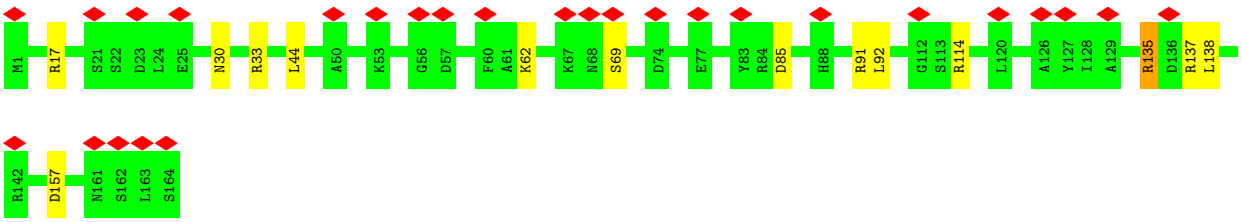




• Molecule 10: R-phycoerythrin alpha chain

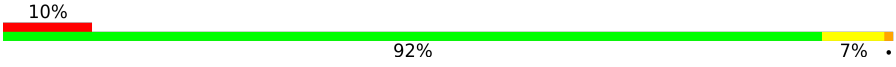
Chain q5:

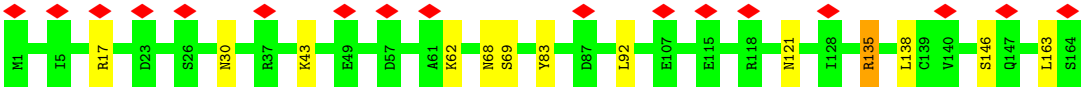




• Molecule 10: R-phycoerythrin alpha chain

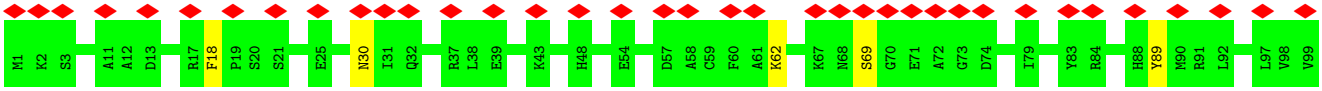
Chain s5:

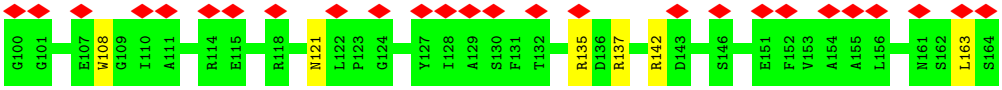




• Molecule 10: R-phycoerythrin alpha chain

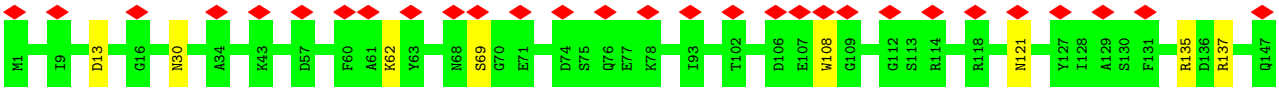
Chain u5:

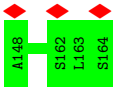




• Molecule 10: R-phycoerythrin alpha chain

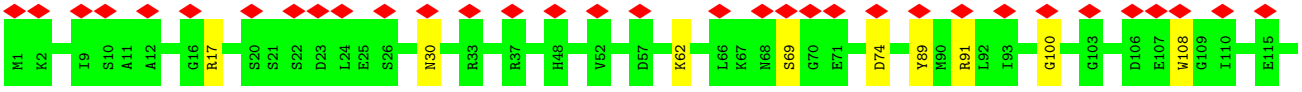
Chain w5:

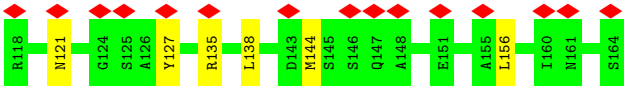




• Molecule 10: R-phycoerythrin alpha chain

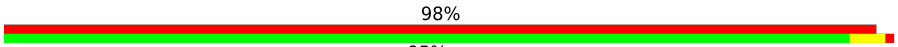
Chain y5:

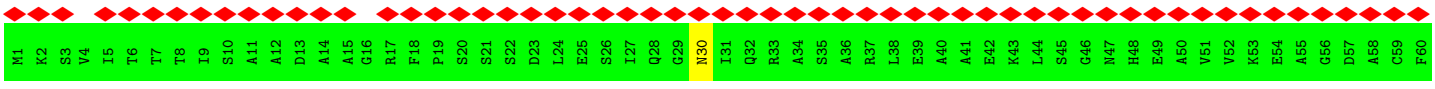


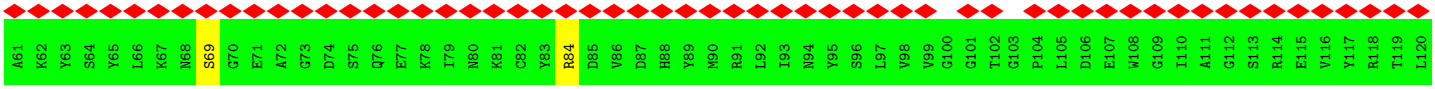


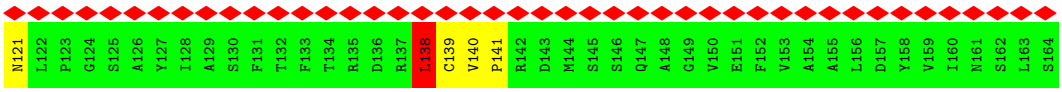
• Molecule 10: R-phycoerythrin alpha chain

Chain i8:



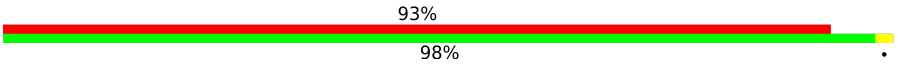


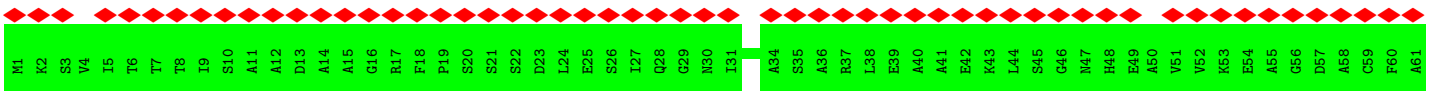




• Molecule 10: R-phycoerythrin alpha chain

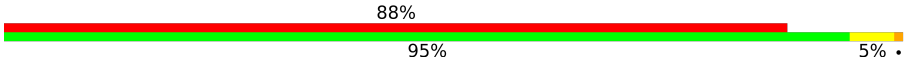
Chain j8:

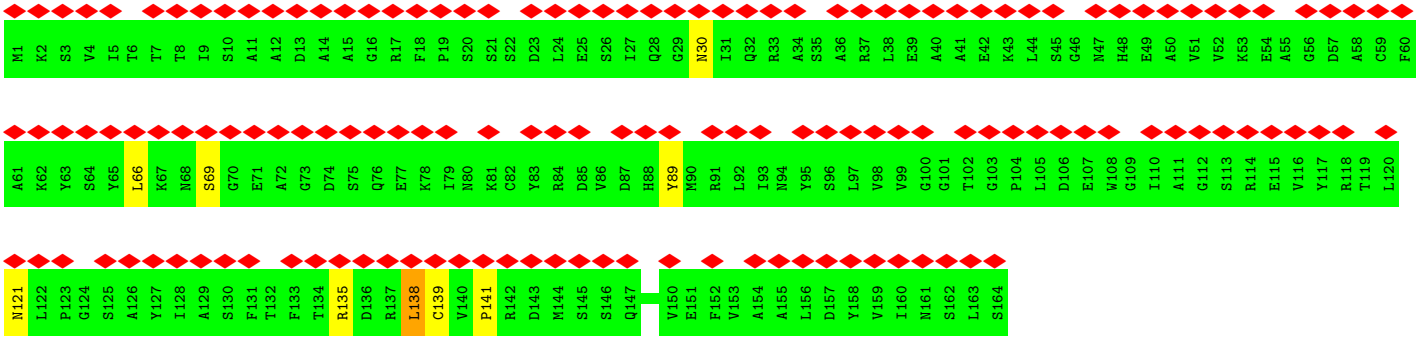




• Molecule 10: R-phycoerythrin alpha chain

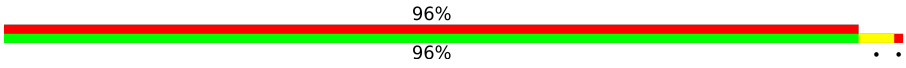
Chain k8:

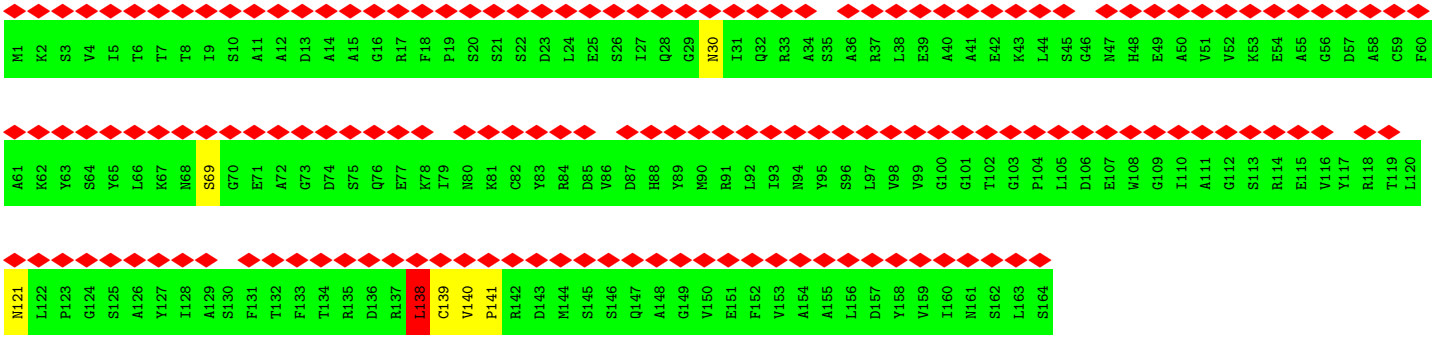




• Molecule 10: R-phycoerythrin alpha chain

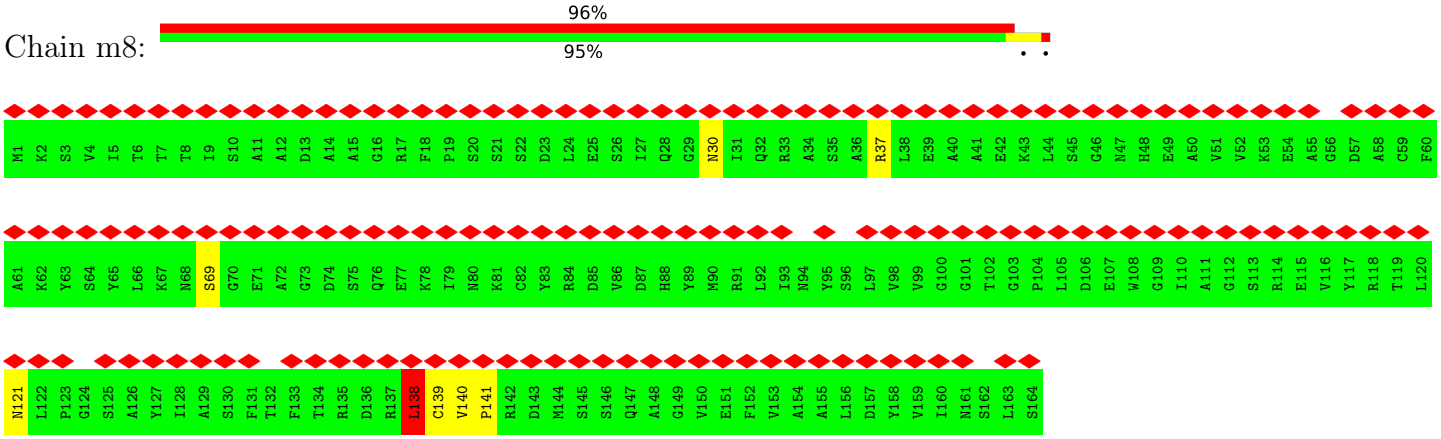
Chain l8:





• Molecule 10: R-phycoerythrin alpha chain

Chain m8:



• Molecule 10: R-phycoerythrin alpha chain

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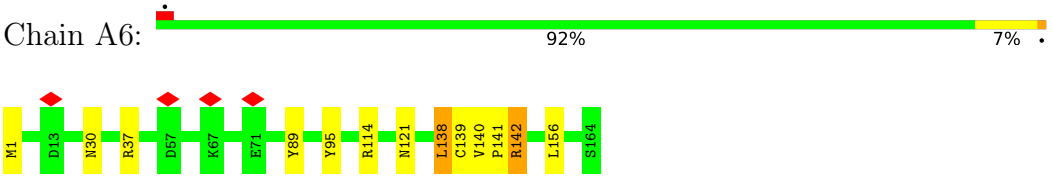

• Molecule 10: R-phycoerythrin alpha chain

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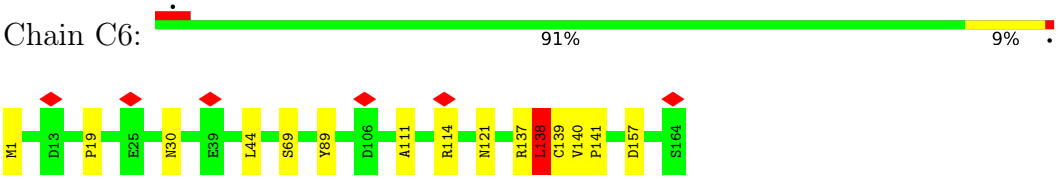

• Molecule 10: R-phycoerythrin alpha chain

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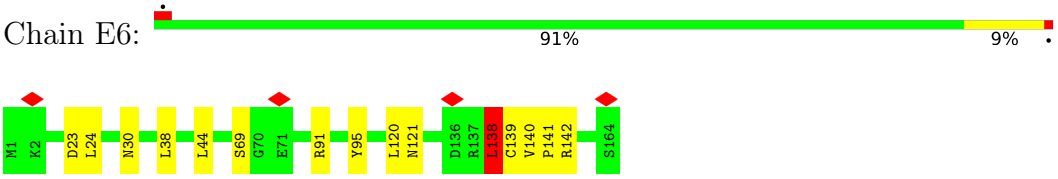
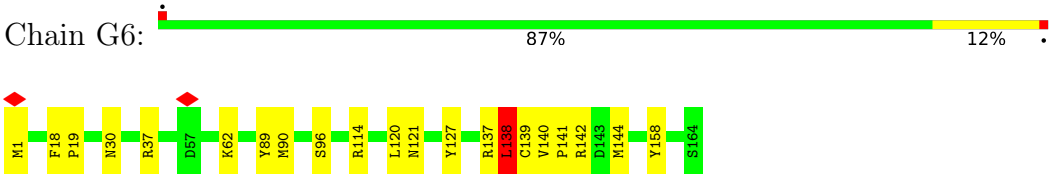


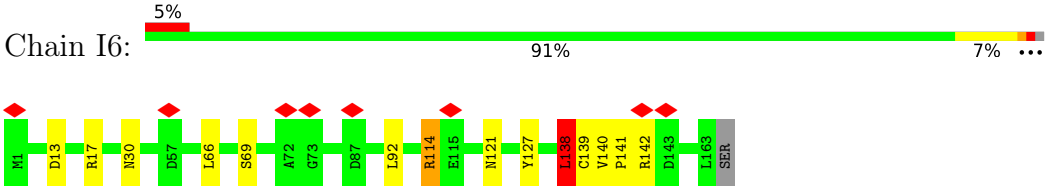
• Molecule 10: R-phycoerythrin alpha chain

Chain G6:



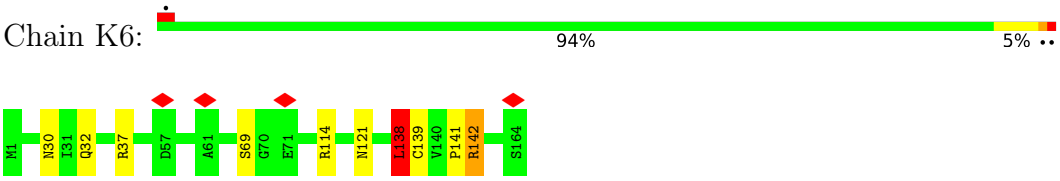
• Molecule 10: R-phycoerythrin alpha chain

Chain I6:



• Molecule 10: R-phycoerythrin alpha chain

Chain K6:



• Molecule 10: R-phycoerythrin alpha chain

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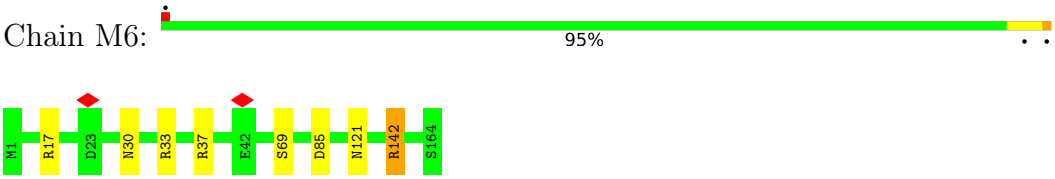

• Molecule 10: R-phycoerythrin alpha chain

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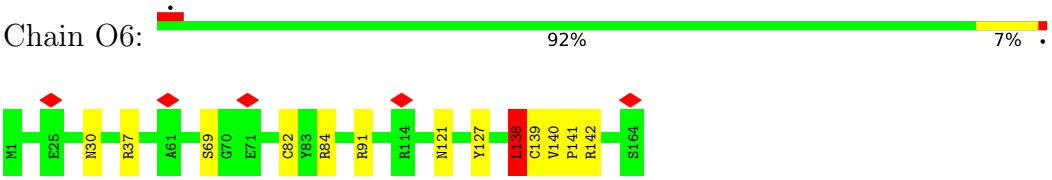
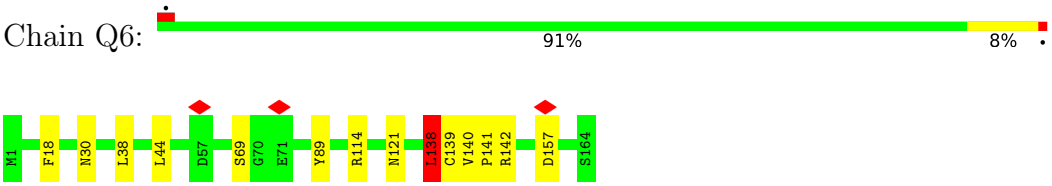


• Molecule 10: R-phycoerythrin alpha chain

Chain Q6:



• Molecule 10: R-phycoerythrin alpha chain

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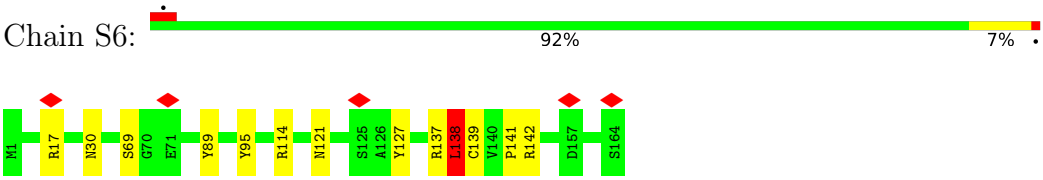
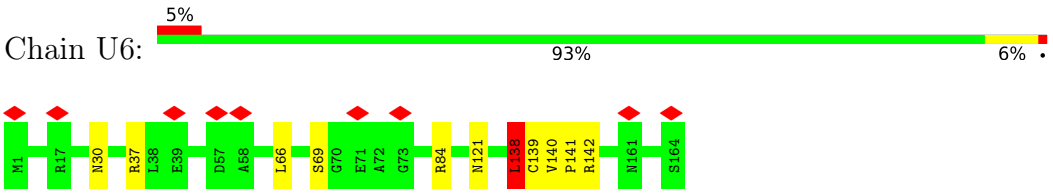


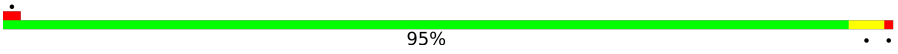
• Molecule 10: R-phycoerythrin alpha chain

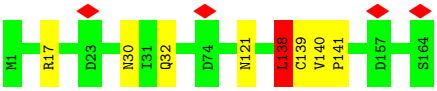
Chain U6:



• Molecule 10: R-phycoerythrin alpha chain

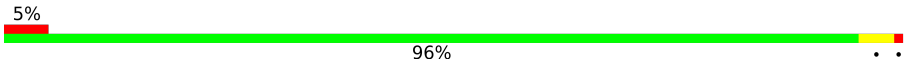
Chain W6:

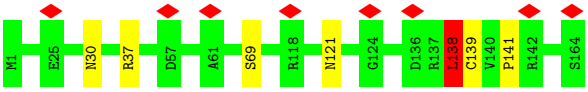




• Molecule 10: R-phycoerythrin alpha chain

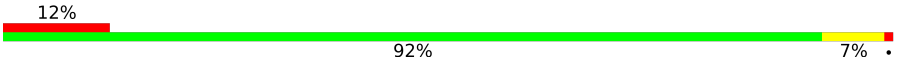
Chain Y6:

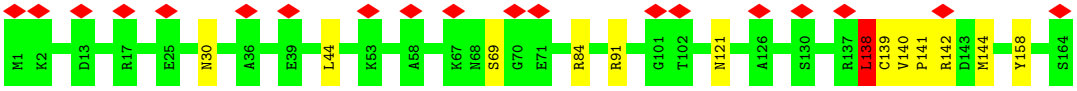




• Molecule 10: R-phycoerythrin alpha chain

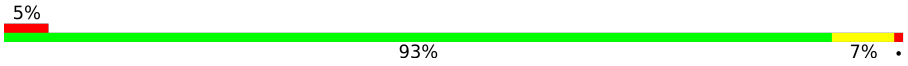
Chain f6:

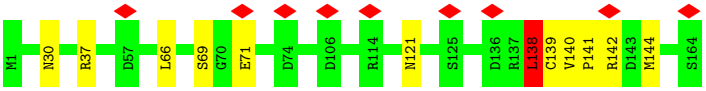




• Molecule 10: R-phycoerythrin alpha chain

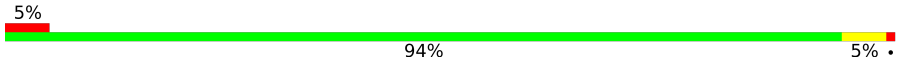
Chain g6:

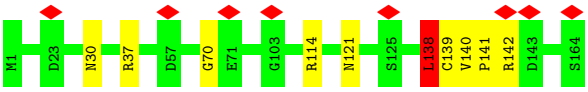




• Molecule 10: R-phycoerythrin alpha chain

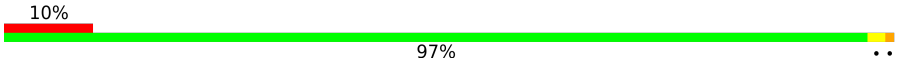
Chain h6:

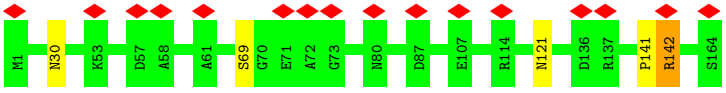




• Molecule 10: R-phycoerythrin alpha chain

Chain i6:





• Molecule 10: R-phycoerythrin alpha chain

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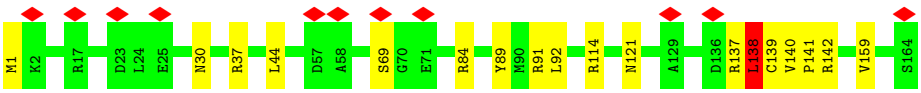
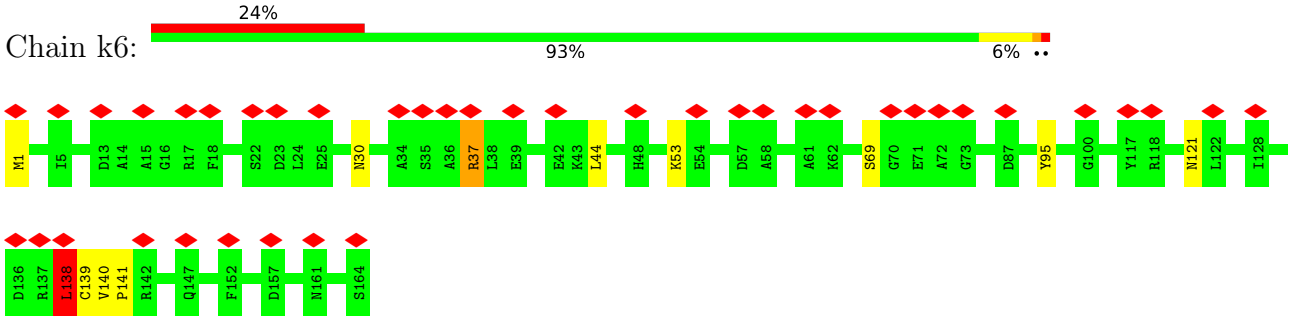


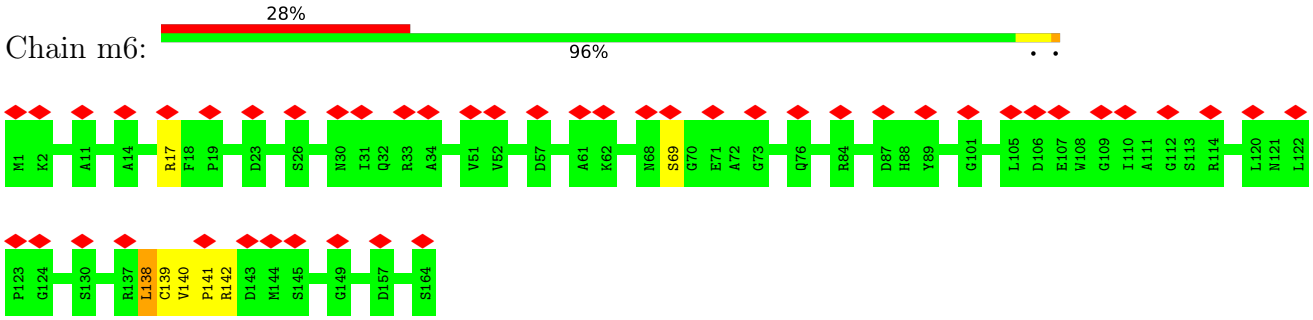
• Molecule 10: R-phycoerythrin alpha chain

Chain k6:



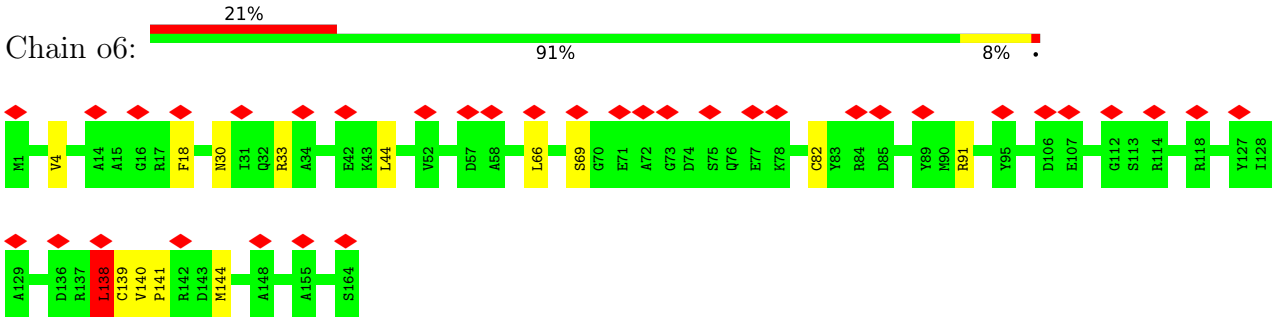
• Molecule 10: R-phycoerythrin alpha chain

Chain m6:



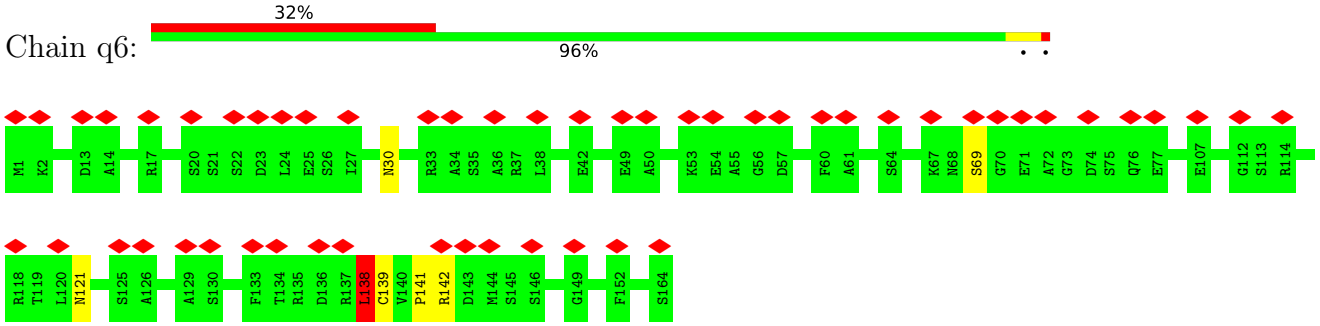
• Molecule 10: R-phycoerythrin alpha chain

Chain o6:



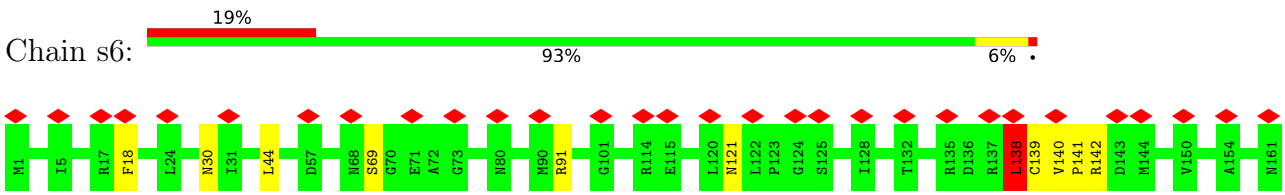
• Molecule 10: R-phycoerythrin alpha chain

Chain q6:



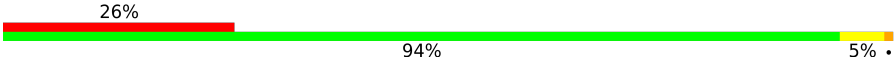
• Molecule 10: R-phycoerythrin alpha chain

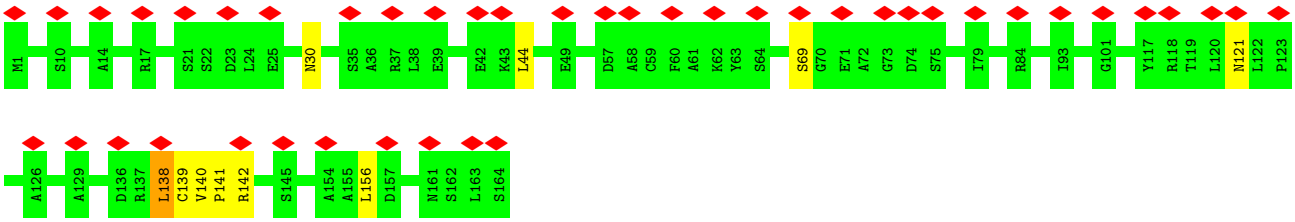
Chain s6:



• Molecule 10: R-phycoerythrin alpha chain

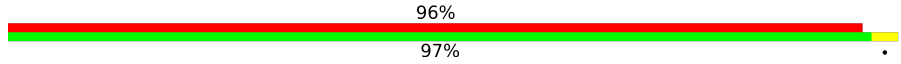
Chain u6:

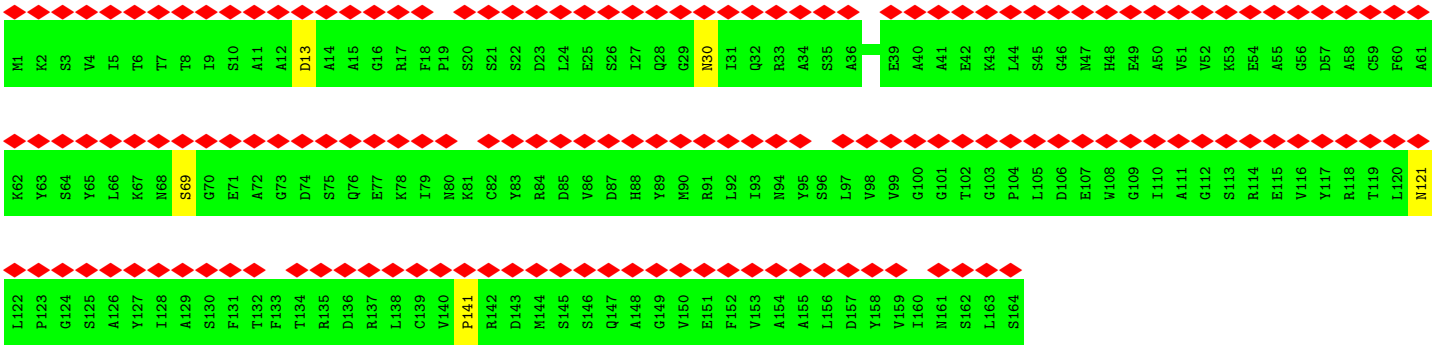




• Molecule 10: R-phycoerythrin alpha chain

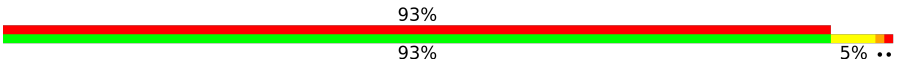
Chain w6:

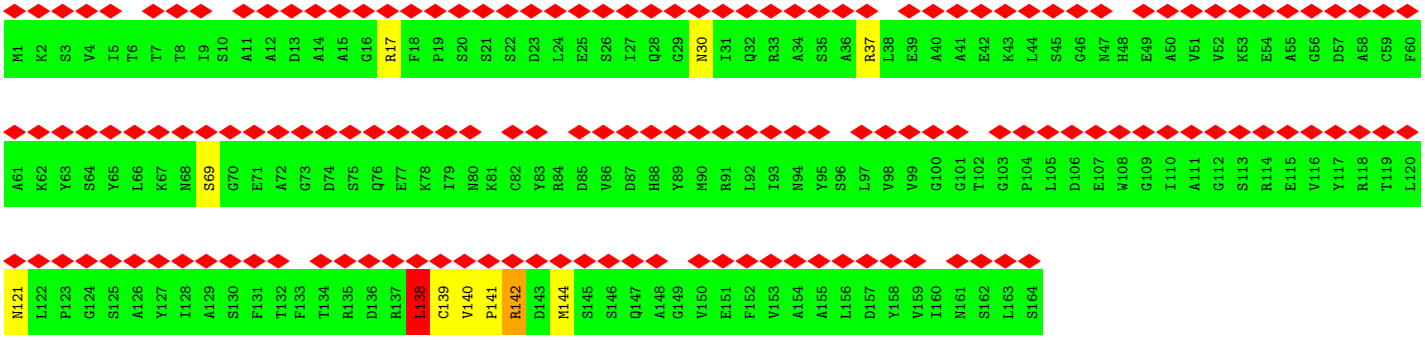




• Molecule 10: R-phycoerythrin alpha chain

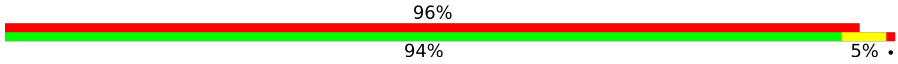
Chain q8:

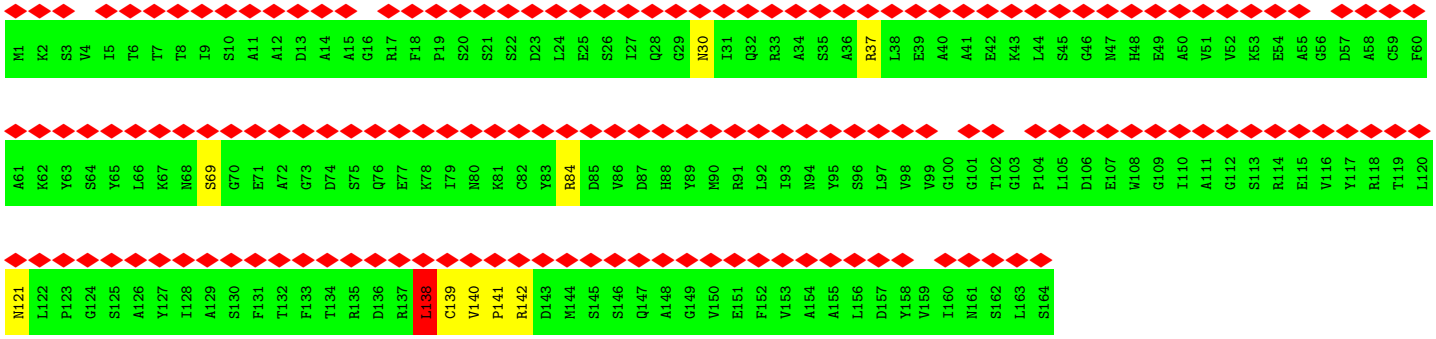




• Molecule 10: R-phycoerythrin alpha chain

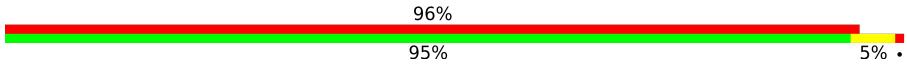
Chain r8:

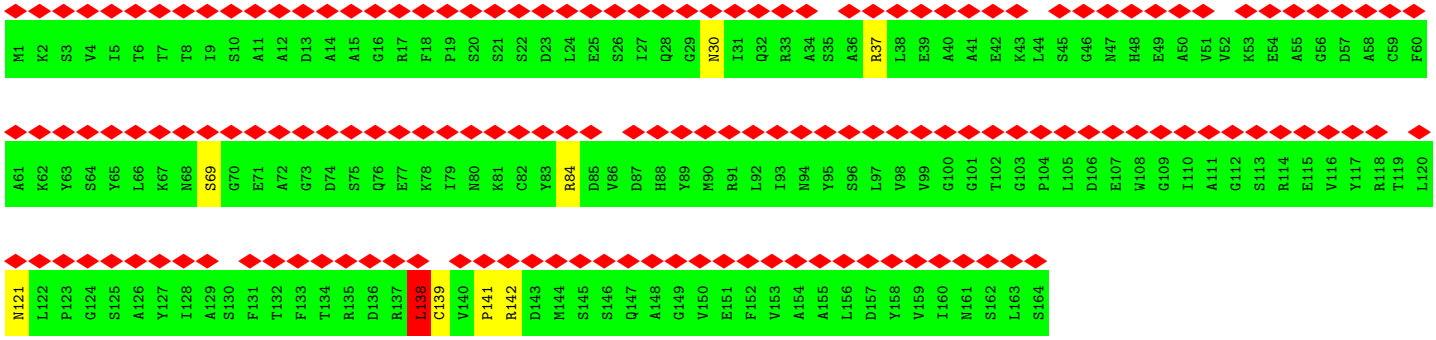




• Molecule 10: R-phycoerythrin alpha chain

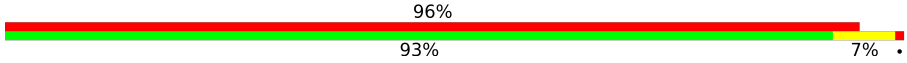
Chain s8:

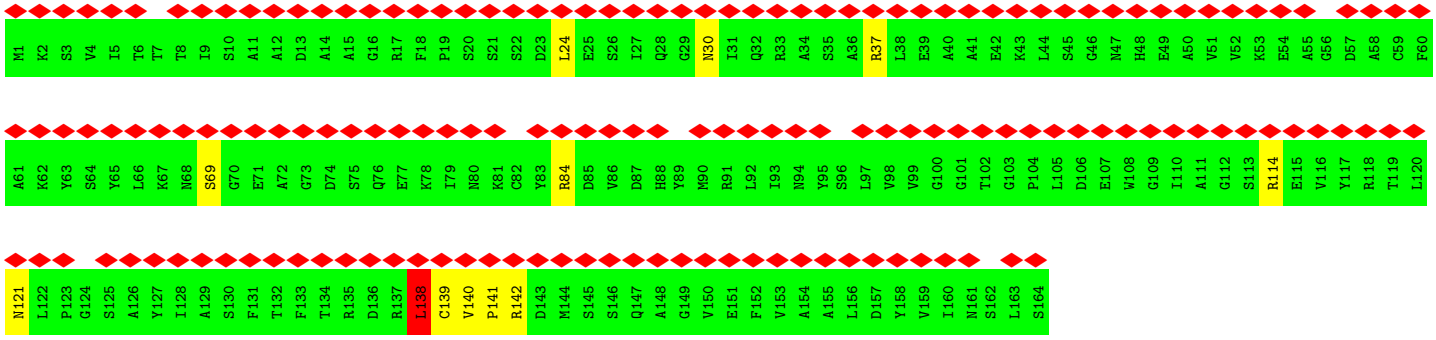




• Molecule 10: R-phycoerythrin alpha chain

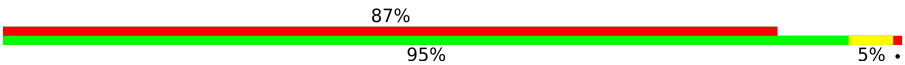
Chain t8:

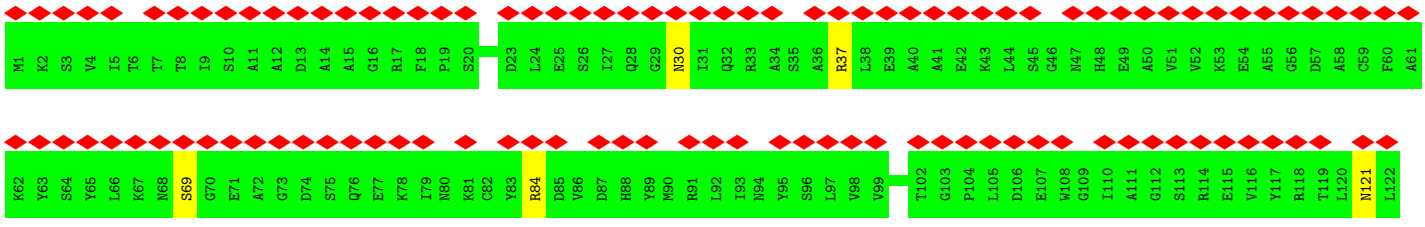


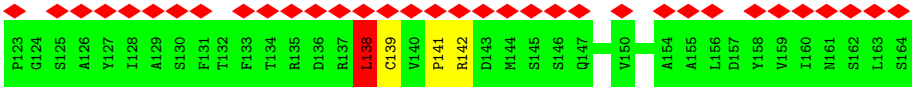


• Molecule 10: R-phycoerythrin alpha chain

Chain u8:

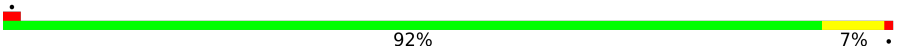


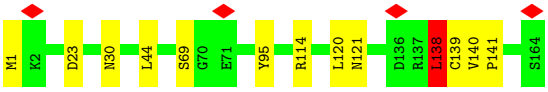




• Molecule 10: R-phycoerythrin alpha chain

Chain A7:



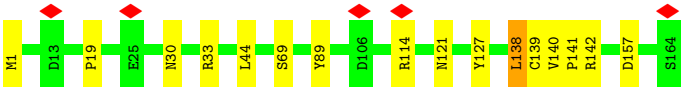


• Molecule 10: R-phycoerythrin alpha chain

Chain C7:

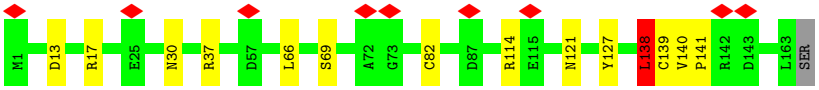
• Molecule 10: R-phycoerythrin alpha chain

Chain E7:



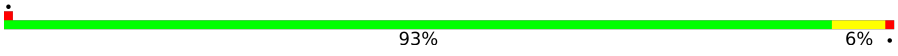
• Molecule 10: R-phycoerythrin alpha chain

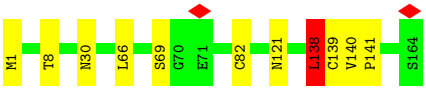
Chain G7:



• Molecule 10: R-phycoerythrin alpha chain

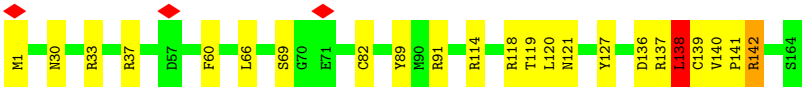
Chain I7:





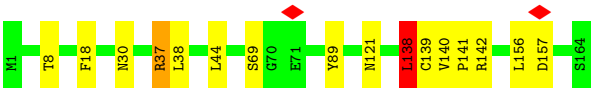
• Molecule 10: R-phycoerythrin alpha chain

Chain K7:



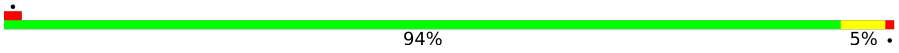
• Molecule 10: R-phycoerythrin alpha chain

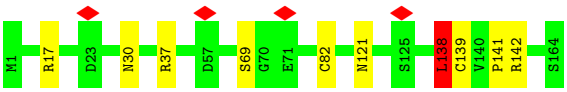
Chain M7:



• Molecule 10: R-phycoerythrin alpha chain

Chain O7:





• Molecule 10: R-phycoerythrin alpha chain

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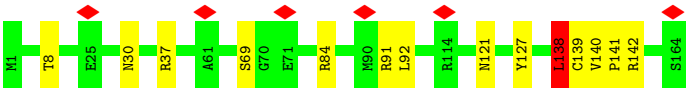
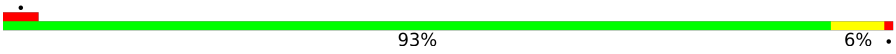
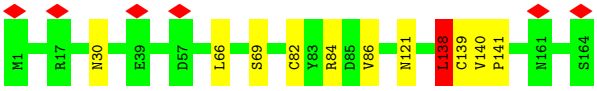


• Molecule 10: R-phycoerythrin alpha chain

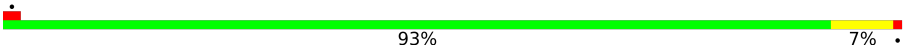
Chain S7:

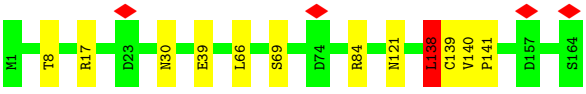




• Molecule 10: R-phycoerythrin alpha chain

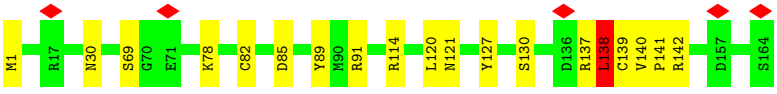
Chain U7:





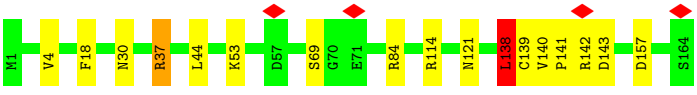
• Molecule 10: R-phycoerythrin alpha chain

Chain W7:



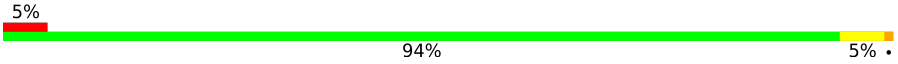
• Molecule 10: R-phycoerythrin alpha chain

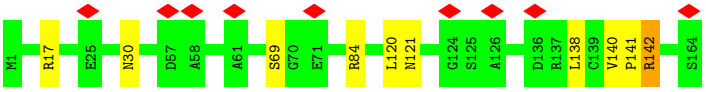
Chain Y7:



• Molecule 10: R-phycoerythrin alpha chain

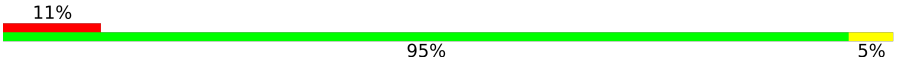
Chain f7:

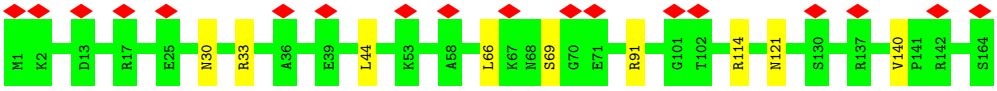




• Molecule 10: R-phycoerythrin alpha chain

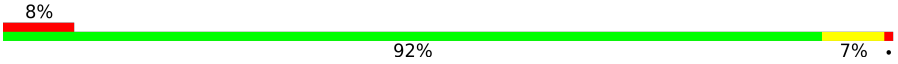
Chain g7:

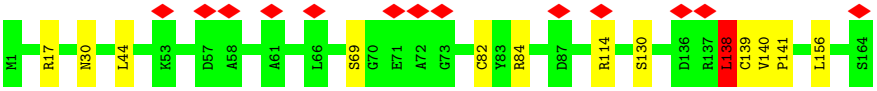




• Molecule 10: R-phycoerythrin alpha chain

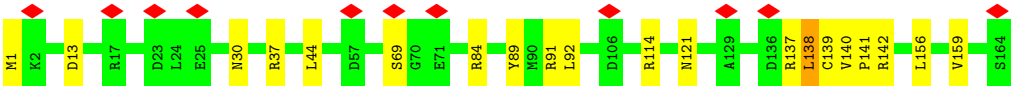
Chain h7:





• Molecule 10: R-phycoerythrin alpha chain

Chain i7:



• Molecule 10: R-phycoerythrin alpha chain

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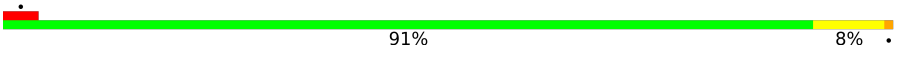
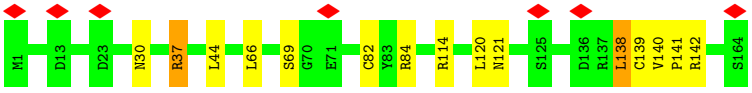
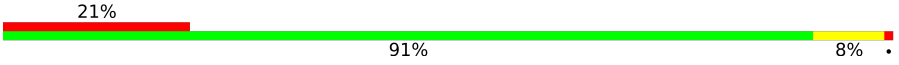
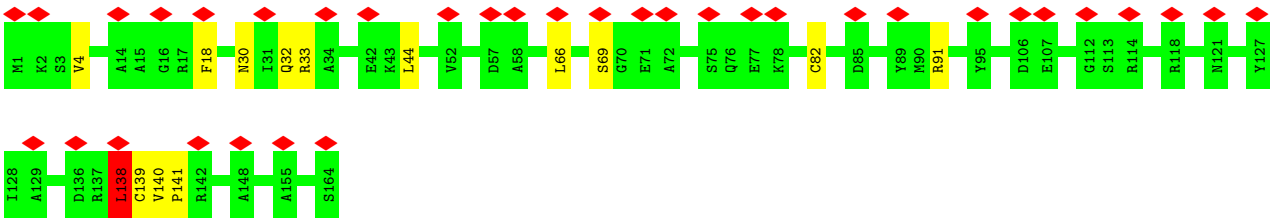




• Molecule 10: R-phycoerythrin alpha chain

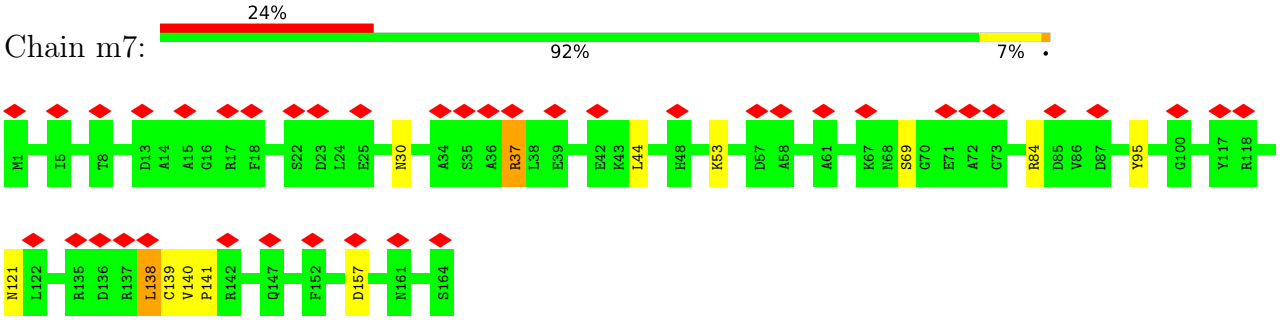
Chain k7:





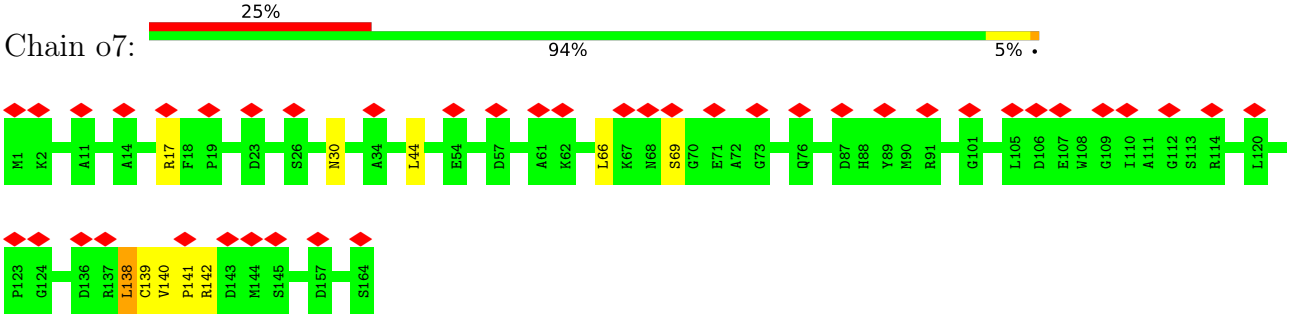
• Molecule 10: R-phycoerythrin alpha chain

Chain m7:



• Molecule 10: R-phycoerythrin alpha chain

Chain o7:



• Molecule 10: R-phycoerythrin alpha chain

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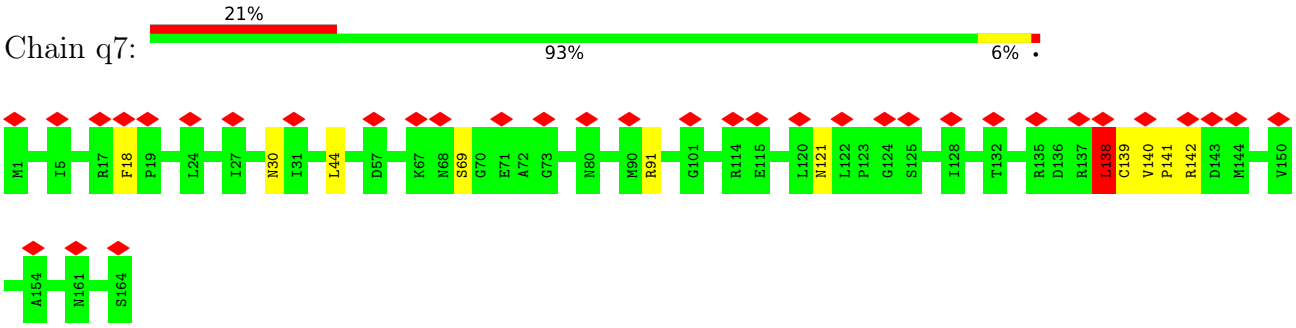
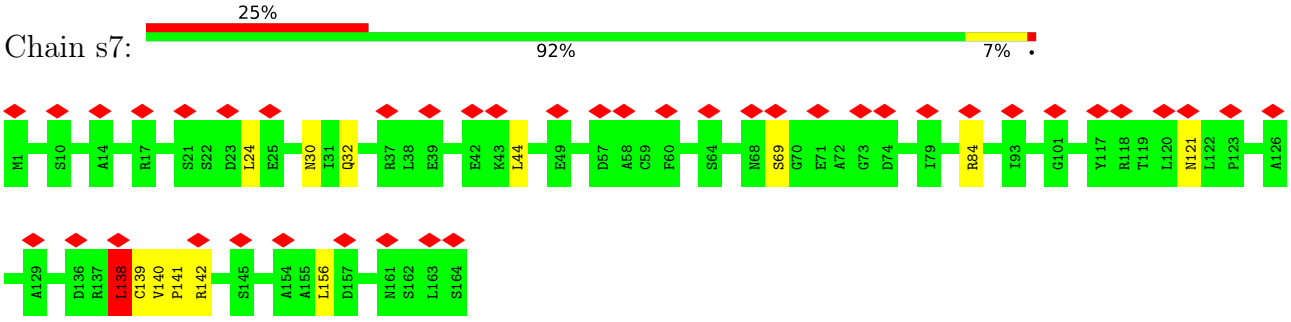


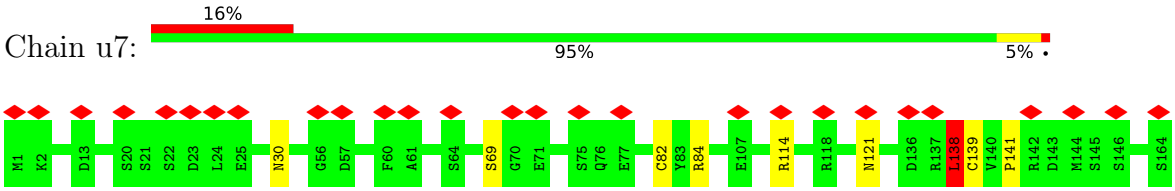
• Molecule 10: R-phycoerythrin alpha chain

Chain s7:



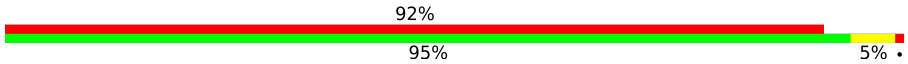
• Molecule 10: R-phycoerythrin alpha chain

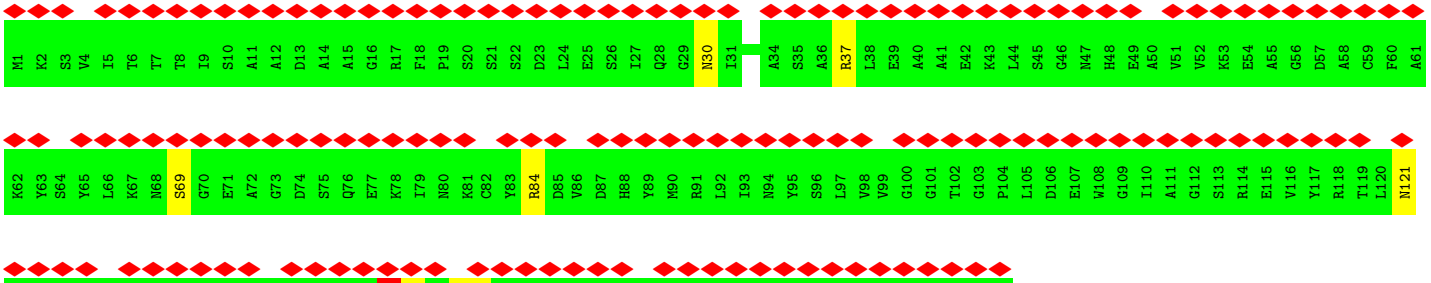
Chain u7:



• Molecule 10: R-phycoerythrin alpha chain

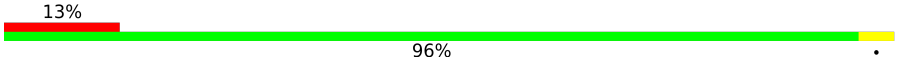
Chain w7:

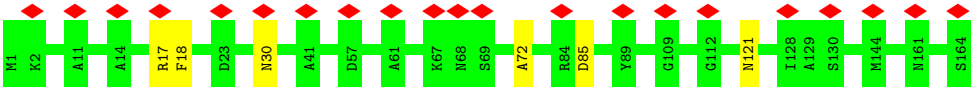




• Molecule 10: R-phycoerythrin alpha chain

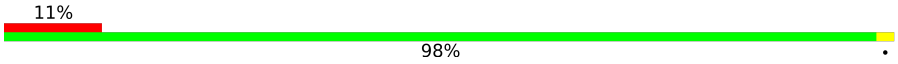
Chain v8:

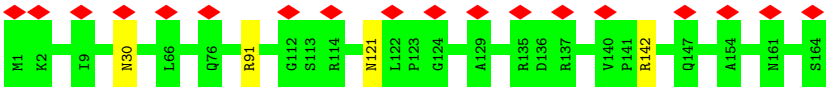




• Molecule 10: R-phycoerythrin alpha chain

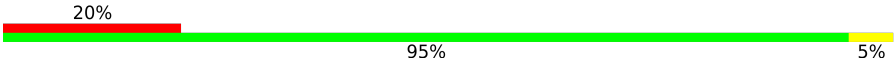
Chain x8:

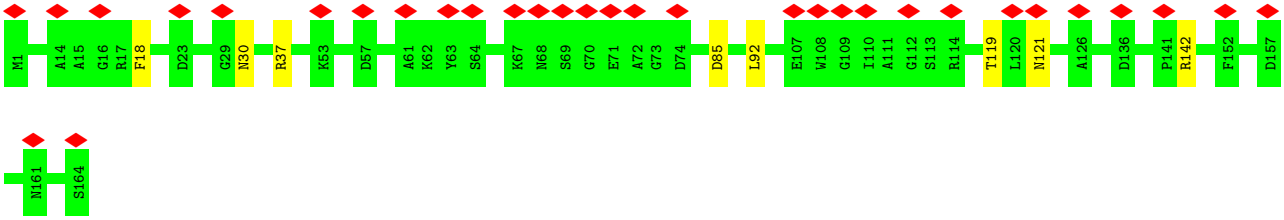




• Molecule 10: R-phycoerythrin alpha chain

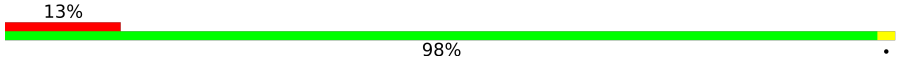
Chain z8:

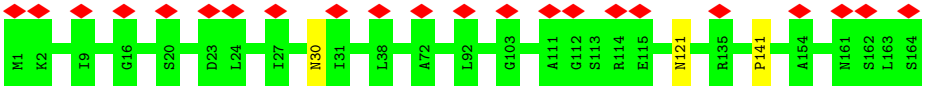




• Molecule 10: R-phycoerythrin alpha chain

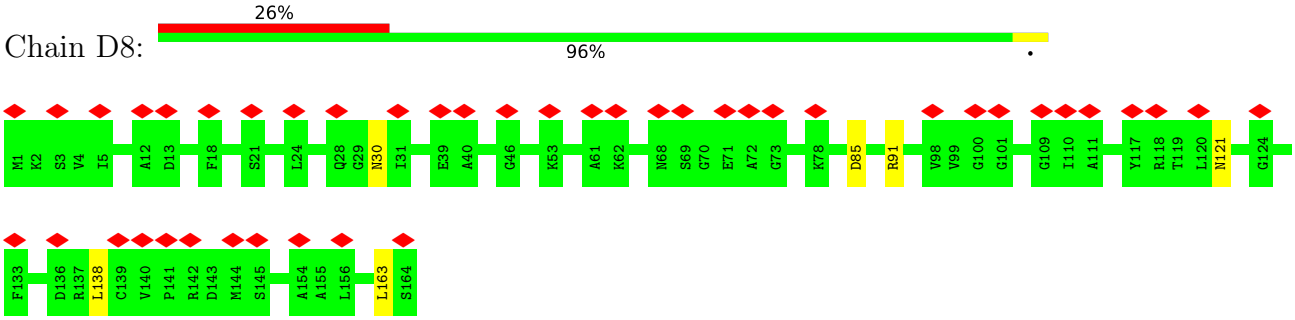
Chain B8:





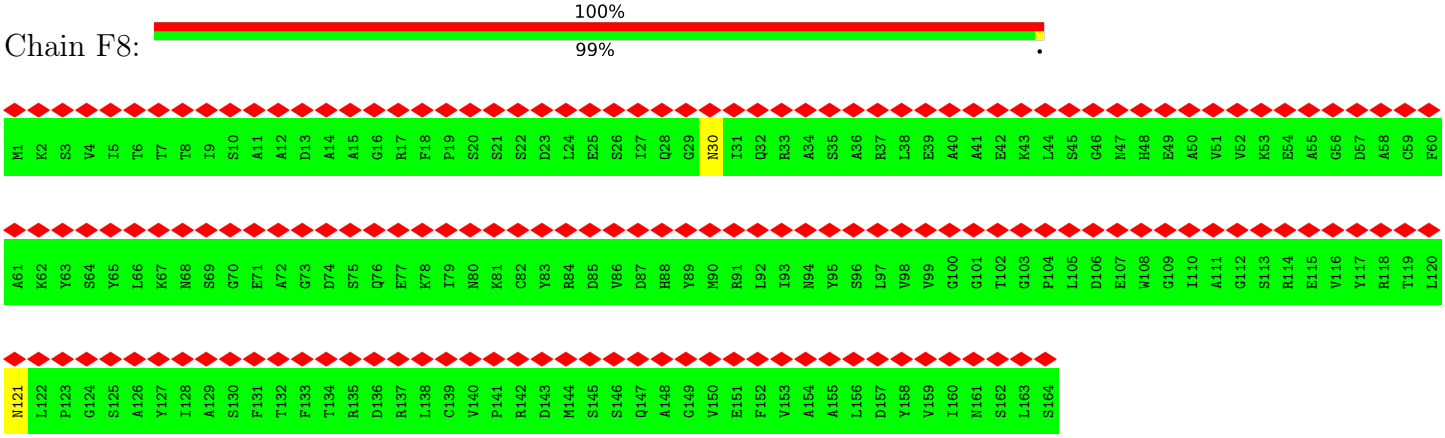
• Molecule 10: R-phycoerythrin alpha chain

Chain D8:



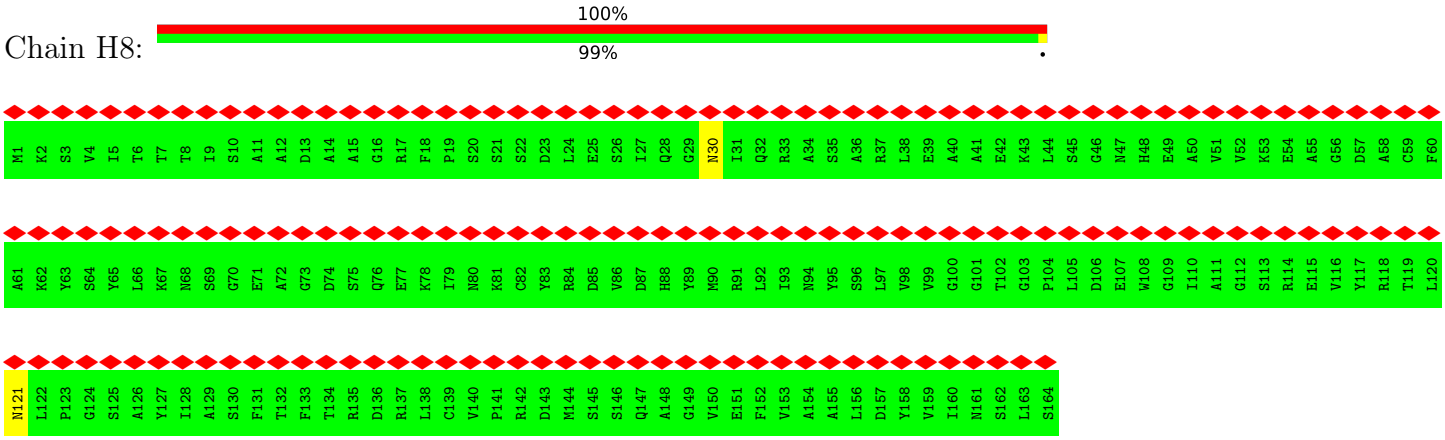
• Molecule 10: R-phycoerythrin alpha chain

Chain F8:



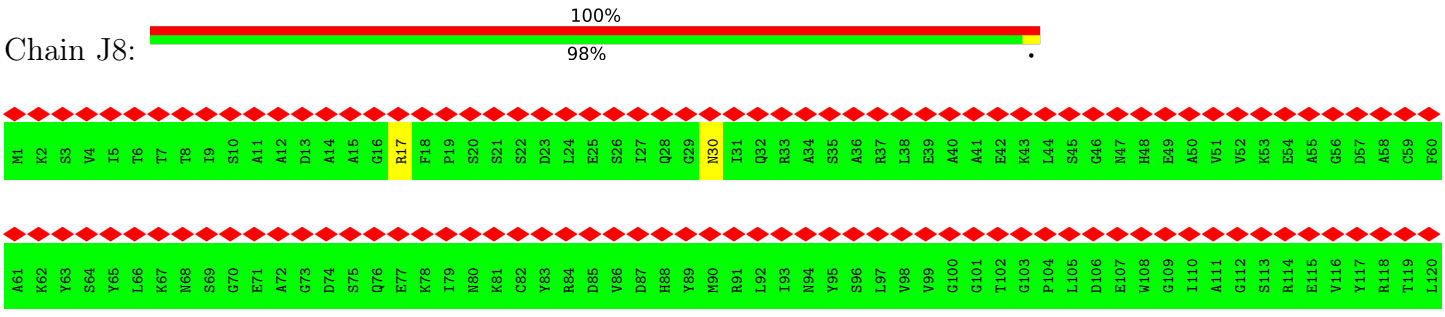
• Molecule 10: R-phycoerythrin alpha chain

Chain H8:



• Molecule 10: R-phycoerythrin alpha chain

Chain J8:



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• Molecule 10: R-phycoerythrin alpha chain

Chain L8:

M1 K2 S3 V4 I5 T6 T7 T8 I9 S10 A11 A12 D13 A14 A15 G16 R17 F18 P19 S20 S21 S22 D23 L24 E25 S26 I27 Q28 G29 N30 I31 Q32 R33 A34 S35 A36 R37 L38 E39 A40 A41 E42 K43 L44 S45 G46 N47 H48 E49 A50 V51 V52 K53 E54 A55 G56 D57 A58 C59 F60

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain N8:

M1 K2 S3 V4 I5 T6 T7 T8 I9 S10 A11 A12 D13 A14 A15 G16 R17 F18 P19 S20 S21 S22 D23 L24 E25 S26 I27 Q28 G29 N30 I31 Q32 R33 A34 S35 A36 R37 L38 E39 A40 A41 E42 K43 L44 S45 G46 N47 H48 E49 A50 V51 V52 K53 E54 A55 G56 D57 A58 C59 F60

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain P8:

M1 K2 S3 V4 I5 T6 T7 T8 I9 S10 A11 A12 D13 A14 A15 G16 R17 F18 P19 S20 S21 S22 D23 L24 E25 S26 I27 Q28 G29 N30 I31 Q32 R33 A34 S35 A36 R37 L38 E39 A40 A41 E42 K43 L44 S45 G46 N47 H48 E49 A50 V51 V52 K53 E54 A55 G56 D57 A58 C59 F60

A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

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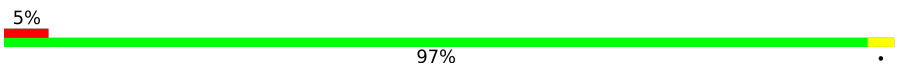
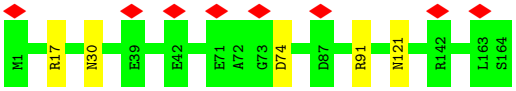
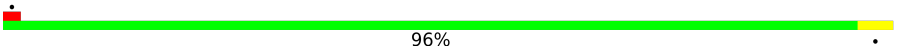
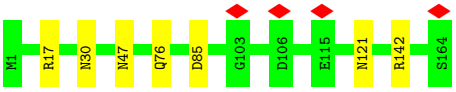




• Molecule 10: R-phycoerythrin alpha chain

Chain o9:





• Molecule 10: R-phycoerythrin alpha chain

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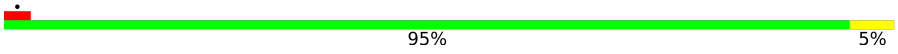
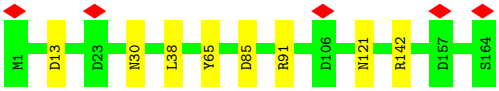
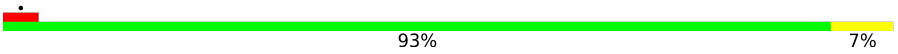
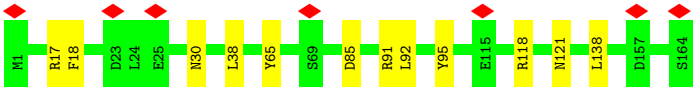




• Molecule 10: R-phycoerythrin alpha chain

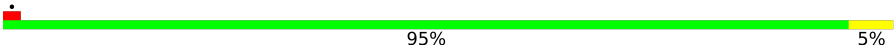
Chain s9:

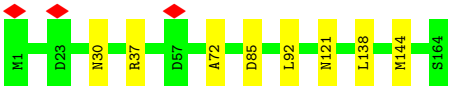




• Molecule 10: R-phycoerythrin alpha chain

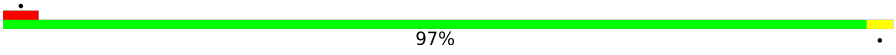
Chain u9:

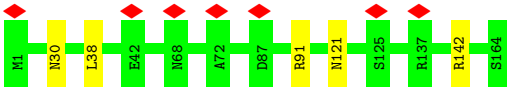




• Molecule 10: R-phycoerythrin alpha chain

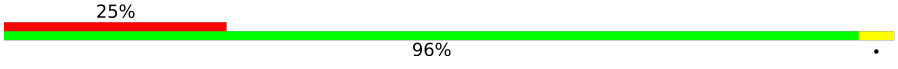
Chain w9:

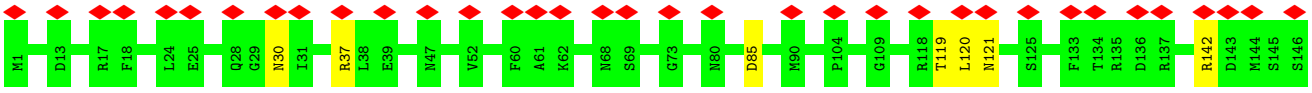


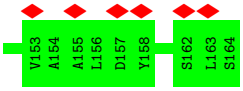


• Molecule 10: R-phycoerythrin alpha chain

Chain y9:

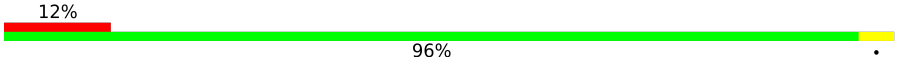


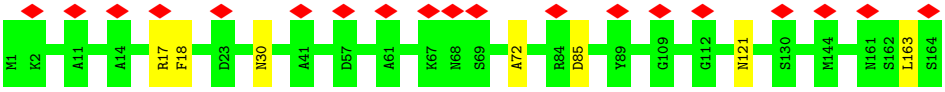




• Molecule 10: R-phycoerythrin alpha chain

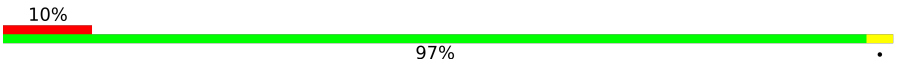
Chain A9:

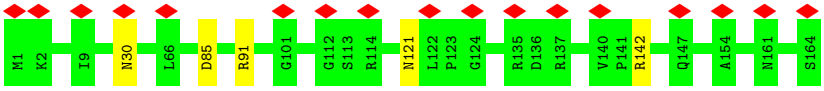




• Molecule 10: R-phycoerythrin alpha chain

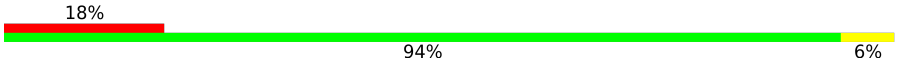
Chain C9:

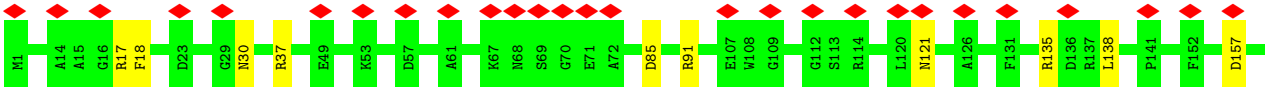




• Molecule 10: R-phycoerythrin alpha chain

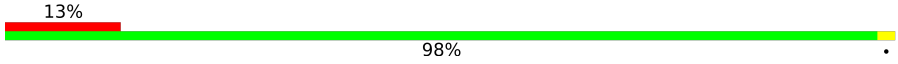
Chain E9:





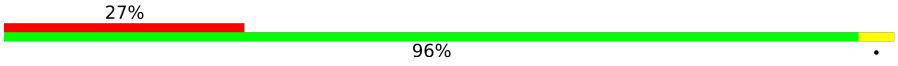
• Molecule 10: R-phycoerythrin alpha chain

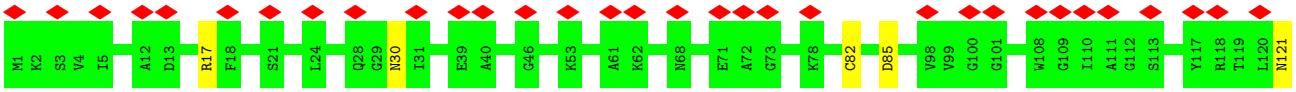
Chain G9:

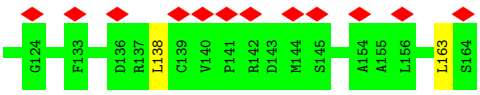


• Molecule 10: R-phycoerythrin alpha chain

Chain I9:

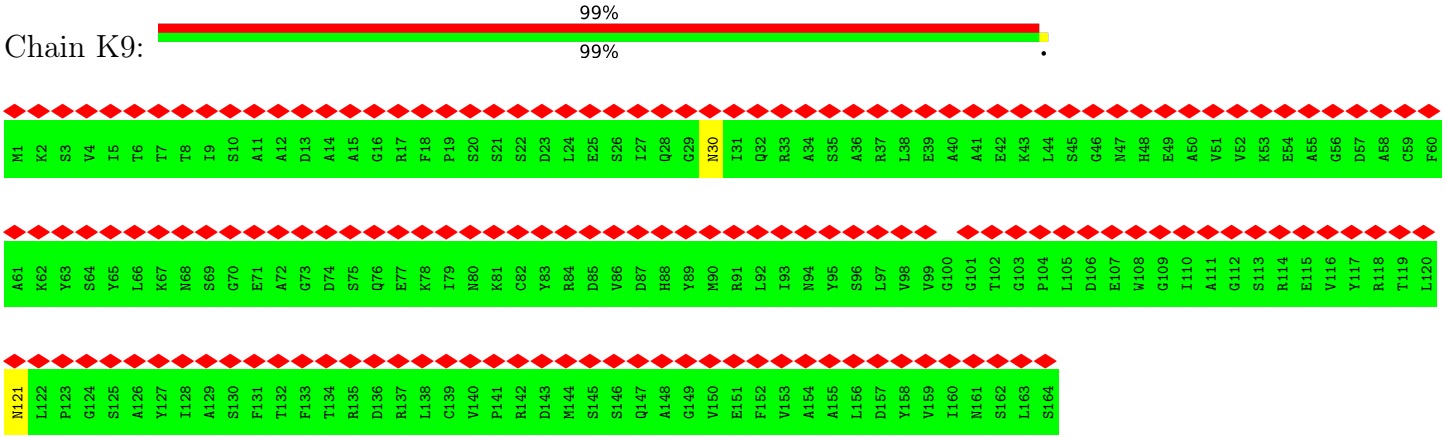






• Molecule 10: R-phycoerythrin alpha chain

Chain K9:



• Molecule 10: R-phycoerythrin alpha chain

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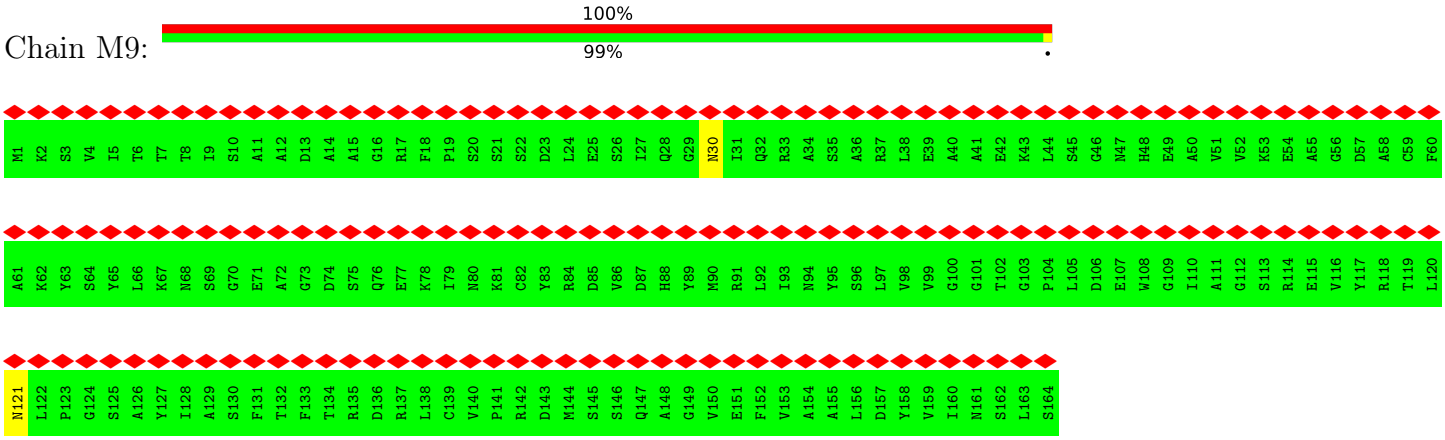

• Molecule 10: R-phycoerythrin alpha chain

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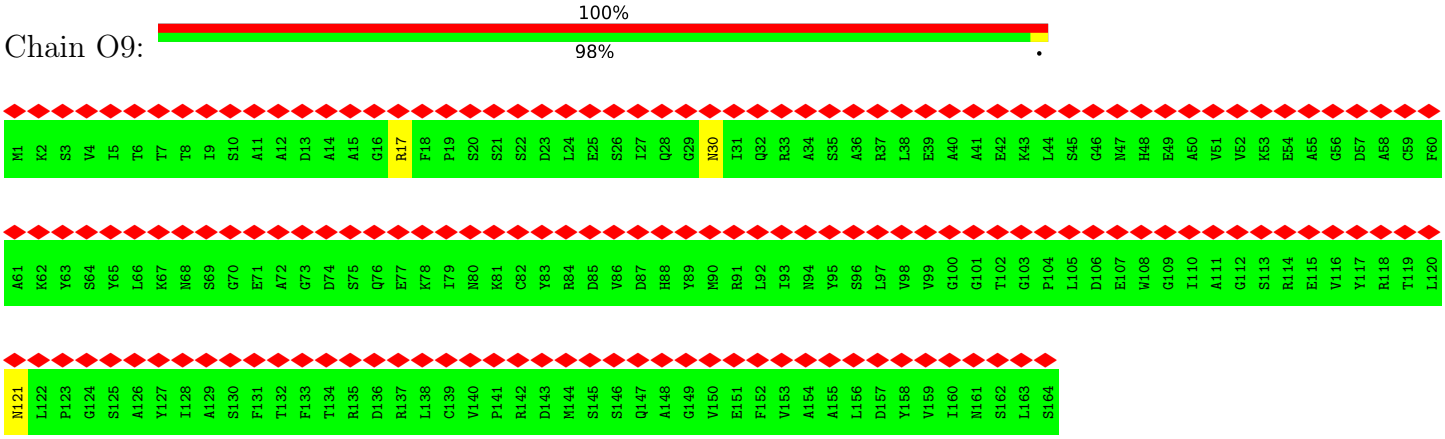

• Molecule 10: R-phycoerythrin alpha chain

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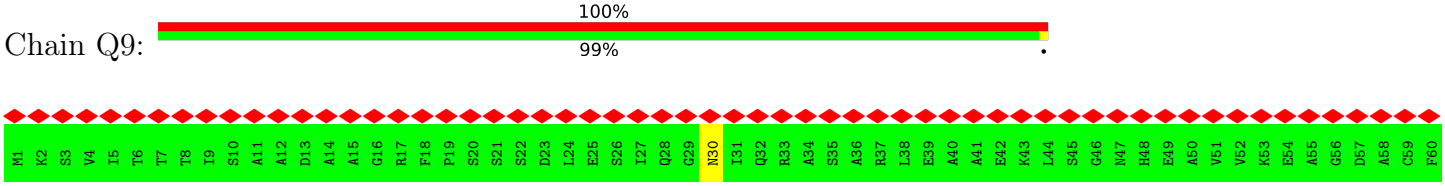

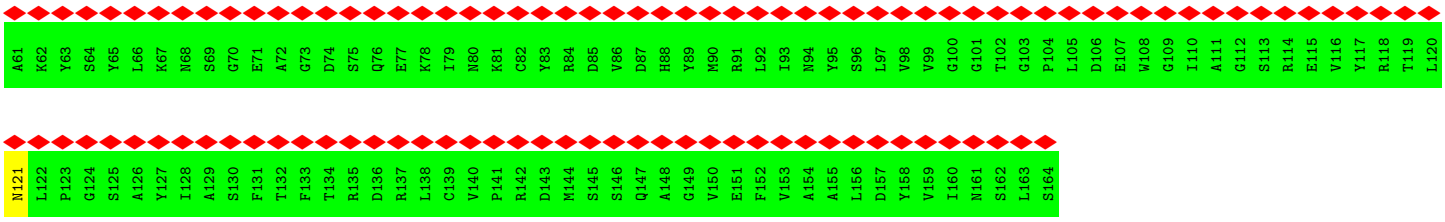

• Molecule 10: R-phycoerythrin alpha chain

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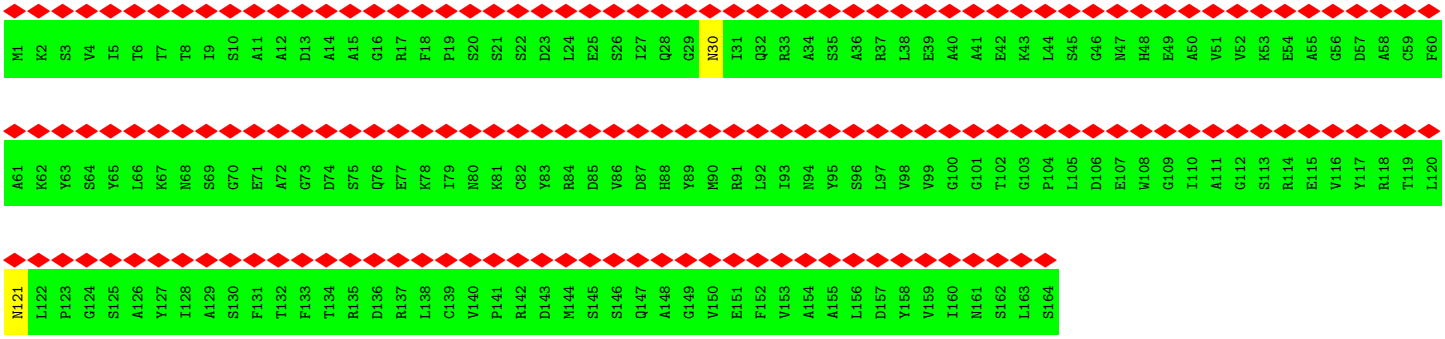

• Molecule 10: R-phycoerythrin alpha chain

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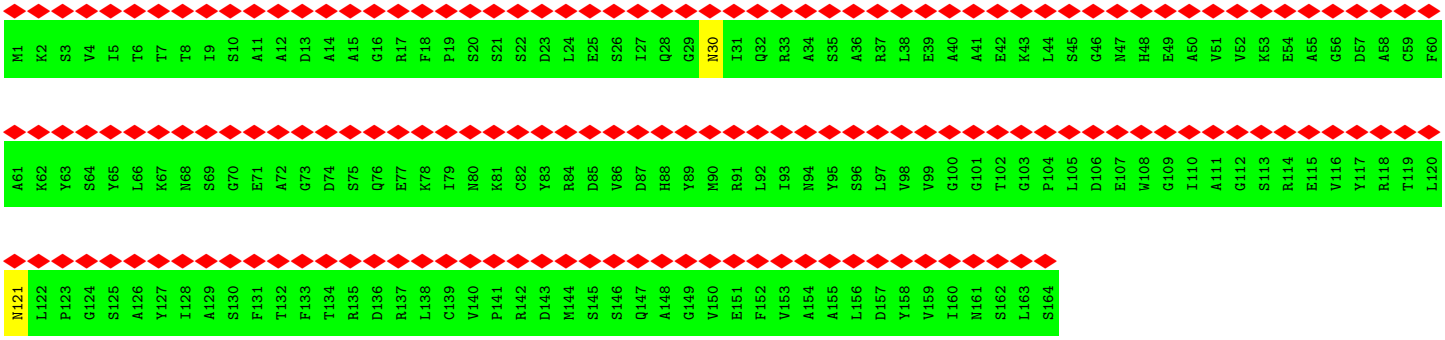
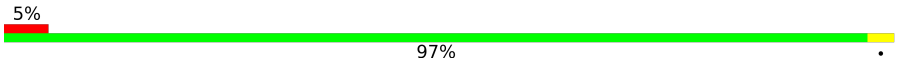
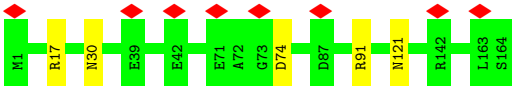


• Molecule 10: R-phycoerythrin alpha chain

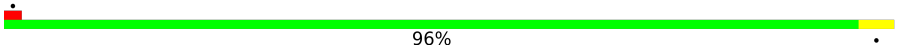
Chain am:

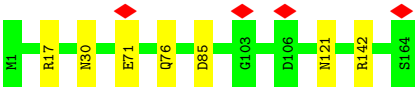




• Molecule 10: R-phycoerythrin alpha chain

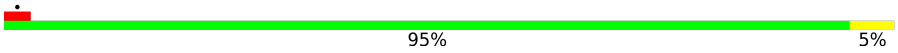
Chain ao:

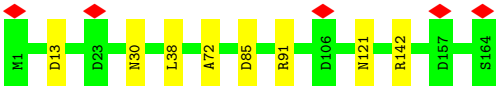




• Molecule 10: R-phycoerythrin alpha chain

Chain aq:





• Molecule 10: R-phycoerythrin alpha chain

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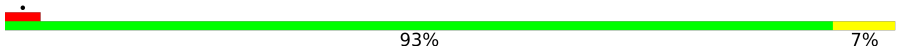

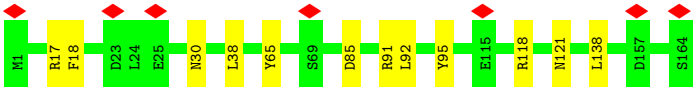

• Molecule 10: R-phycoerythrin alpha chain

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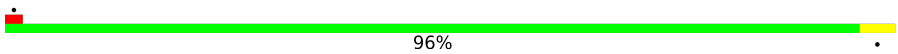

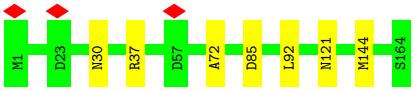

• Molecule 10: R-phycoerythrin alpha chain

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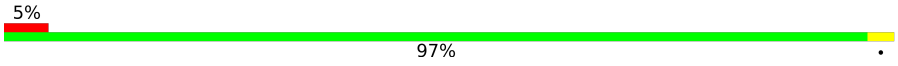

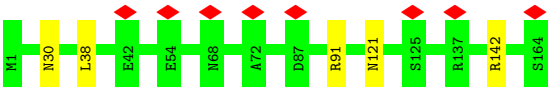

• Molecule 10: R-phycoerythrin alpha chain

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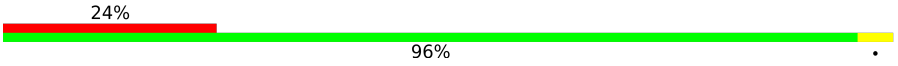
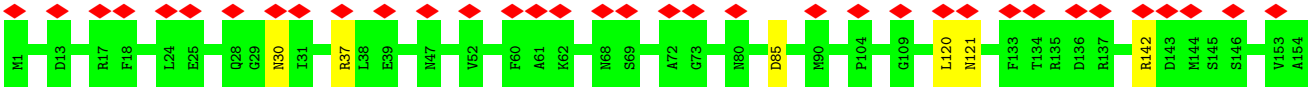
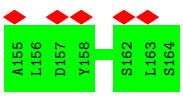
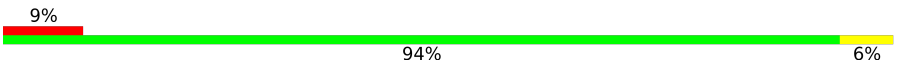


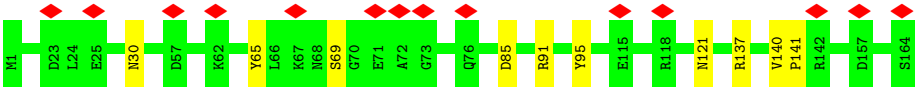




• Molecule 10: R-phycoerythrin alpha chain

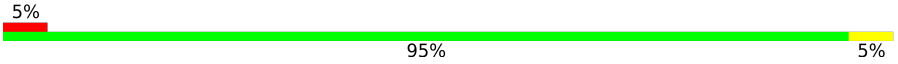
Chain aA:

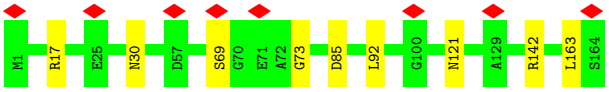




• Molecule 10: R-phycoerythrin alpha chain

Chain aC:





• Molecule 10: R-phycoerythrin alpha chain

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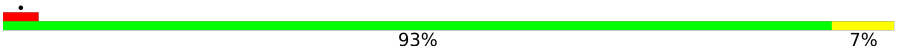
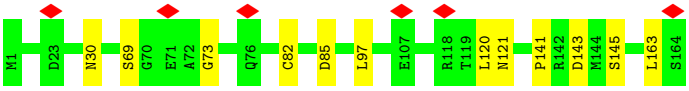
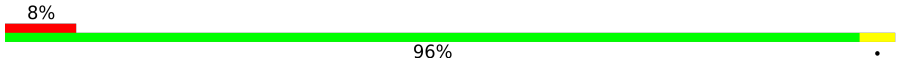
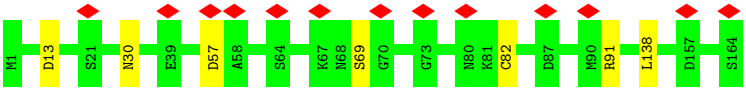




• Molecule 10: R-phycoerythrin alpha chain

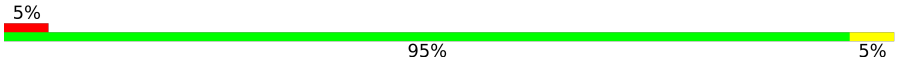
Chain aG:

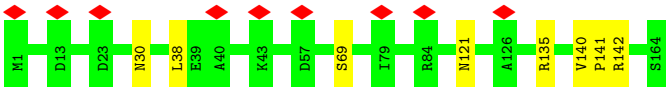




• Molecule 10: R-phycoerythrin alpha chain

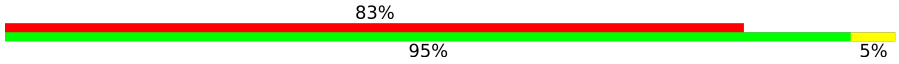
Chain aI:

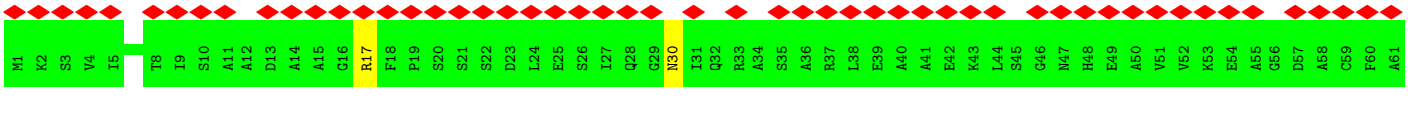


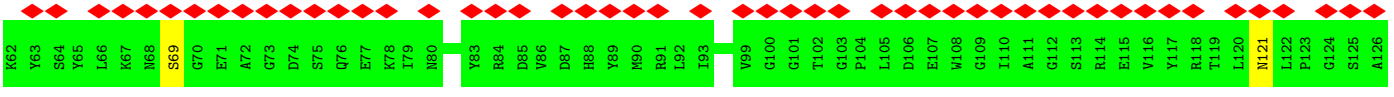


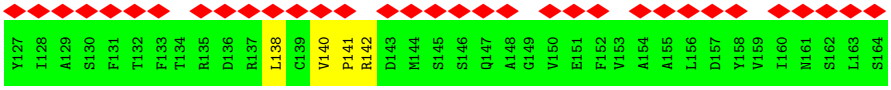
• Molecule 10: R-phycoerythrin alpha chain

Chain aK:



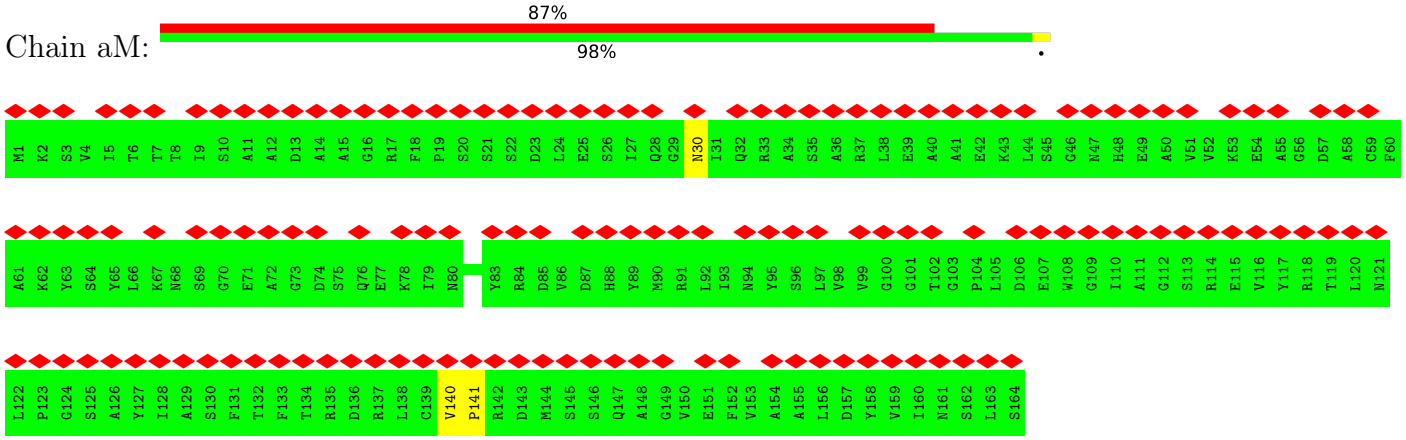






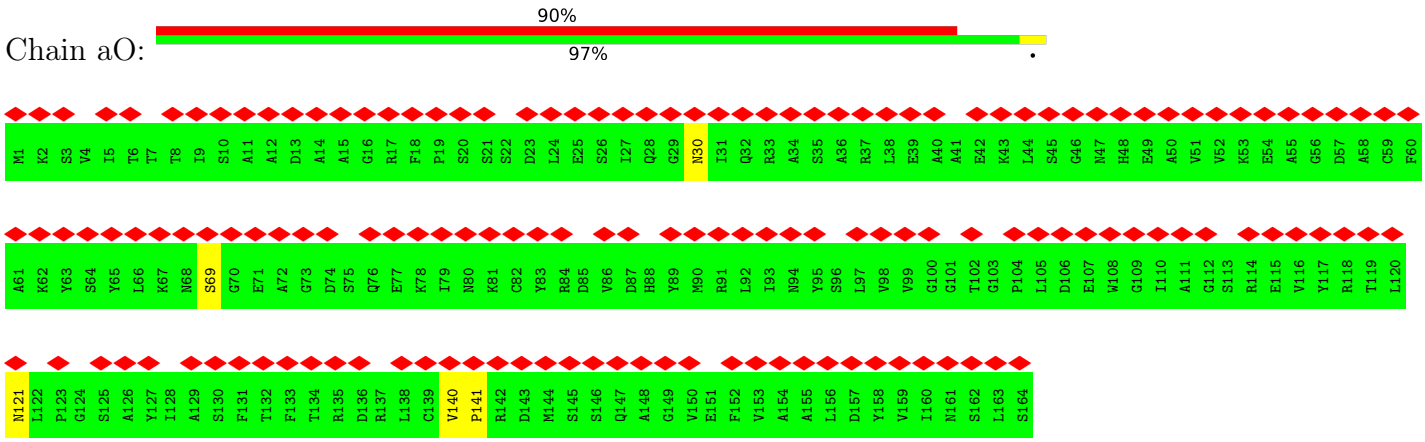
• Molecule 10: R-phycoerythrin alpha chain

Chain aM:



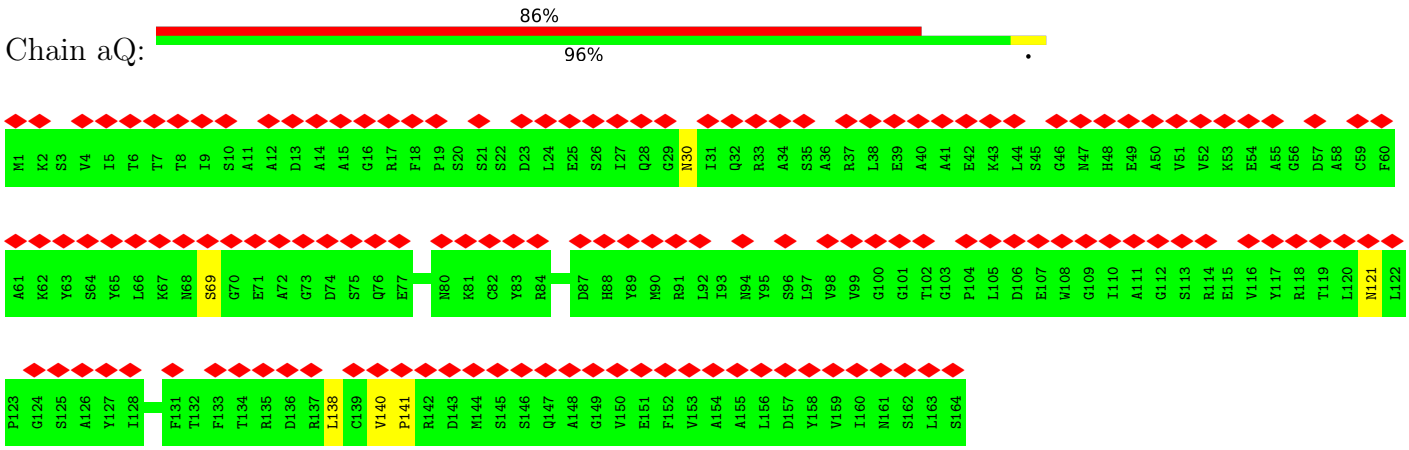
• Molecule 10: R-phycoerythrin alpha chain

Chain aO:



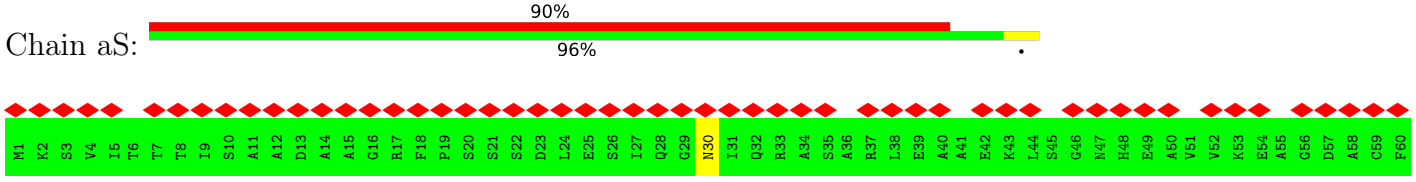
• Molecule 10: R-phycoerythrin alpha chain

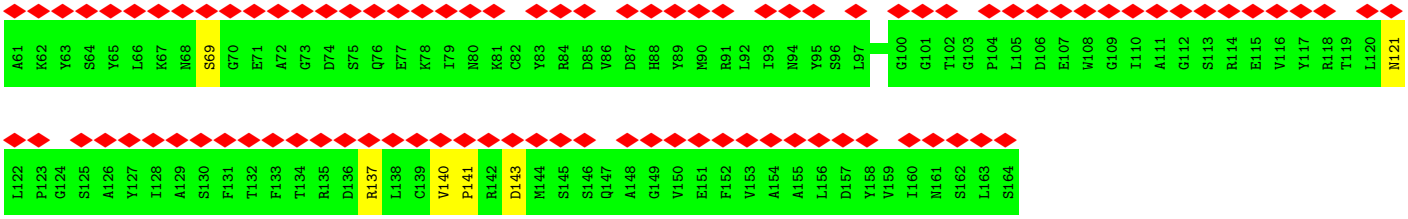
Chain aQ:



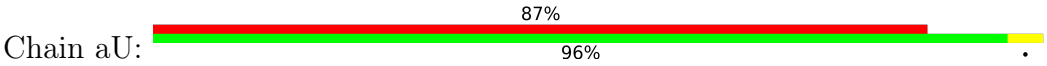
• Molecule 10: R-phycoerythrin alpha chain

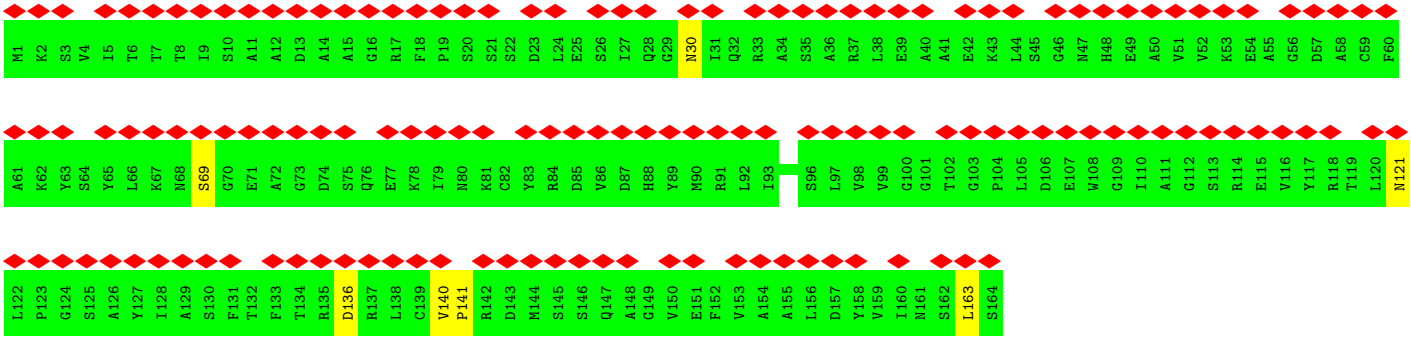
Chain aS:



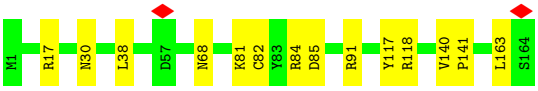


• Molecule 10: R-phycoerythrin alpha chain

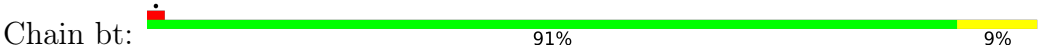




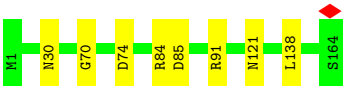
• Molecule 10: R-phycoerythrin alpha chain



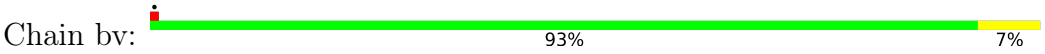
• Molecule 10: R-phycoerythrin alpha chain

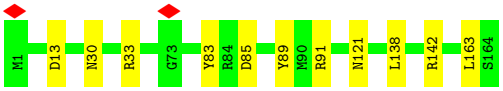


• Molecule 10: R-phycoerythrin alpha chain



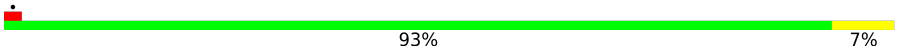
• Molecule 10: R-phycoerythrin alpha chain

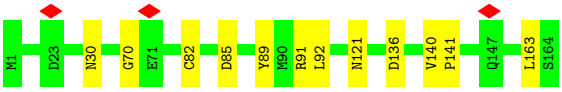




• Molecule 10: R-phycoerythrin alpha chain

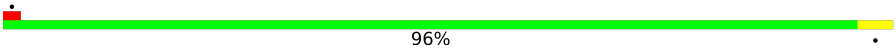
Chain bw:

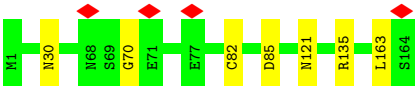




• Molecule 10: R-phycoerythrin alpha chain

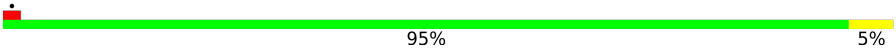
Chain bx:

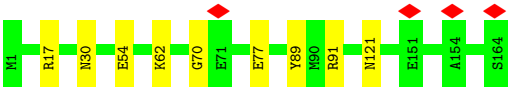




• Molecule 10: R-phycoerythrin alpha chain

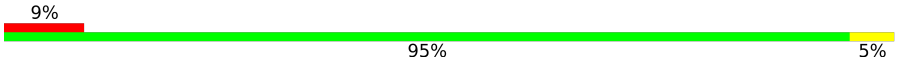
Chain by:

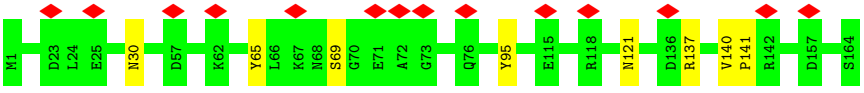




• Molecule 10: R-phycoerythrin alpha chain

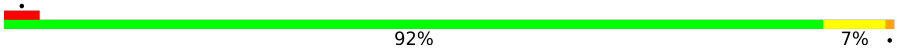
Chain bA:

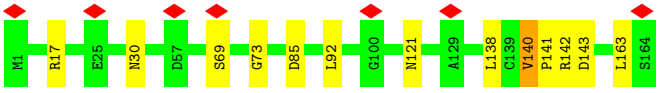




• Molecule 10: R-phycoerythrin alpha chain

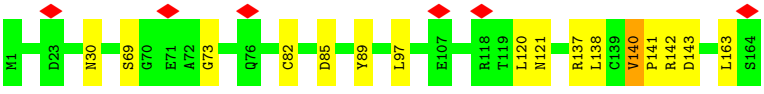
Chain bC:





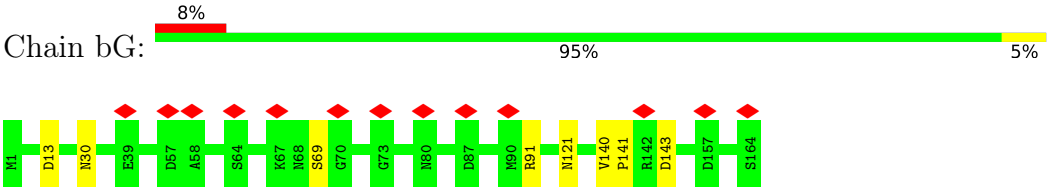
• Molecule 10: R-phycoerythrin alpha chain

Chain bE:



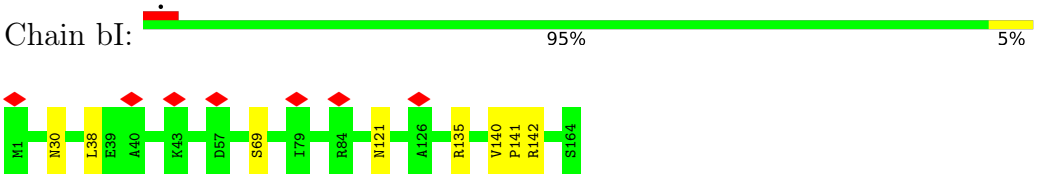
• Molecule 10: R-phycoerythrin alpha chain

Chain bG:



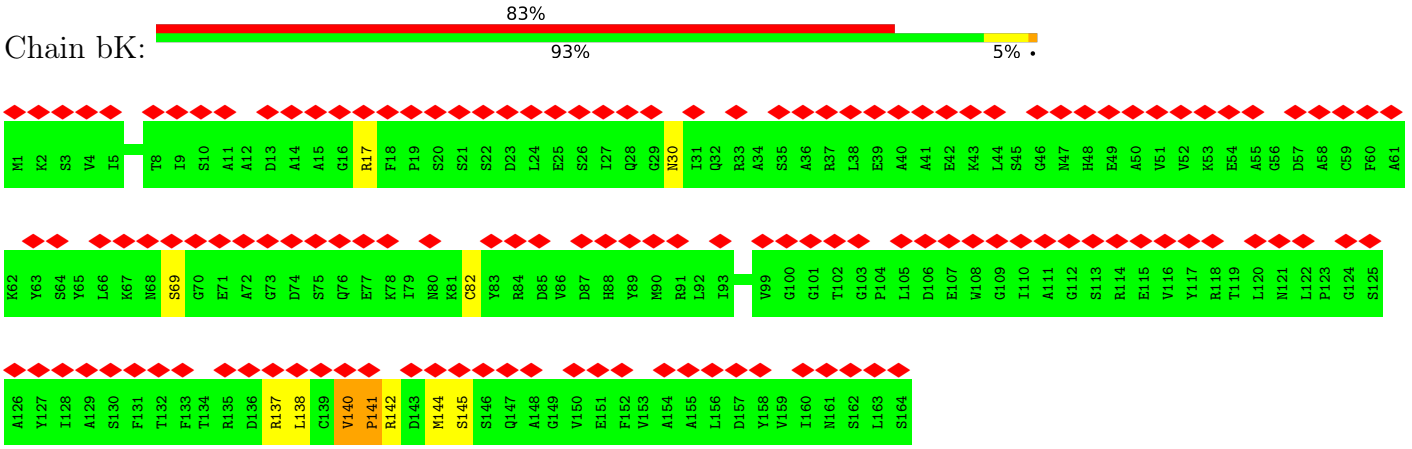
• Molecule 10: R-phycoerythrin alpha chain

Chain bI:



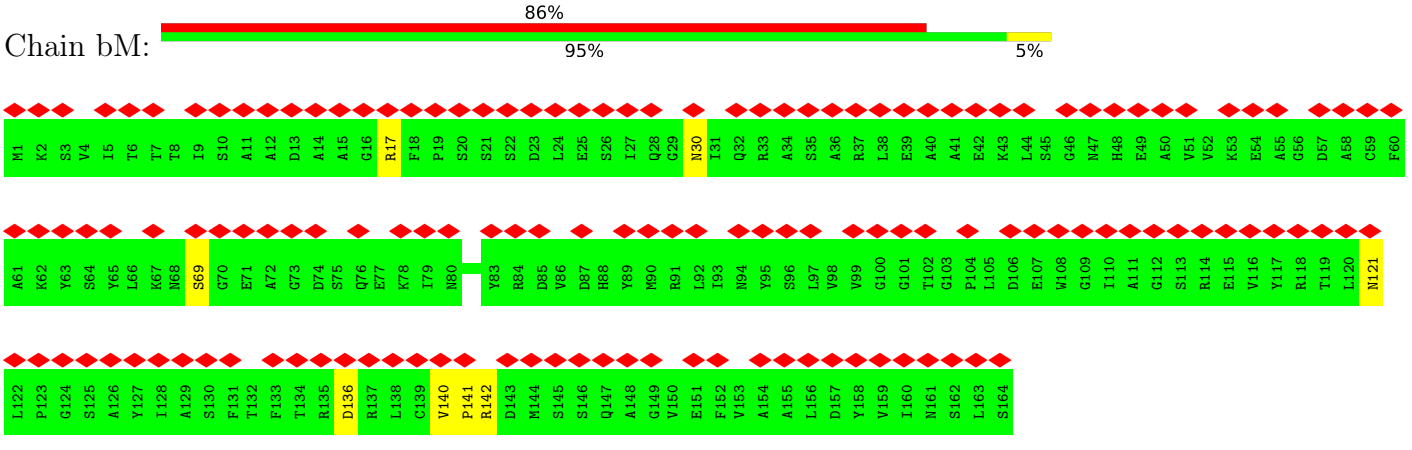
• Molecule 10: R-phycoerythrin alpha chain

Chain bK:



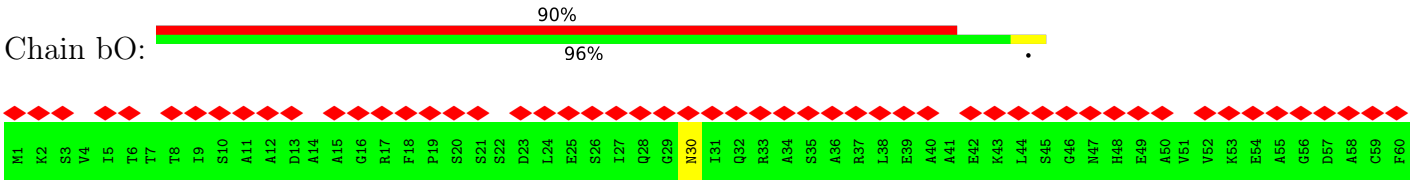
• Molecule 10: R-phycoerythrin alpha chain

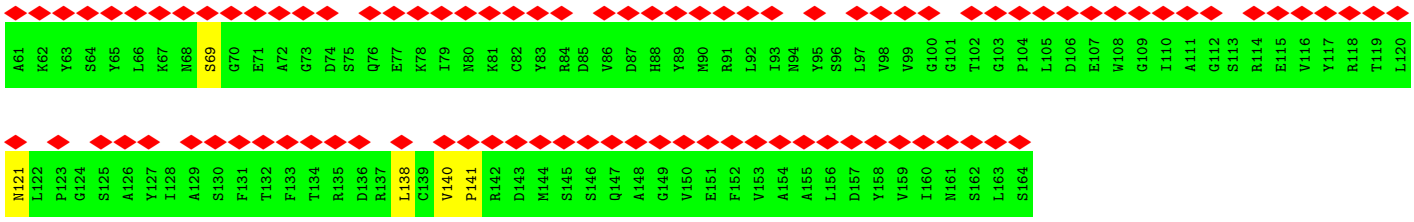
Chain bM:



• Molecule 10: R-phycoerythrin alpha chain

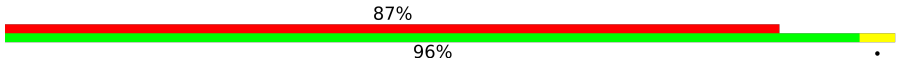
Chain bO:

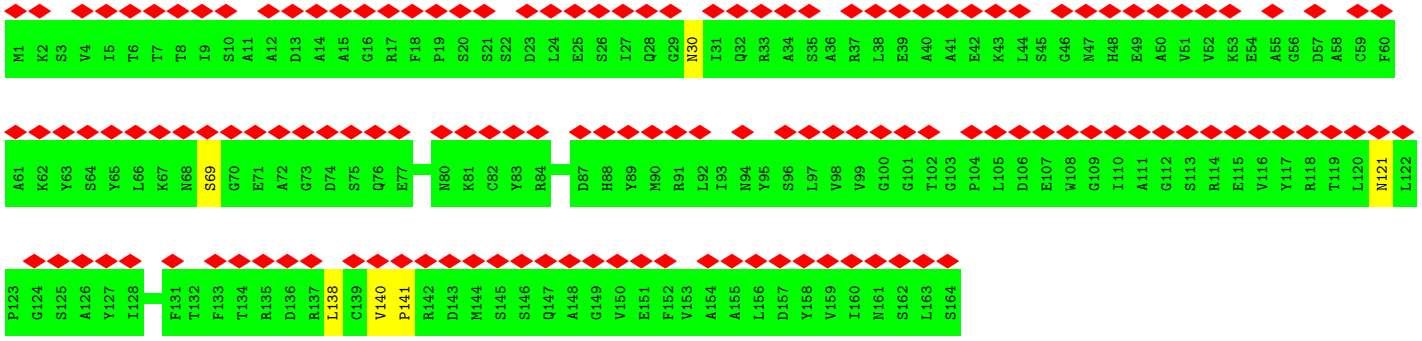




• Molecule 10: R-phycoerythrin alpha chain

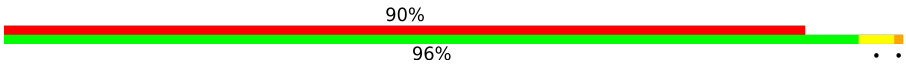
Chain bQ:

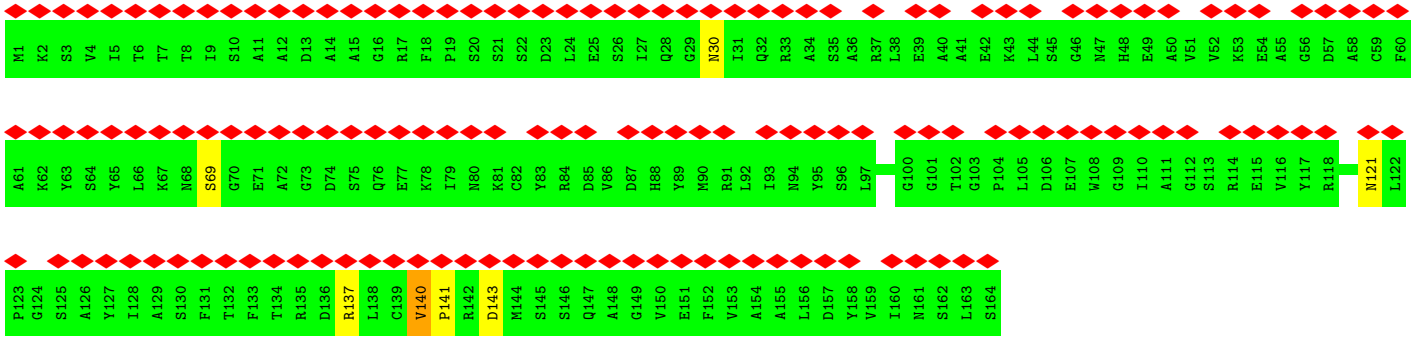




• Molecule 10: R-phycoerythrin alpha chain

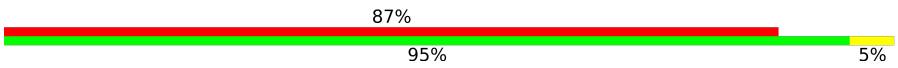
Chain bS:

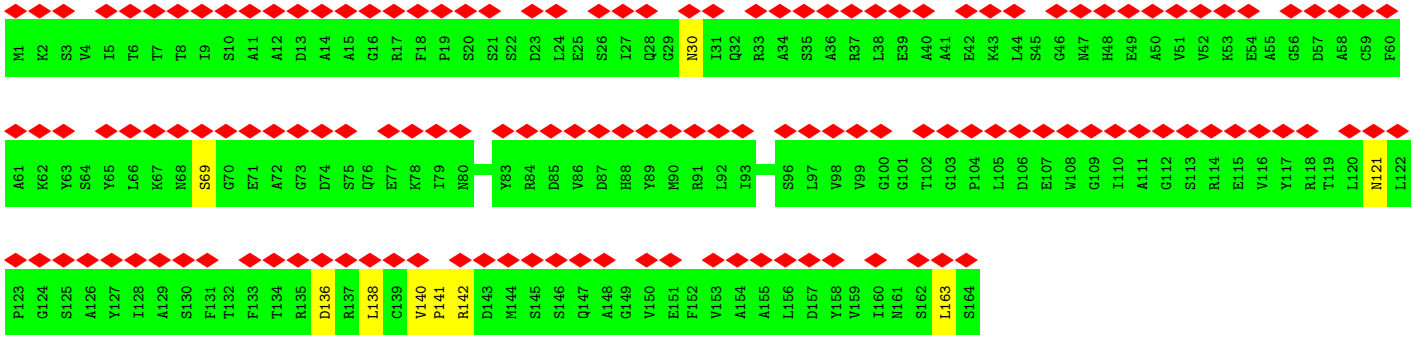




• Molecule 10: R-phycoerythrin alpha chain

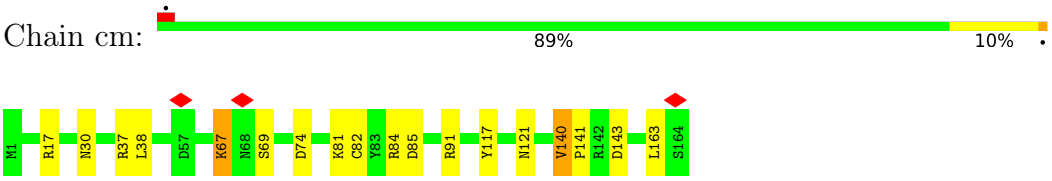
Chain bU:





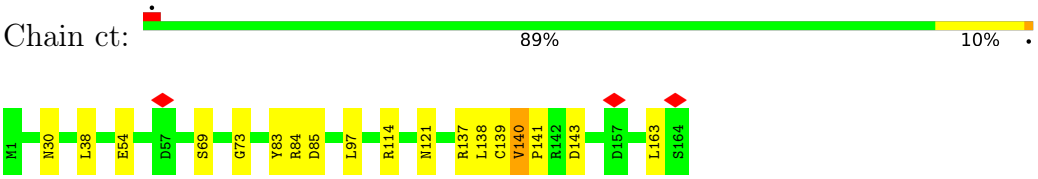
• Molecule 10: R-phycoerythrin alpha chain

Chain cm:



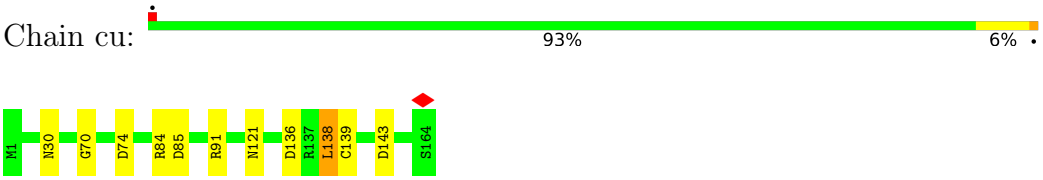
• Molecule 10: R-phycoerythrin alpha chain

Chain ct:



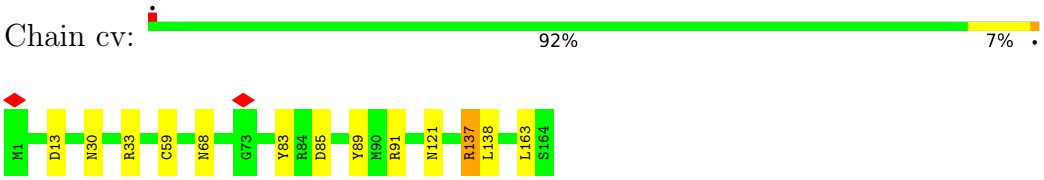
• Molecule 10: R-phycoerythrin alpha chain

Chain cu:



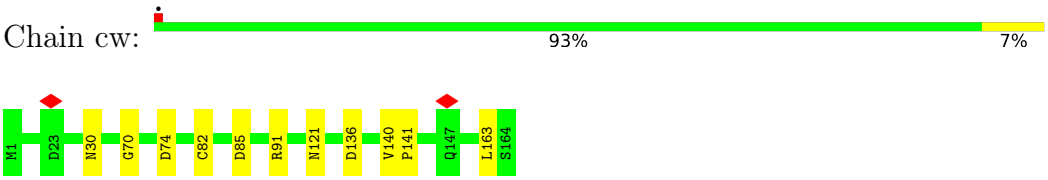
• Molecule 10: R-phycoerythrin alpha chain

Chain cv:



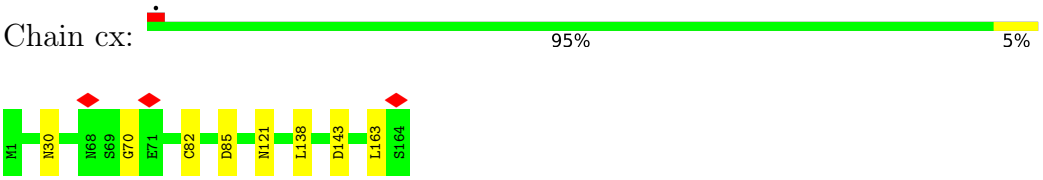
• Molecule 10: R-phycoerythrin alpha chain

Chain cw:



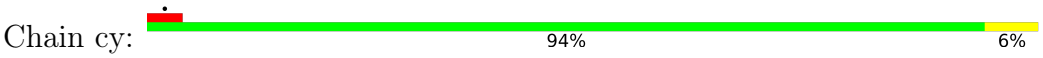
• Molecule 10: R-phycoerythrin alpha chain

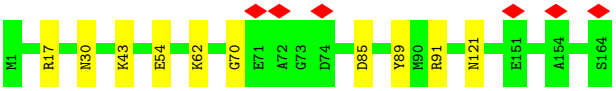
Chain cx:



• Molecule 10: R-phycoerythrin alpha chain

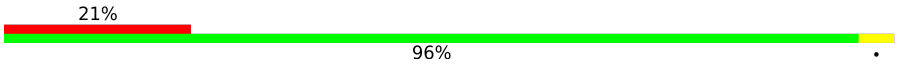
Chain cy:

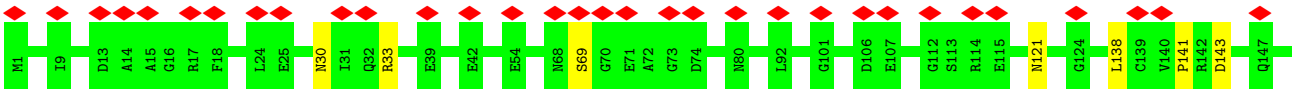




• Molecule 10: R-phycoerythrin alpha chain

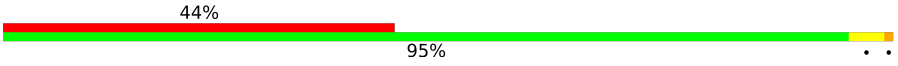
Chain cA:

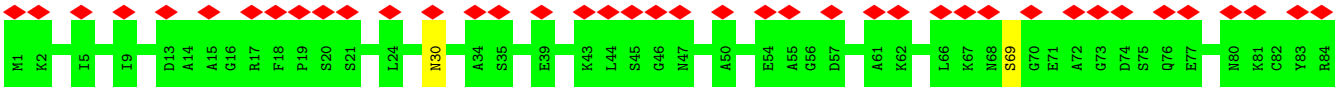


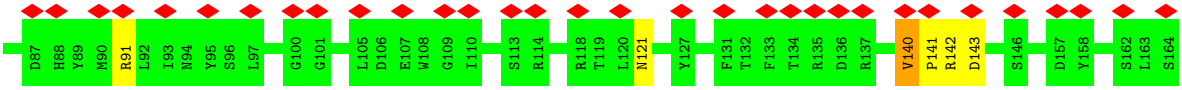


• Molecule 10: R-phycoerythrin alpha chain

Chain cC:

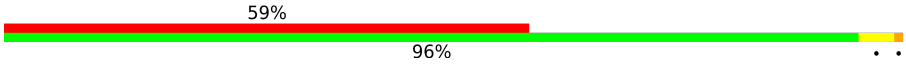


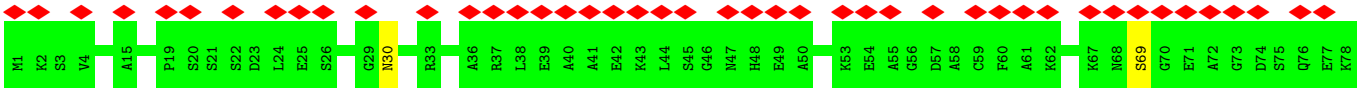


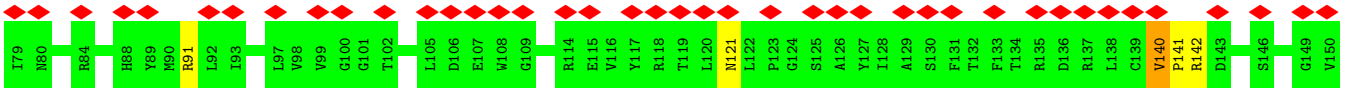


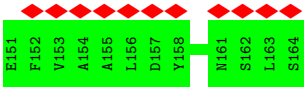
• Molecule 10: R-phycoerythrin alpha chain

Chain cD:



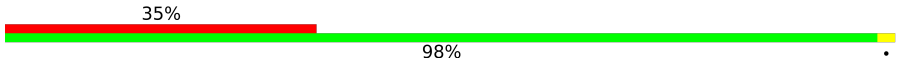


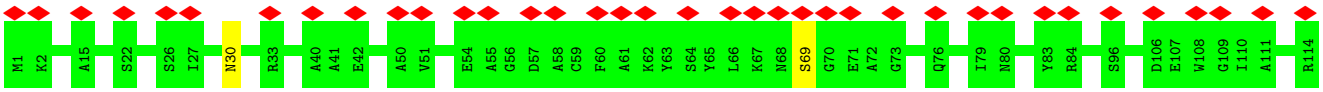


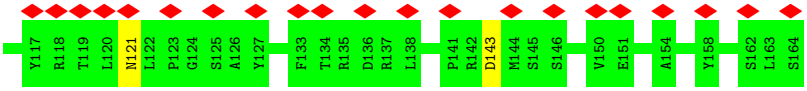


• Molecule 10: R-phycoerythrin alpha chain

Chain cG:

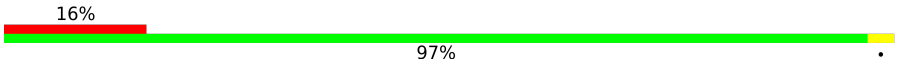


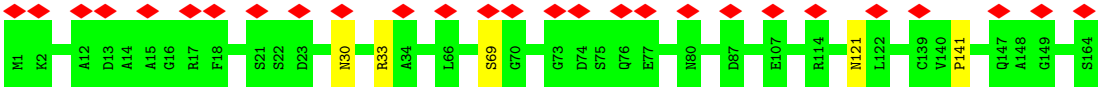




• Molecule 10: R-phycoerythrin alpha chain

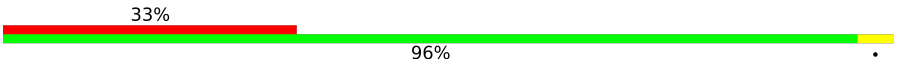
Chain cI:

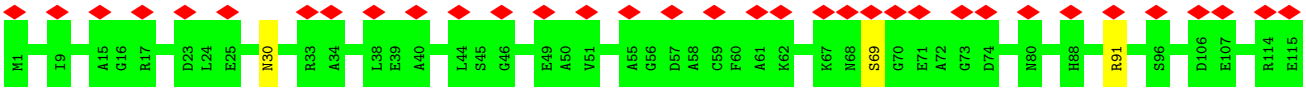


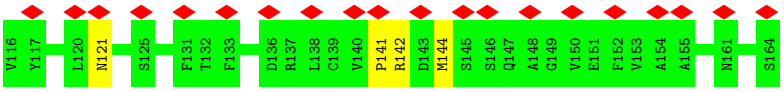


• Molecule 10: R-phycoerythrin alpha chain

Chain cK:

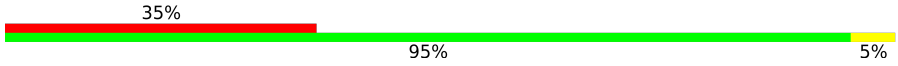


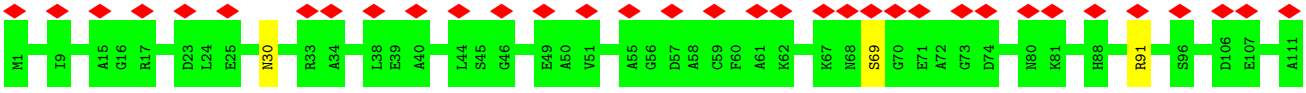


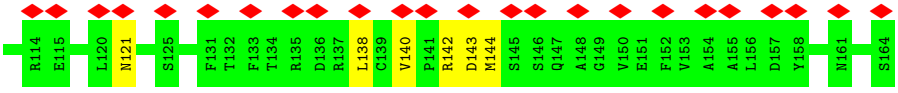


• Molecule 10: R-phycoerythrin alpha chain

Chain cS:







• Molecule 10: R-phycoerythrin alpha chain

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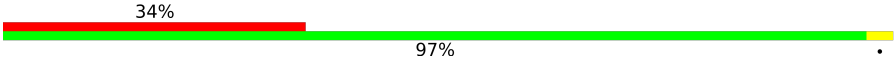

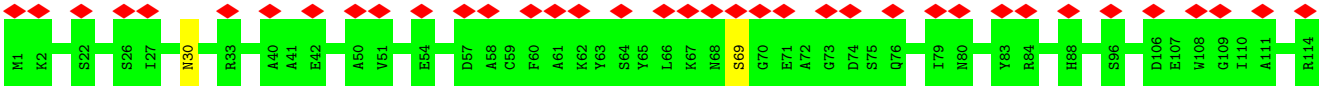

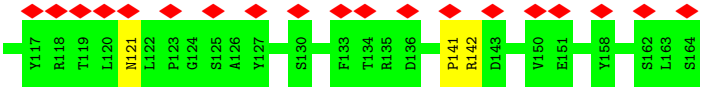

• Molecule 10: R-phycoerythrin alpha chain

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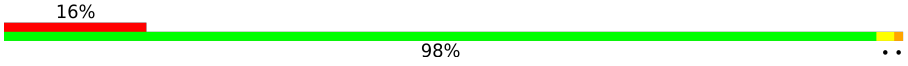
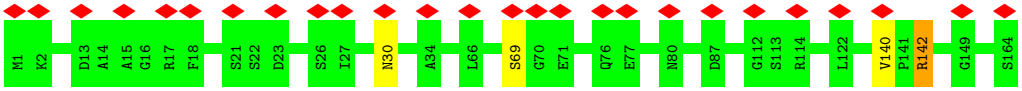
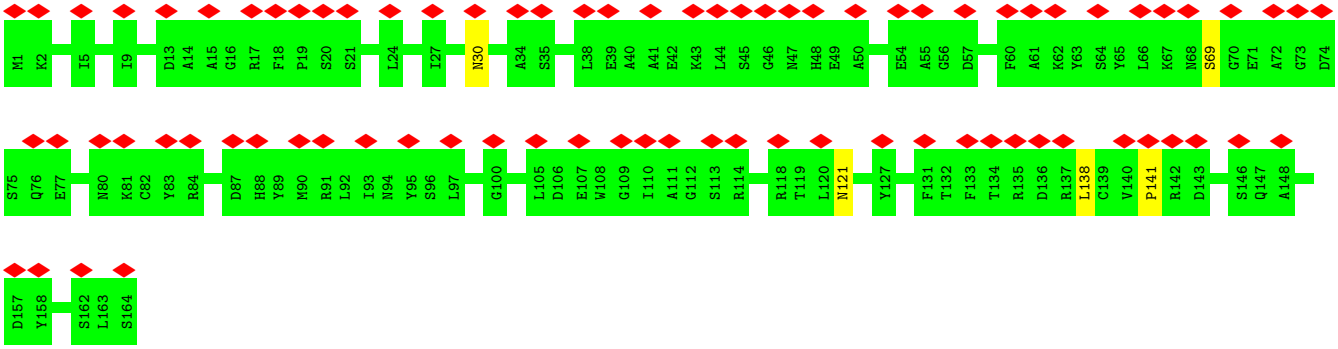
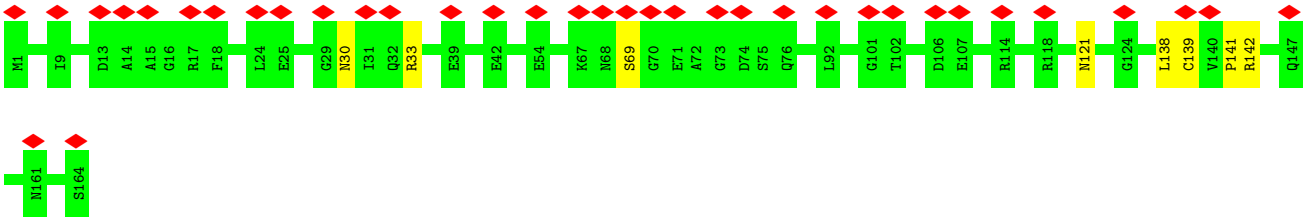




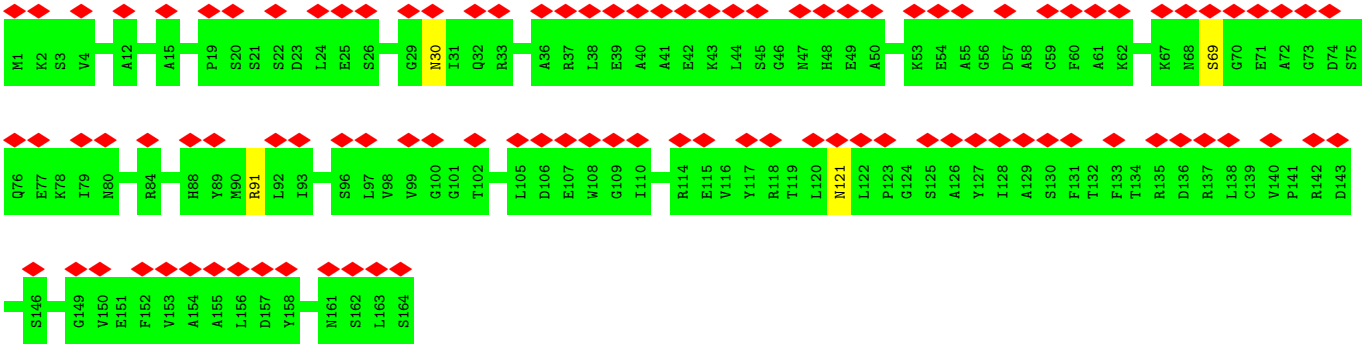
• Molecule 10: R-phycoerythrin alpha chain



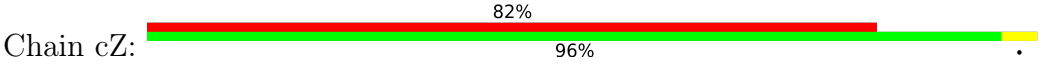
• Molecule 10: R-phycoerythrin alpha chain

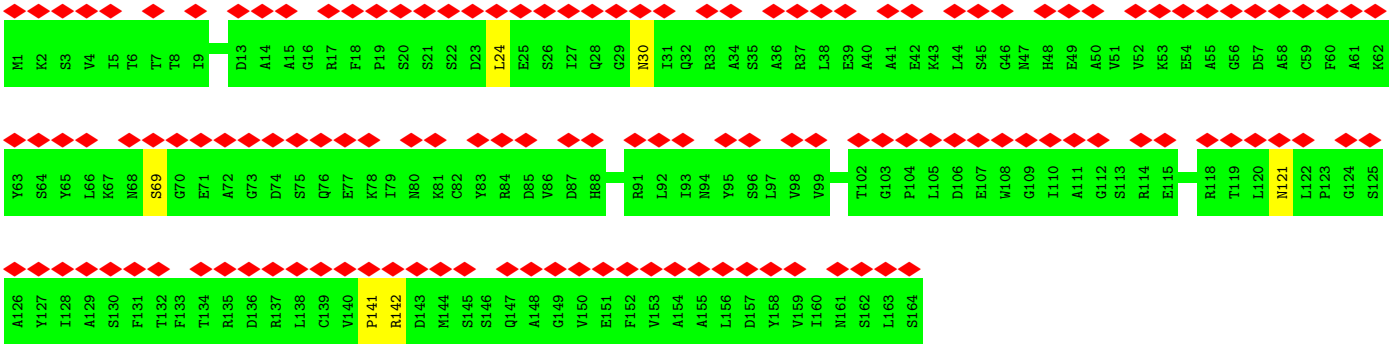


• Molecule 10: R-phycoerythrin alpha chain



• Molecule 10: R-phycoerythrin alpha chain





• Molecule 10: R-phycoerythrin alpha chain

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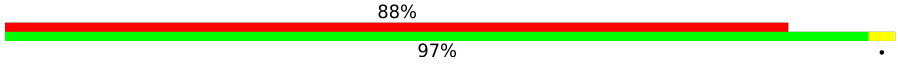

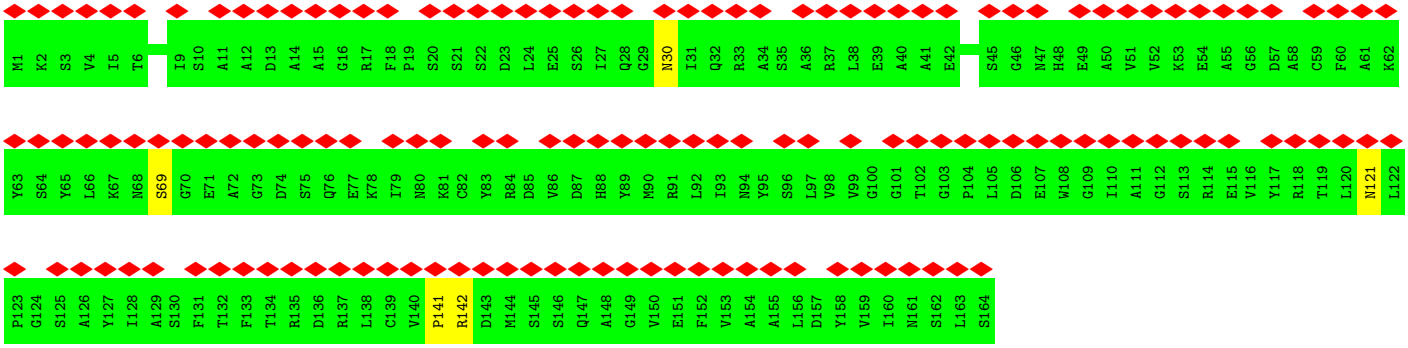

• Molecule 10: R-phycoerythrin alpha chain

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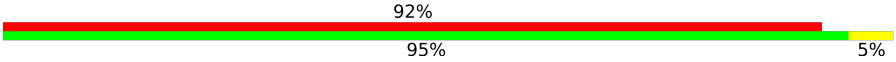
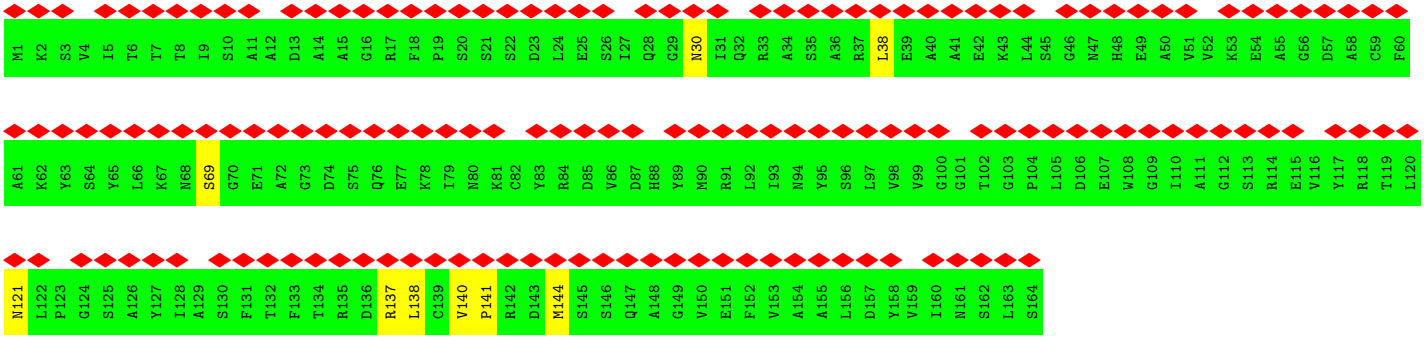
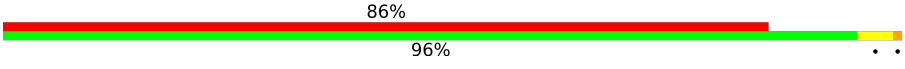
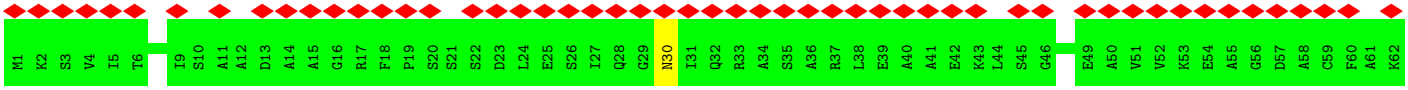


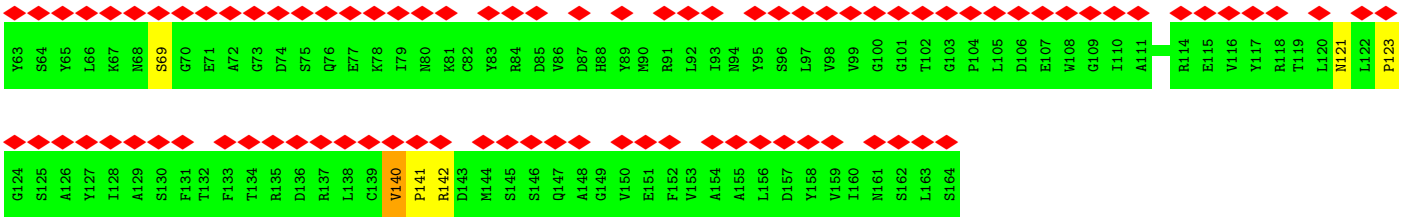


• Molecule 10: R-phycoerythrin alpha chain

Chain dc:







• Molecule 10: R-phycoerythrin alpha chain

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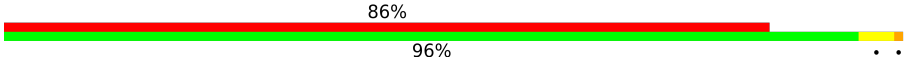
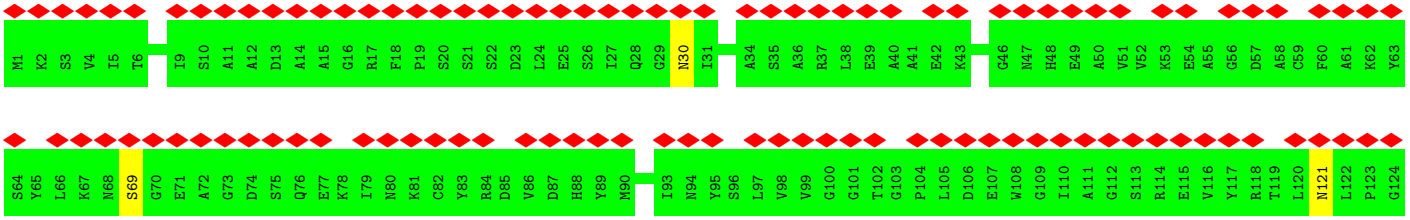
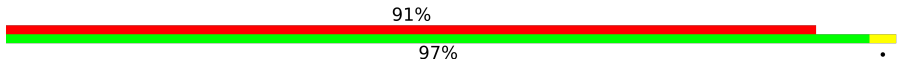
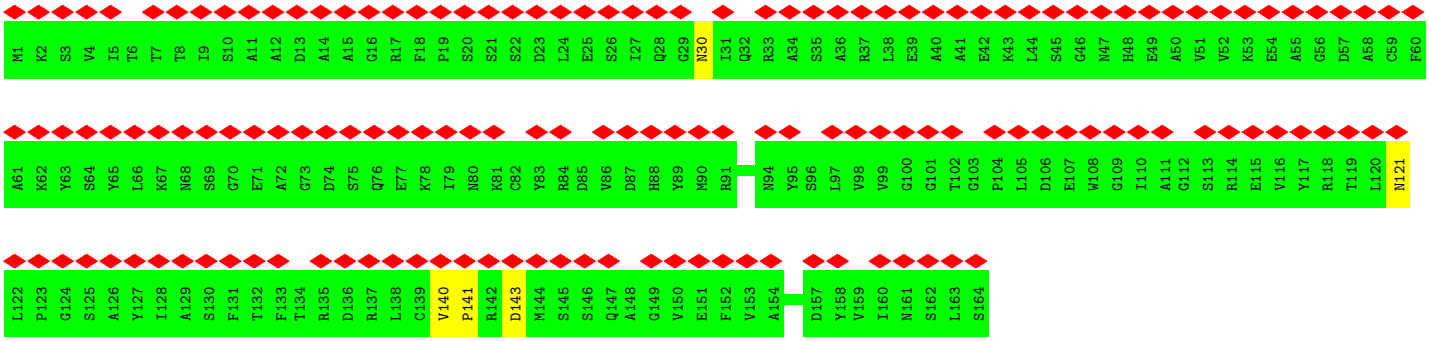




• Molecule 10: R-phycoerythrin alpha chain

Chain dg:





• Molecule 10: R-phycoerythrin alpha chain

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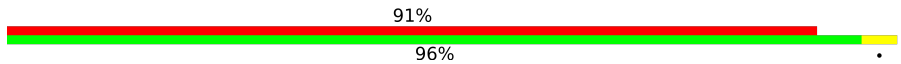
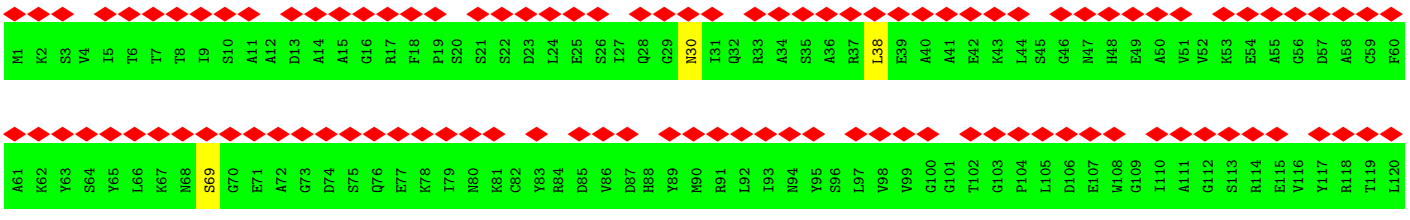
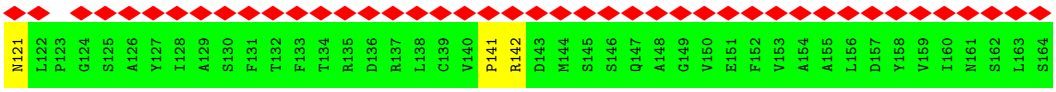
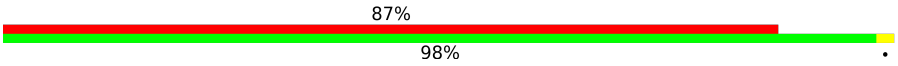


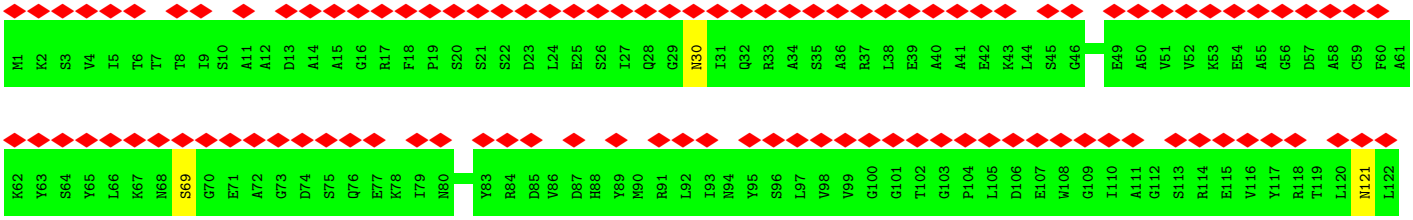


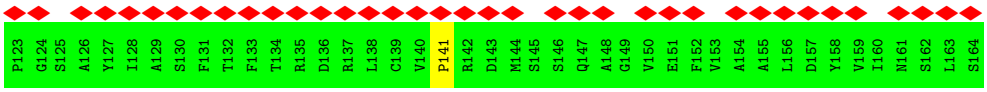


• Molecule 10: R-phycoerythrin alpha chain

Chain dm:

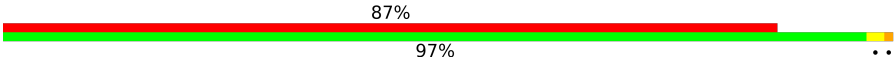


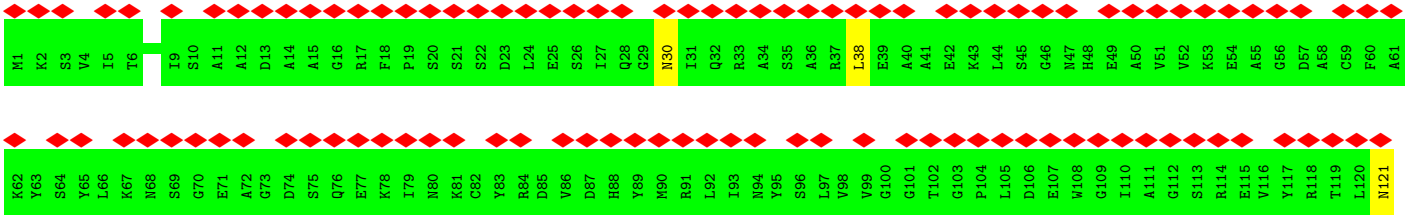


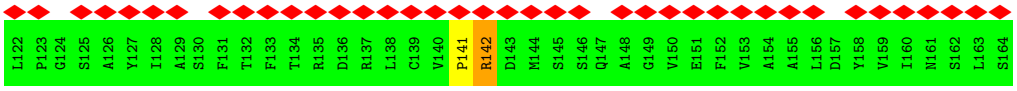


• Molecule 10: R-phycoerythrin alpha chain

Chain do:







• Molecule 10: R-phycoerythrin alpha chain

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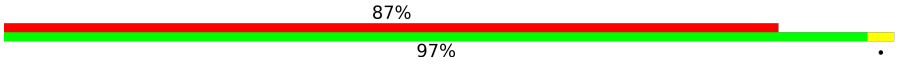
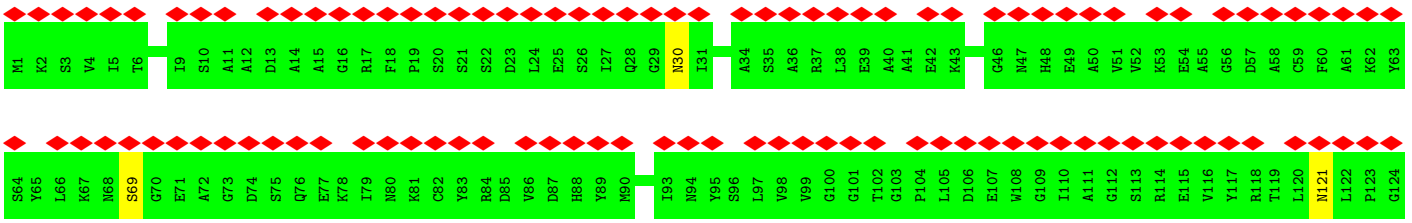
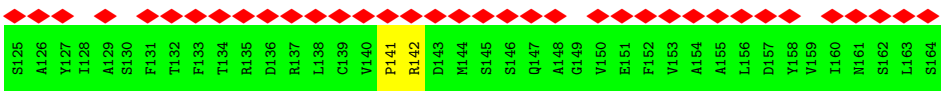
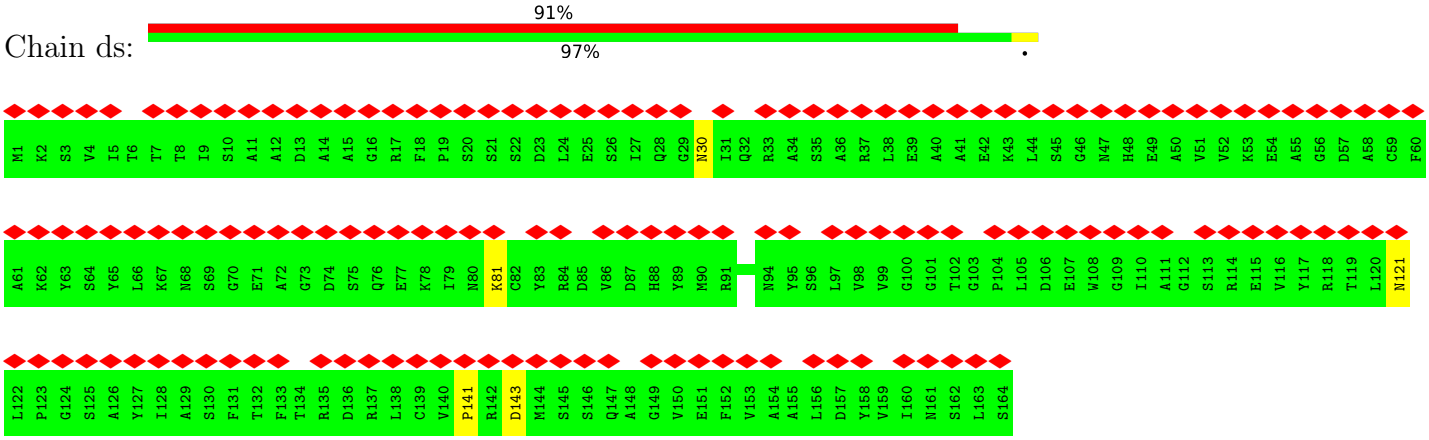






• Molecule 10: R-phycoerythrin alpha chain

Chain ds:



• Molecule 10: R-phycoerythrin alpha chain

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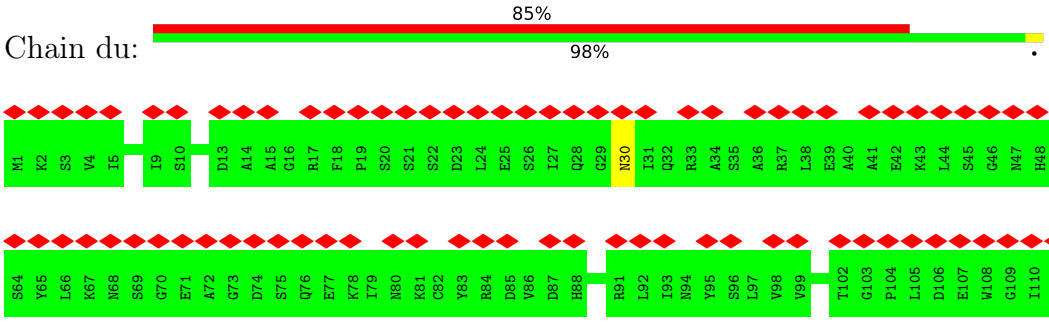
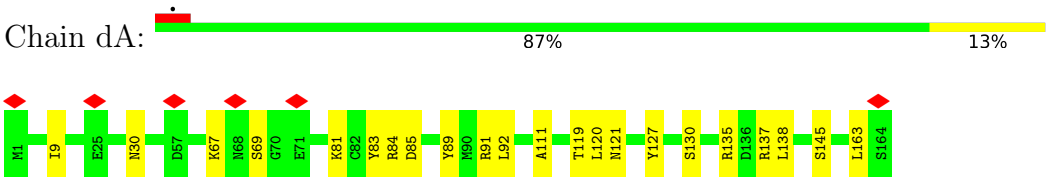


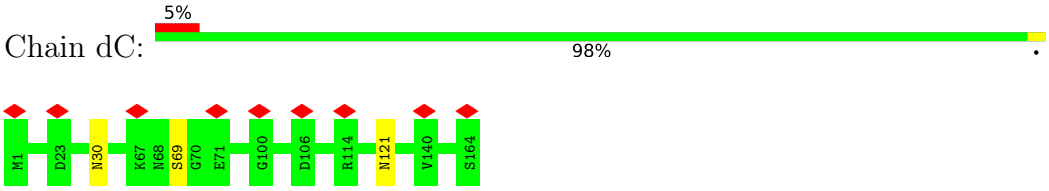
• Molecule 10: R-phycoerythrin alpha chain

Chain dA:



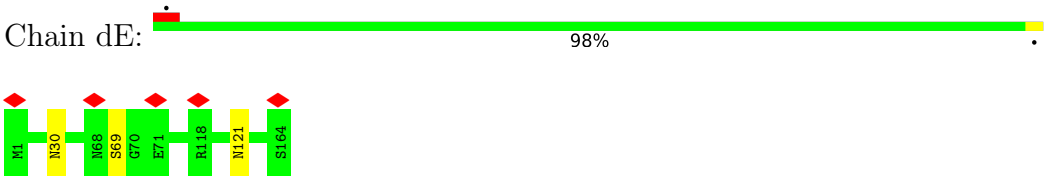
• Molecule 10: R-phycoerythrin alpha chain

Chain dC:



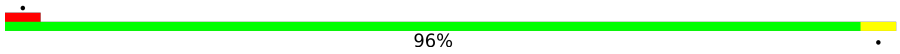
• Molecule 10: R-phycoerythrin alpha chain

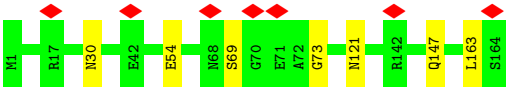
Chain dE:



• Molecule 10: R-phycoerythrin alpha chain

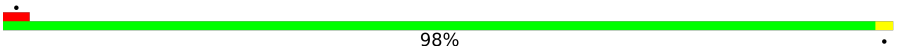
Chain dG:

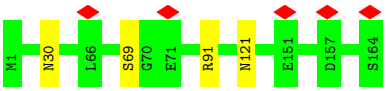




• Molecule 10: R-phycoerythrin alpha chain

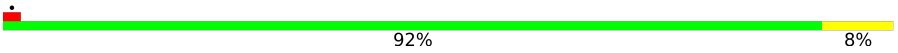
Chain dI:

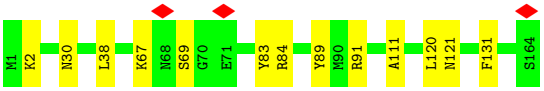




• Molecule 10: R-phycoerythrin alpha chain

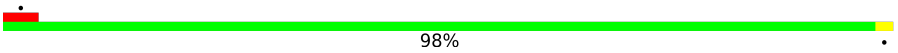
Chain dJ:

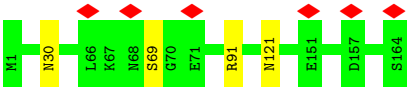




• Molecule 10: R-phycoerythrin alpha chain

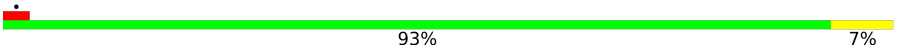
Chain dM:

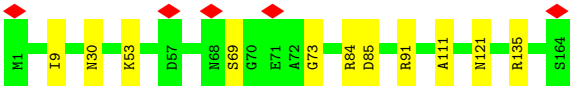




• Molecule 10: R-phycoerythrin alpha chain

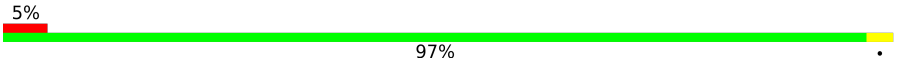
Chain dO:

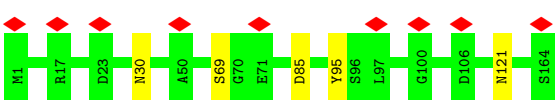




• Molecule 10: R-phycoerythrin alpha chain

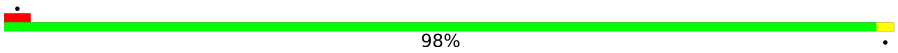
Chain dQ:

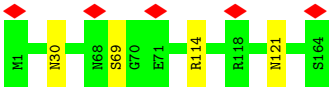




• Molecule 10: R-phycoerythrin alpha chain

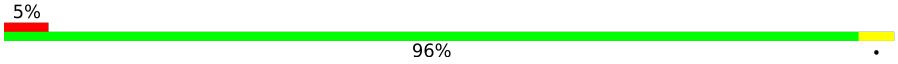
Chain dS:

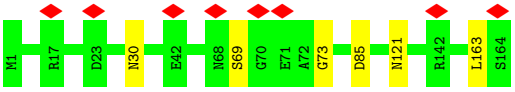




• Molecule 10: R-phycoerythrin alpha chain

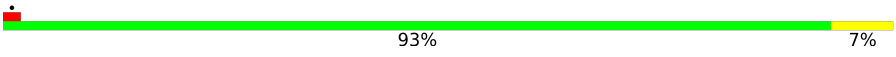
Chain dU:

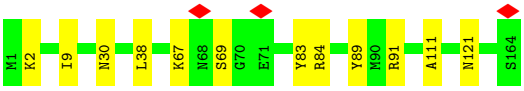




• Molecule 10: R-phycoerythrin alpha chain

Chain dW:





• Molecule 10: R-phycoerythrin alpha chain

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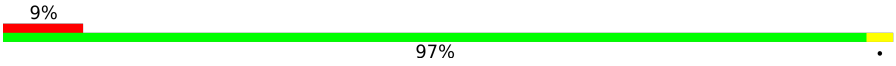
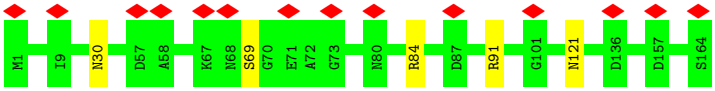
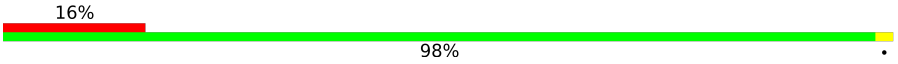
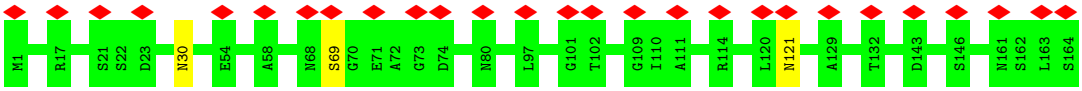




• Molecule 10: R-phycoerythrin alpha chain

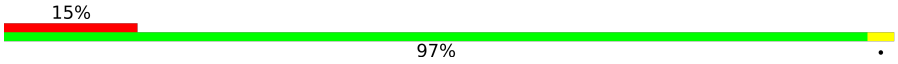
Chain ea:

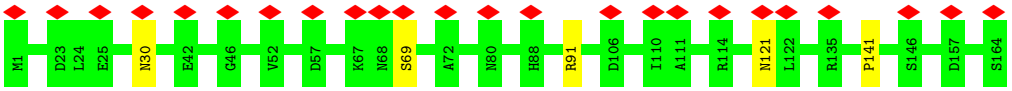




• Molecule 10: R-phycoerythrin alpha chain

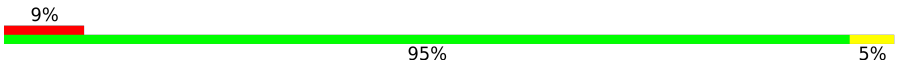
Chain ed:

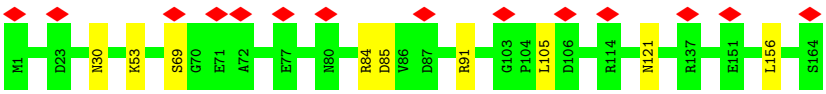




• Molecule 10: R-phycoerythrin alpha chain

Chain ef:





• Molecule 10: R-phycoerythrin alpha chain

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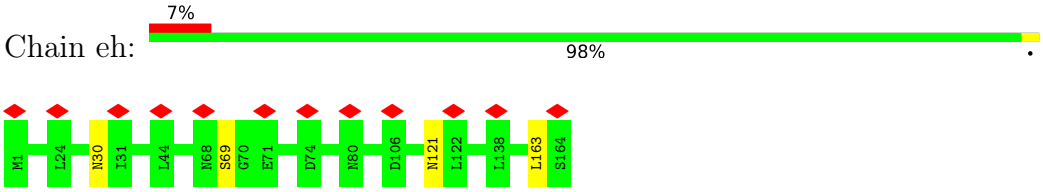

• Molecule 10: R-phycoerythrin alpha chain

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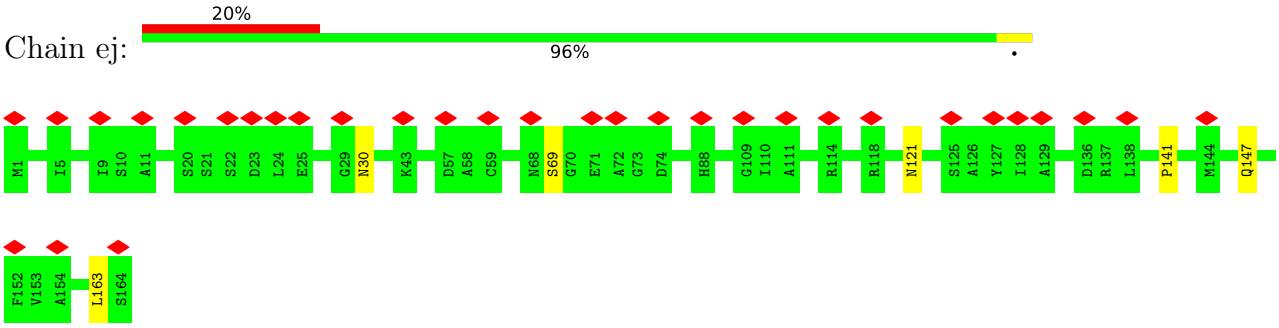
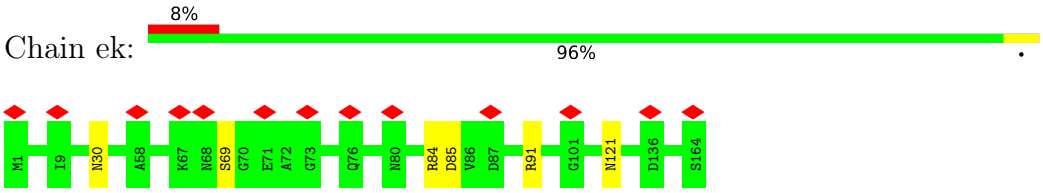


• Molecule 10: R-phycoerythrin alpha chain

Chain ek:



• Molecule 10: R-phycoerythrin alpha chain

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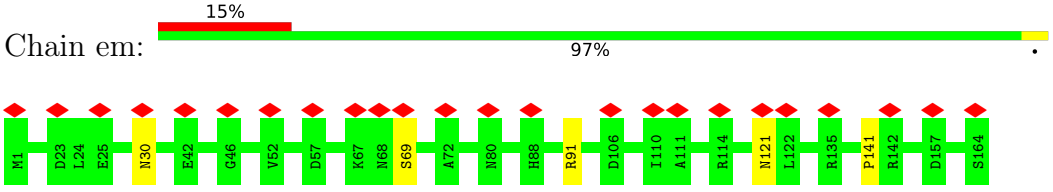
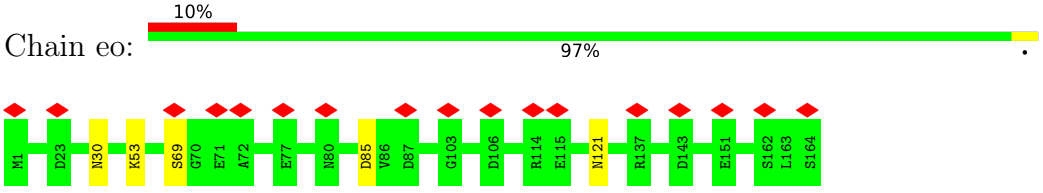


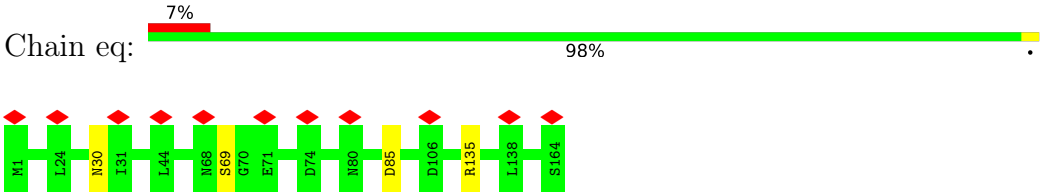
• Molecule 10: R-phycoerythrin alpha chain

Chain eo:



• Molecule 10: R-phycoerythrin alpha chain

Chain eq:



• Molecule 10: R-phycoerythrin alpha chain

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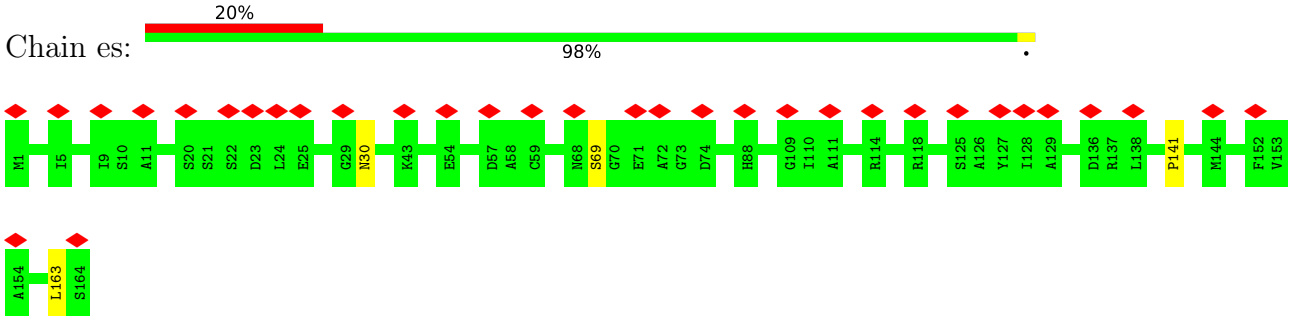
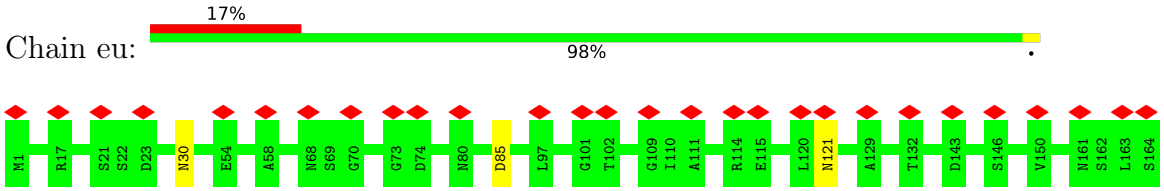


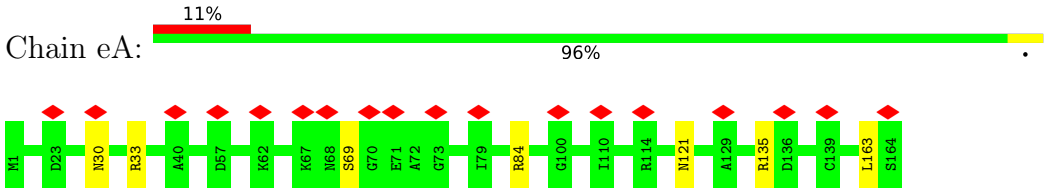
• Molecule 10: R-phycoerythrin alpha chain

Chain eu:



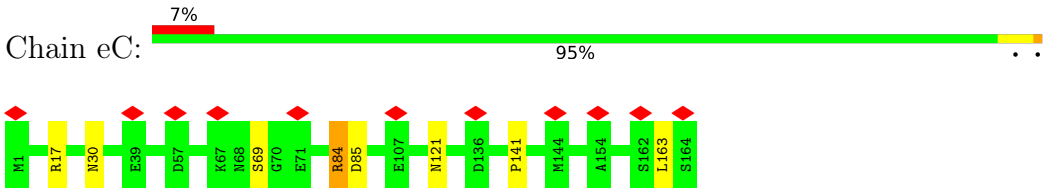
• Molecule 10: R-phycoerythrin alpha chain

Chain eA:



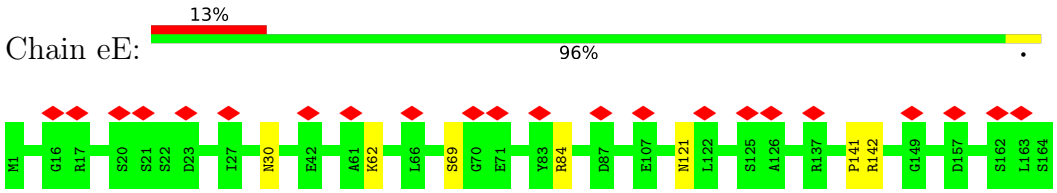
• Molecule 10: R-phycoerythrin alpha chain

Chain eC:



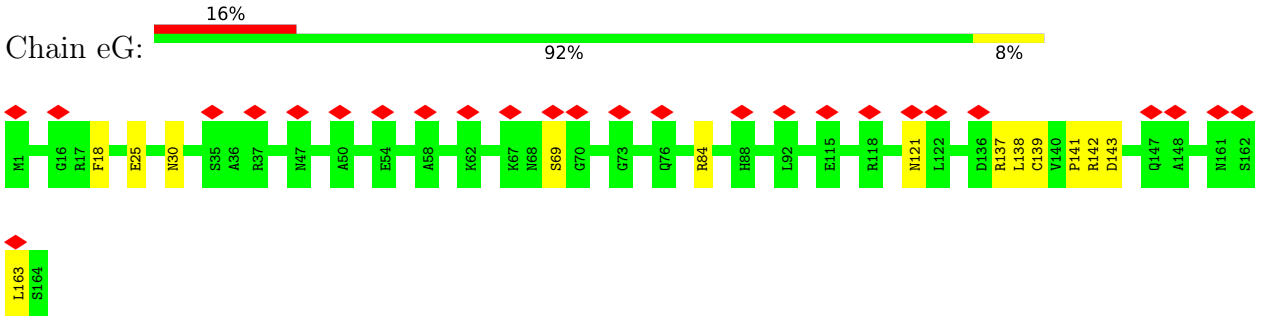
• Molecule 10: R-phycoerythrin alpha chain

Chain eE:



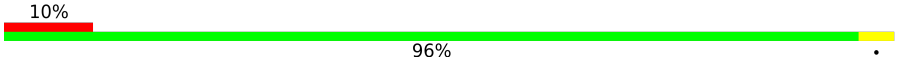
• Molecule 10: R-phycoerythrin alpha chain

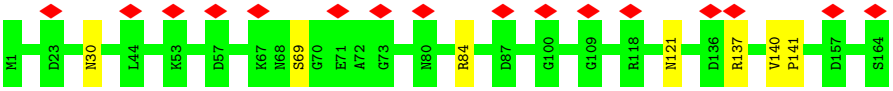
Chain eG:



• Molecule 10: R-phycoerythrin alpha chain

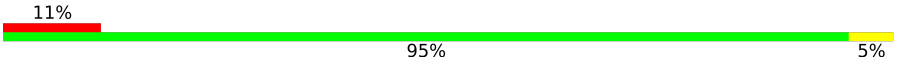
Chain eI:

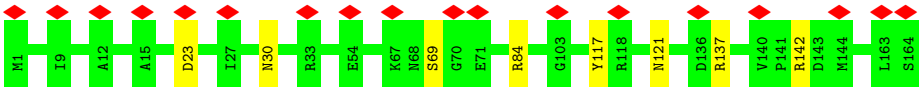




• Molecule 10: R-phycoerythrin alpha chain

Chain eK:





• Molecule 10: R-phycoerythrin alpha chain

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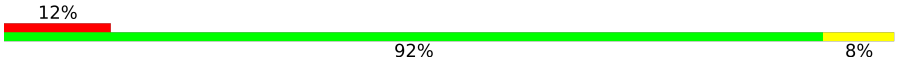
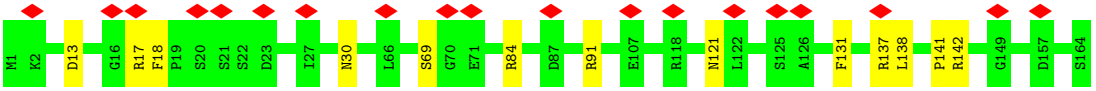
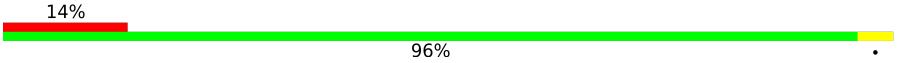
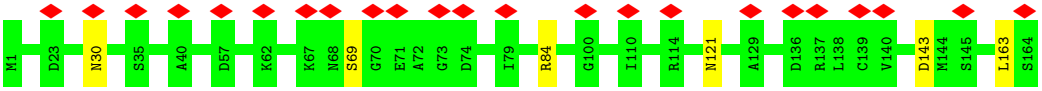




• Molecule 10: R-phycoerythrin alpha chain

Chain eO:





• Molecule 10: R-phycoerythrin alpha chain

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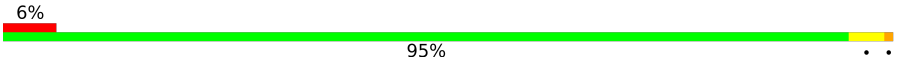
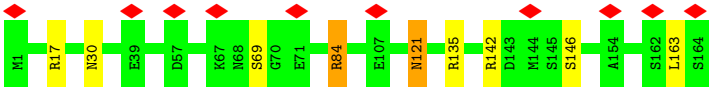
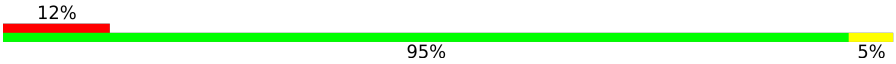
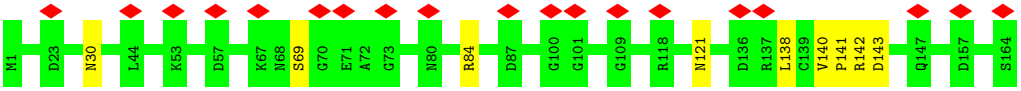




• Molecule 10: R-phycoerythrin alpha chain

Chain eS:





• Molecule 10: R-phycoerythrin alpha chain

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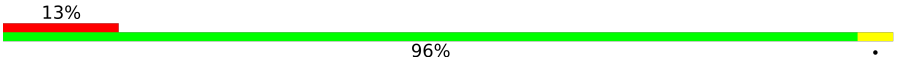
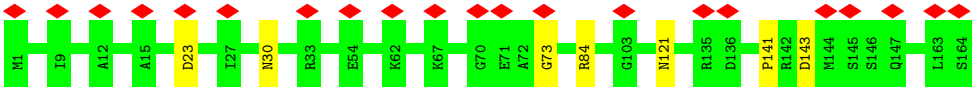
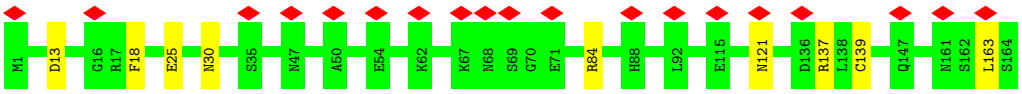
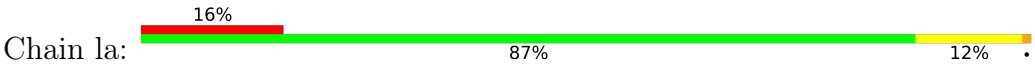


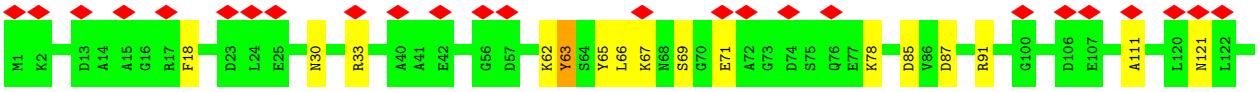


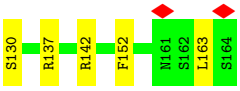
• Molecule 10: R-phycoerythrin alpha chain



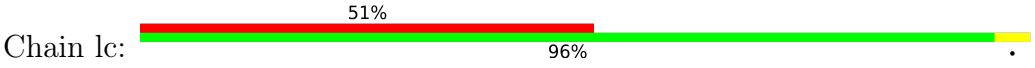
• Molecule 10: R-phycoerythrin alpha chain

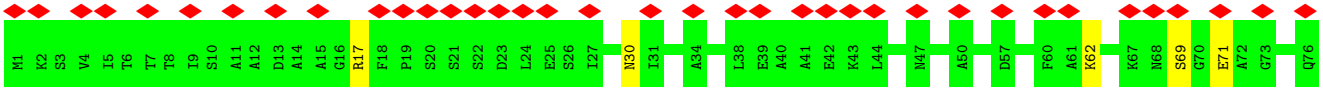


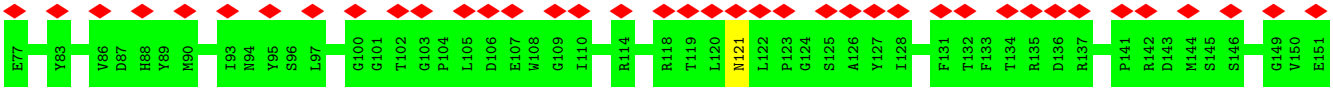


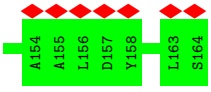


• Molecule 10: R-phycoerythrin alpha chain

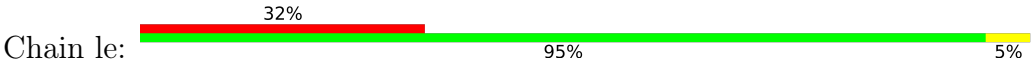


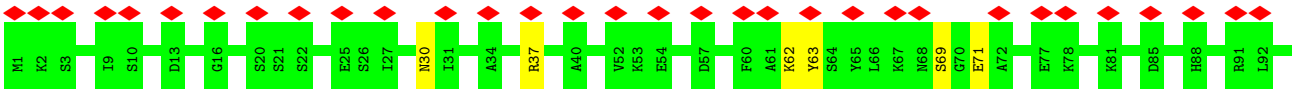


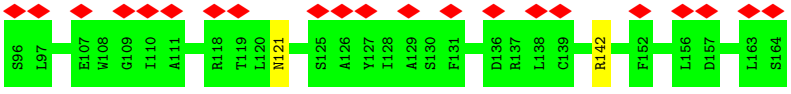




• Molecule 10: R-phycoerythrin alpha chain

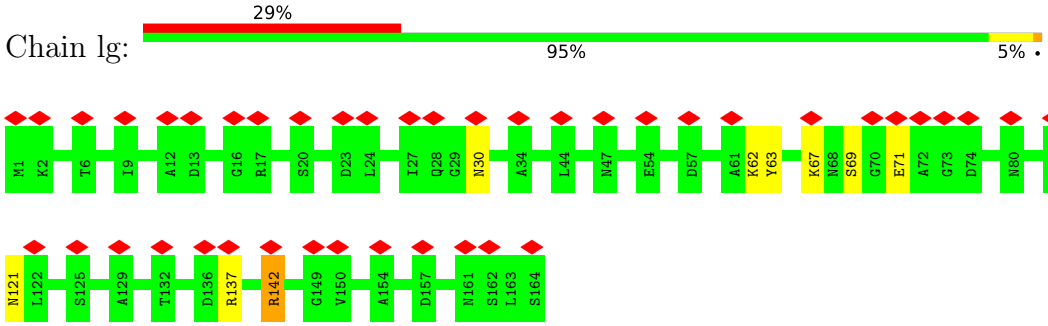






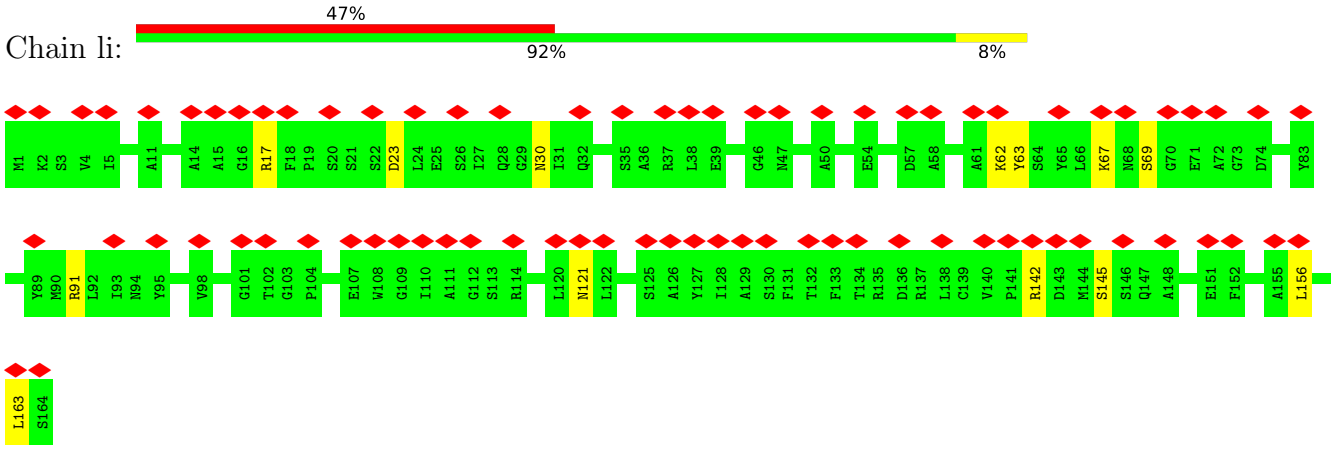
• Molecule 10: R-phycoerythrin alpha chain

Chain lg:



• Molecule 10: R-phycoerythrin alpha chain

Chain li:



• Molecule 10: R-phycoerythrin alpha chain

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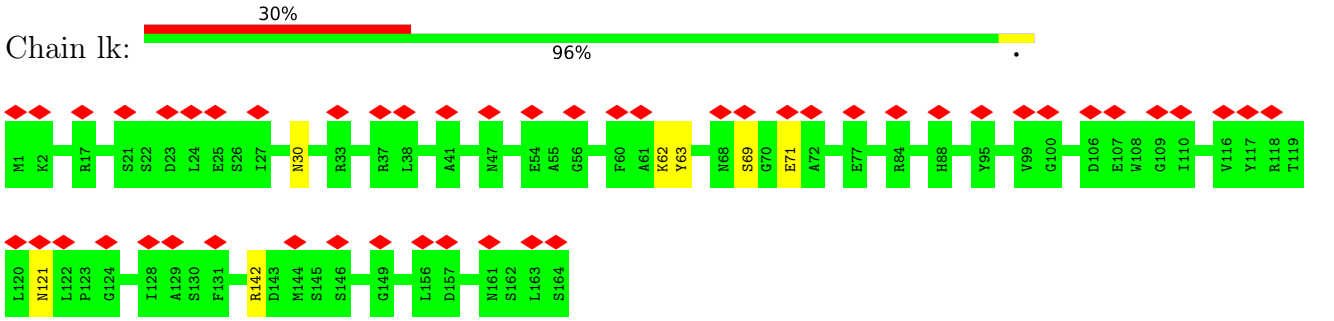

• Molecule 10: R-phycoerythrin alpha chain

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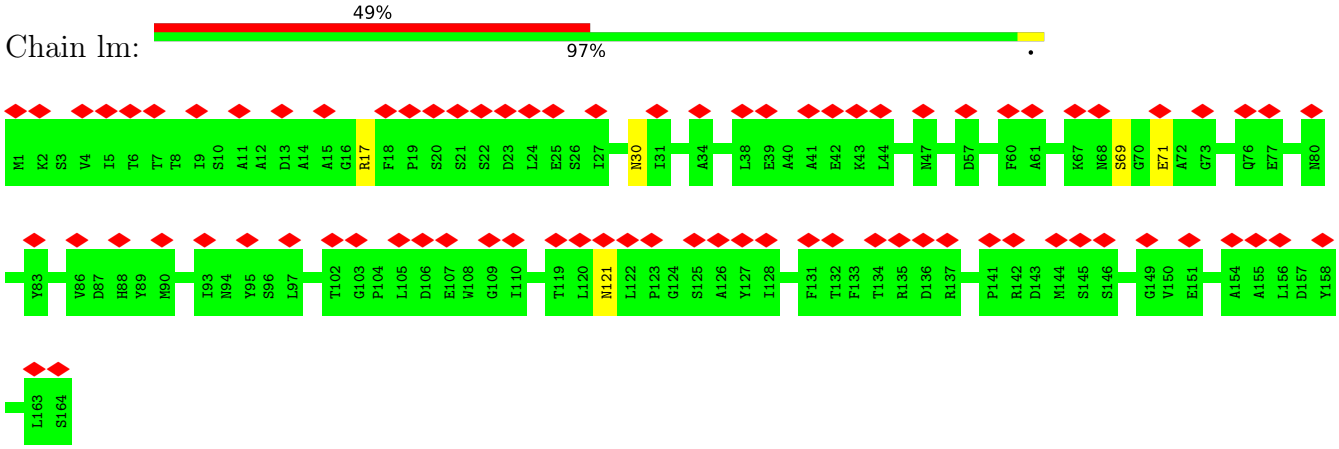

• Molecule 10: R-phycoerythrin alpha chain

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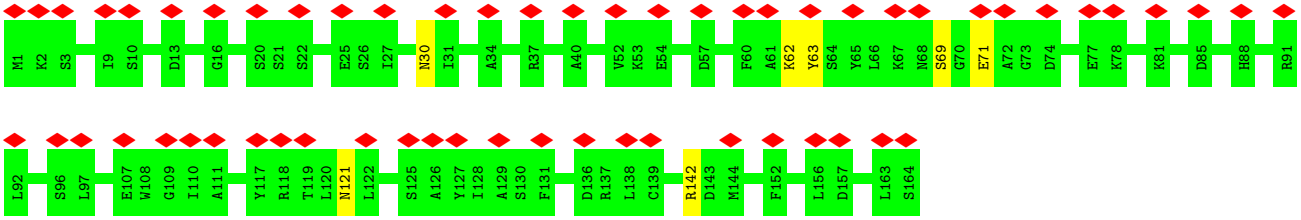

• Molecule 10: R-phycoerythrin alpha chain

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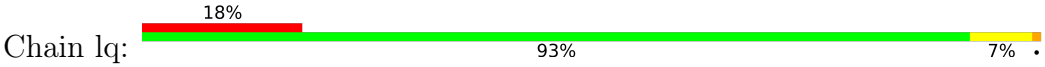

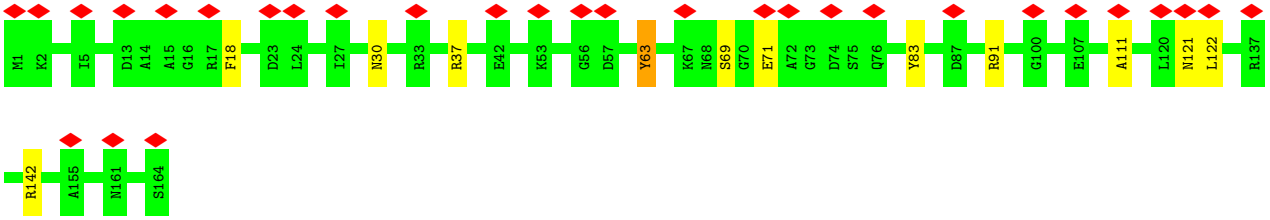

• Molecule 10: R-phycoerythrin alpha chain

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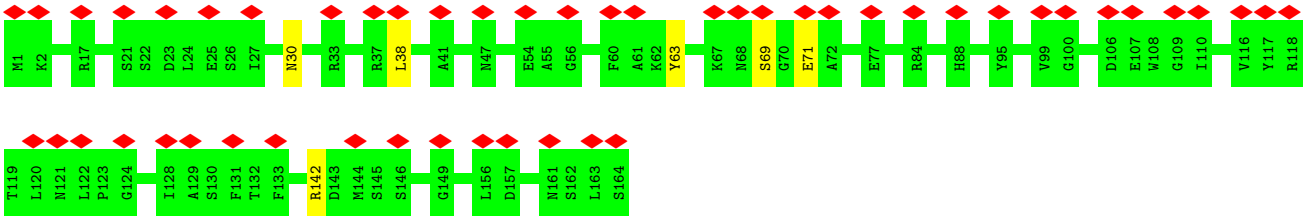

• Molecule 10: R-phycoerythrin alpha chain

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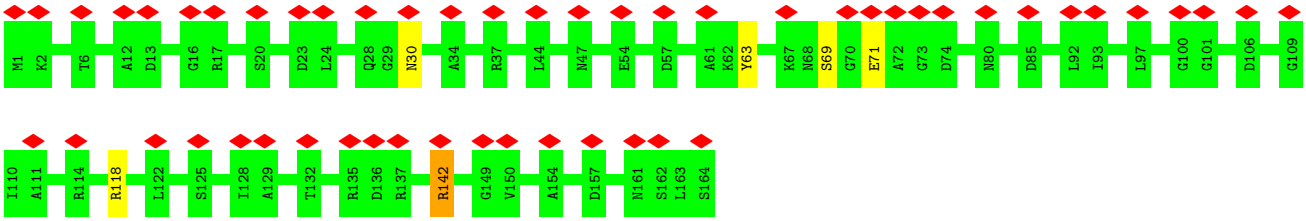

• Molecule 10: R-phycoerythrin alpha chain

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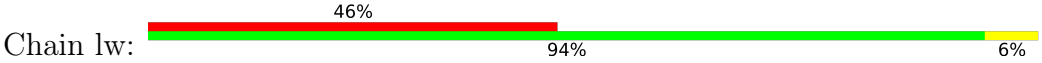

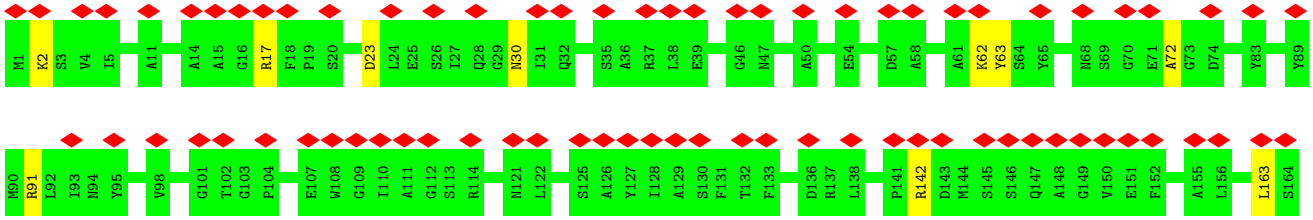

• Molecule 10: R-phycoerythrin alpha chain

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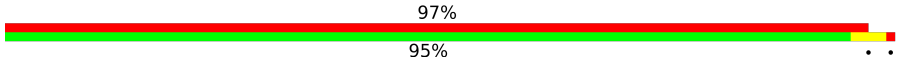

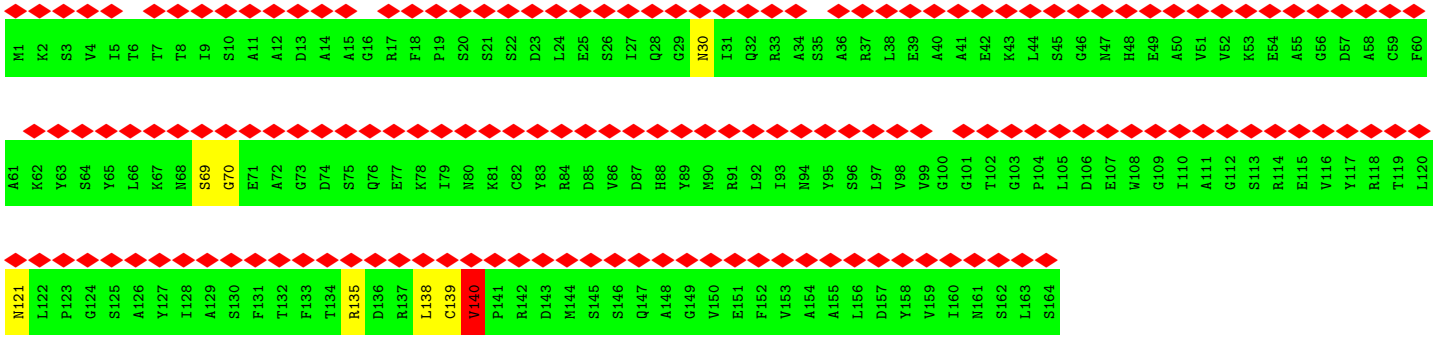

• Molecule 10: R-phycoerythrin alpha chain

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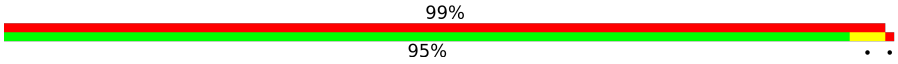

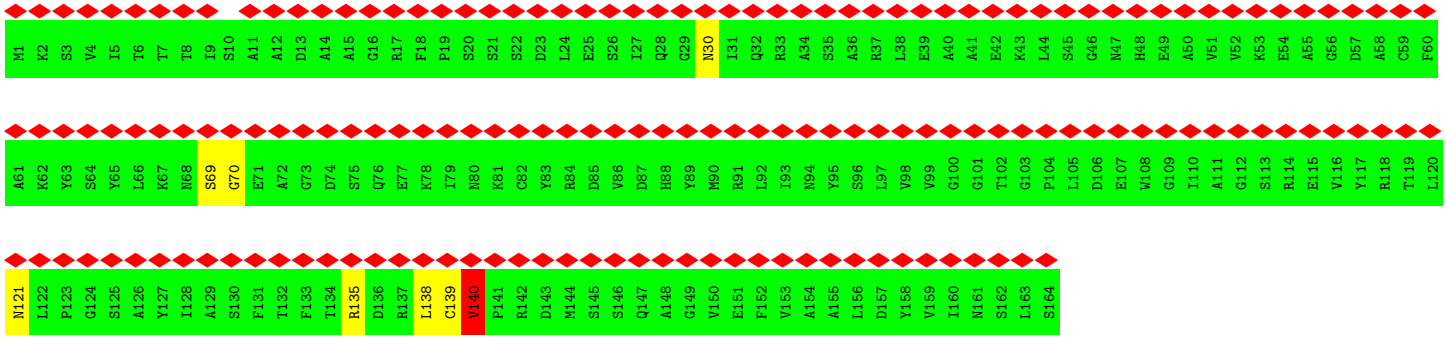

• Molecule 10: R-phycoerythrin alpha chain

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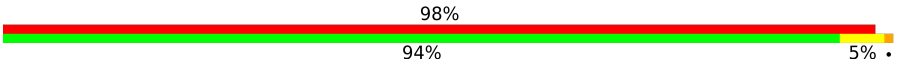

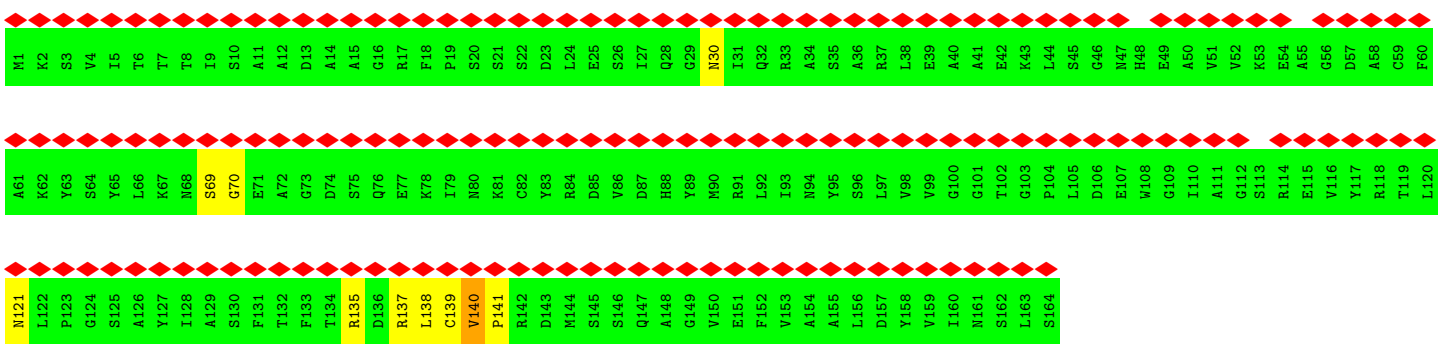

• Molecule 10: R-phycoerythrin alpha chain

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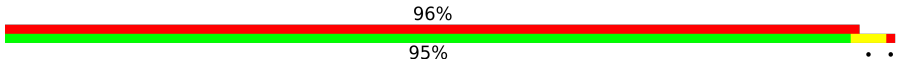

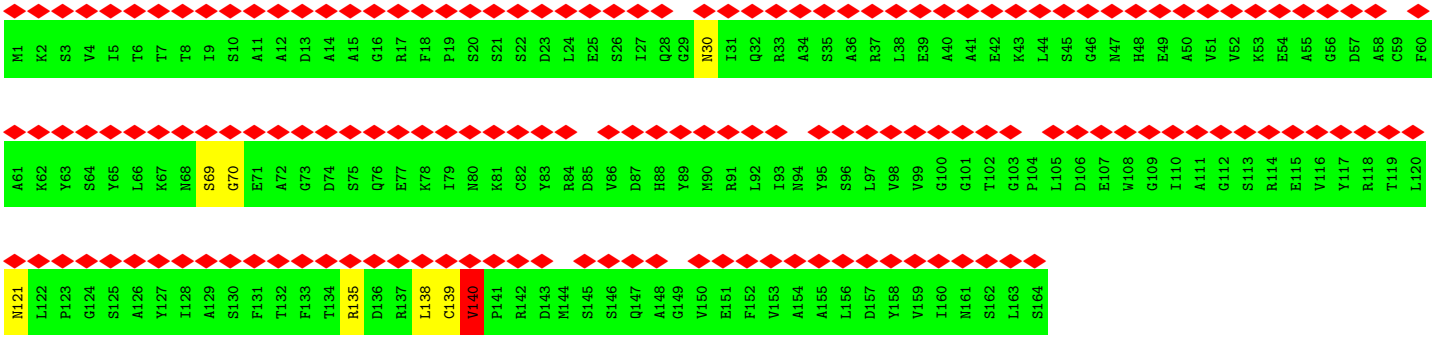

• Molecule 10: R-phycoerythrin alpha chain

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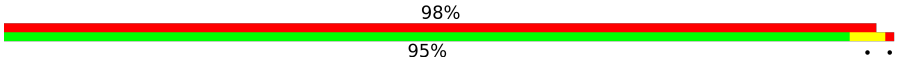
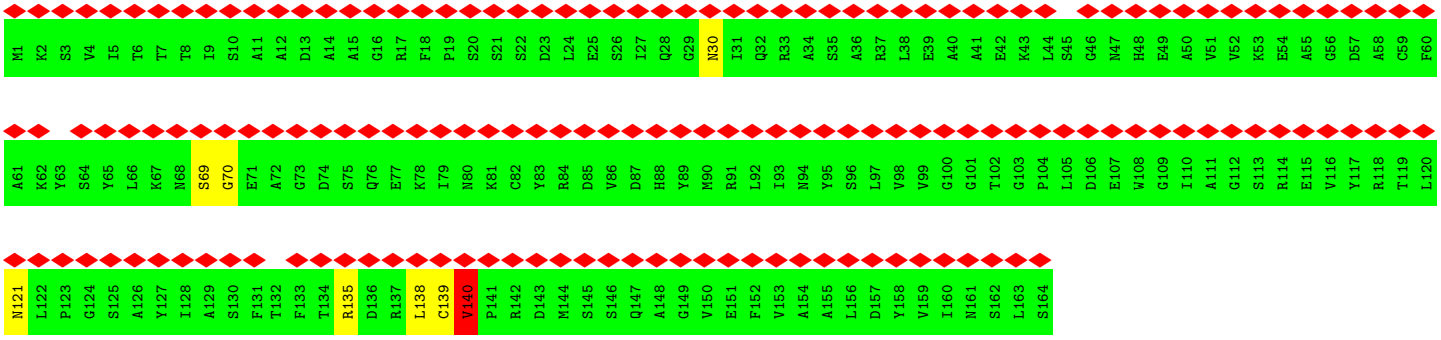
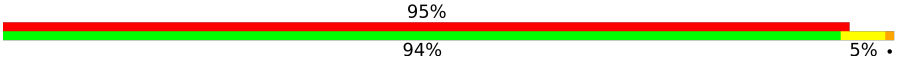
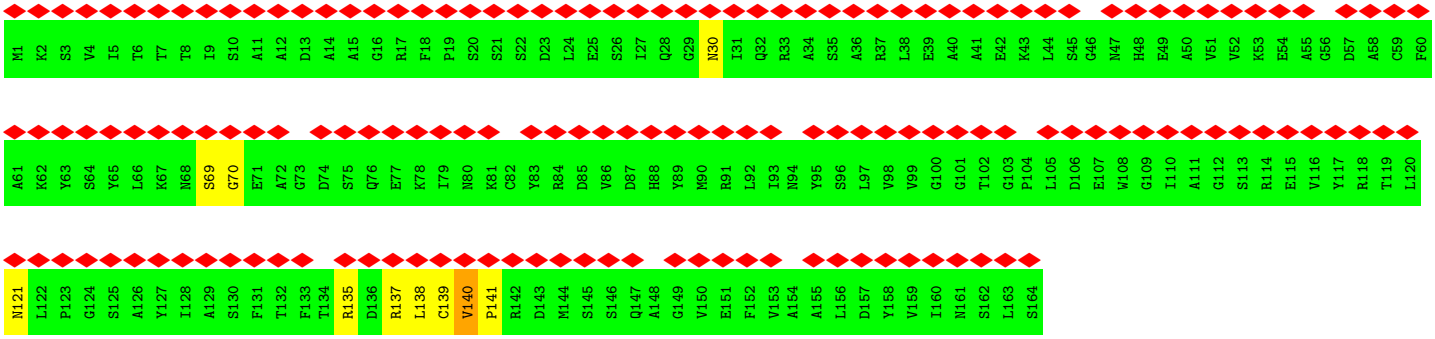




• Molecule 10: R-phycoerythrin alpha chain

Chain fl:





• Molecule 10: R-phycoerythrin alpha chain

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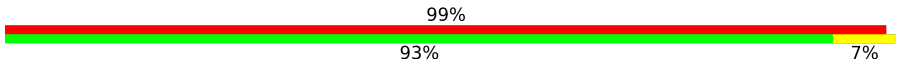
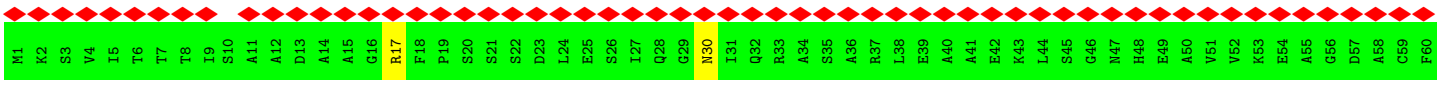
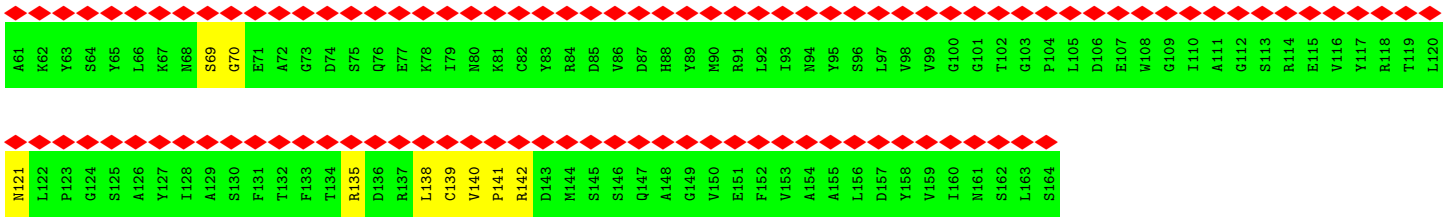
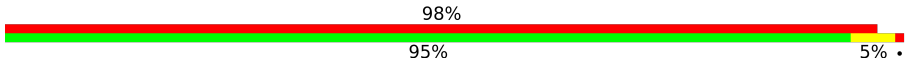


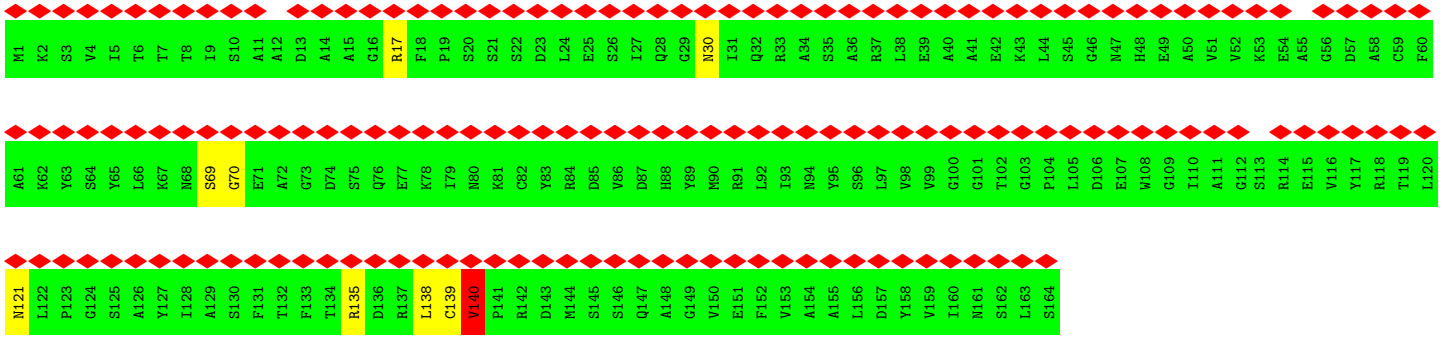




• Molecule 10: R-phycoerythrin alpha chain

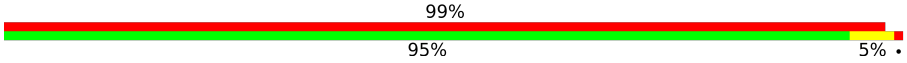
Chain fp:

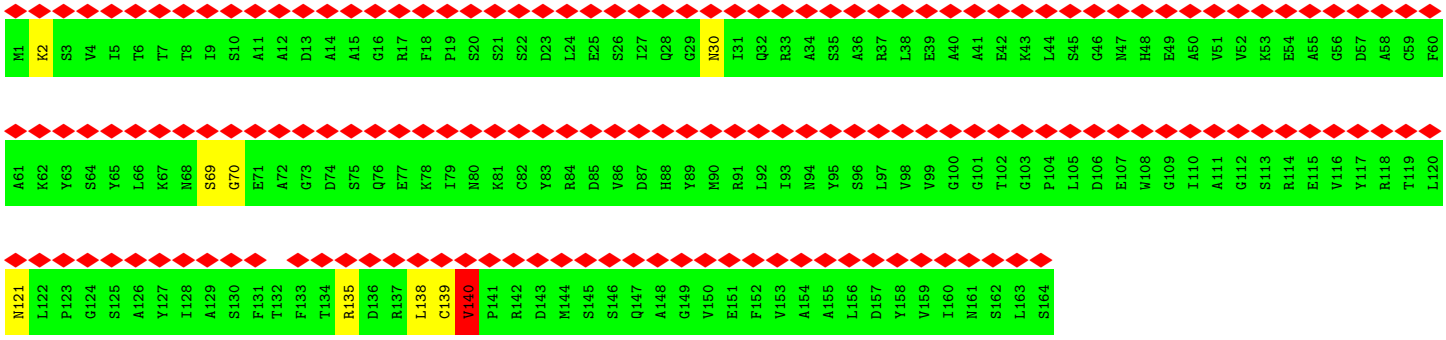




• Molecule 10: R-phycoerythrin alpha chain

Chain fr:





• Molecule 10: R-phycoerythrin alpha chain

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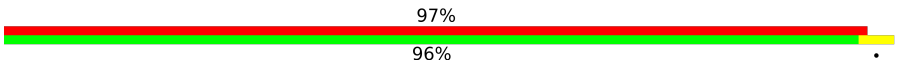
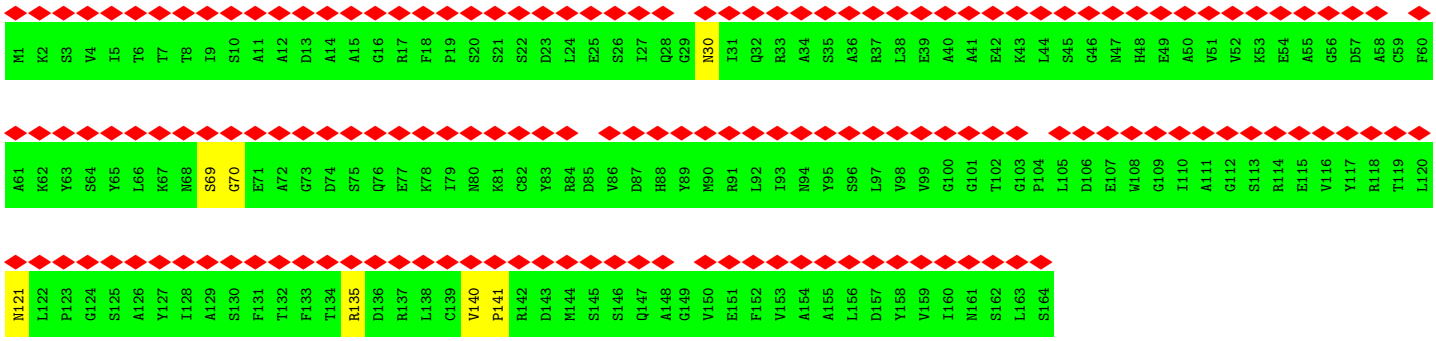
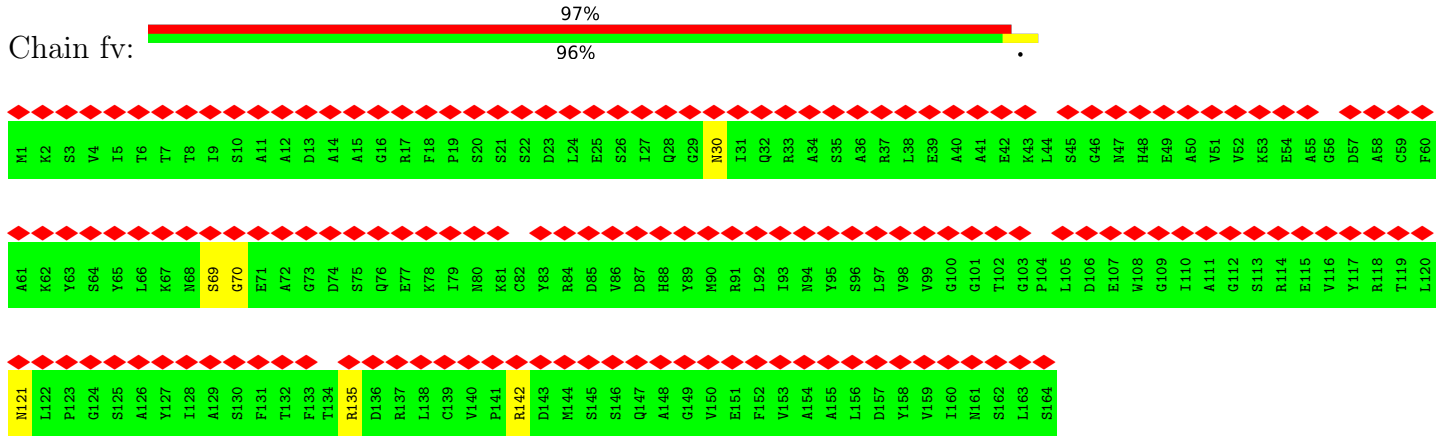




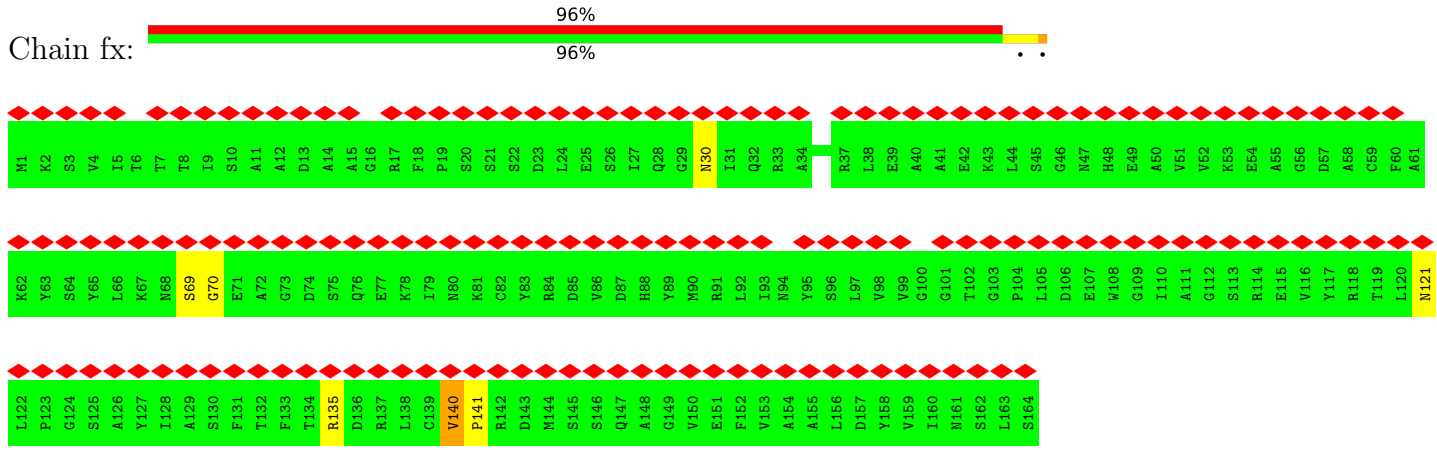
• Molecule 10: R-phycoerythrin alpha chain

Chain fv:



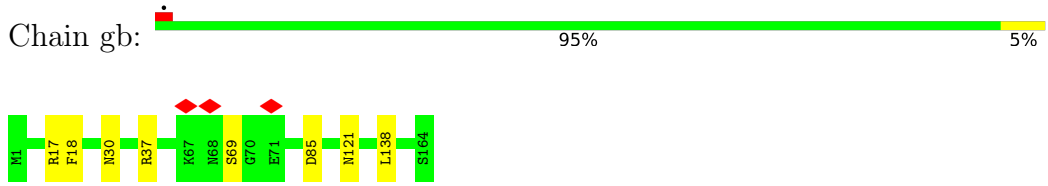
• Molecule 10: R-phycoerythrin alpha chain

Chain fx:



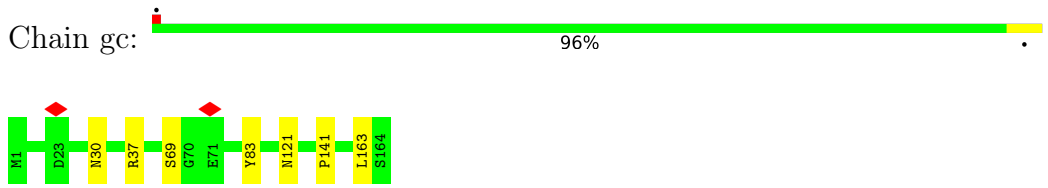
• Molecule 10: R-phycoerythrin alpha chain

Chain gb:



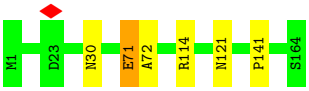
• Molecule 10: R-phycoerythrin alpha chain

Chain gc:



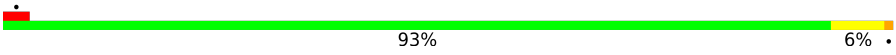
• Molecule 10: R-phycoerythrin alpha chain

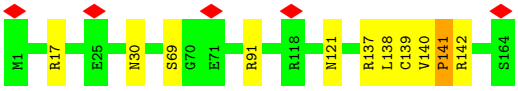
Chain gf:



• Molecule 10: R-phycoerythrin alpha chain

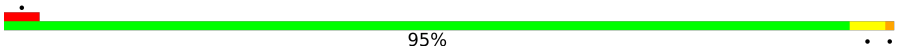
Chain gh:

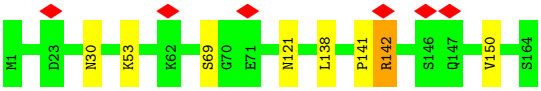




• Molecule 10: R-phycoerythrin alpha chain

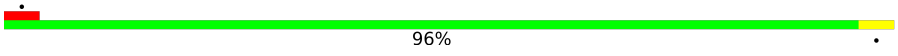
Chain gj:

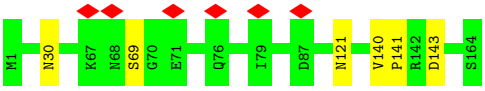




• Molecule 10: R-phycoerythrin alpha chain

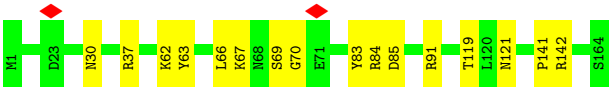
Chain gl:





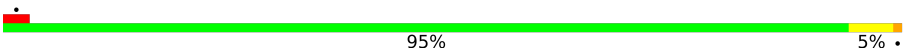
• Molecule 10: R-phycoerythrin alpha chain

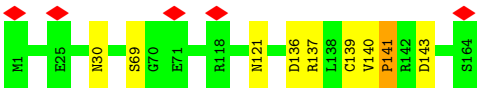
Chain gm:



• Molecule 10: R-phycoerythrin alpha chain

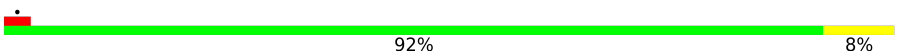
Chain go:

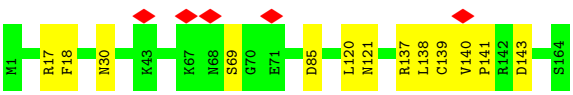




• Molecule 10: R-phycoerythrin alpha chain

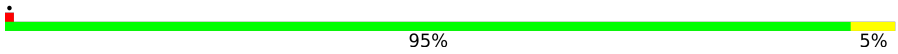
Chain gq:

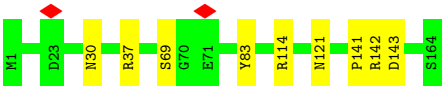




• Molecule 10: R-phycoerythrin alpha chain

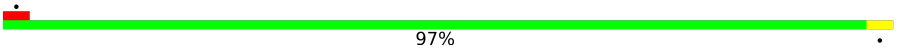
Chain gs:

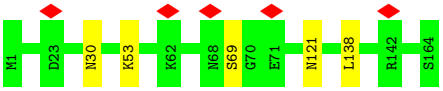




• Molecule 10: R-phycoerythrin alpha chain

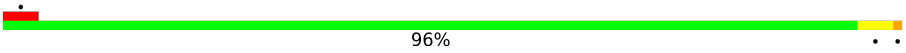
Chain gu:

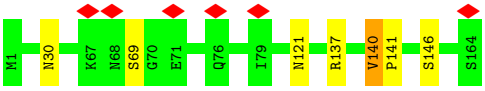




• Molecule 10: R-phycoerythrin alpha chain

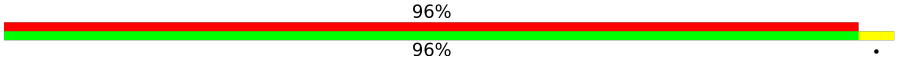
Chain gw:

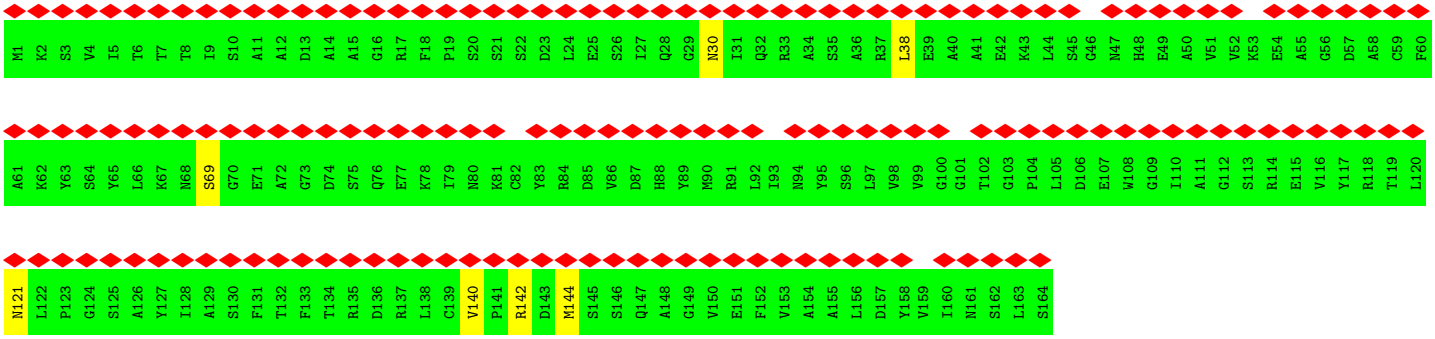




• Molecule 10: R-phycoerythrin alpha chain

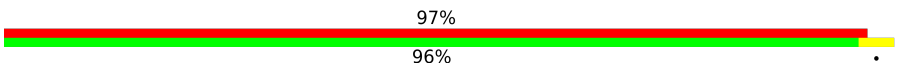
Chain hA:

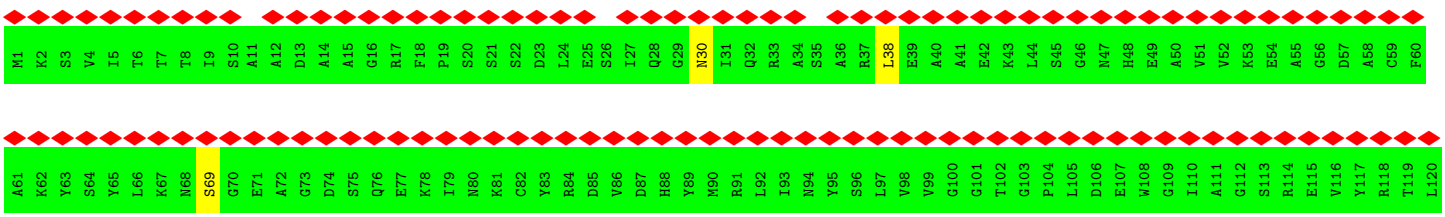


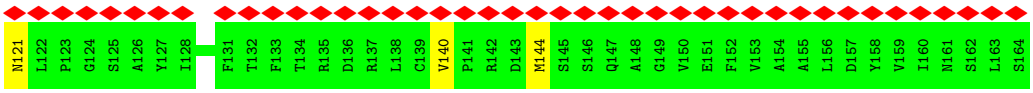


• Molecule 10: R-phycoerythrin alpha chain

Chain hC:

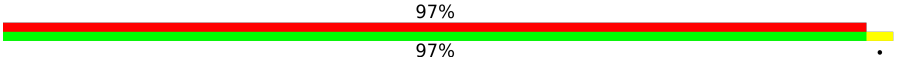


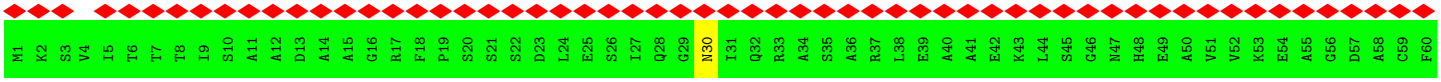


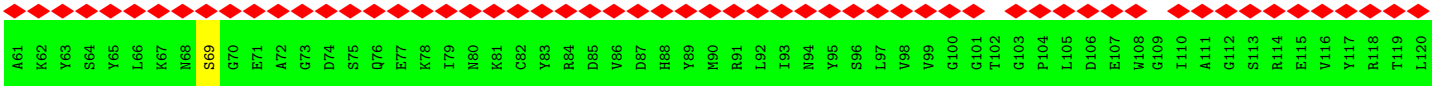


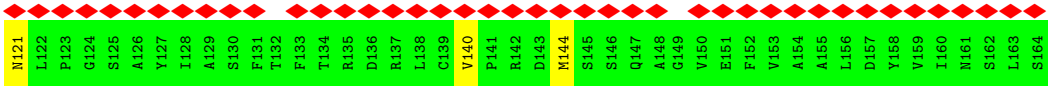
• Molecule 10: R-phycoerythrin alpha chain

Chain hE:



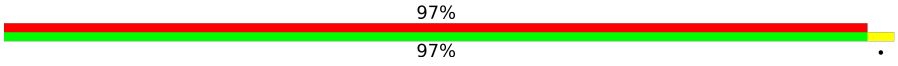


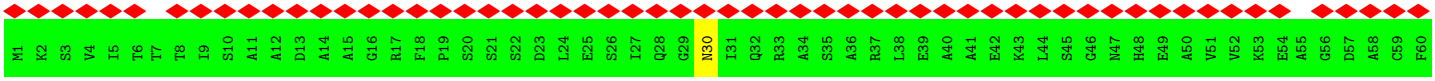


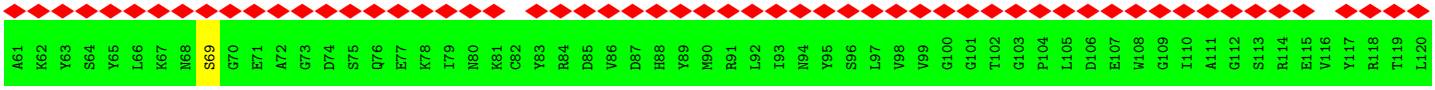


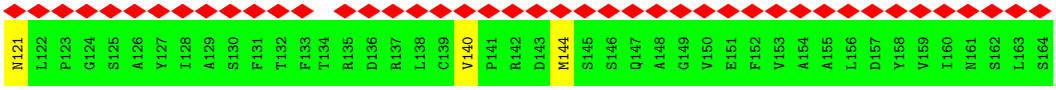
• Molecule 10: R-phycoerythrin alpha chain

Chain hF:



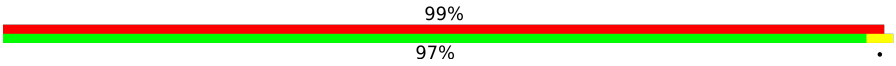


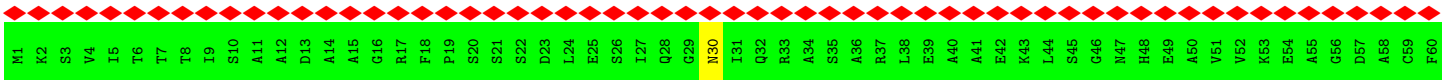


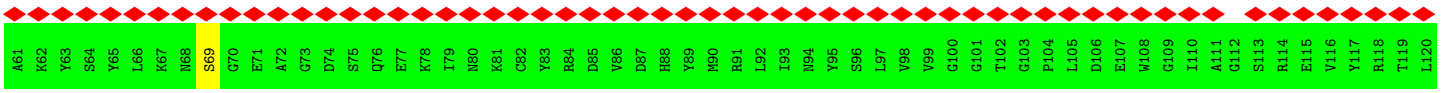


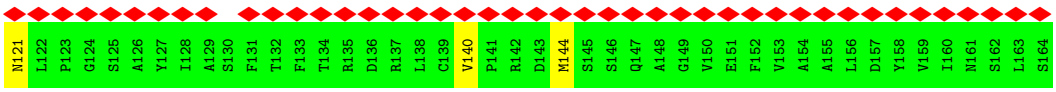
• Molecule 10: R-phycoerythrin alpha chain

Chain hI:



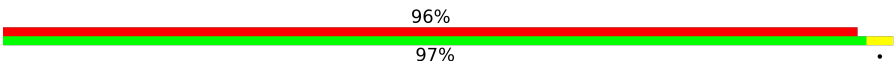






• Molecule 10: R-phycoerythrin alpha chain

Chain hK:



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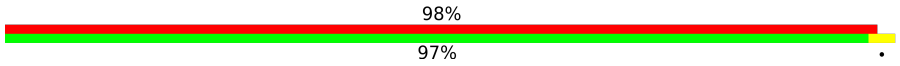
A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain hM:



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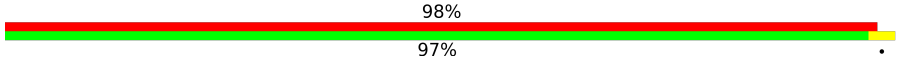
A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

N121 L122 P123 G124 S125 A126 Y127 I128 A129 S130 F131 T132 F133 T134 R135 D136 R137 L138 C139 V140 P141 R142 D143 M144 S145 S146 Q147 A148 G149 V150 E151 F152 V153 A154 A155 L156 D157 Y158 V159 I160 N161 S162 L163 S164

• Molecule 10: R-phycoerythrin alpha chain

Chain hO:



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A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

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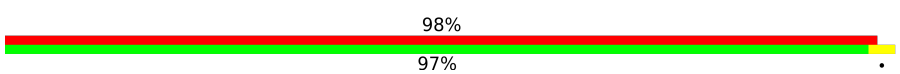
• Molecule 10: R-phycoerythrin alpha chain

Chain hQ:



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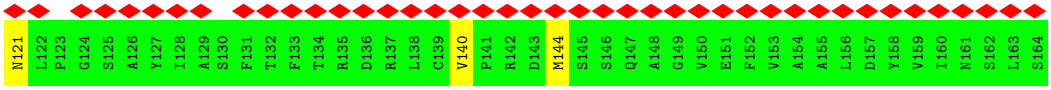
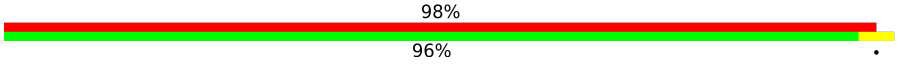
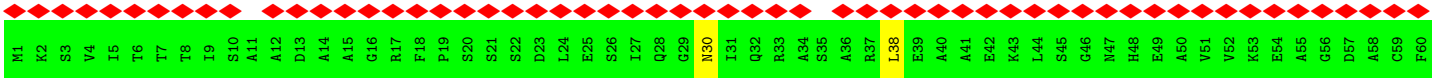
A61 K62 Y63 S64 Y65 L66 K67 N68 S69 G70 E71 A72 G73 D74 S75 Q76 E77 K78 I79 N80 K81 C82 Y83 R84 D85 V86 D87 H88 Y89 M90 R91 L92 I93 N94 Y95 S96 L97 V98 V99 G100 G101 T102 G103 P104 L105 D106 E107 W108 G109 I110 A111 G112 S113 R114 E115 V116 Y117 R118 T119 L120

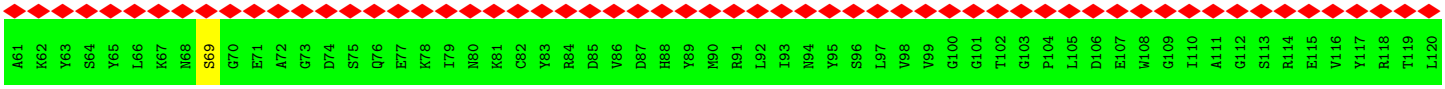


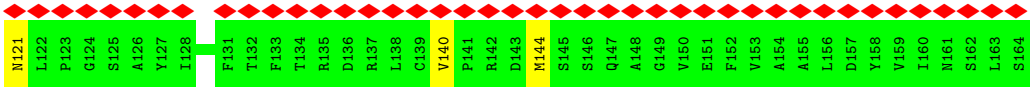
• Molecule 10: R-phycoerythrin alpha chain

Chain hS:



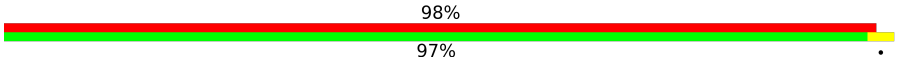


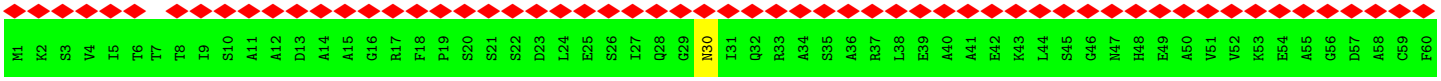


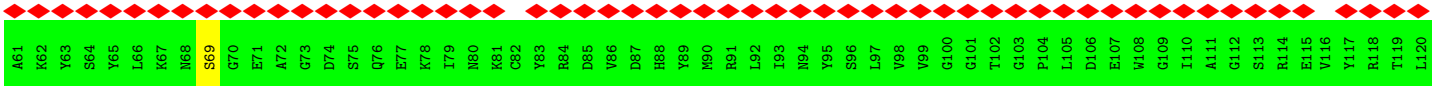


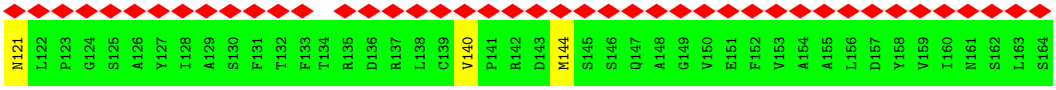
• Molecule 10: R-phycoerythrin alpha chain

Chain hU:



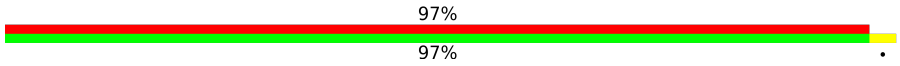


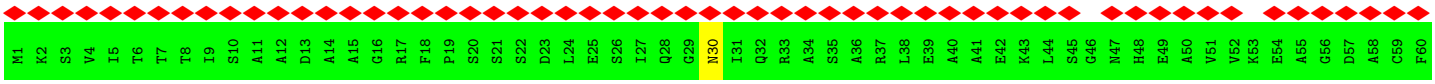


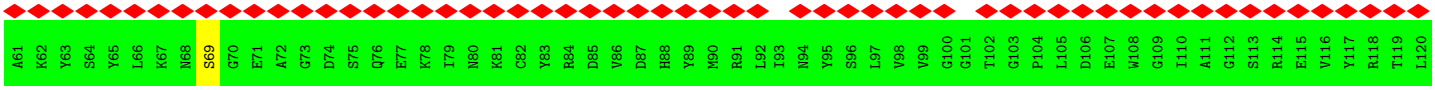


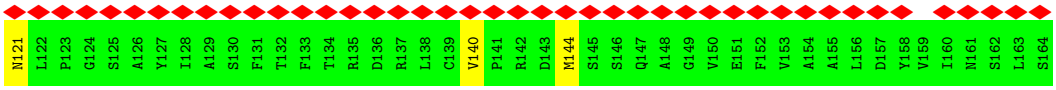
• Molecule 10: R-phycoerythrin alpha chain

Chain hW:



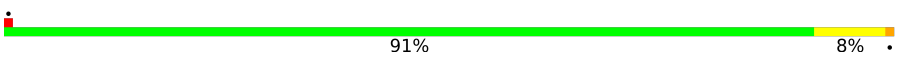


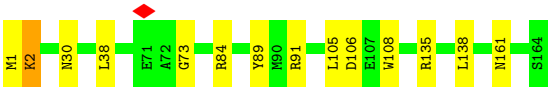




• Molecule 10: R-phycoerythrin alpha chain

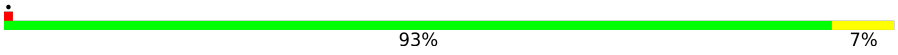
Chain iA:

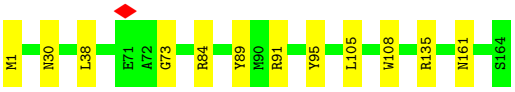




• Molecule 10: R-phycoerythrin alpha chain

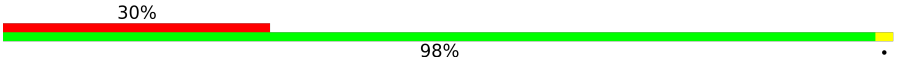
Chain iB:

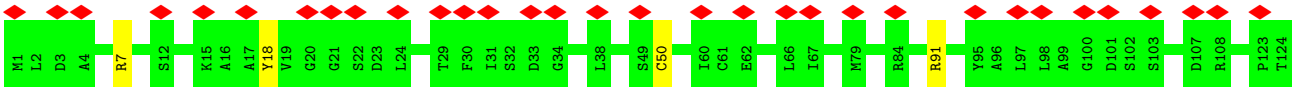


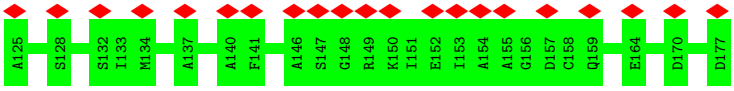


• Molecule 11: R-phycoerythrin beta chain

Chain f2:

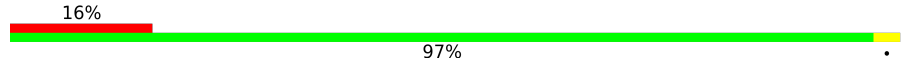


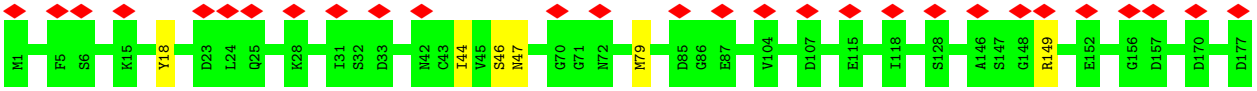




• Molecule 11: R-phycoerythrin beta chain

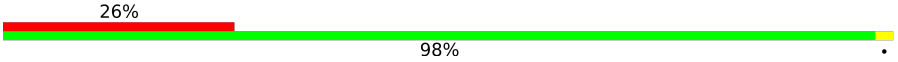
Chain h2:

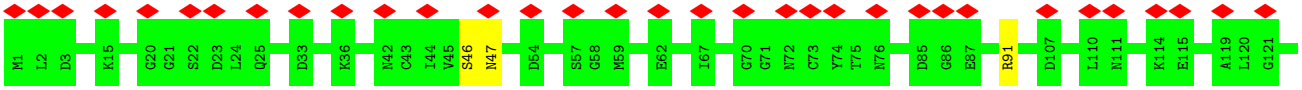


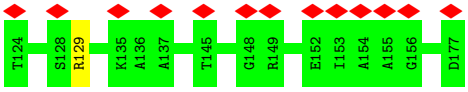


• Molecule 11: R-phycoerythrin beta chain

Chain j2:

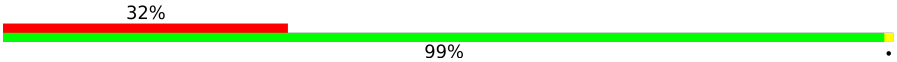


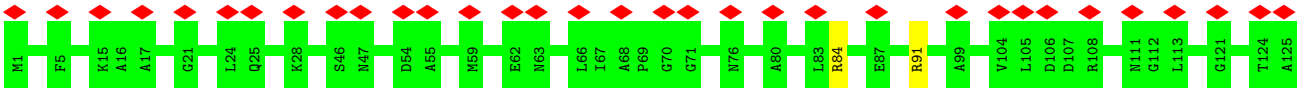


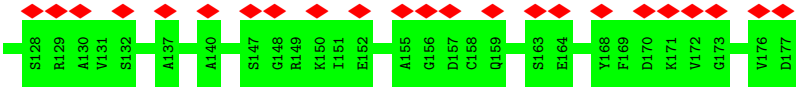


• Molecule 11: R-phycoerythrin beta chain

Chain l2:

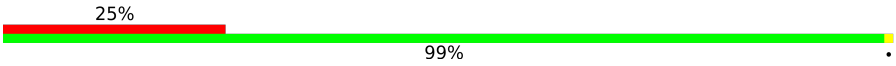


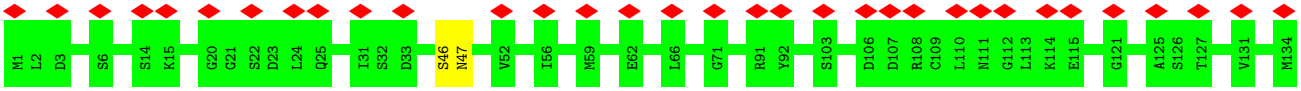


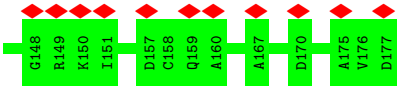


• Molecule 11: R-phycoerythrin beta chain

Chain n2:

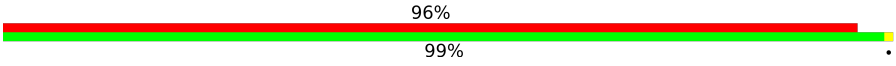


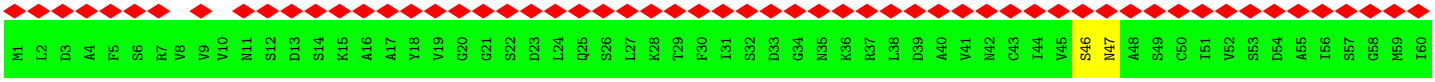


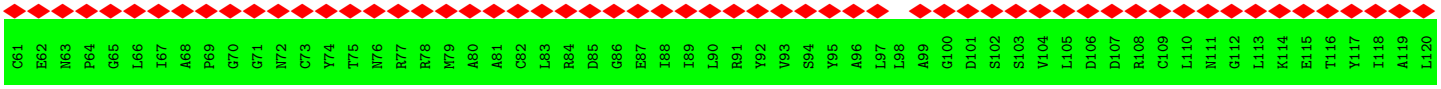


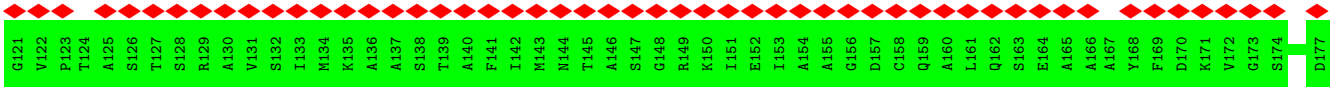
• Molecule 11: R-phycoerythrin beta chain

Chain p2:



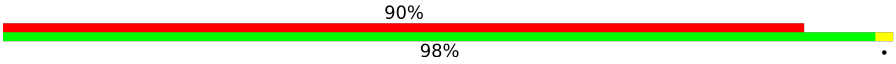


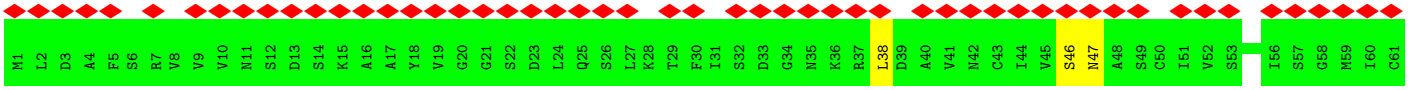


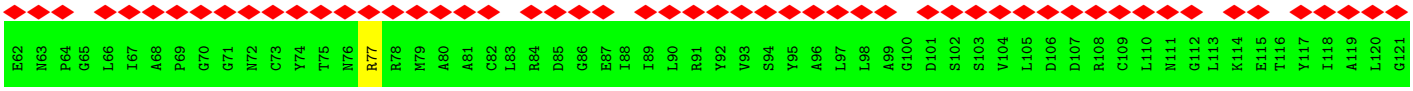


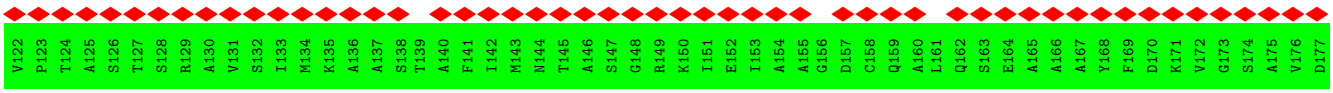
• Molecule 11: R-phycoerythrin beta chain

Chain r2:



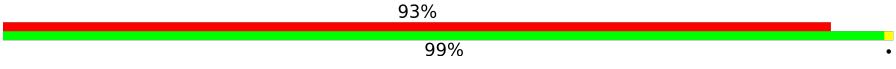


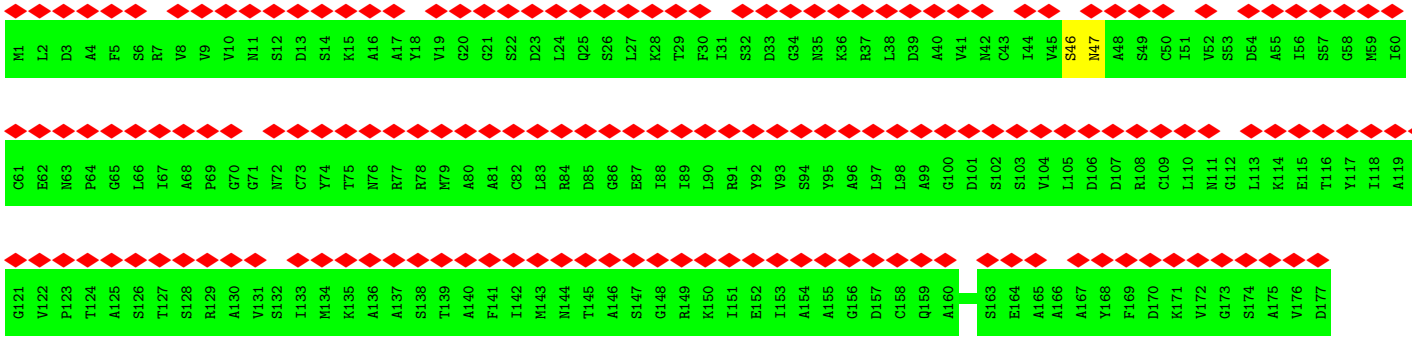




• Molecule 11: R-phycoerythrin beta chain

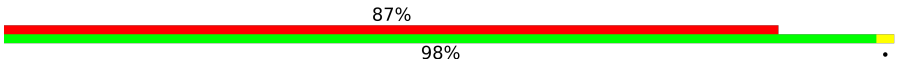
Chain t2:

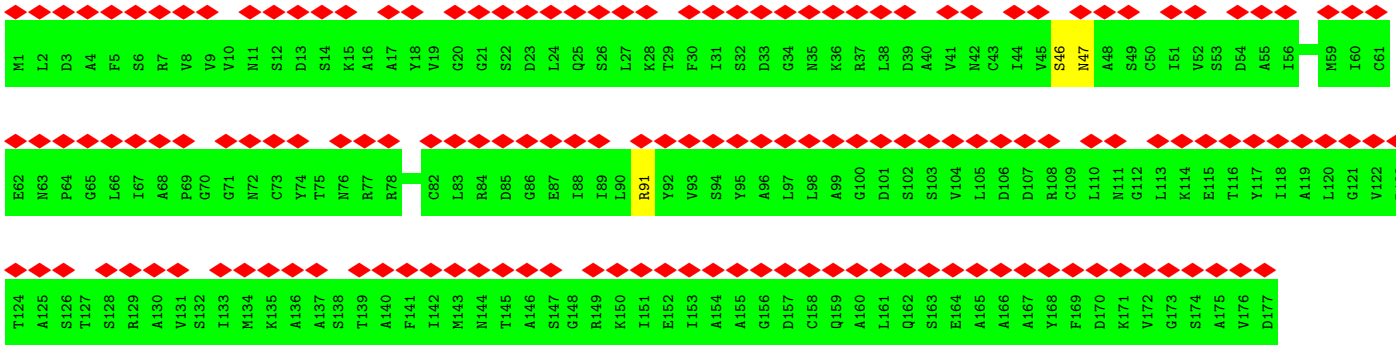




• Molecule 11: R-phycoerythrin beta chain

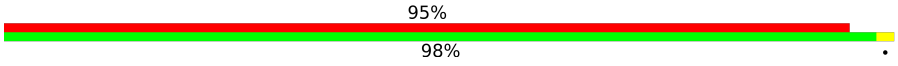
Chain v2:

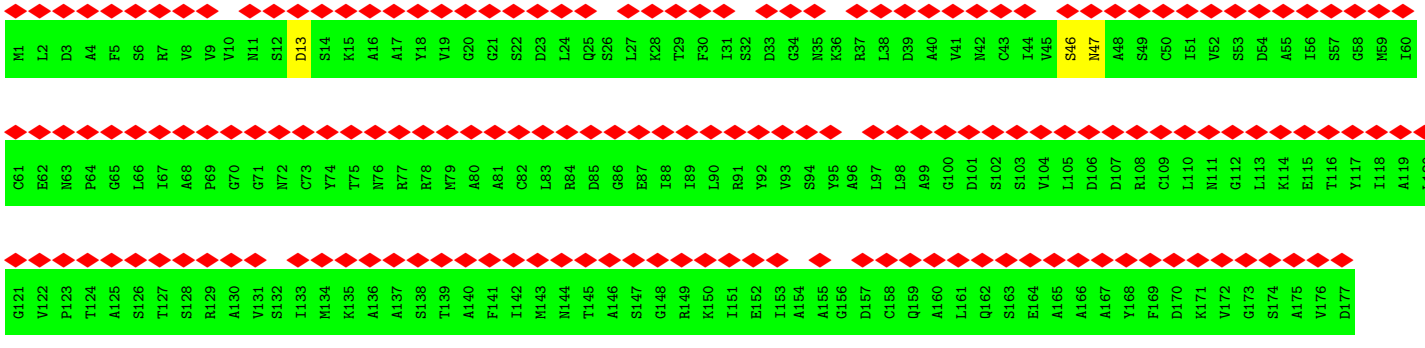




• Molecule 11: R-phycoerythrin beta chain

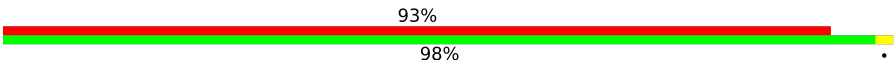
Chain x2:

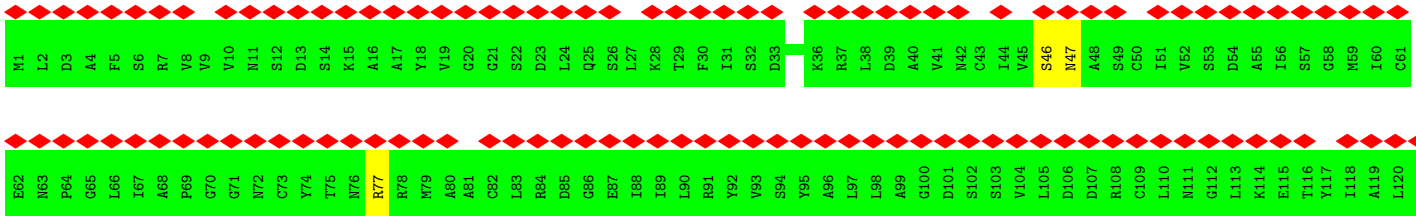


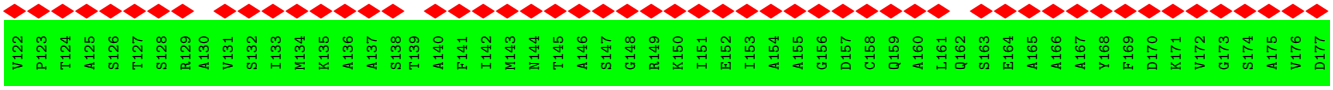


• Molecule 11: R-phycoerythrin beta chain

Chain z2:

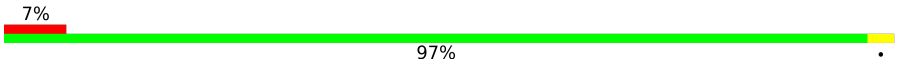


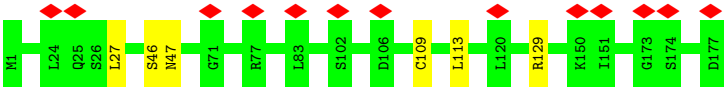




• Molecule 11: R-phycoerythrin beta chain

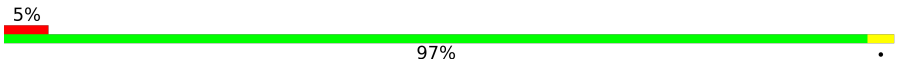
Chain F2:

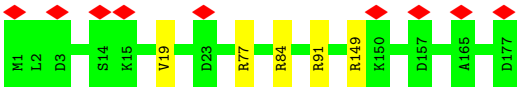




• Molecule 11: R-phycoerythrin beta chain

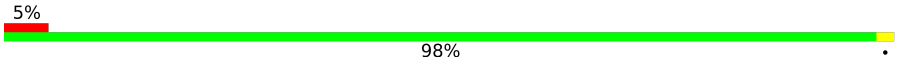
Chain H2:

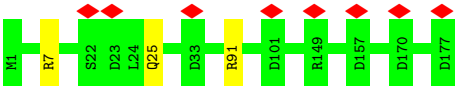




• Molecule 11: R-phycoerythrin beta chain

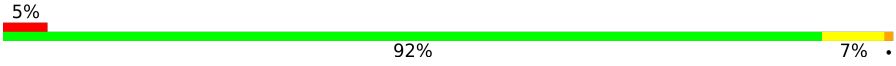
Chain J2:

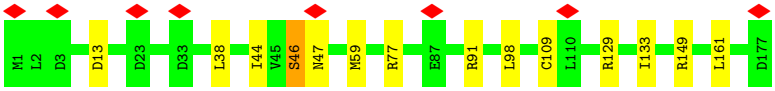




• Molecule 11: R-phycoerythrin beta chain

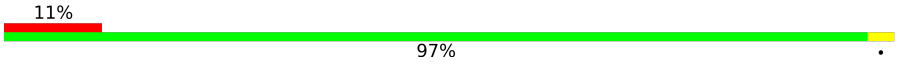
Chain L2:

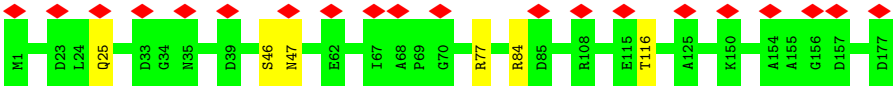




• Molecule 11: R-phycoerythrin beta chain

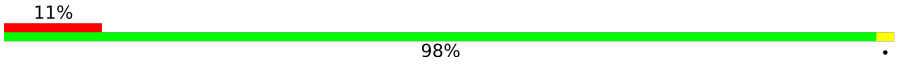
Chain N2:

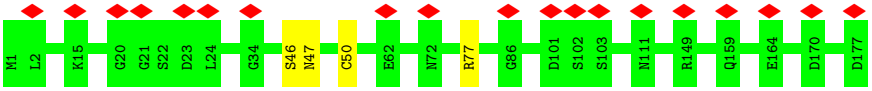




• Molecule 11: R-phycoerythrin beta chain

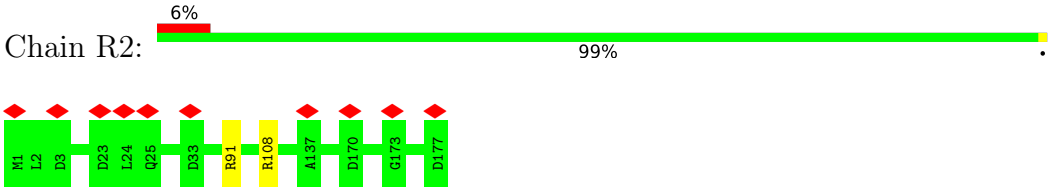
Chain P2:





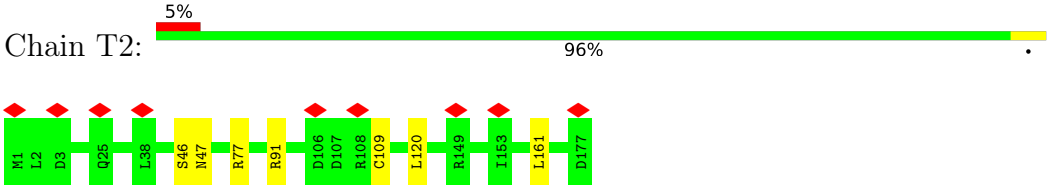
• Molecule 11: R-phycoerythrin beta chain

Chain R2:



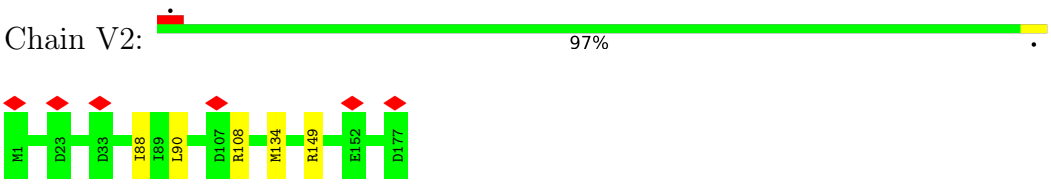
• Molecule 11: R-phycoerythrin beta chain

Chain T2:



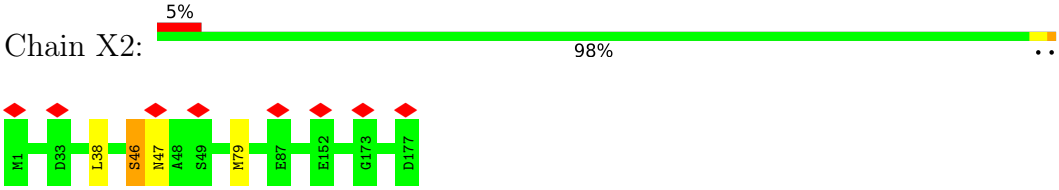
• Molecule 11: R-phycoerythrin beta chain

Chain V2:



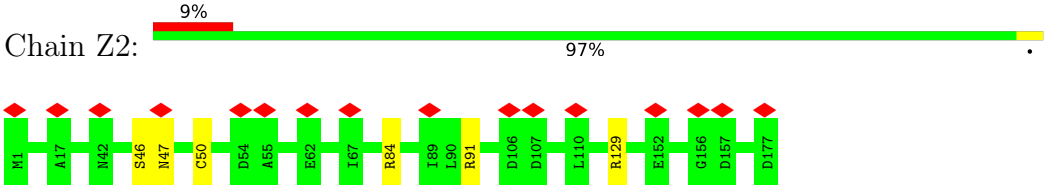
• Molecule 11: R-phycoerythrin beta chain

Chain X2:



• Molecule 11: R-phycoerythrin beta chain

Chain Z2:



• Molecule 11: R-phycoerythrin beta chain

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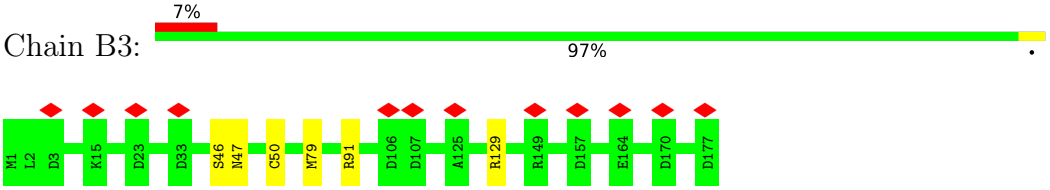
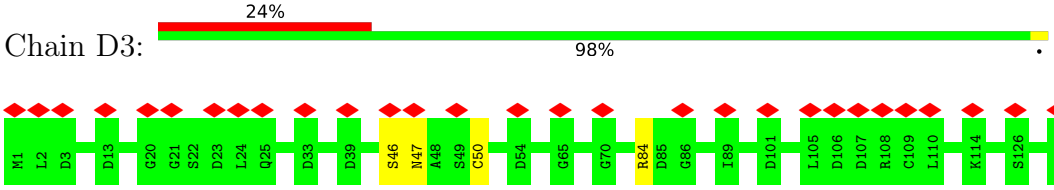
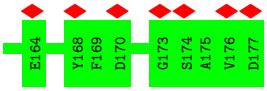


• Molecule 11: R-phycoerythrin beta chain

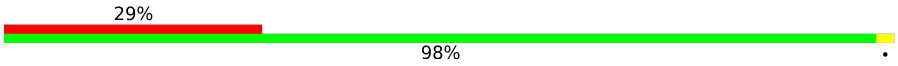
Chain D3:

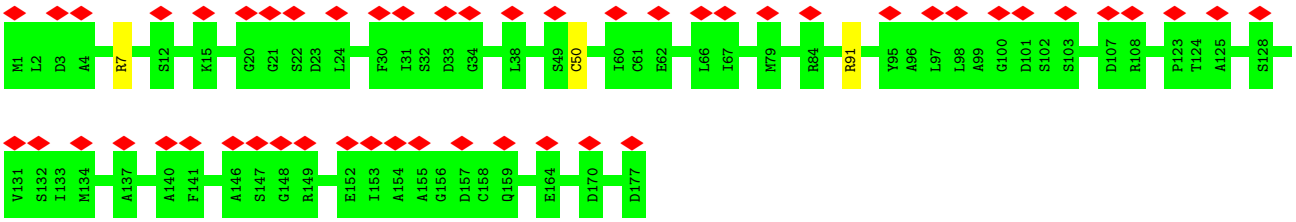




• Molecule 11: R-phycoerythrin beta chain

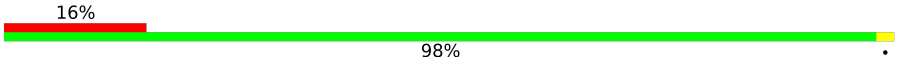
Chain F3:

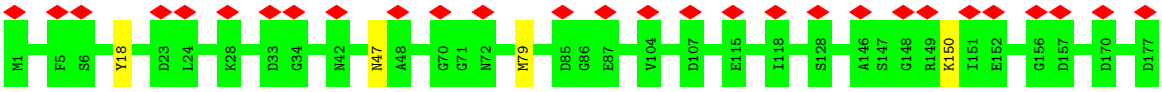




• Molecule 11: R-phycoerythrin beta chain

Chain H3:





• Molecule 11: R-phycoerythrin beta chain

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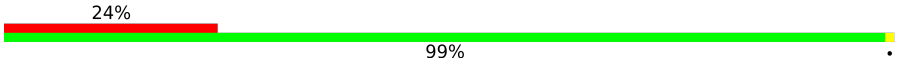
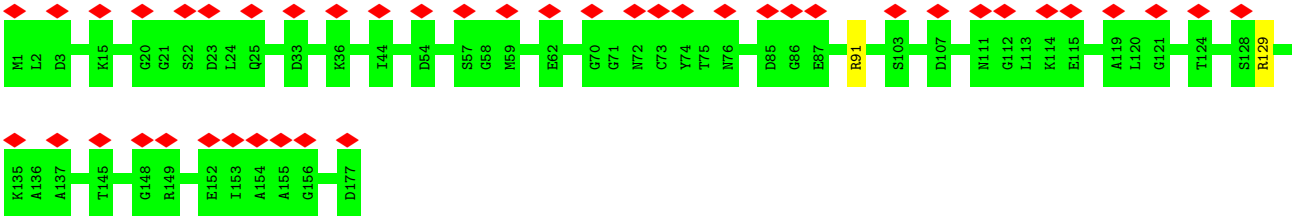
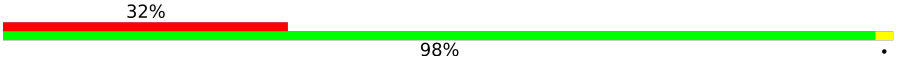
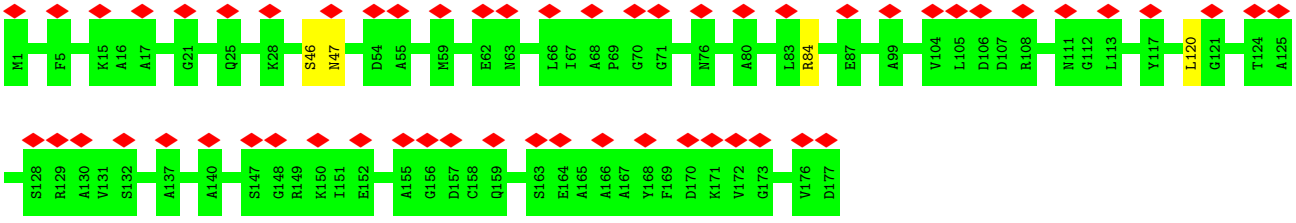




• Molecule 11: R-phycoerythrin beta chain

Chain L3:





• Molecule 11: R-phycoerythrin beta chain

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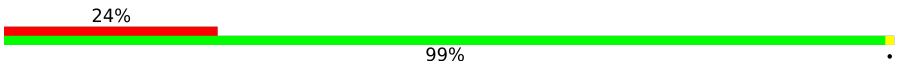

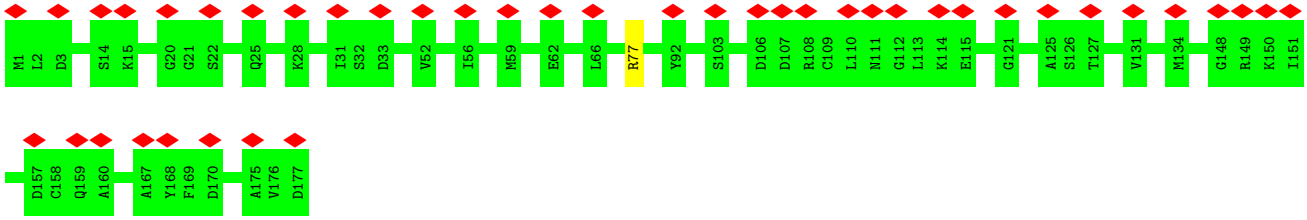

• Molecule 11: R-phycoerythrin beta chain

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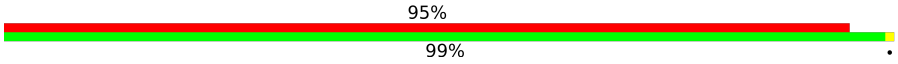
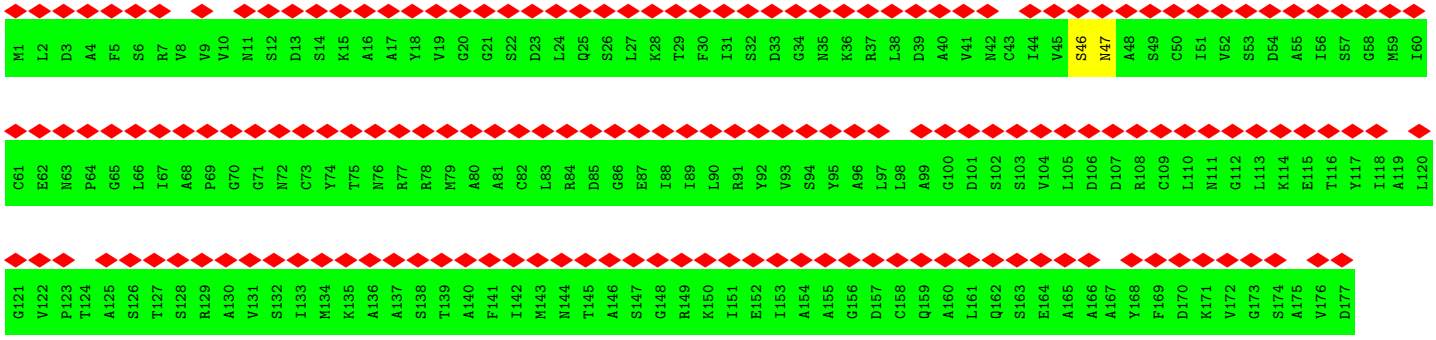
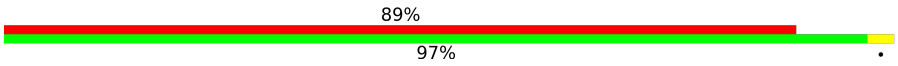
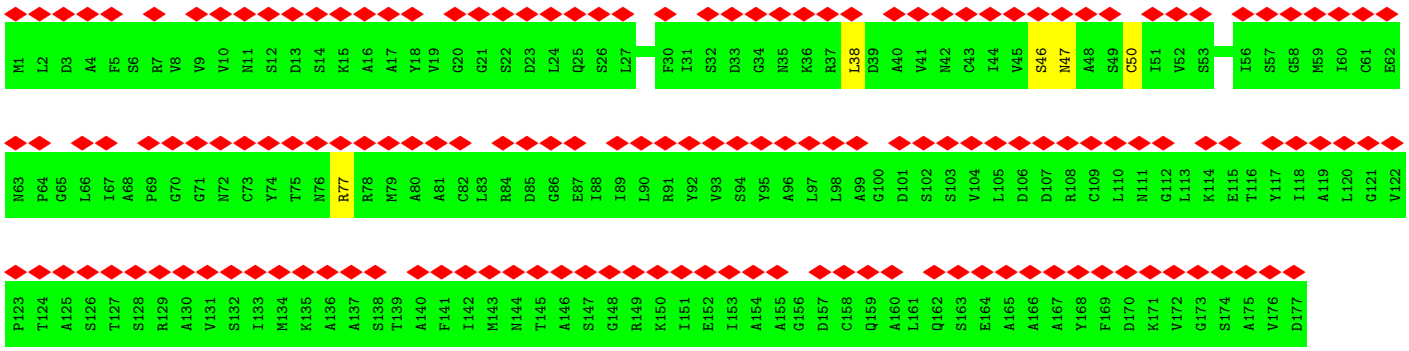




• Molecule 11: R-phycoerythrin beta chain

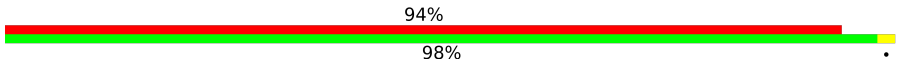
Chain R3:

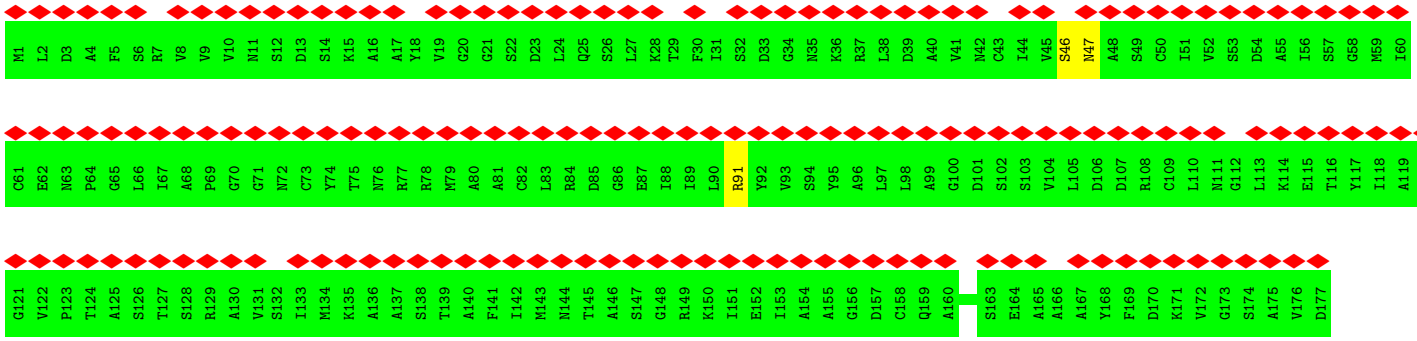




• Molecule 11: R-phycoerythrin beta chain

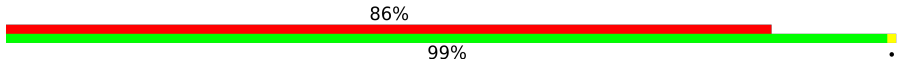
Chain T3:

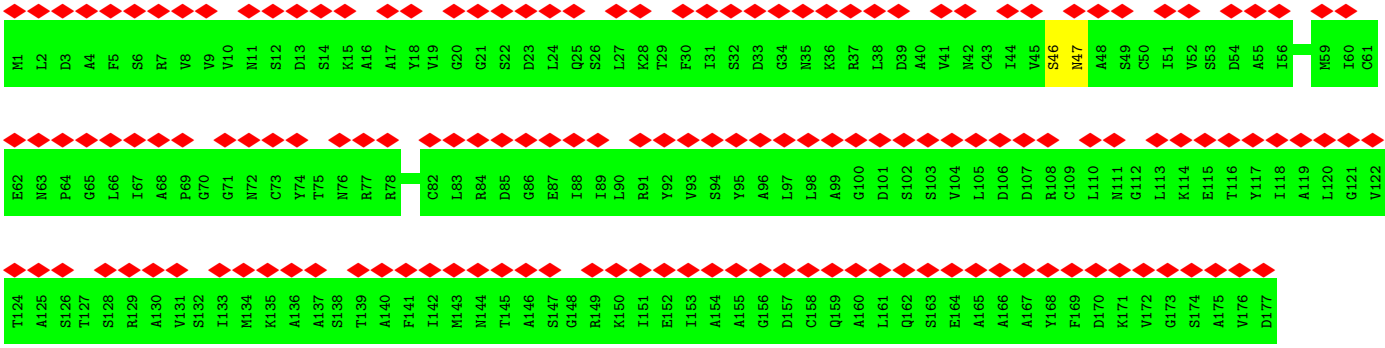




• Molecule 11: R-phycoerythrin beta chain

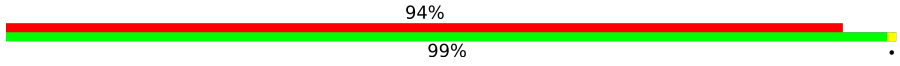
Chain V3:

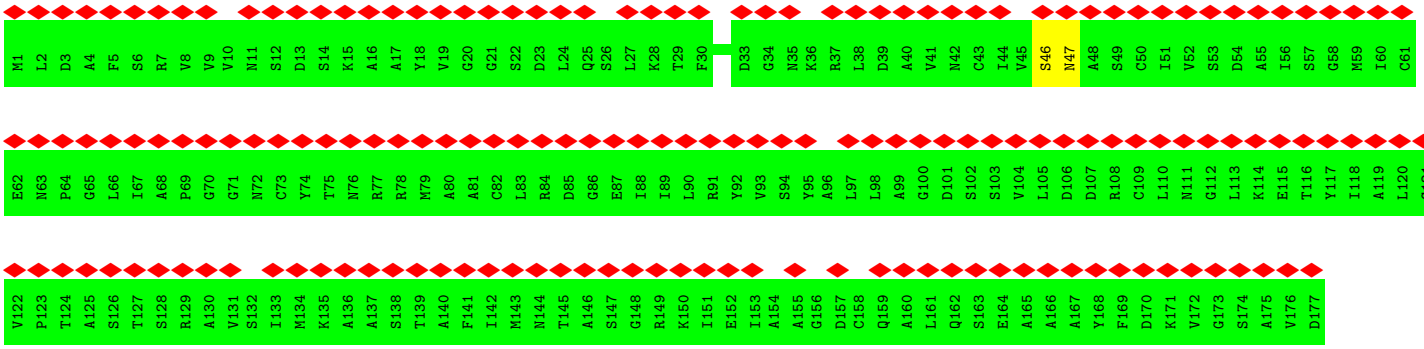




• Molecule 11: R-phycoerythrin beta chain

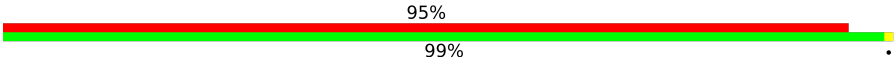
Chain X3:

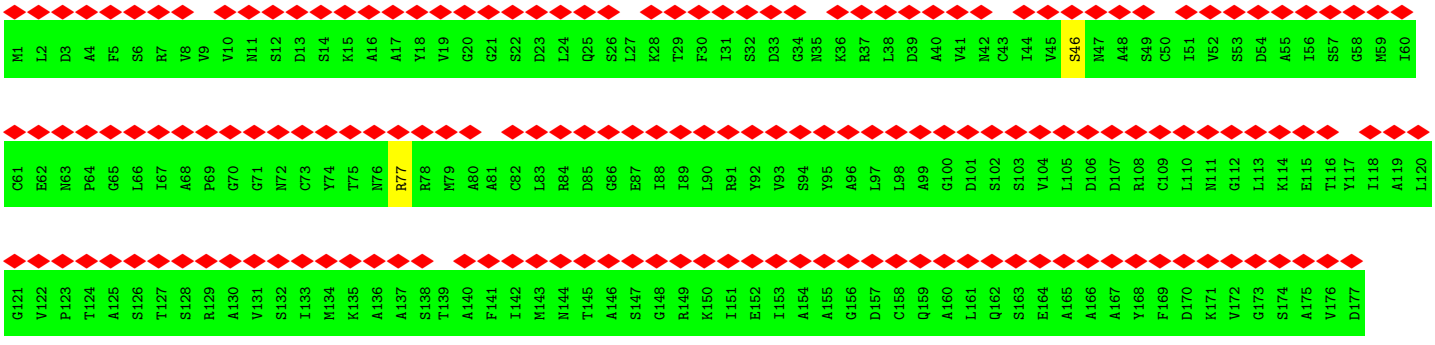




• Molecule 11: R-phycoerythrin beta chain

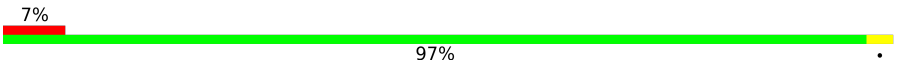
Chain Z3:

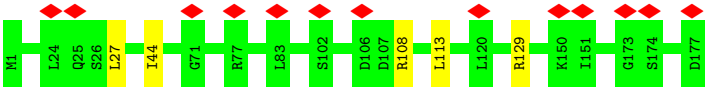




• Molecule 11: R-phycoerythrin beta chain

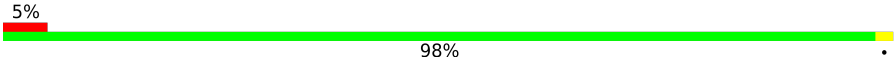
Chain f3:

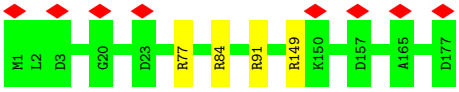




• Molecule 11: R-phycoerythrin beta chain

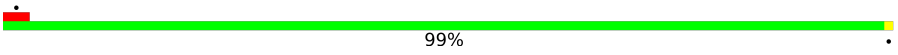
Chain h3:

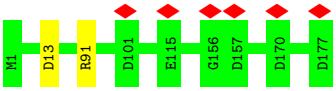




• Molecule 11: R-phycoerythrin beta chain

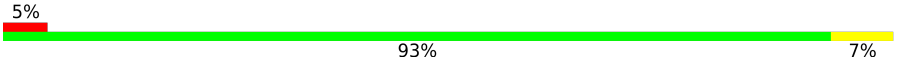
Chain j3:

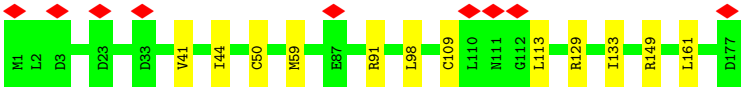




• Molecule 11: R-phycoerythrin beta chain

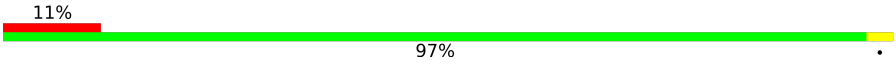
Chain l3:

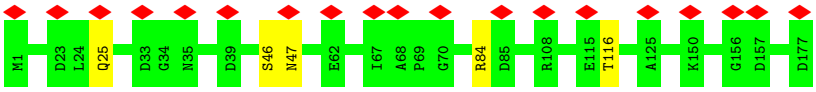




• Molecule 11: R-phycoerythrin beta chain

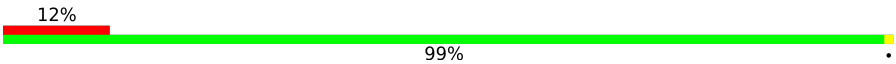
Chain n3:





• Molecule 11: R-phycoerythrin beta chain

Chain p3:



• Molecule 11: R-phycoerythrin beta chain

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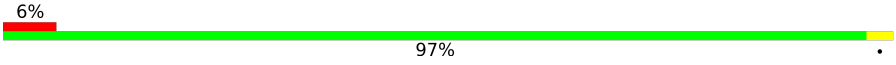
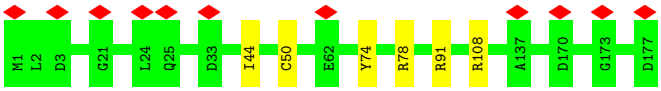
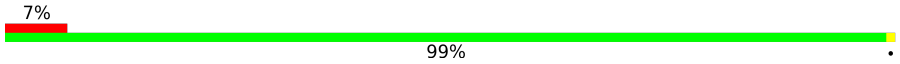
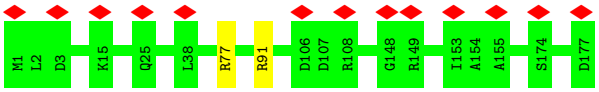




• Molecule 11: R-phycoerythrin beta chain

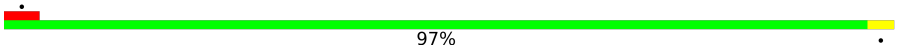
Chain t3:

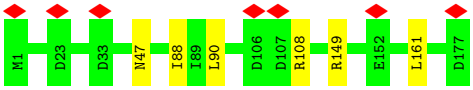




• Molecule 11: R-phycoerythrin beta chain

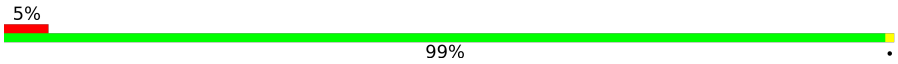
Chain v3:

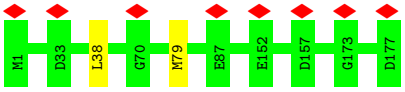




• Molecule 11: R-phycoerythrin beta chain

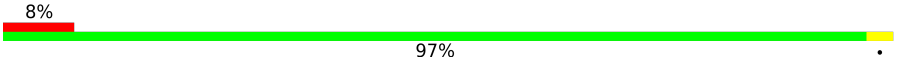
Chain x3:

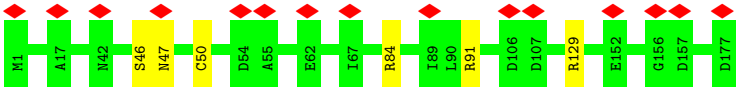




• Molecule 11: R-phycoerythrin beta chain

Chain z3:





• Molecule 11: R-phycoerythrin beta chain

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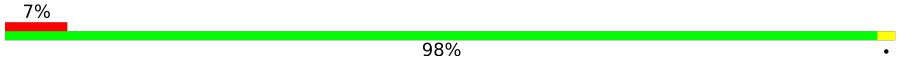

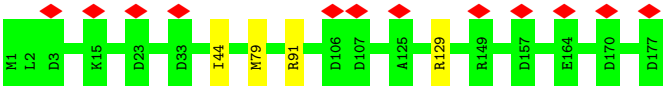

• Molecule 11: R-phycoerythrin beta chain

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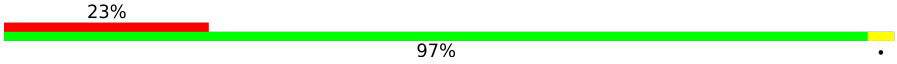
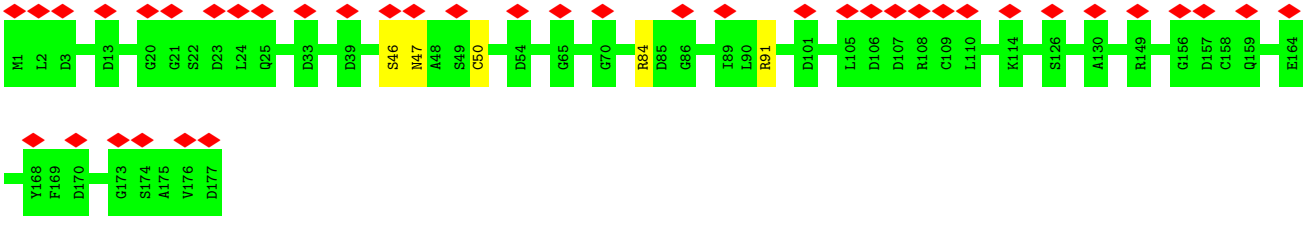
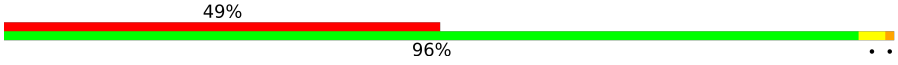
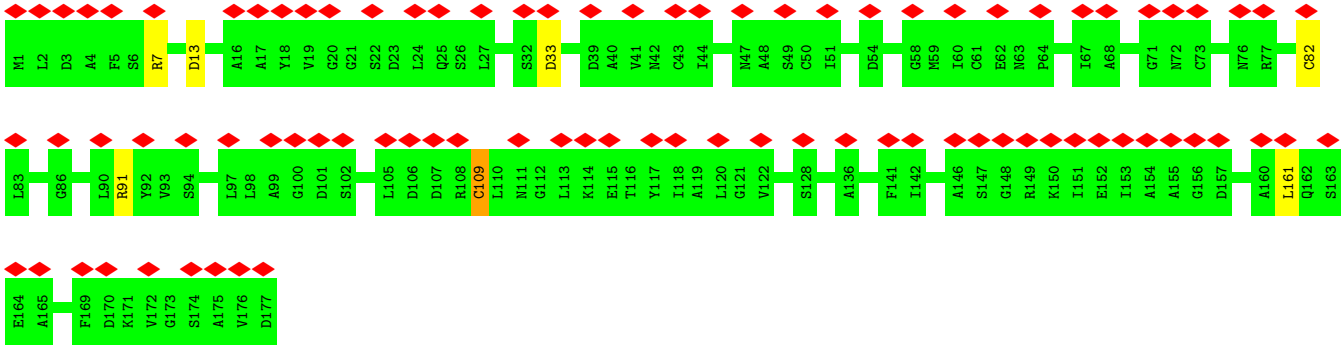




• Molecule 11: R-phycoerythrin beta chain

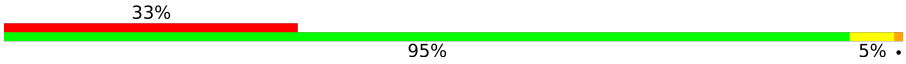
Chain F4:

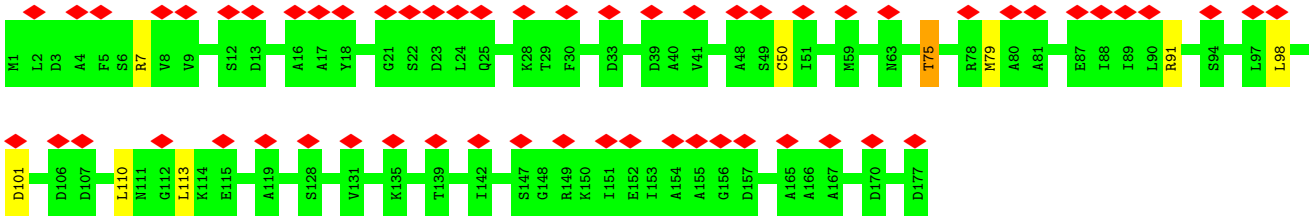




• Molecule 11: R-phycoerythrin beta chain

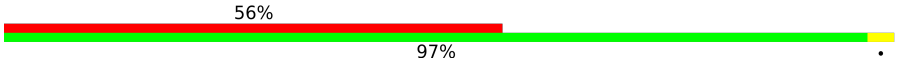
Chain H4:

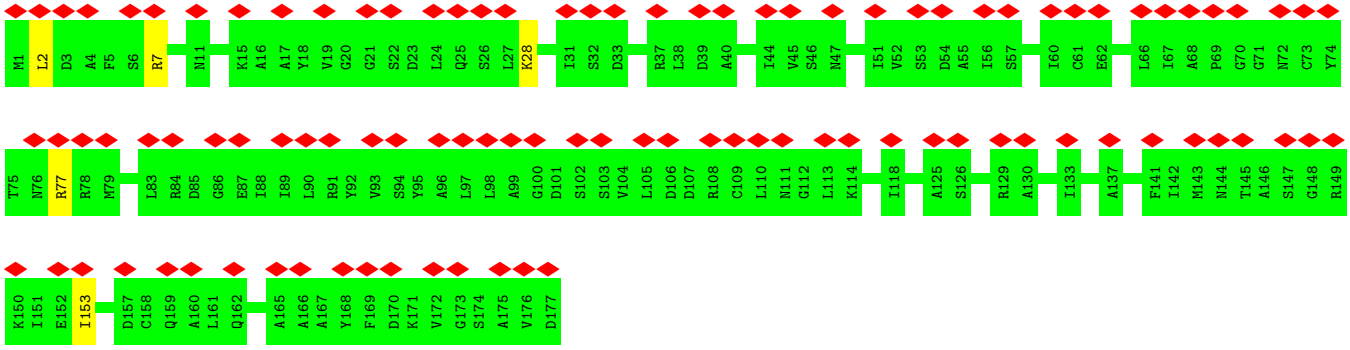




• Molecule 11: R-phycoerythrin beta chain

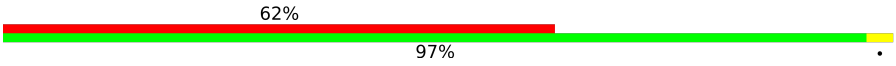
Chain J4:

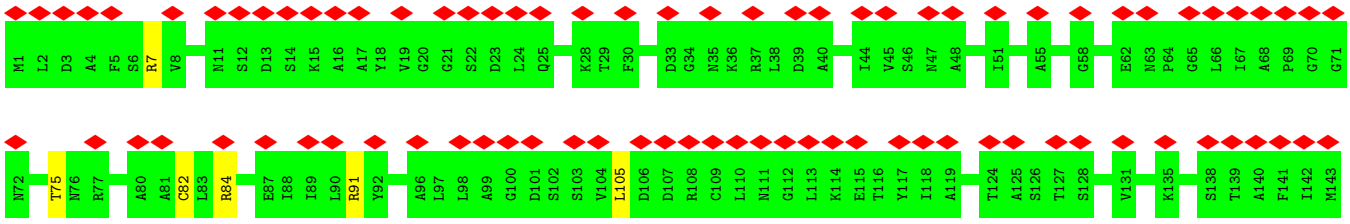


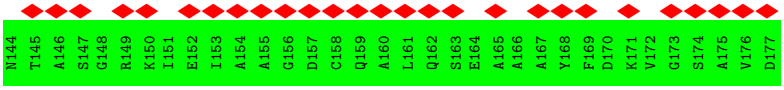


• Molecule 11: R-phycoerythrin beta chain

Chain L4:







• Molecule 11: R-phycoerythrin beta chain

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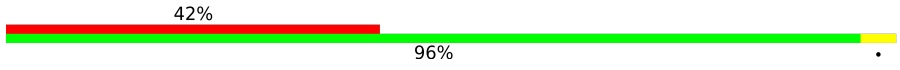

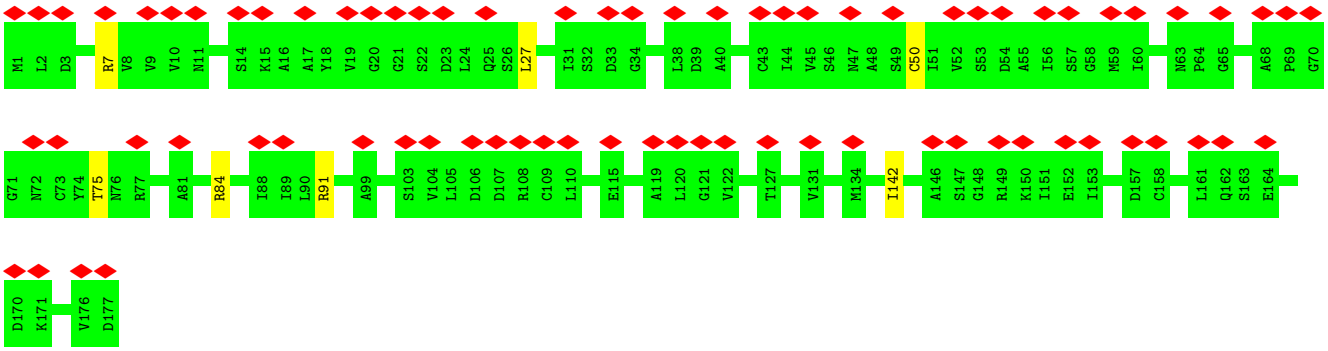

• Molecule 11: R-phycoerythrin beta chain

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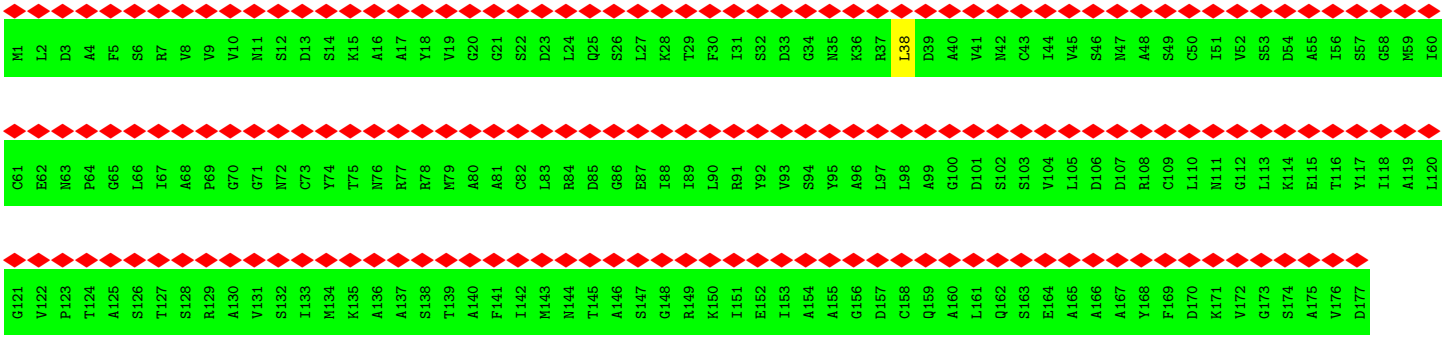

• Molecule 11: R-phycoerythrin beta chain

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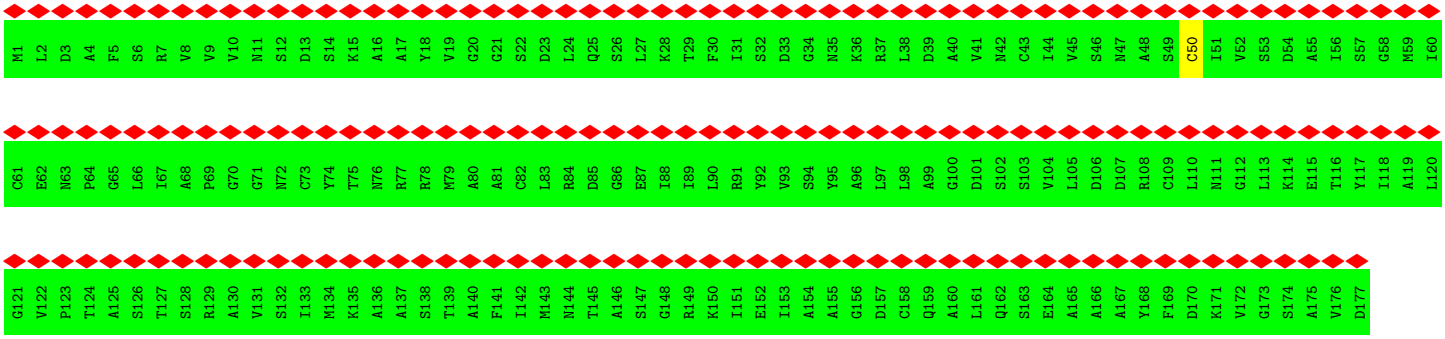

• Molecule 11: R-phycoerythrin beta chain

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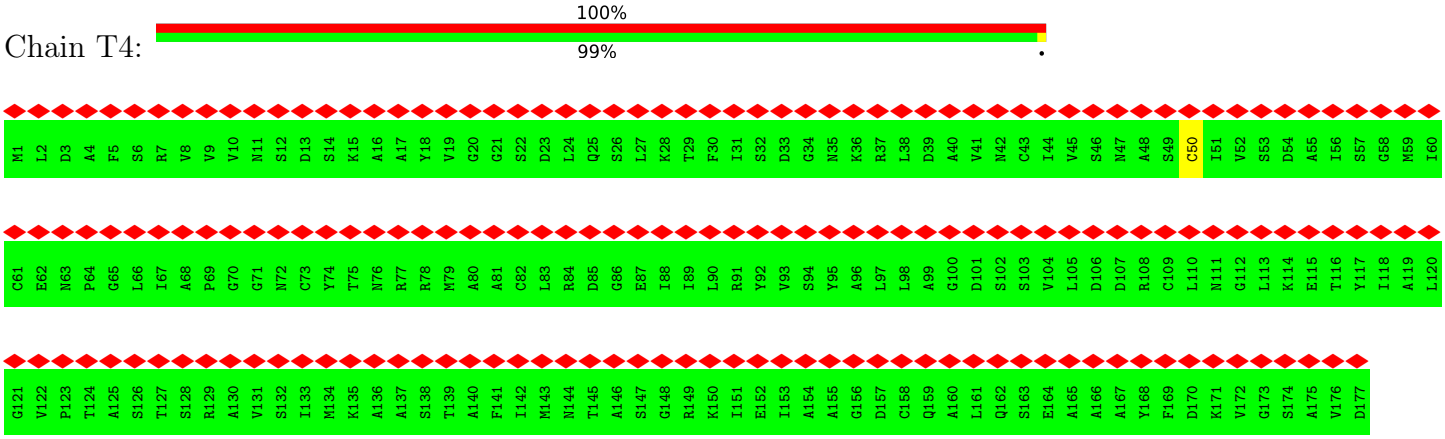

• Molecule 11: R-phycoerythrin beta chain

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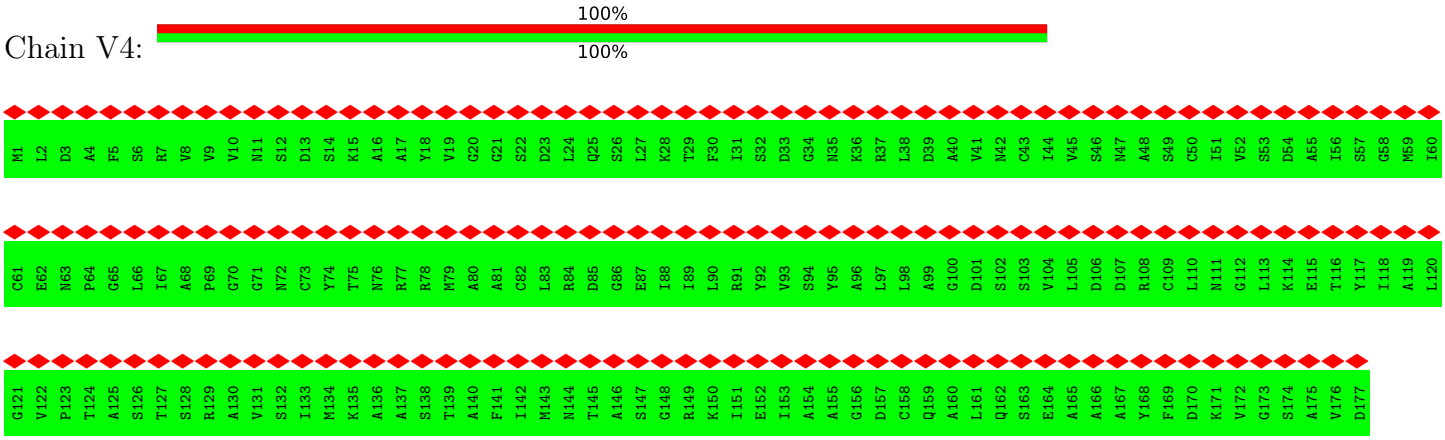

• Molecule 11: R-phycoerythrin beta chain

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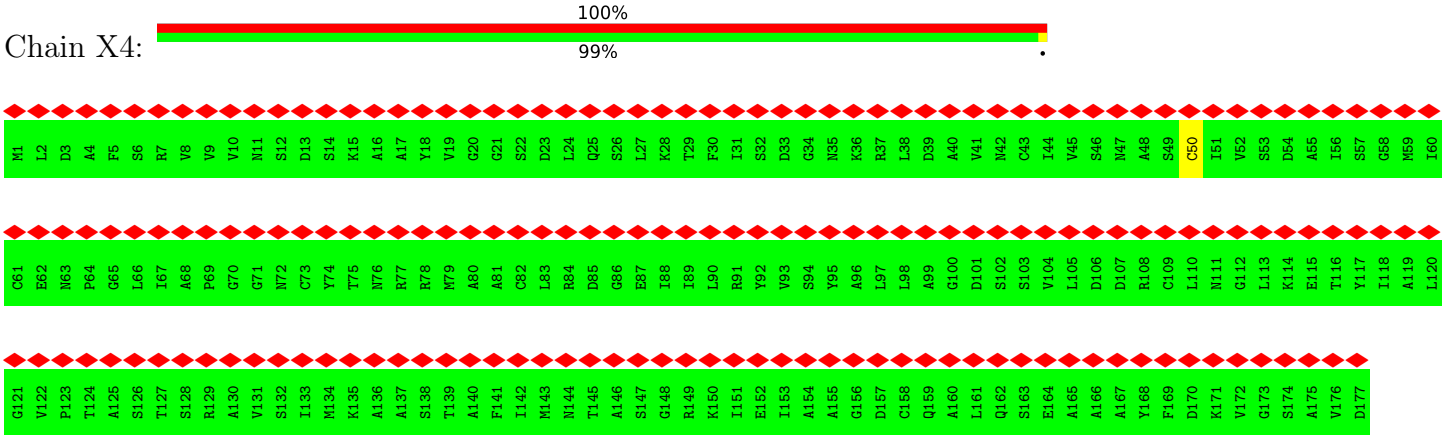

• Molecule 11: R-phycoerythrin beta chain

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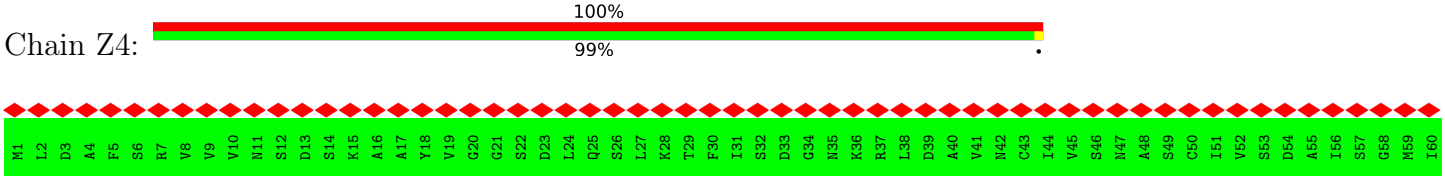

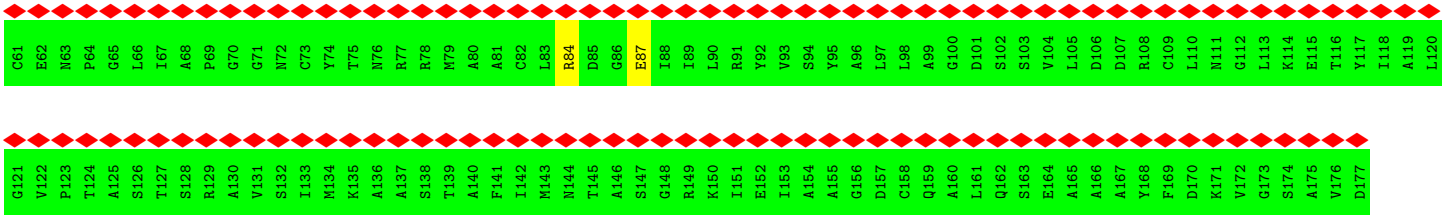

• Molecule 11: R-phycoerythrin beta chain

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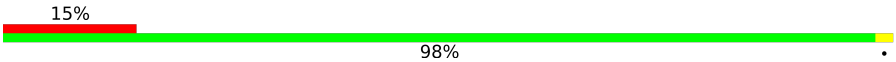

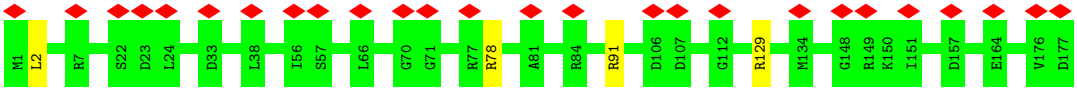

• Molecule 11: R-phycoerythrin beta chain

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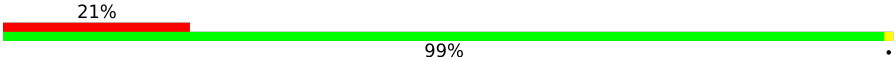

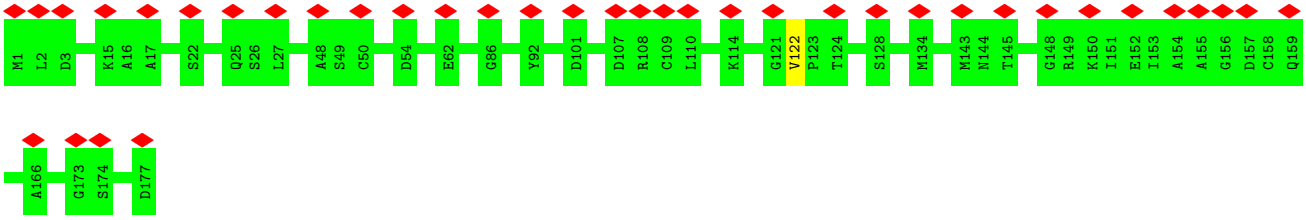

• Molecule 11: R-phycoerythrin beta chain

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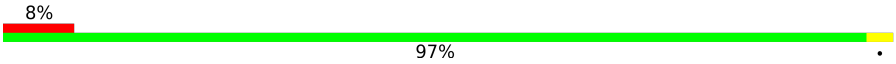

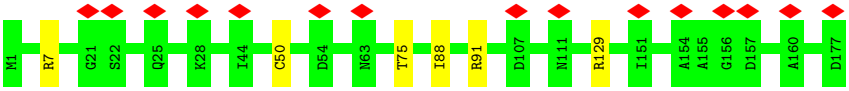

• Molecule 11: R-phycoerythrin beta chain

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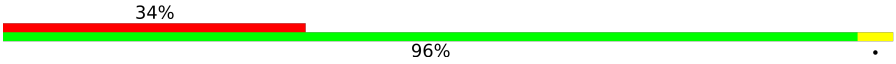

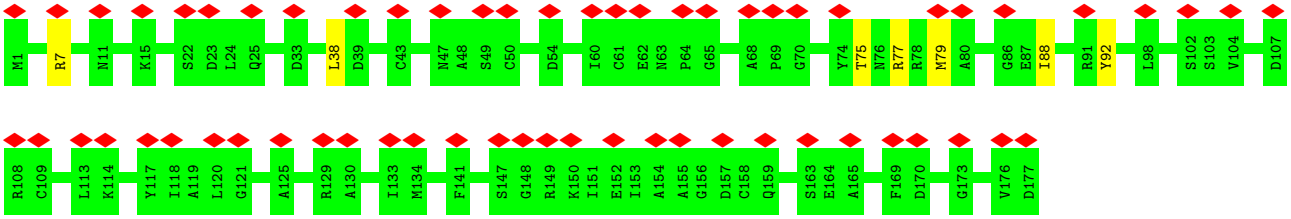

• Molecule 11: R-phycoerythrin beta chain

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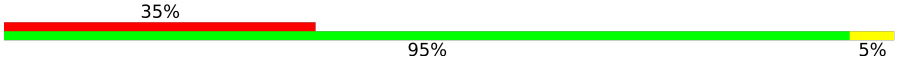
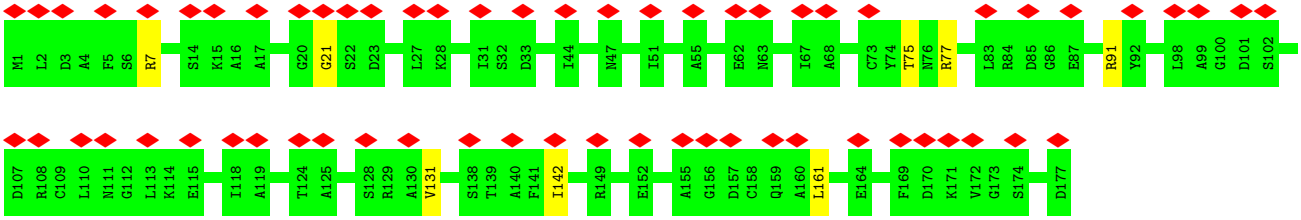
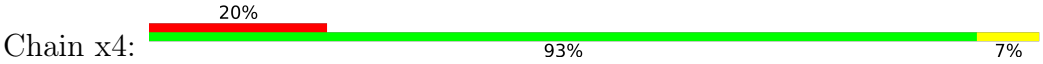
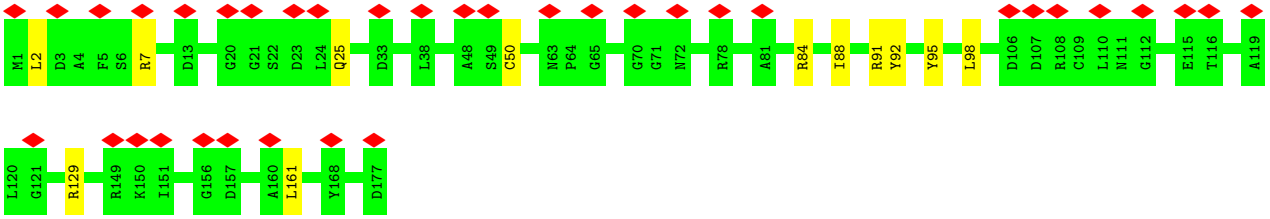


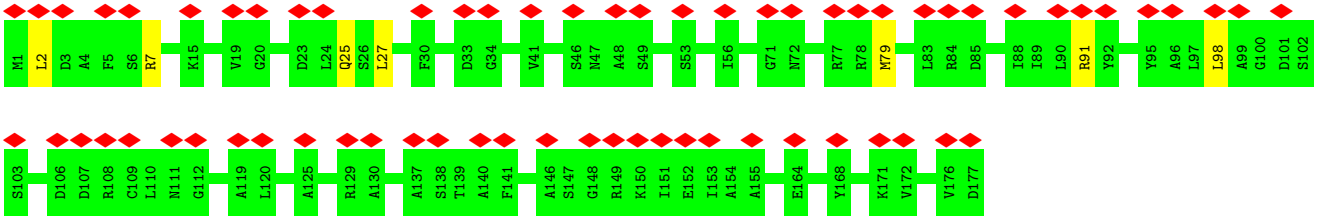


• Molecule 11: R-phycoerythrin beta chain

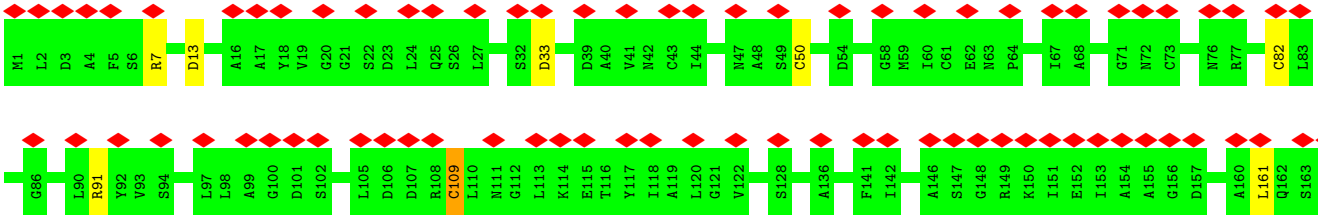




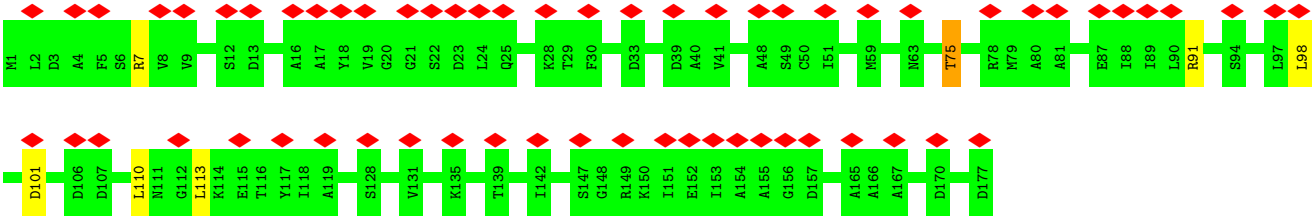
• Molecule 11: R-phycoerythrin beta chain



• Molecule 11: R-phycoerythrin beta chain

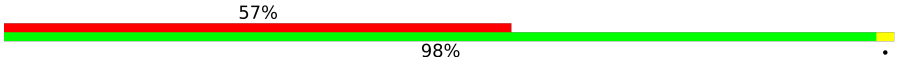


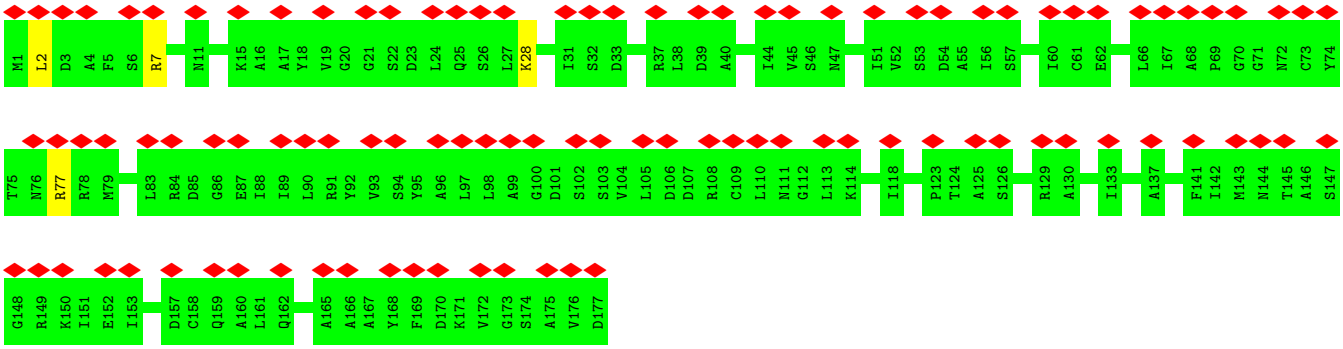
• Molecule 11: R-phycoerythrin beta chain



• Molecule 11: R-phycoerythrin beta chain

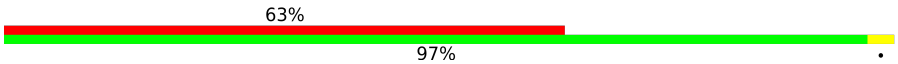
Chain F5:

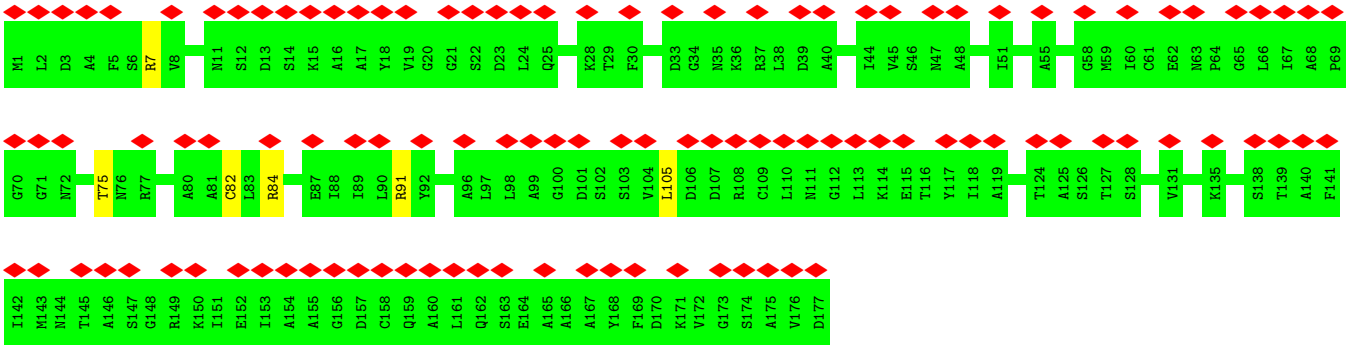




• Molecule 11: R-phycoerythrin beta chain

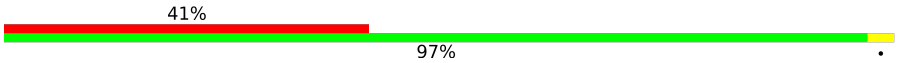
Chain H5:

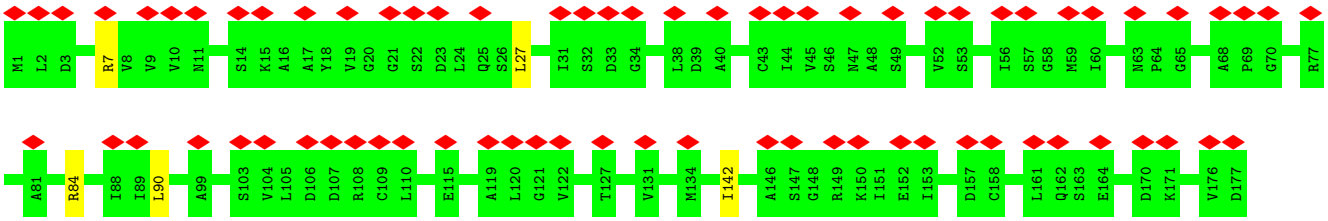




• Molecule 11: R-phycoerythrin beta chain

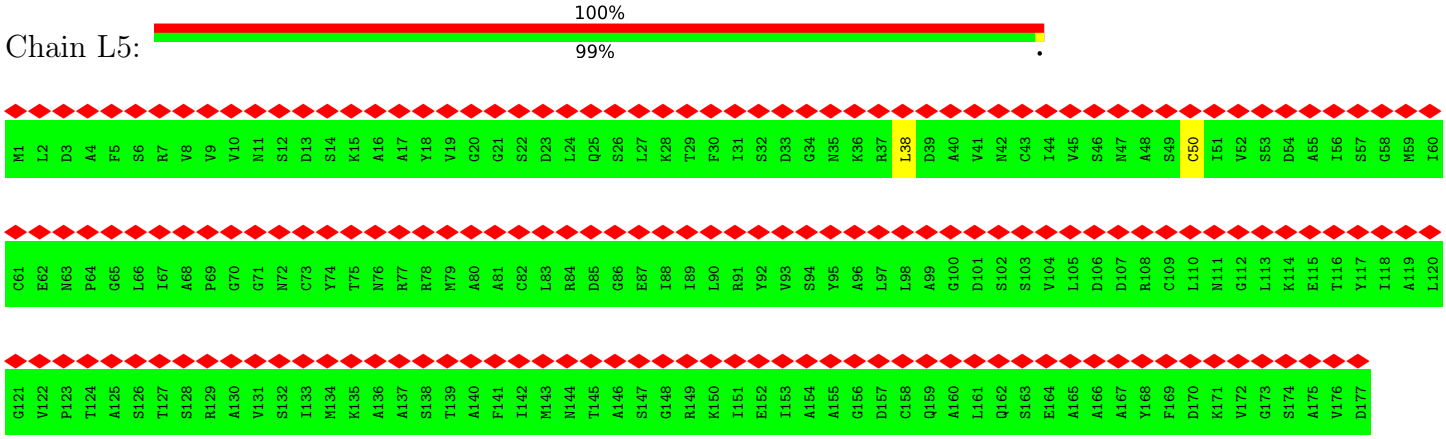
Chain J5:





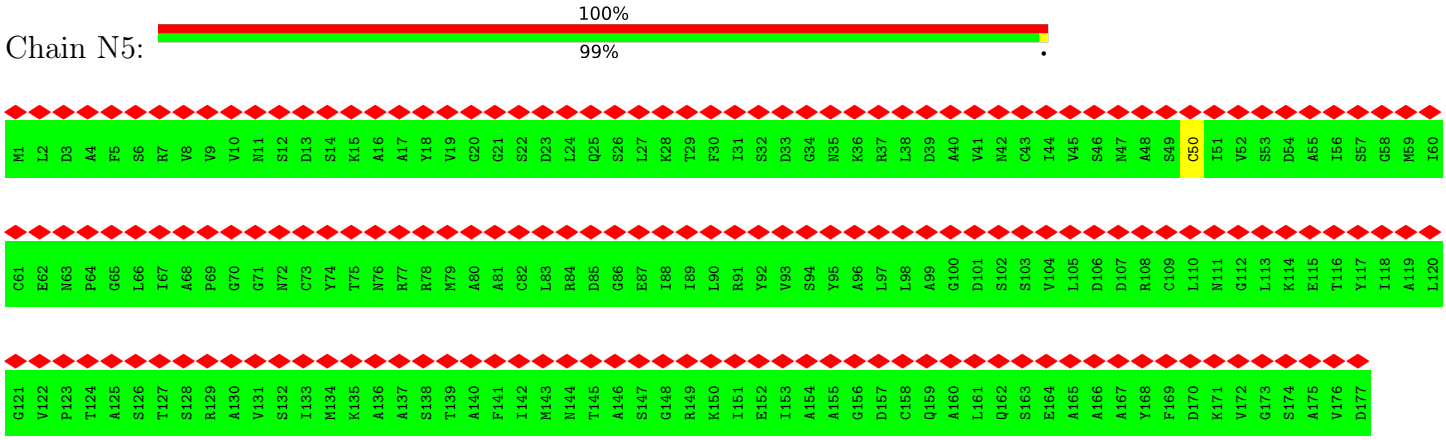
• Molecule 11: R-phycoerythrin beta chain

Chain L5:



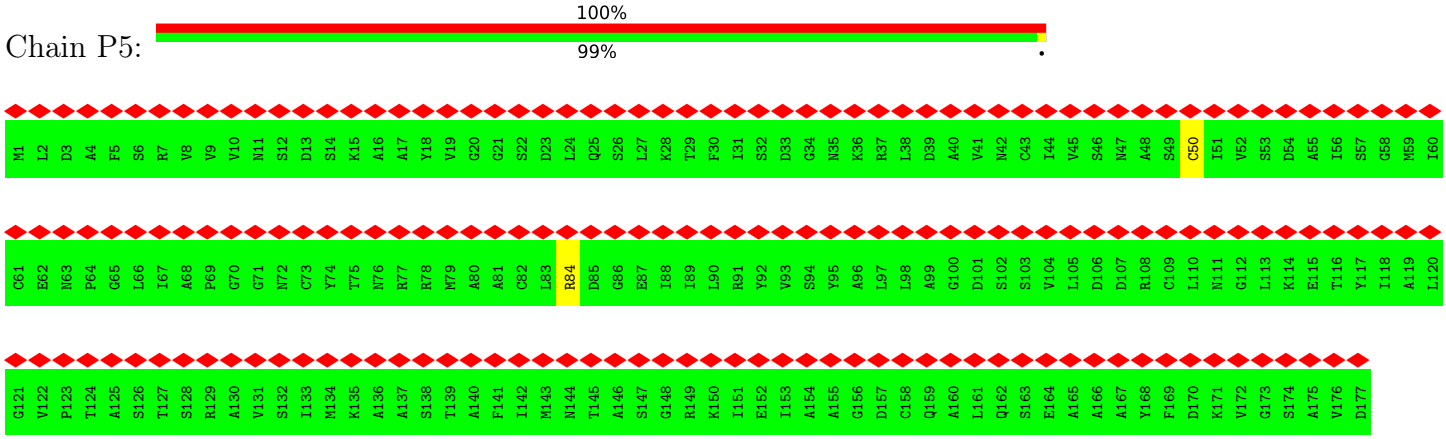
• Molecule 11: R-phycoerythrin beta chain

Chain N5:



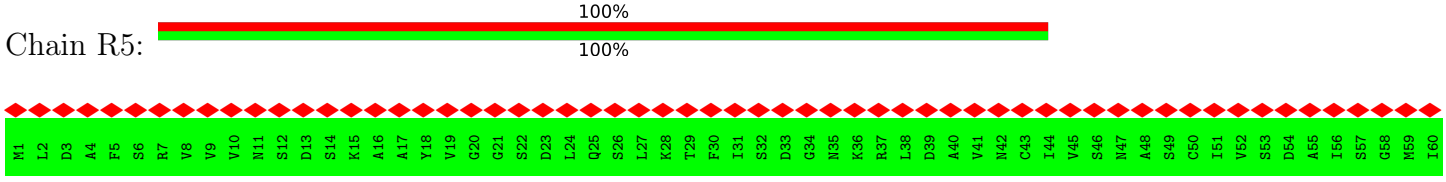
• Molecule 11: R-phycoerythrin beta chain

Chain P5:



• Molecule 11: R-phycoerythrin beta chain

Chain R5:



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G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain T5:

M1 L2 D3 A4 F5 S6 R7 V8 V9 V10 N11 S12 D13 S14 K15 A16 A17 Y18 V19 G20 G21 S22 D23 L24 Q25 S26 L27 K28 T29 F30 I31 S32 D33 G34 N35 K36 R37 L38 D39 A40 V41 N42 C43 I44 V45 S46 N47 A48 S49 C50 I51 V52 S53 D54 A55 I56 S57 G58 M59 I60

C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain V5:

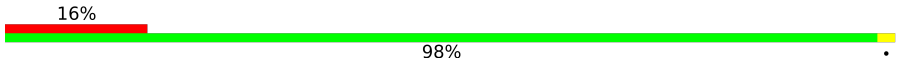
M1 L2 D3 A4 F5 S6 R7 V8 V9 V10 N11 S12 D13 S14 K15 A16 A17 Y18 V19 G20 G21 S22 D23 L24 Q25 S26 L27 K28 T29 F30 I31 S32 D33 G34 N35 K36 R37 L38 D39 A40 V41 N42 C43 I44 V45 S46 N47 A48 S49 C50 I51 V52 S53 D54 A55 I56 S57 G58 M59 I60

C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain n5:



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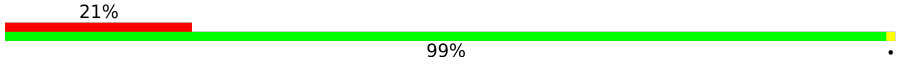
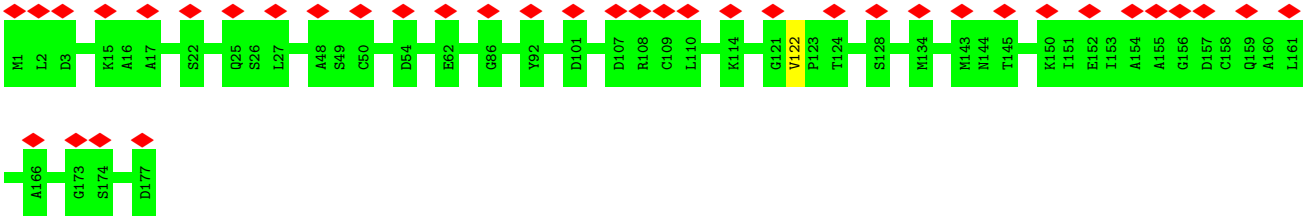
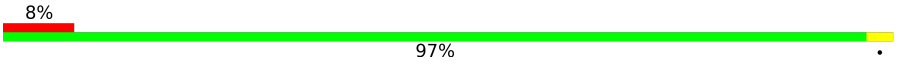
• Molecule 11: R-phycoerythrin beta chain

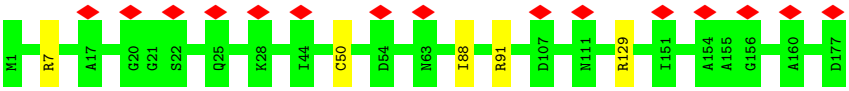
Chain p5:



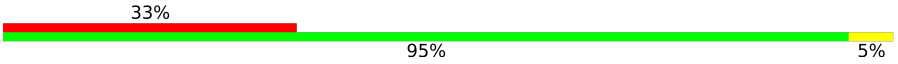


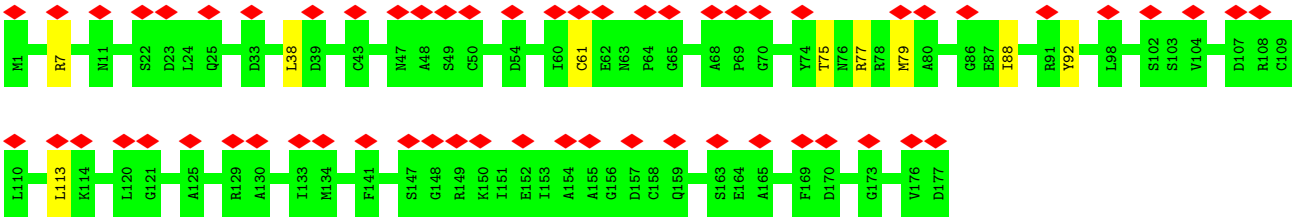
• Molecule 11: R-phycoerythrin beta chain



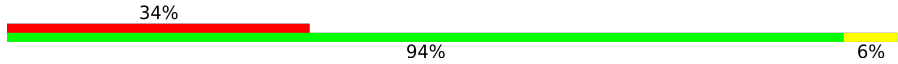


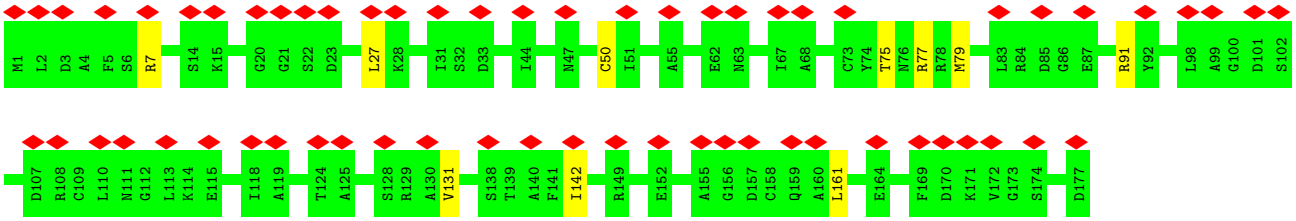
• Molecule 11: R-phycoerythrin beta chain



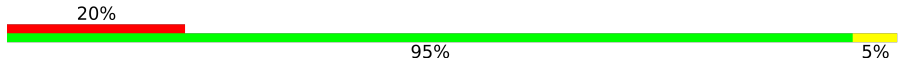


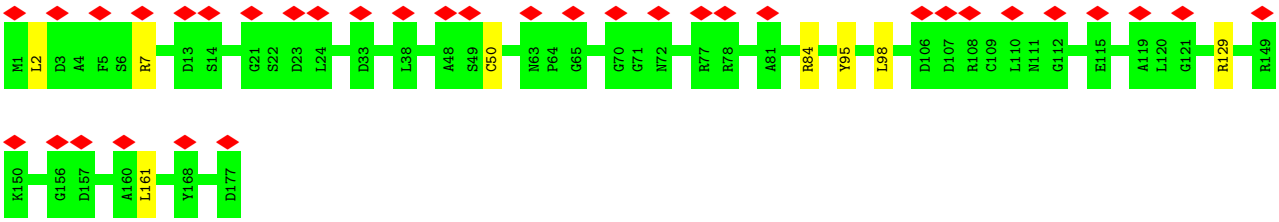
• Molecule 11: R-phycoerythrin beta chain





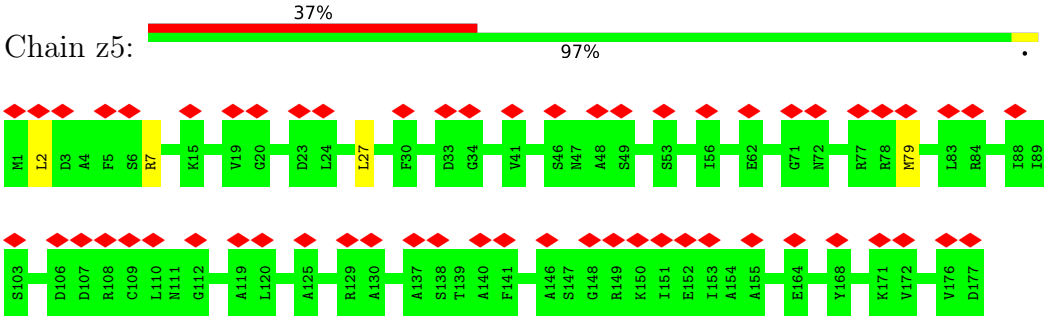
• Molecule 11: R-phycoerythrin beta chain





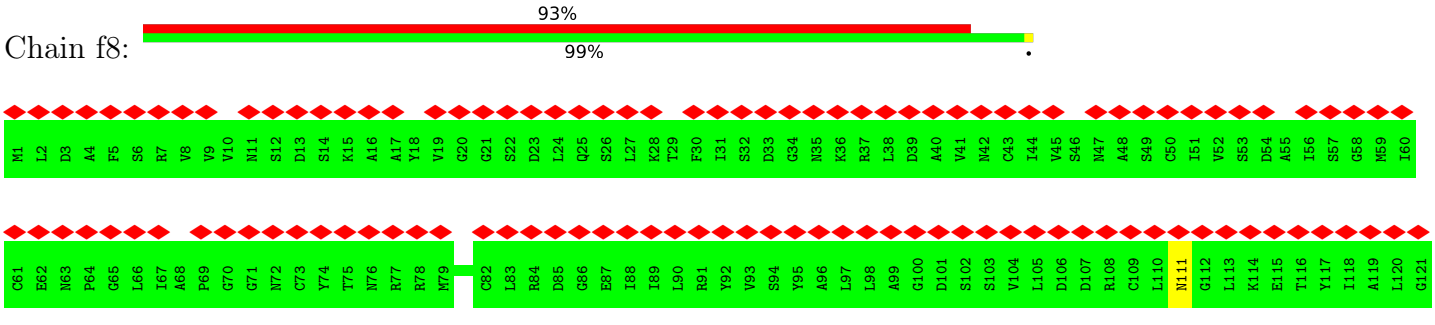
• Molecule 11: R-phycoerythrin beta chain

Chain z5:



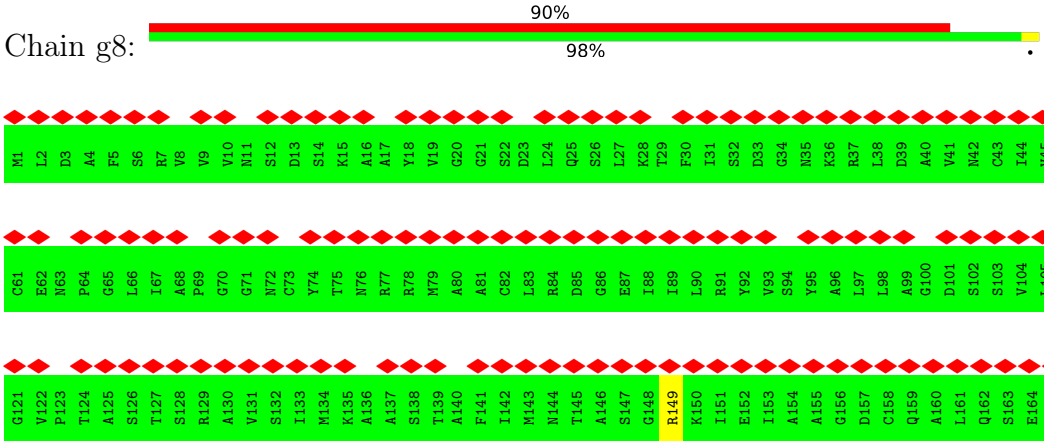
• Molecule 11: R-phycoerythrin beta chain

Chain f8:



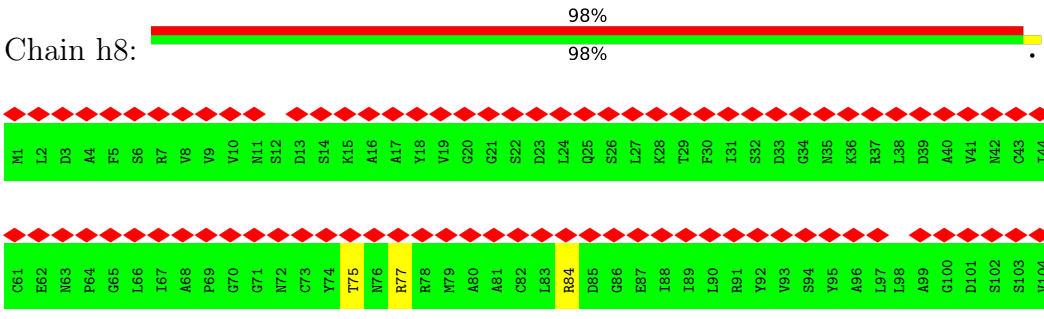
• Molecule 11: R-phycoerythrin beta chain

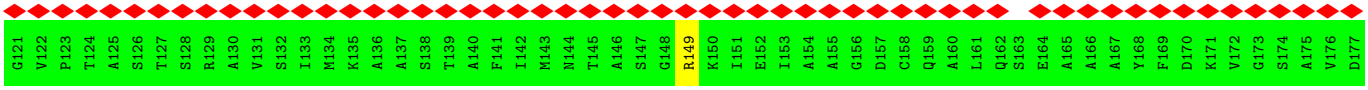
Chain g8:



• Molecule 11: R-phycoerythrin beta chain

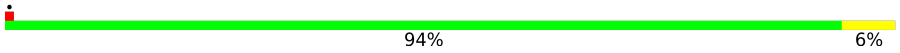
Chain h8:





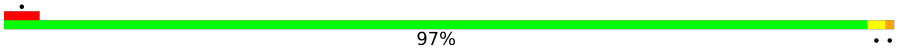
• Molecule 11: R-phycoerythrin beta chain

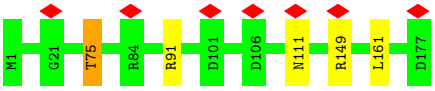
Chain B6:



• Molecule 11: R-phycoerythrin beta chain

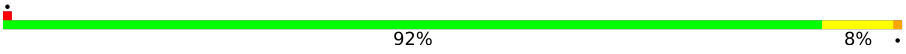
Chain D6:

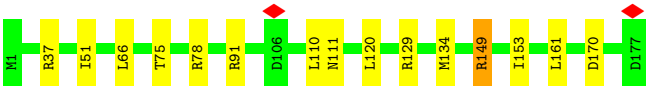




• Molecule 11: R-phycoerythrin beta chain

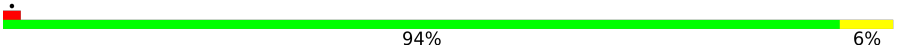
Chain F6:

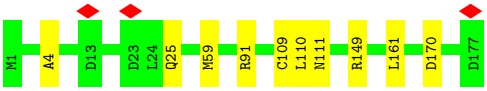




• Molecule 11: R-phycoerythrin beta chain

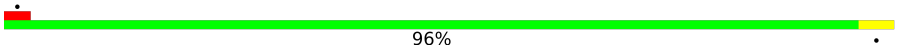
Chain H6:

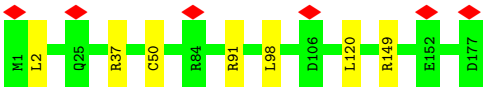




• Molecule 11: R-phycoerythrin beta chain

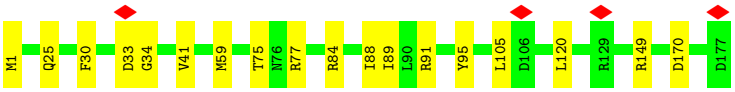
Chain J6:





• Molecule 11: R-phycoerythrin beta chain

Chain L6:



• Molecule 11: R-phycoerythrin beta chain

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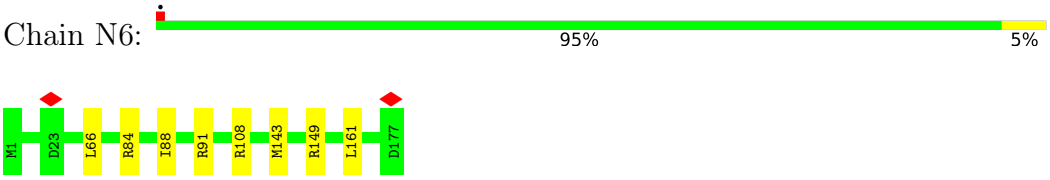

• Molecule 11: R-phycoerythrin beta chain

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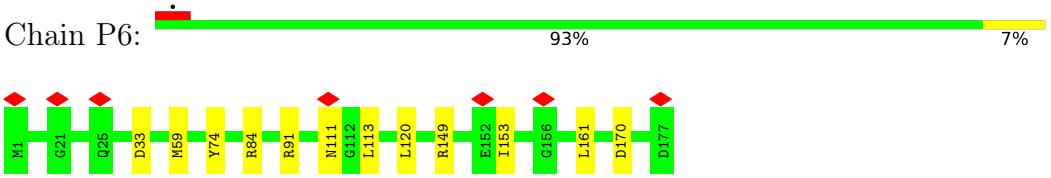
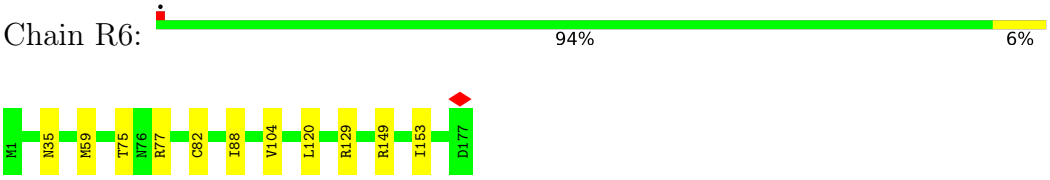


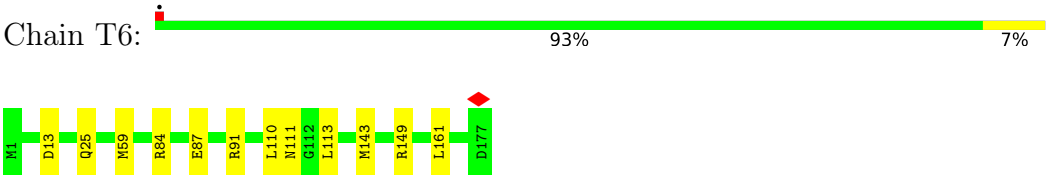
• Molecule 11: R-phycoerythrin beta chain

Chain R6:



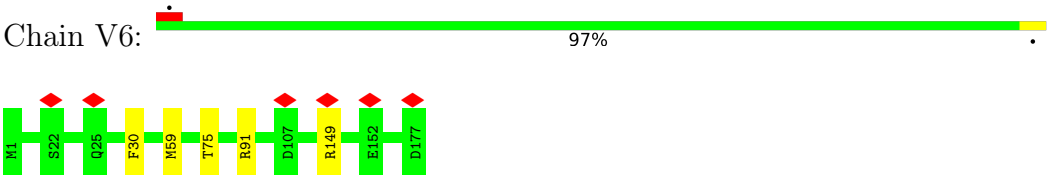
• Molecule 11: R-phycoerythrin beta chain

Chain T6:



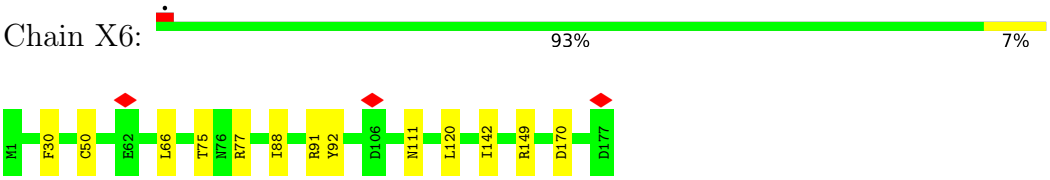
• Molecule 11: R-phycoerythrin beta chain

Chain V6:



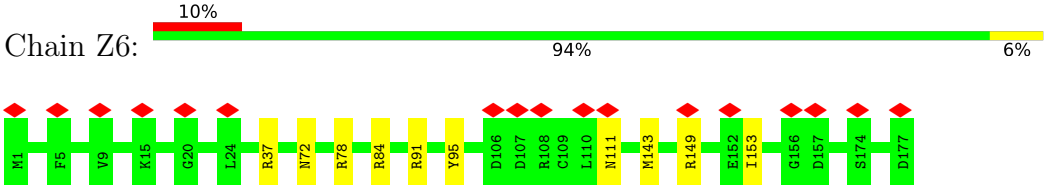
• Molecule 11: R-phycoerythrin beta chain

Chain X6:



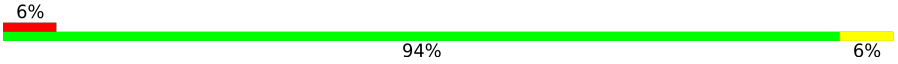
• Molecule 11: R-phycoerythrin beta chain

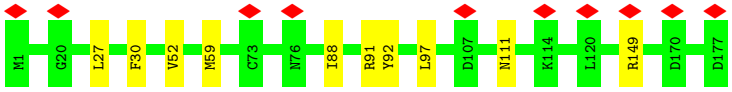
Chain Z6:



• Molecule 11: R-phycoerythrin beta chain

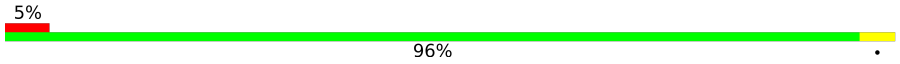
Chain a6:





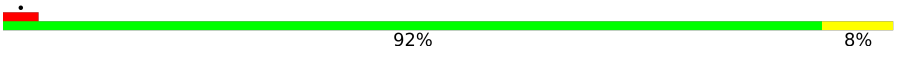
• Molecule 11: R-phycoerythrin beta chain

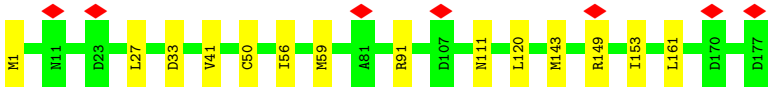
Chain b6:



• Molecule 11: R-phycoerythrin beta chain

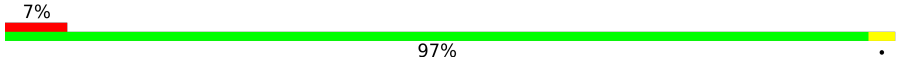
Chain c6:





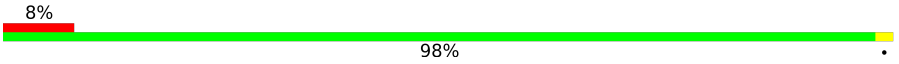
• Molecule 11: R-phycoerythrin beta chain

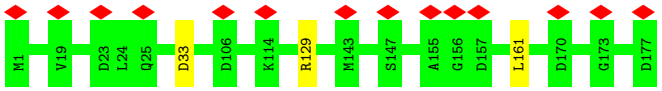
Chain d6:



• Molecule 11: R-phycoerythrin beta chain

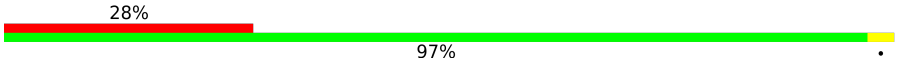
Chain e6:

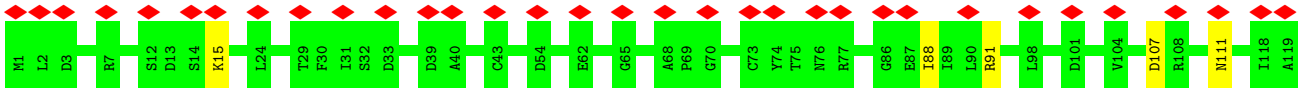


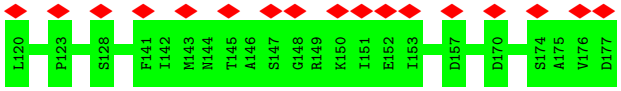


• Molecule 11: R-phycoerythrin beta chain

Chain l6:

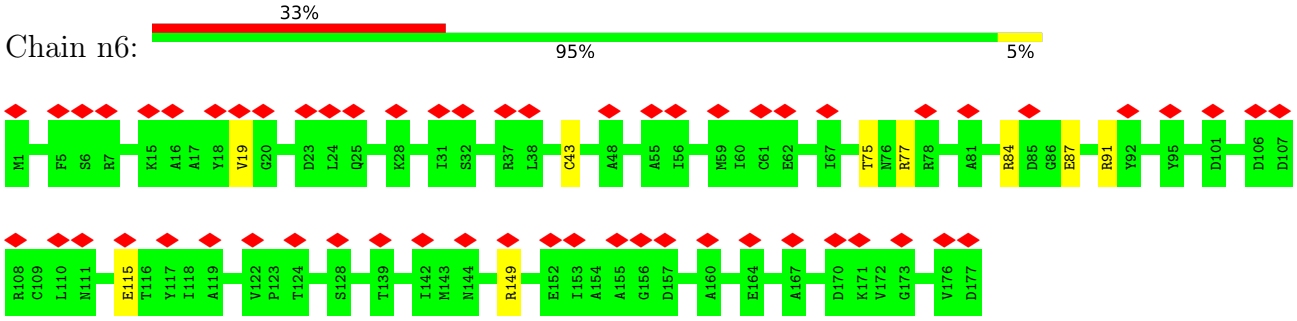






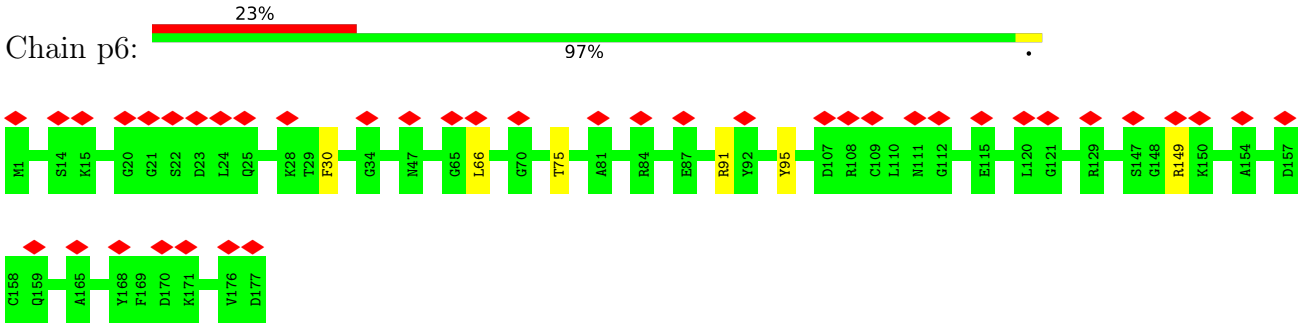
• Molecule 11: R-phycoerythrin beta chain

Chain n6:



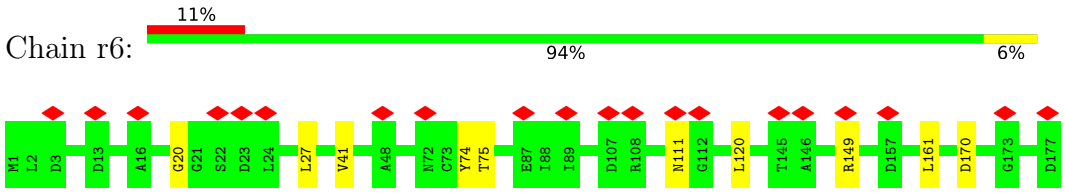
• Molecule 11: R-phycoerythrin beta chain

Chain p6:



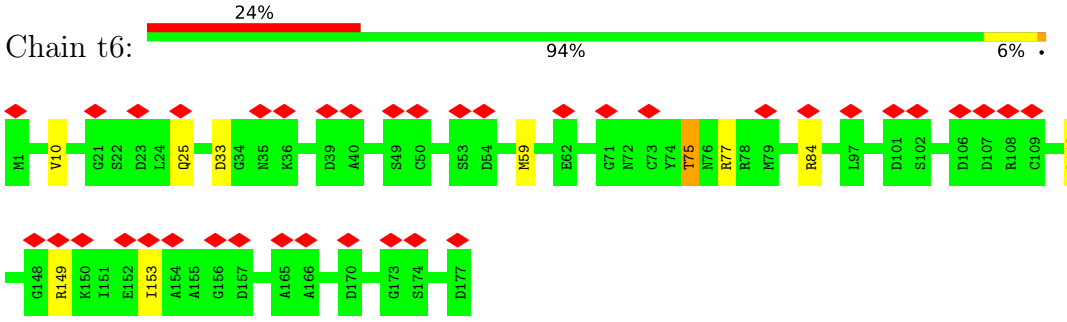
• Molecule 11: R-phycoerythrin beta chain

Chain r6:



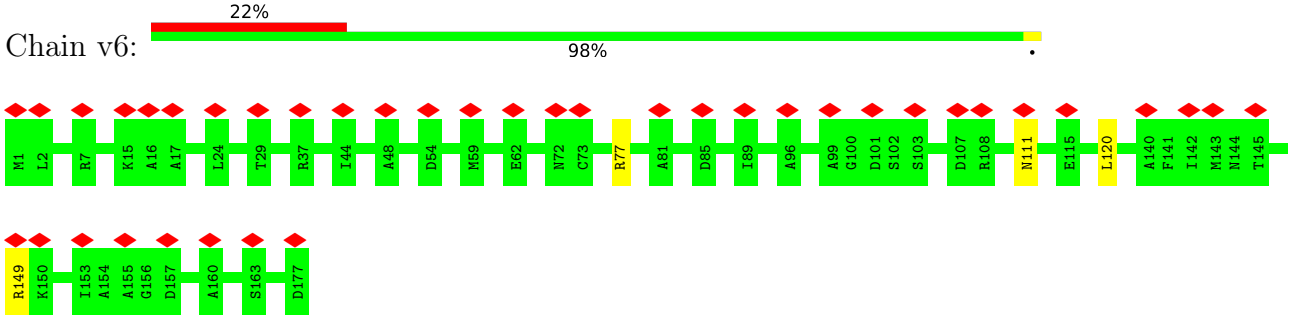
• Molecule 11: R-phycoerythrin beta chain

Chain t6:



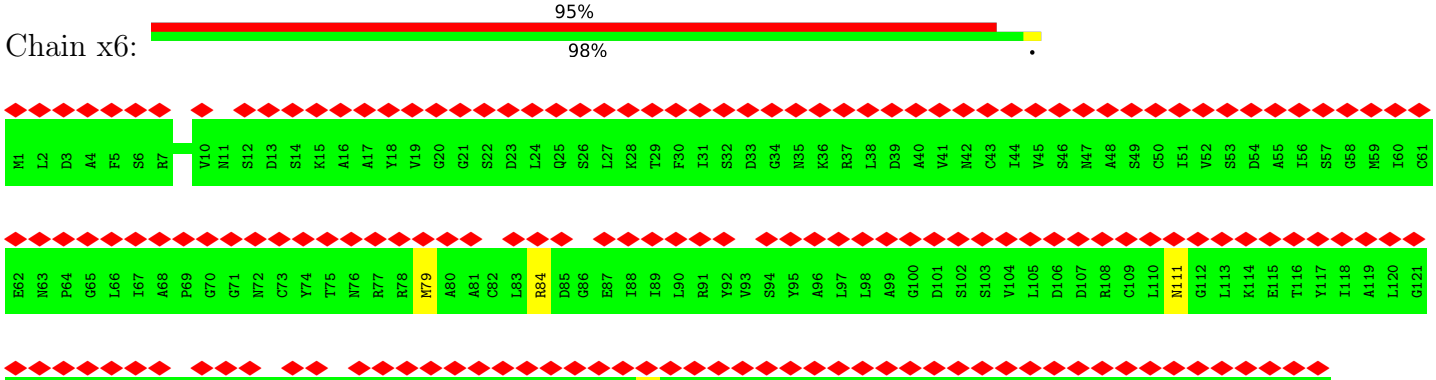
• Molecule 11: R-phycoerythrin beta chain

Chain v6:



• Molecule 11: R-phycoerythrin beta chain

Chain x6:



• Molecule 11: R-phycoerythrin beta chain

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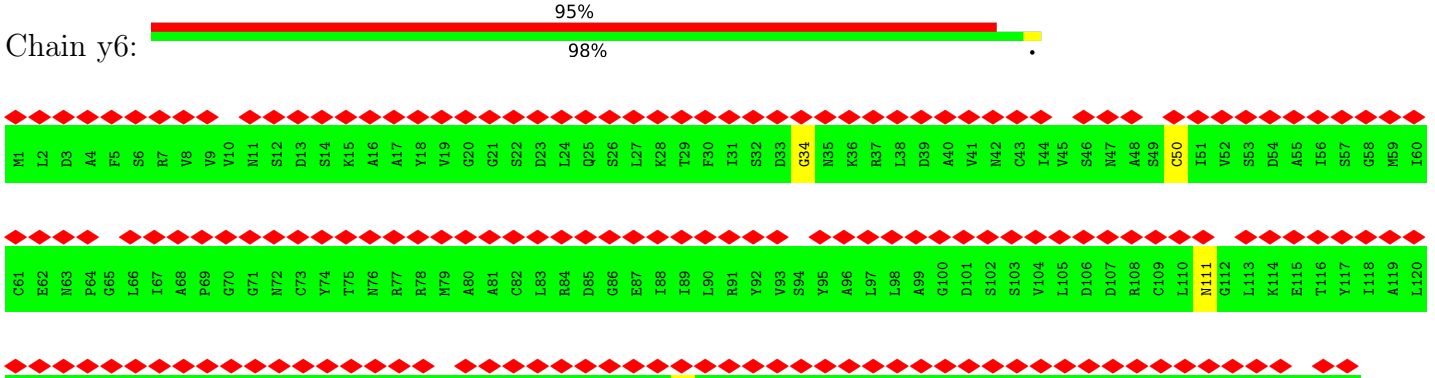

• Molecule 11: R-phycoerythrin beta chain

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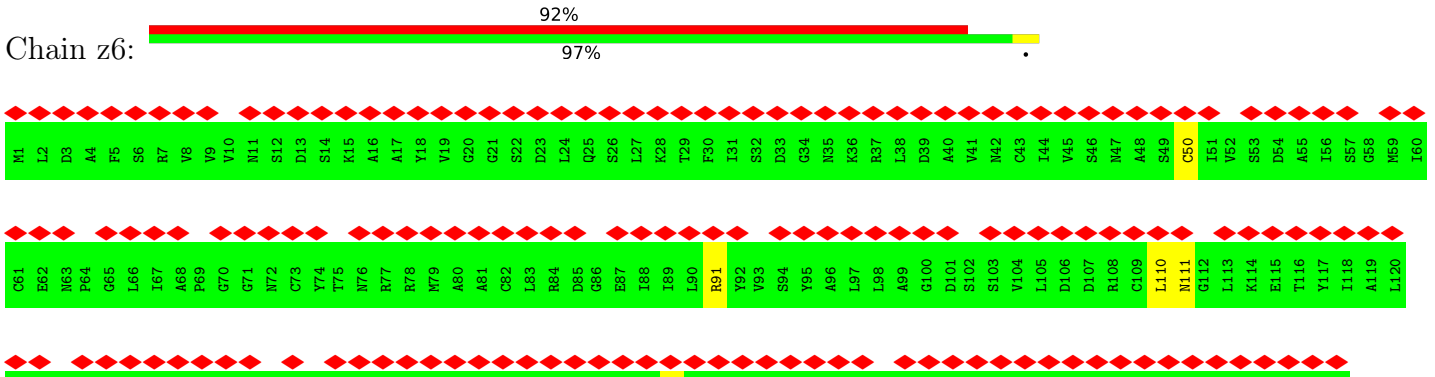
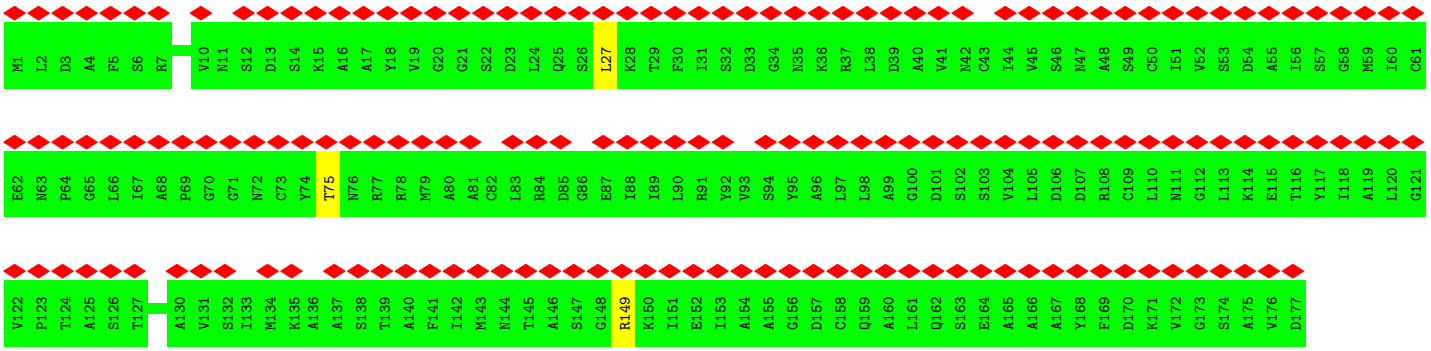


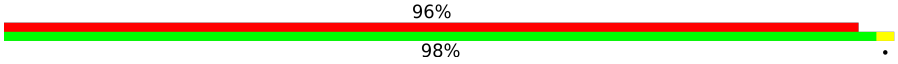
• Molecule 11: R-phycoerythrin beta chain

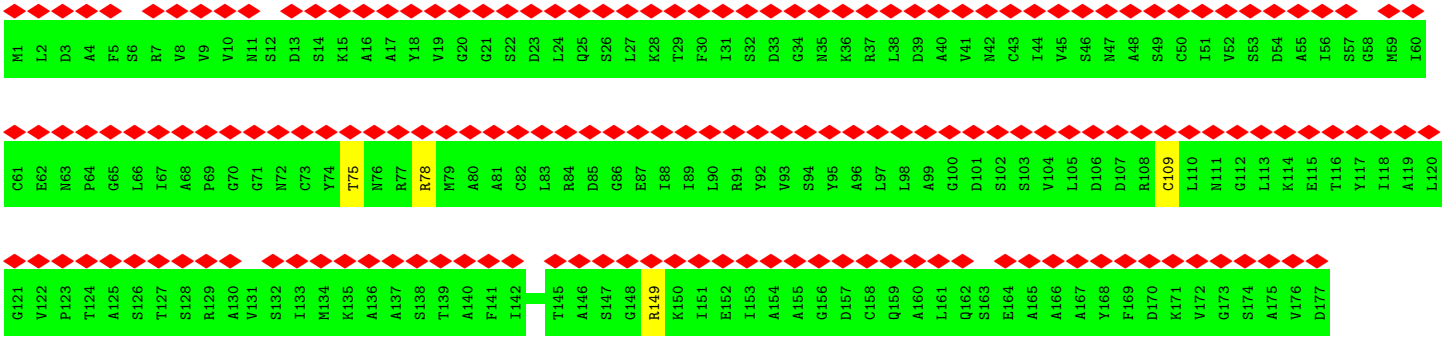
Chain n8:



• Molecule 11: R-phycoerythrin beta chain

Chain o8:





• Molecule 11: R-phycoerythrin beta chain

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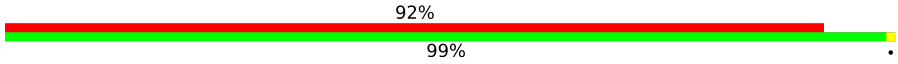
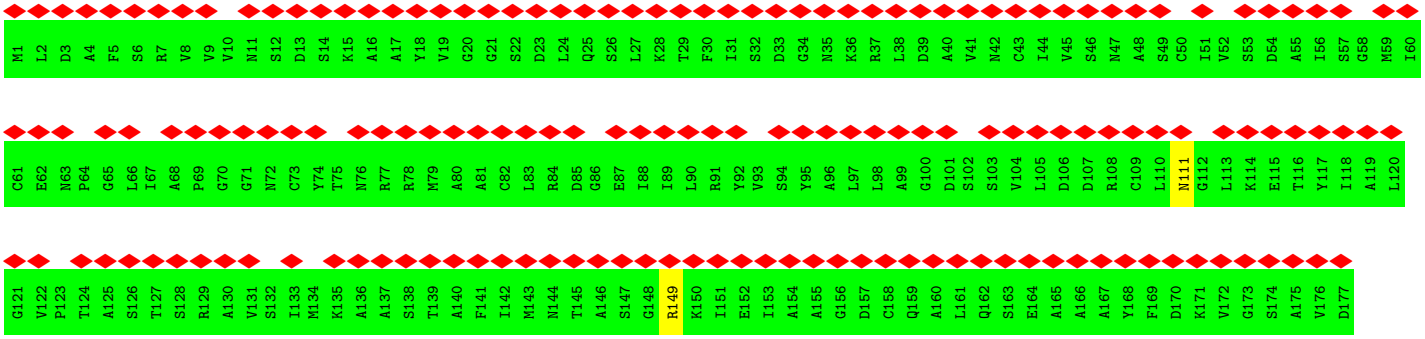
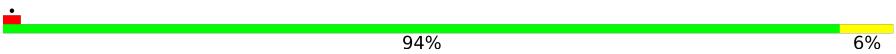
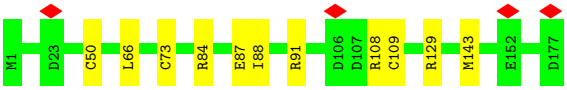




• Molecule 11: R-phycoerythrin beta chain

Chain B7:





• Molecule 11: R-phycoerythrin beta chain

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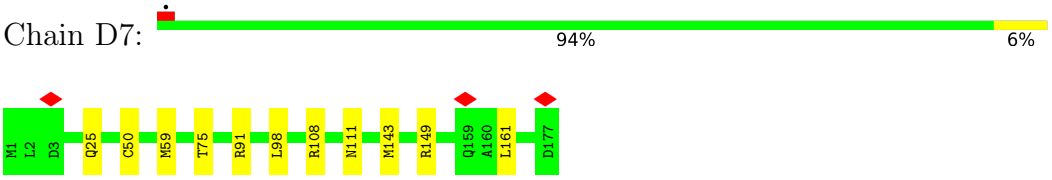

• Molecule 11: R-phycoerythrin beta chain

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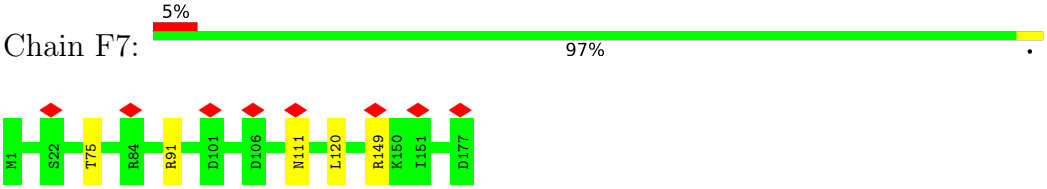

• Molecule 11: R-phycoerythrin beta chain

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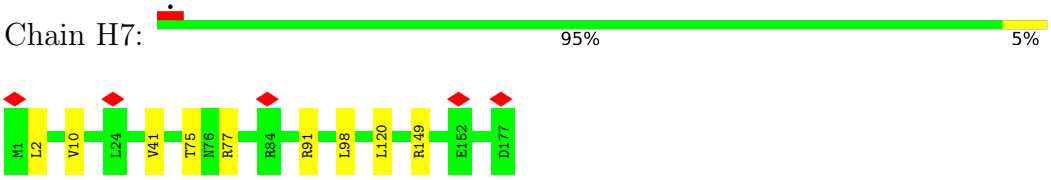
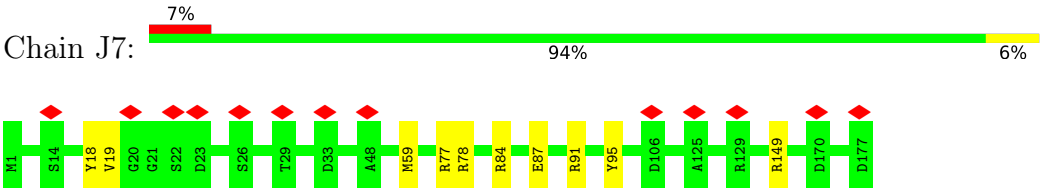


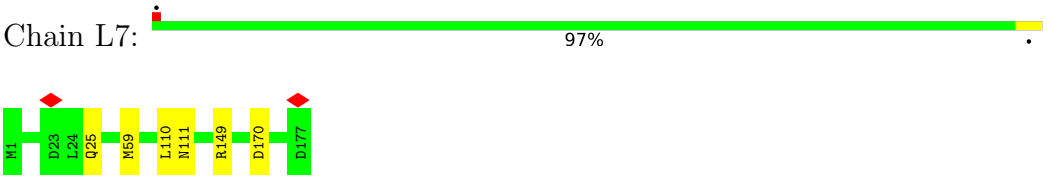
• Molecule 11: R-phycoerythrin beta chain

Chain J7:



• Molecule 11: R-phycoerythrin beta chain

Chain L7:



• Molecule 11: R-phycoerythrin beta chain

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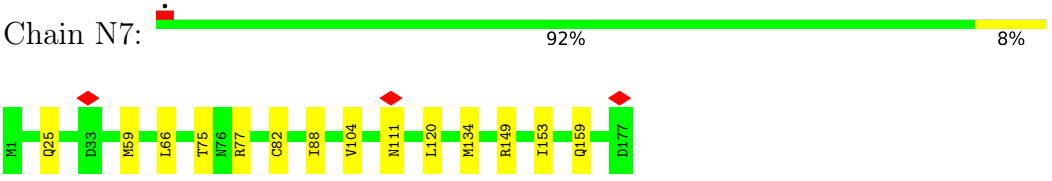

• Molecule 11: R-phycoerythrin beta chain

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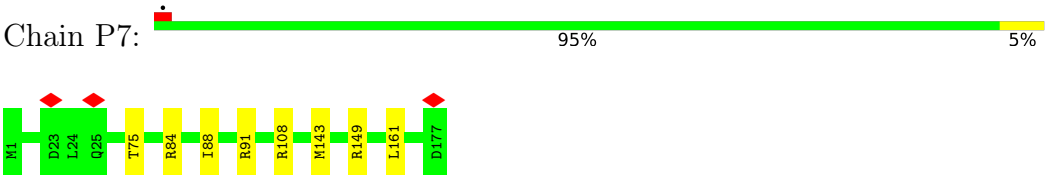

• Molecule 11: R-phycoerythrin beta chain

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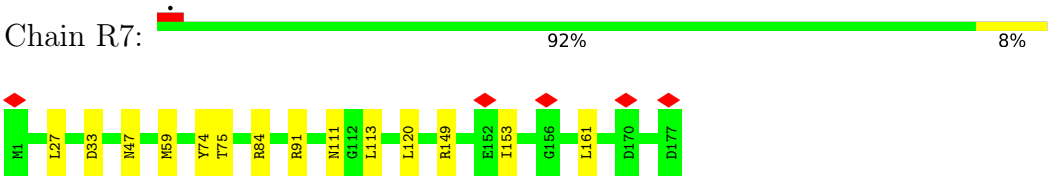
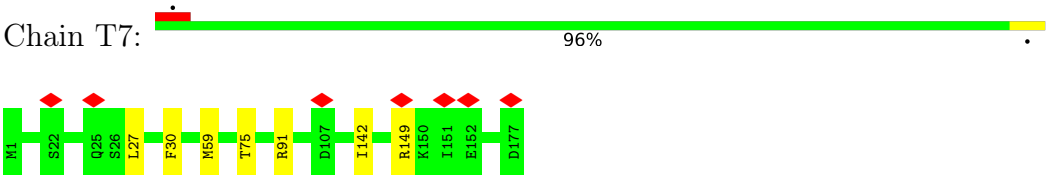


• Molecule 11: R-phycoerythrin beta chain

Chain T7:



• Molecule 11: R-phycoerythrin beta chain

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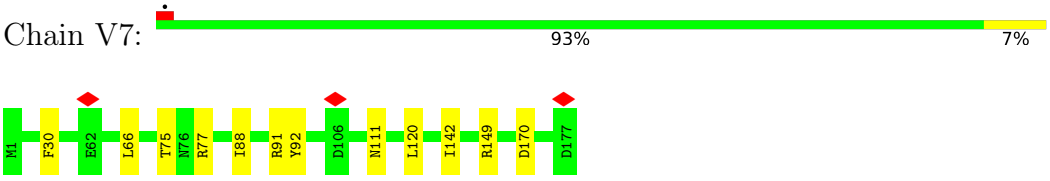
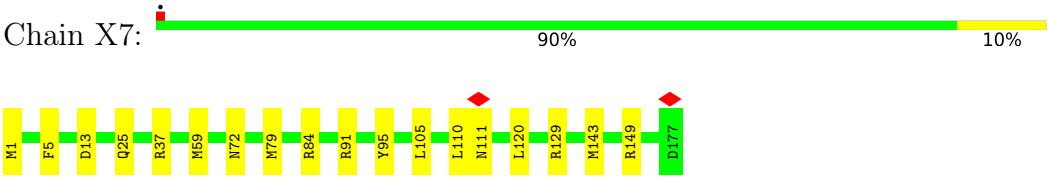


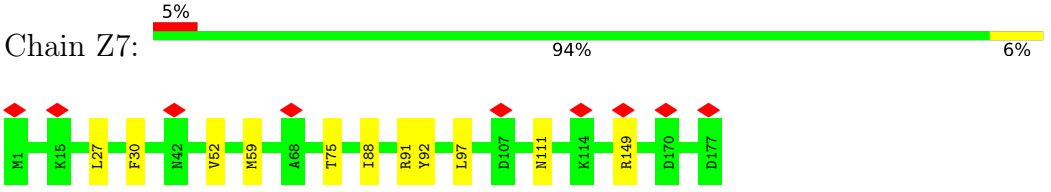
• Molecule 11: R-phycoerythrin beta chain

Chain X7:



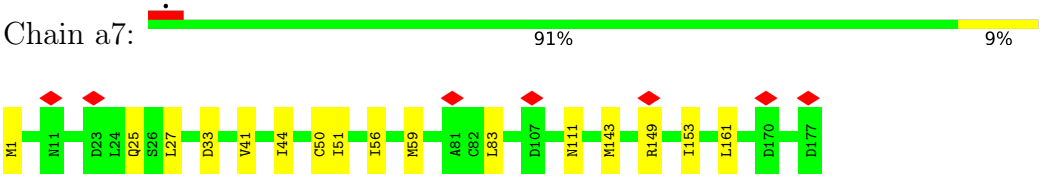
• Molecule 11: R-phycoerythrin beta chain

Chain Z7:



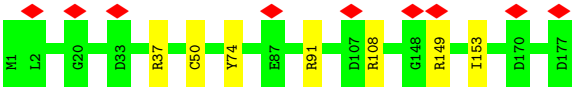
• Molecule 11: R-phycoerythrin beta chain

Chain a7:



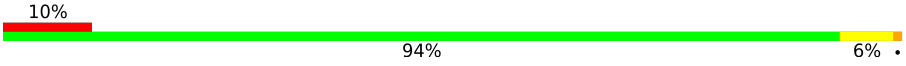
• Molecule 11: R-phycoerythrin beta chain

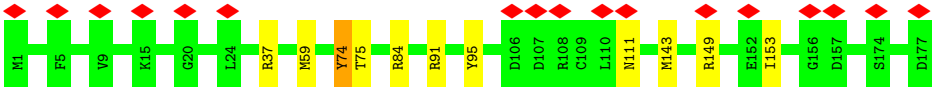
Chain b7:



• Molecule 11: R-phycoerythrin beta chain

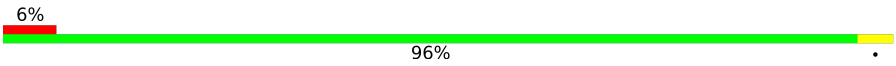
Chain c7:

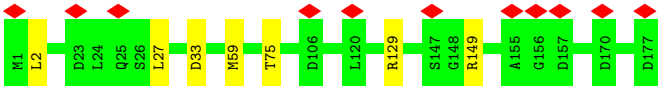




• Molecule 11: R-phycoerythrin beta chain

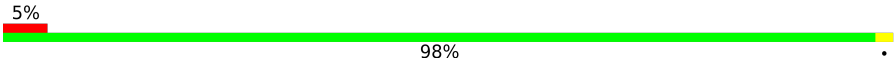
Chain d7:

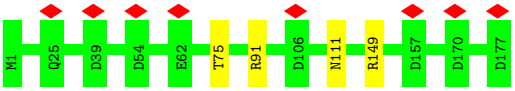




• Molecule 11: R-phycoerythrin beta chain

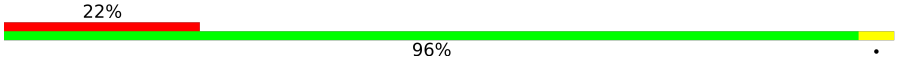
Chain e7:

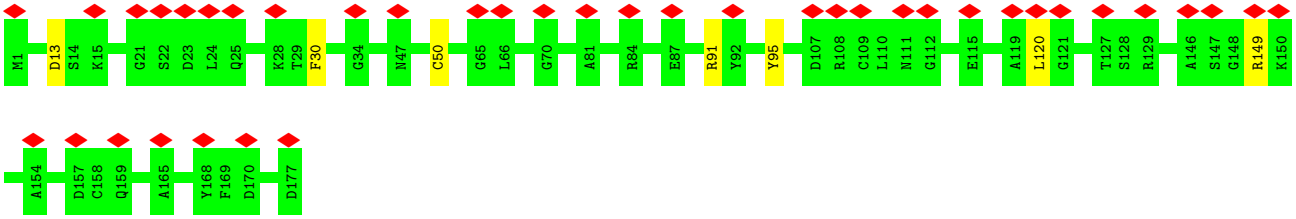




• Molecule 11: R-phycoerythrin beta chain

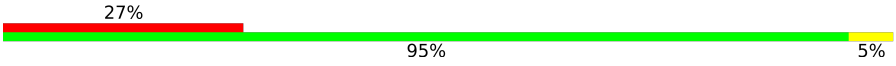
Chain l7:

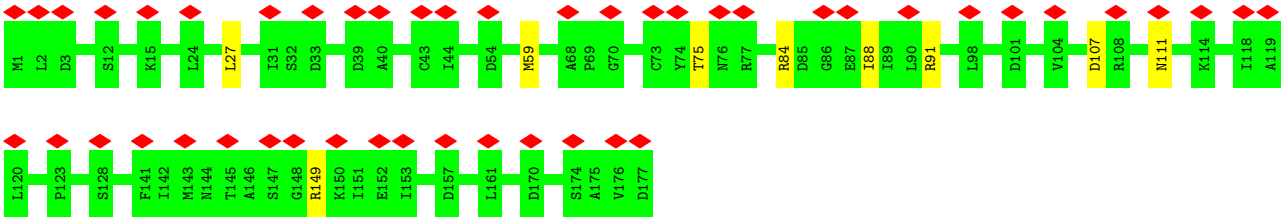




• Molecule 11: R-phycoerythrin beta chain

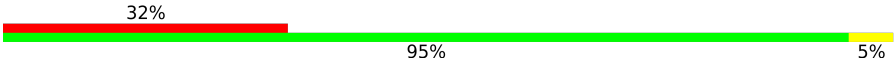
Chain n7:

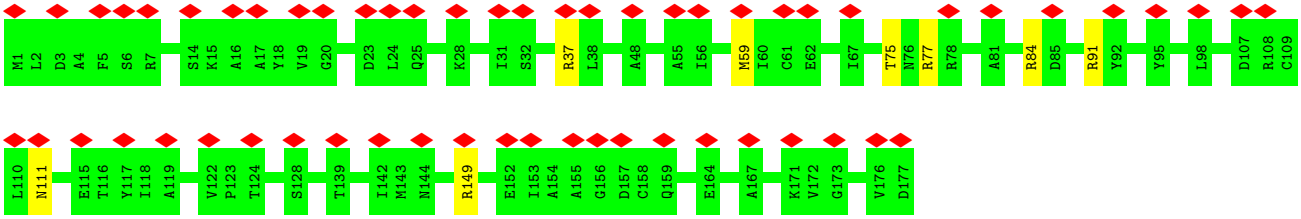




• Molecule 11: R-phycoerythrin beta chain

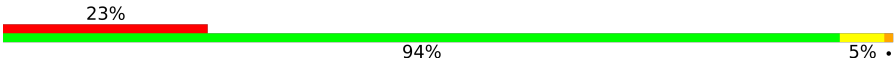
Chain p7:

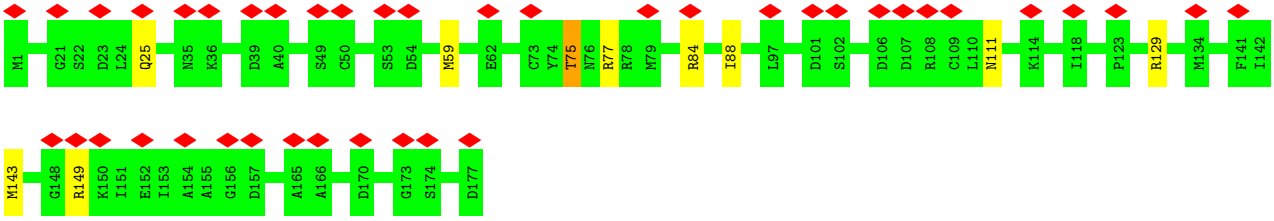




• Molecule 11: R-phycoerythrin beta chain

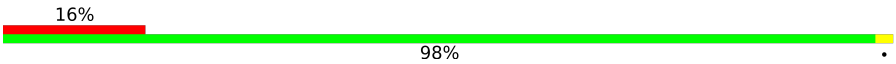
Chain r7:

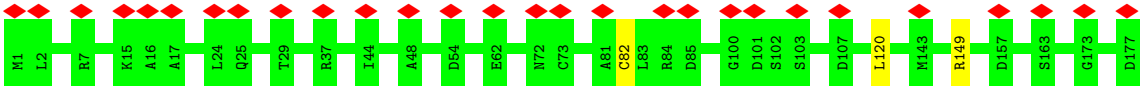




• Molecule 11: R-phycoerythrin beta chain

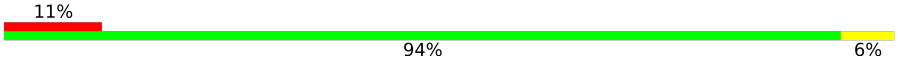
Chain t7:

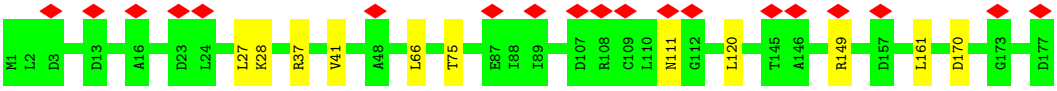




• Molecule 11: R-phycoerythrin beta chain

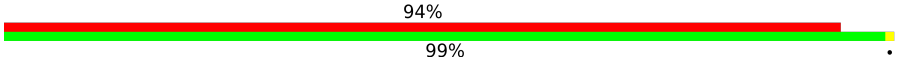
Chain v7:

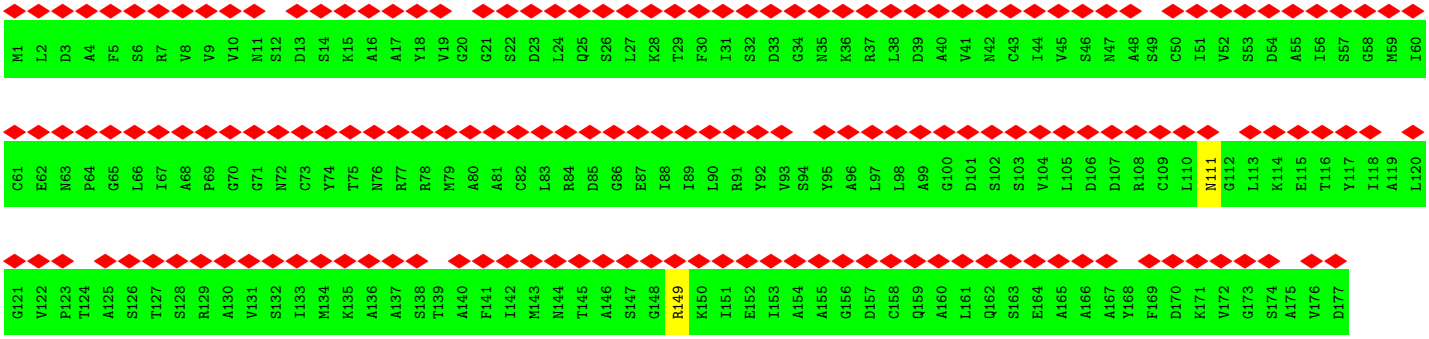




• Molecule 11: R-phycoerythrin beta chain

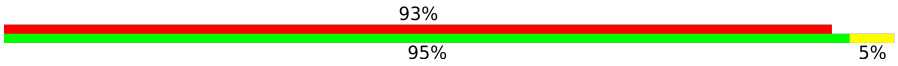
Chain x7:

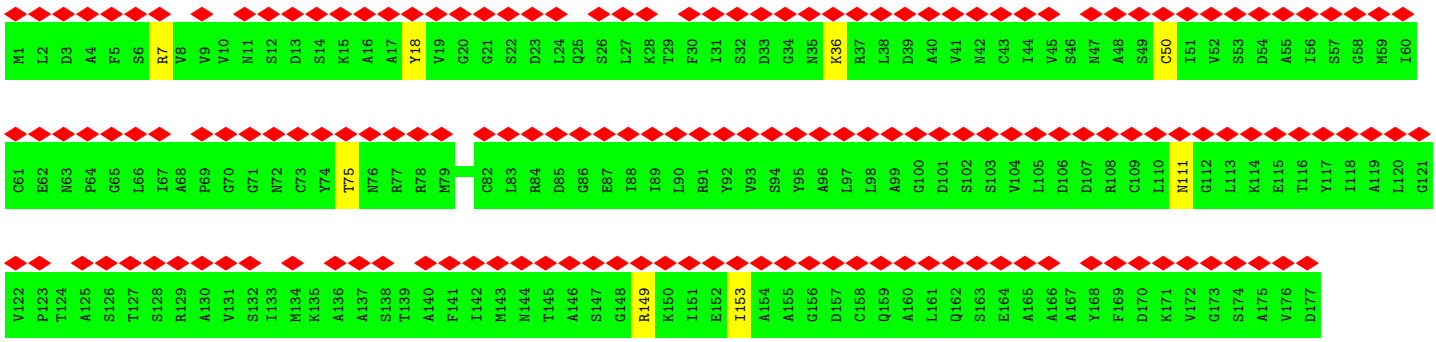




• Molecule 11: R-phycoerythrin beta chain

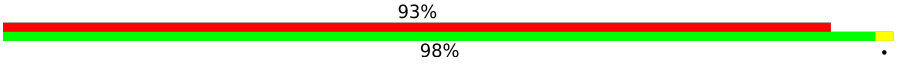
Chain y7:

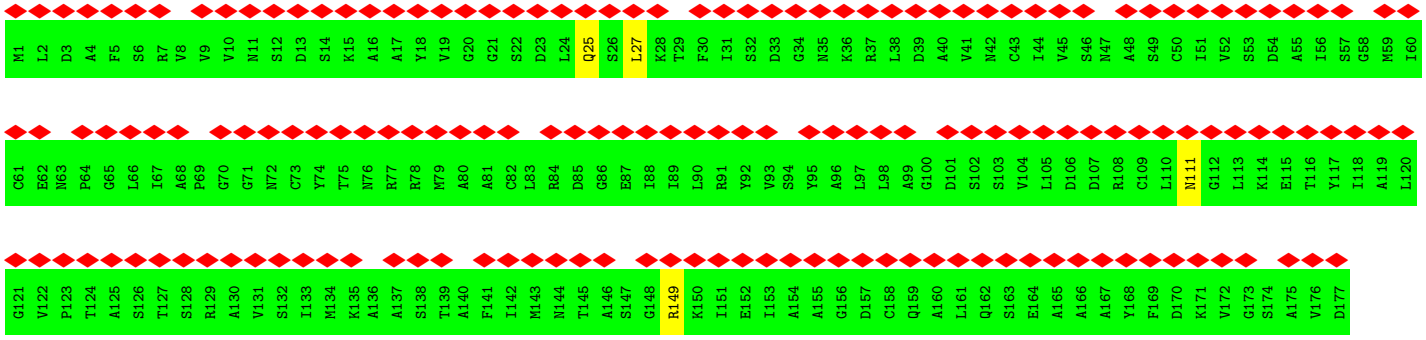




• Molecule 11: R-phycoerythrin beta chain

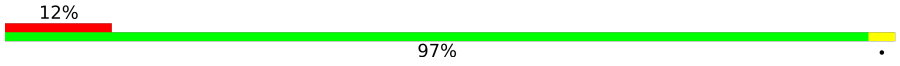
Chain z7:

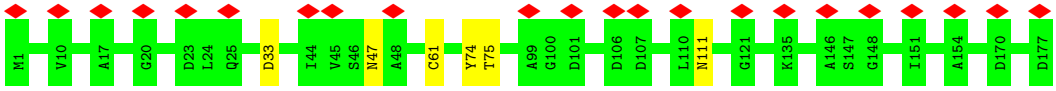




• Molecule 11: R-phycoerythrin beta chain

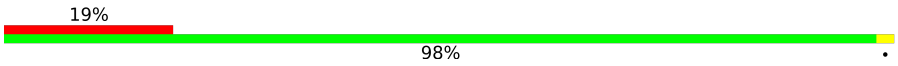
Chain w8:

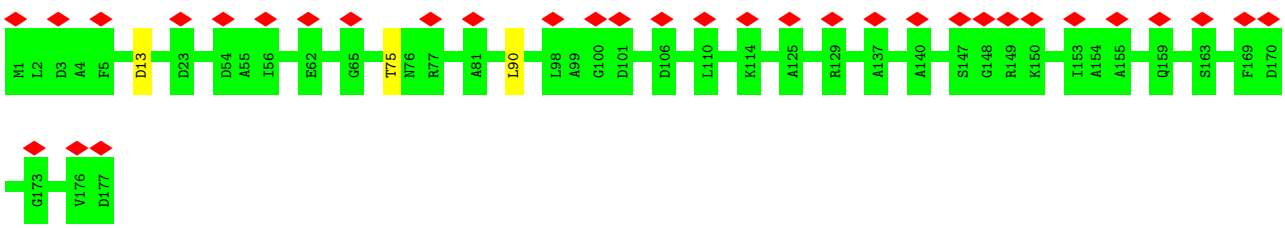




• Molecule 11: R-phycoerythrin beta chain

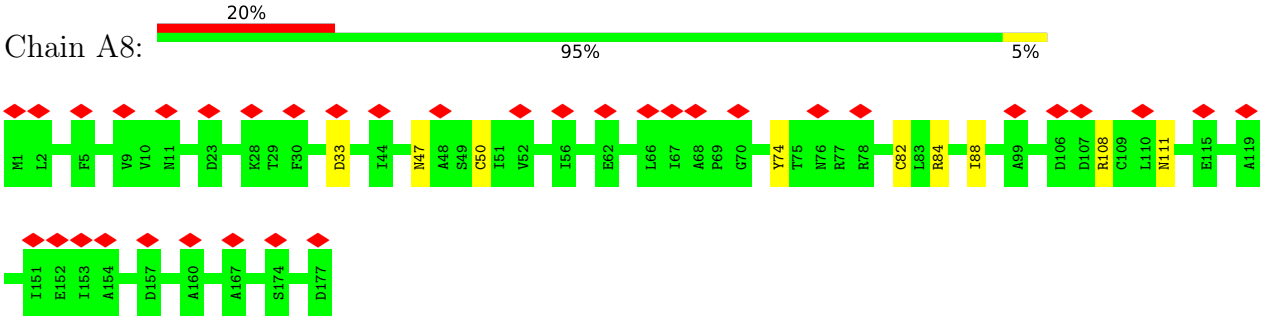
Chain y8:





• Molecule 11: R-phycoerythrin beta chain

Chain A8:



• Molecule 11: R-phycoerythrin beta chain

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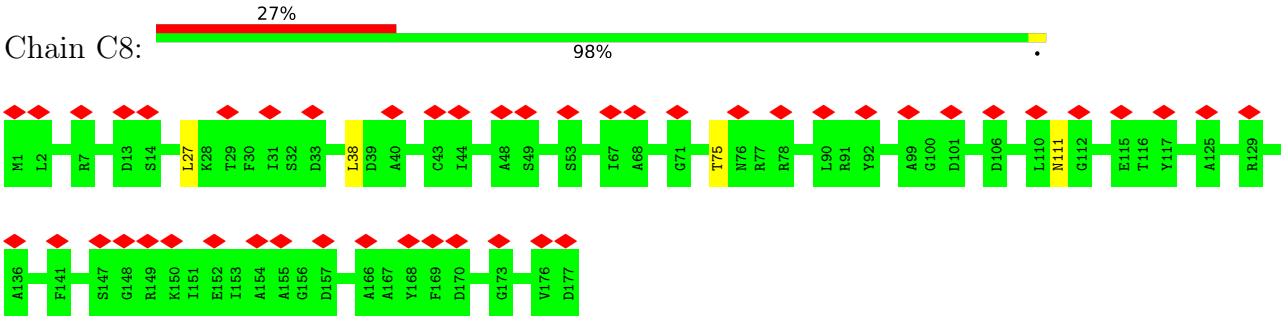
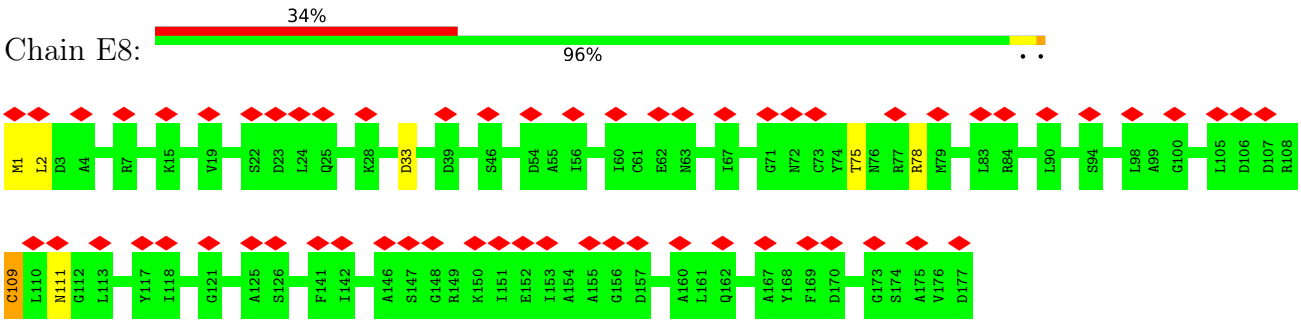


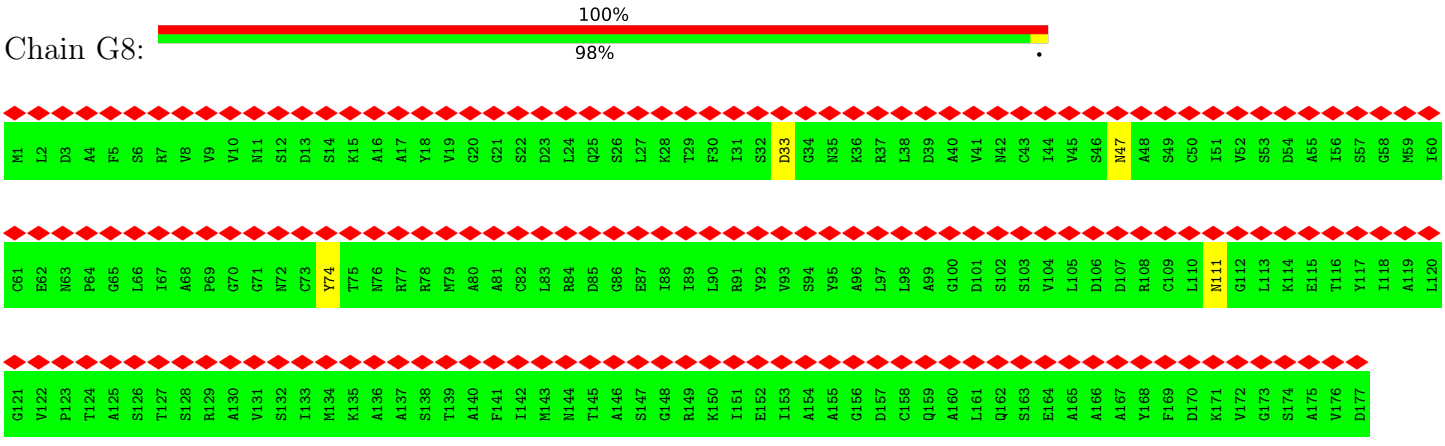
• Molecule 11: R-phycoerythrin beta chain

Chain E8:



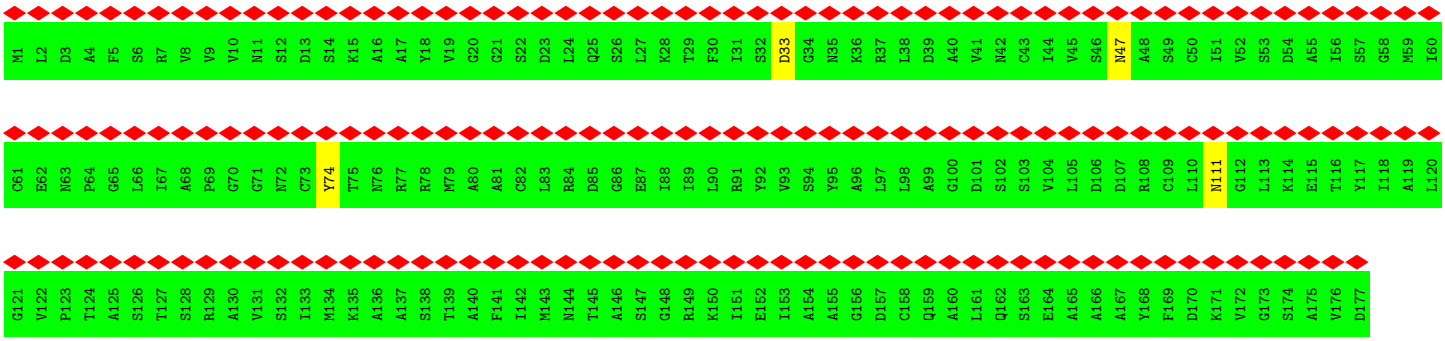
• Molecule 11: R-phycoerythrin beta chain

Chain G8:



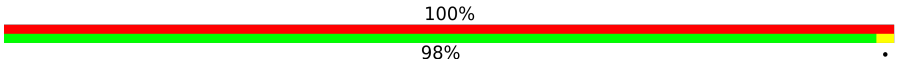
• Molecule 11: R-phycoerythrin beta chain

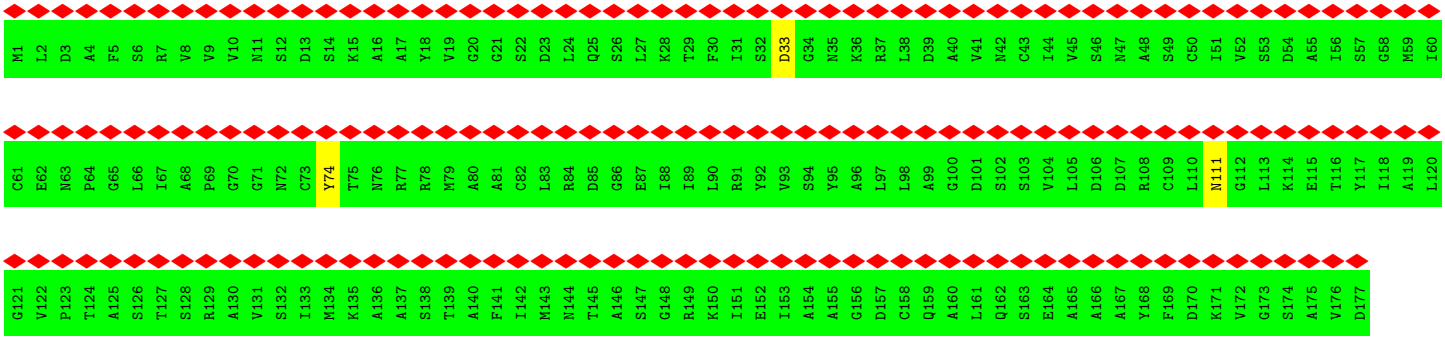
Chain I8:



• Molecule 11: R-phycoerythrin beta chain

Chain K8:





• Molecule 11: R-phycoerythrin beta chain

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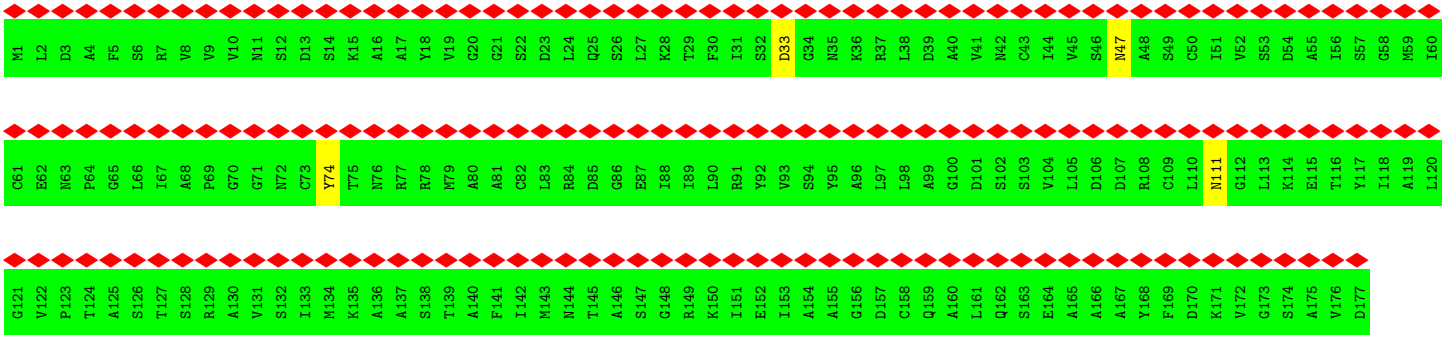
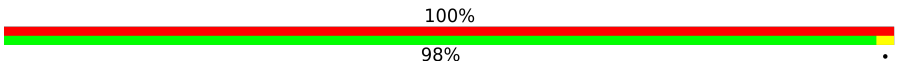
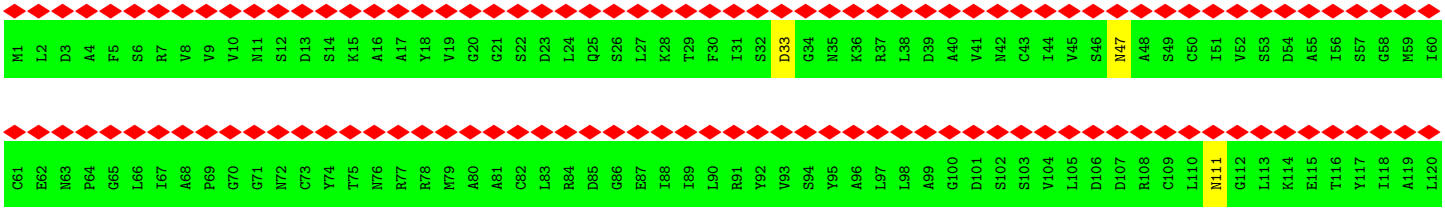
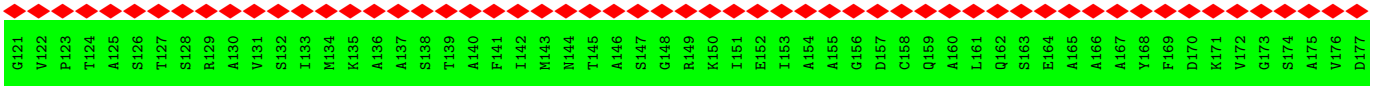


• Molecule 11: R-phycoerythrin beta chain

Chain O8:

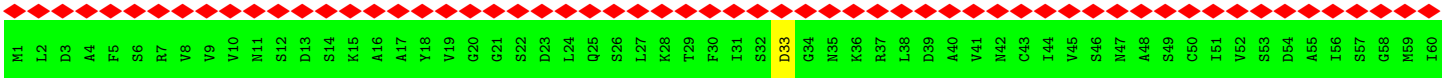


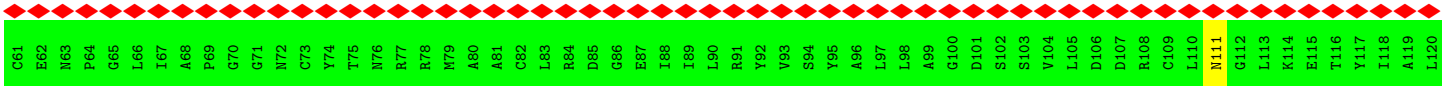


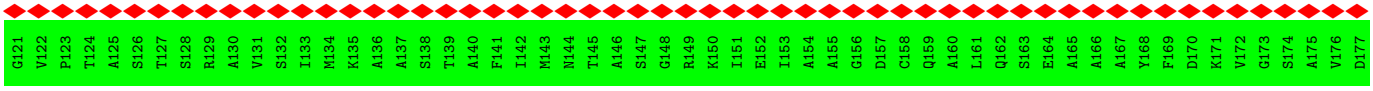


• Molecule 11: R-phycoerythrin beta chain

Chain Q8:

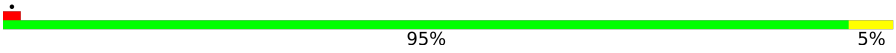


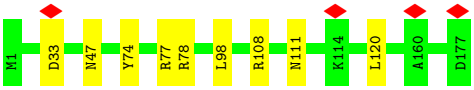




• Molecule 11: R-phycoerythrin beta chain

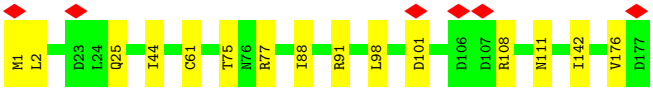
Chain n9:





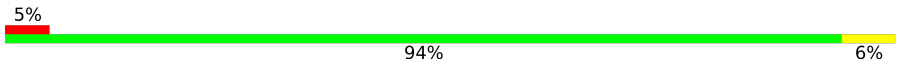
• Molecule 11: R-phycoerythrin beta chain

Chain p9:



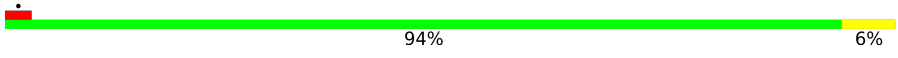
• Molecule 11: R-phycoerythrin beta chain

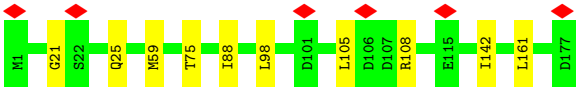
Chain r9:



• Molecule 11: R-phycoerythrin beta chain

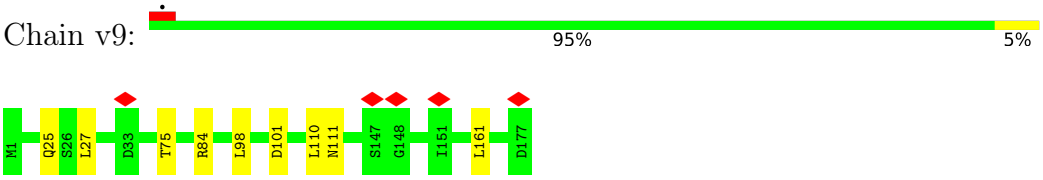
Chain t9:





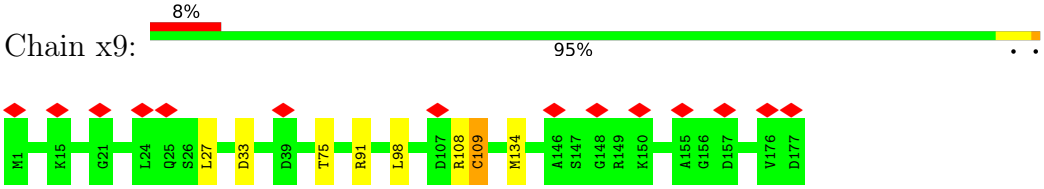
• Molecule 11: R-phycoerythrin beta chain

Chain v9:



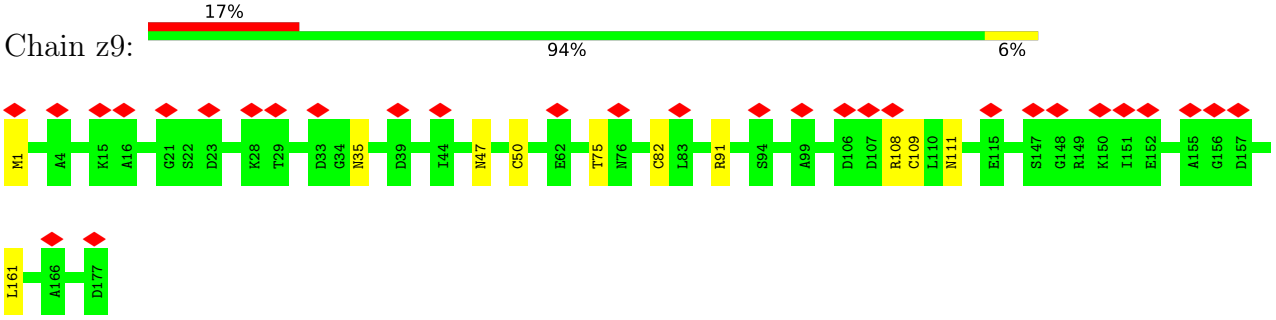
• Molecule 11: R-phycoerythrin beta chain

Chain x9:



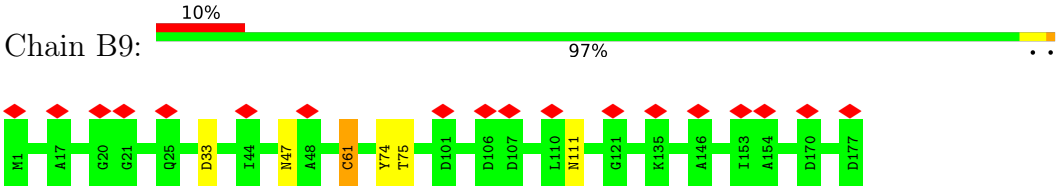
• Molecule 11: R-phycoerythrin beta chain

Chain z9:



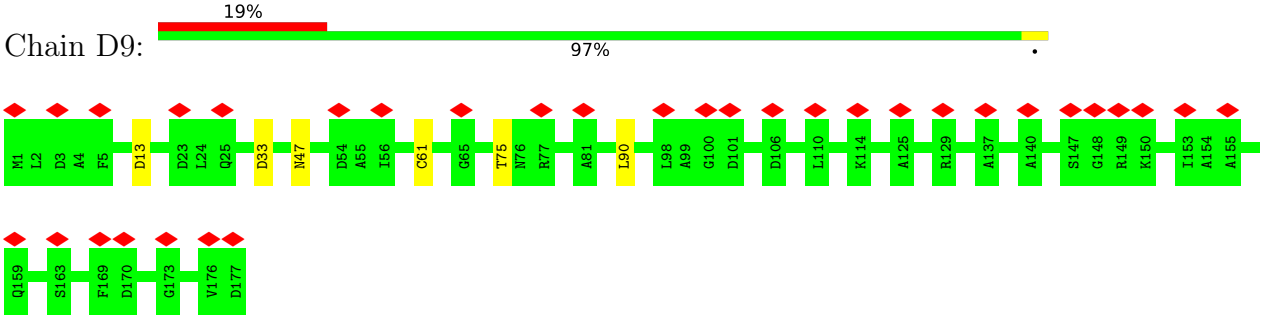
• Molecule 11: R-phycoerythrin beta chain

Chain B9:



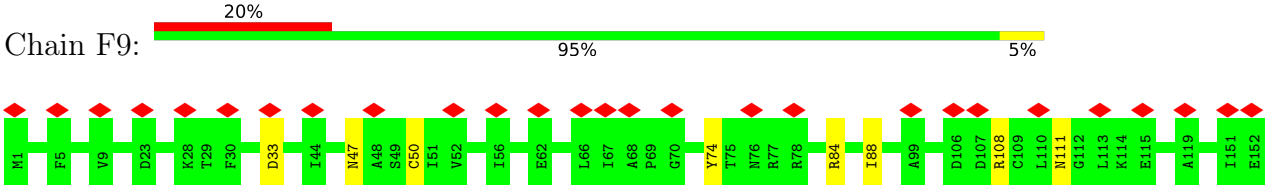
• Molecule 11: R-phycoerythrin beta chain

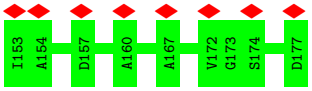
Chain D9:



• Molecule 11: R-phycoerythrin beta chain

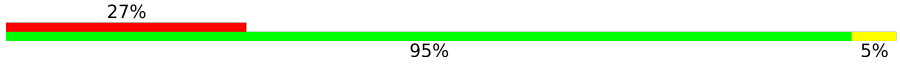
Chain F9:

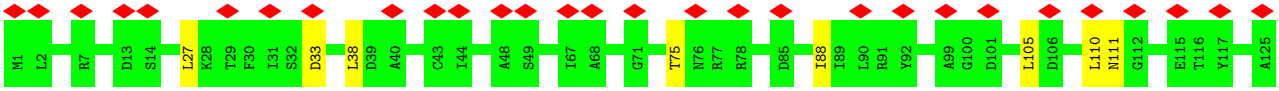


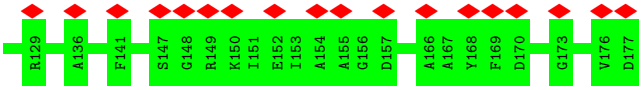


• Molecule 11: R-phycoerythrin beta chain

Chain H9:

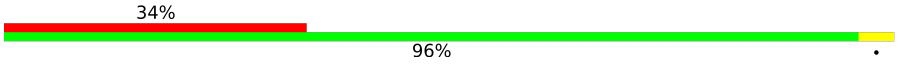


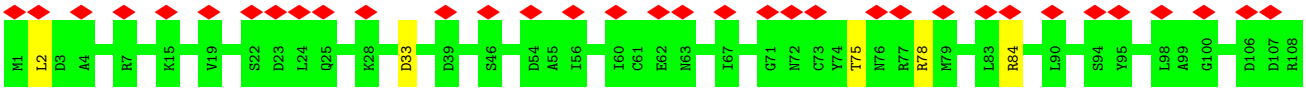


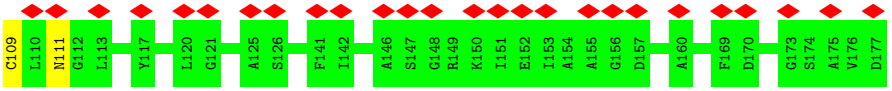


• Molecule 11: R-phycoerythrin beta chain

Chain J9:

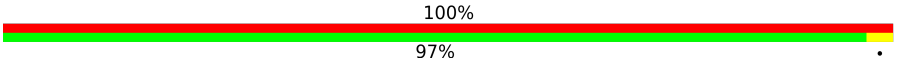


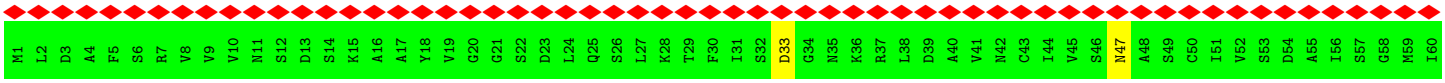


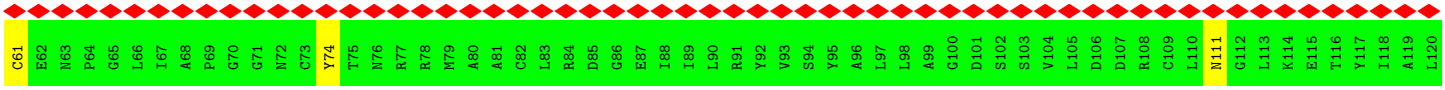


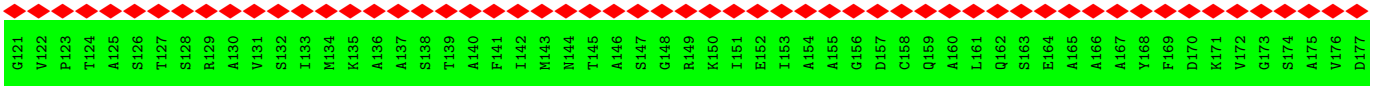
• Molecule 11: R-phycoerythrin beta chain

Chain L9:



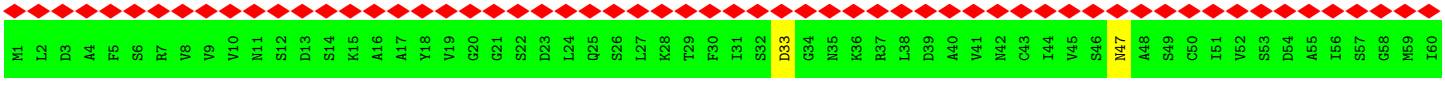






• Molecule 11: R-phycoerythrin beta chain

Chain N9:



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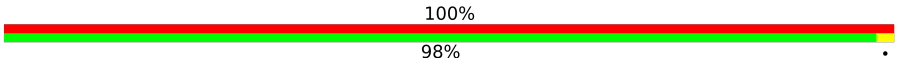
G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain P9:



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C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain R9:

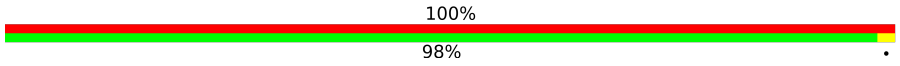
M1 L2 D3 A4 F5 S6 R7 V8 V9 V10 N11 S12 D13 S14 K15 A16 A17 Y18 V19 G20 G21 S22 D23 L24 Q25 S26 L27 K28 T29 F30 I31 S32 D33 G34 N35 K36 R37 L38 D39 A40 V41 N42 C43 I44 V45 S46 N47 A48 S49 C50 I51 V52 S53 D54 A55 I56 S57 G58 M59 I60

C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain T9:



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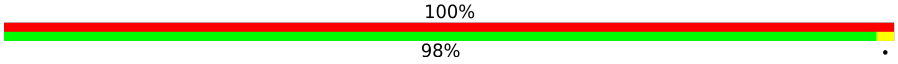
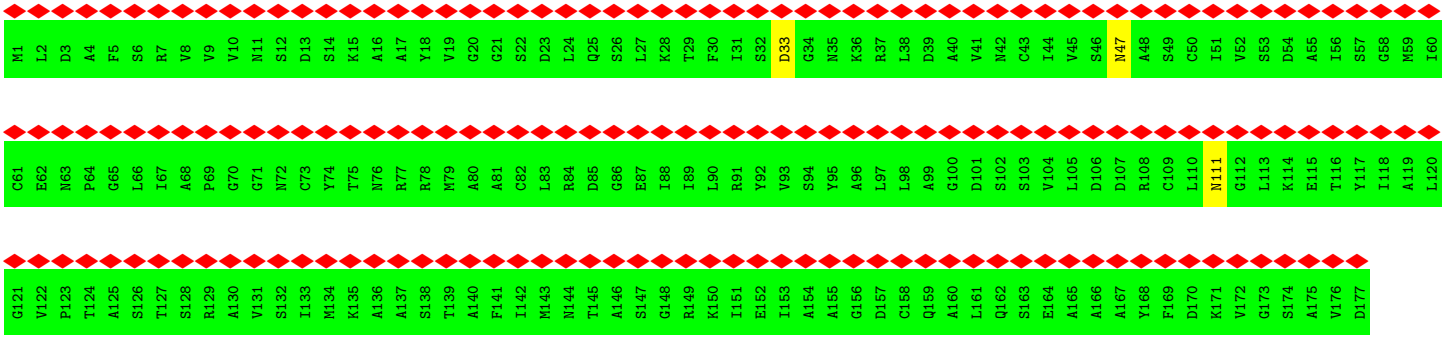
C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain V9:



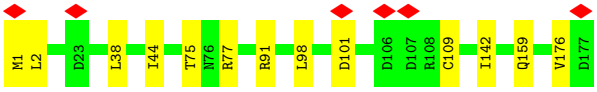


• Molecule 11: R-phycoerythrin beta chain

Chain an:

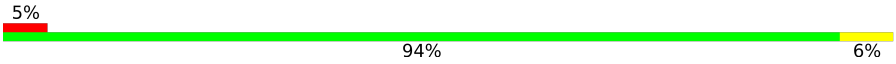
• Molecule 11: R-phycoerythrin beta chain

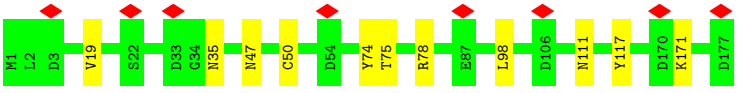
Chain ap:



• Molecule 11: R-phycoerythrin beta chain

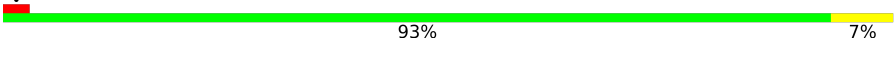
Chain ar:

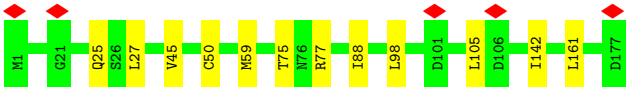




• Molecule 11: R-phycoerythrin beta chain

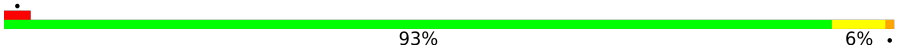
Chain at:





• Molecule 11: R-phycoerythrin beta chain

Chain av:



• Molecule 11: R-phycoerythrin beta chain

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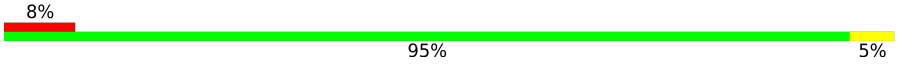
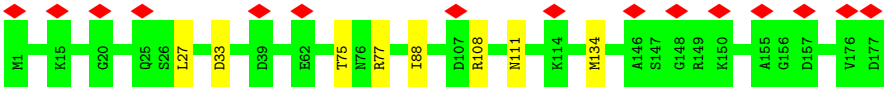
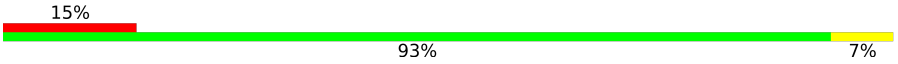
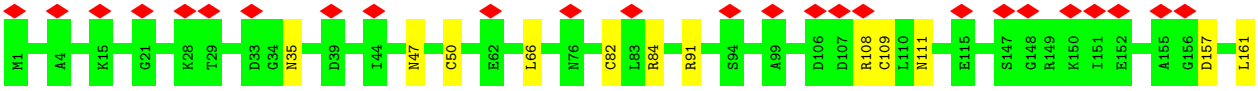




• Molecule 11: R-phycoerythrin beta chain

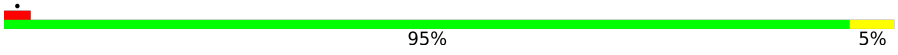
Chain az:

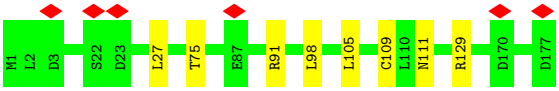




• Molecule 11: R-phycoerythrin beta chain

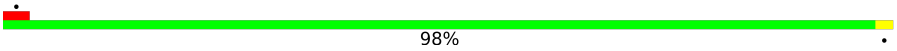
Chain aB:

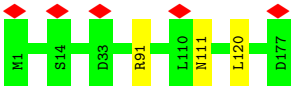




• Molecule 11: R-phycoerythrin beta chain

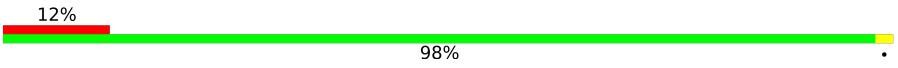
Chain aD:

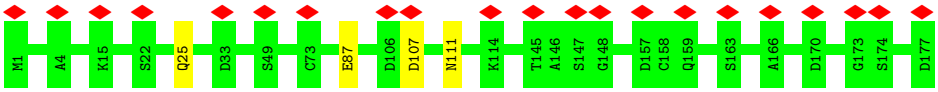




• Molecule 11: R-phycoerythrin beta chain

Chain aF:





• Molecule 11: R-phycoerythrin beta chain

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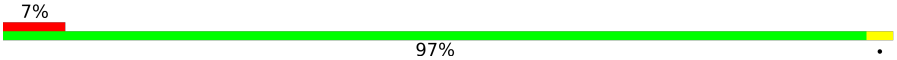
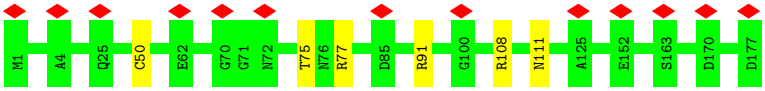
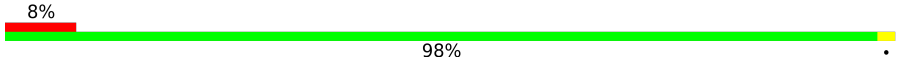
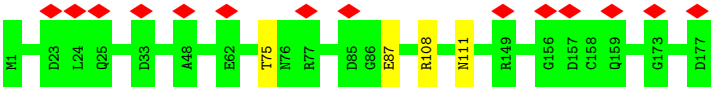




• Molecule 11: R-phycoerythrin beta chain

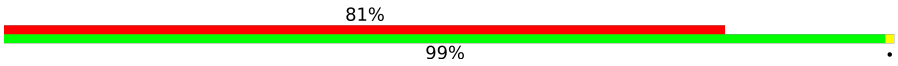
Chain aJ:

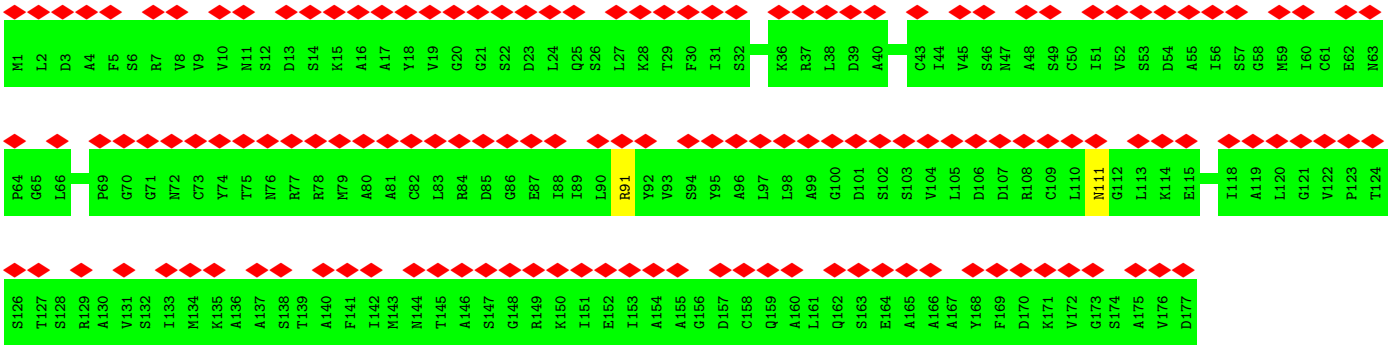




• Molecule 11: R-phycoerythrin beta chain

Chain aL:





• Molecule 11: R-phycoerythrin beta chain

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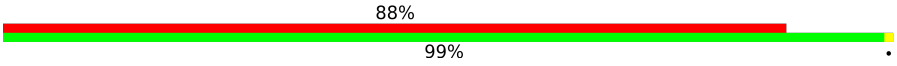

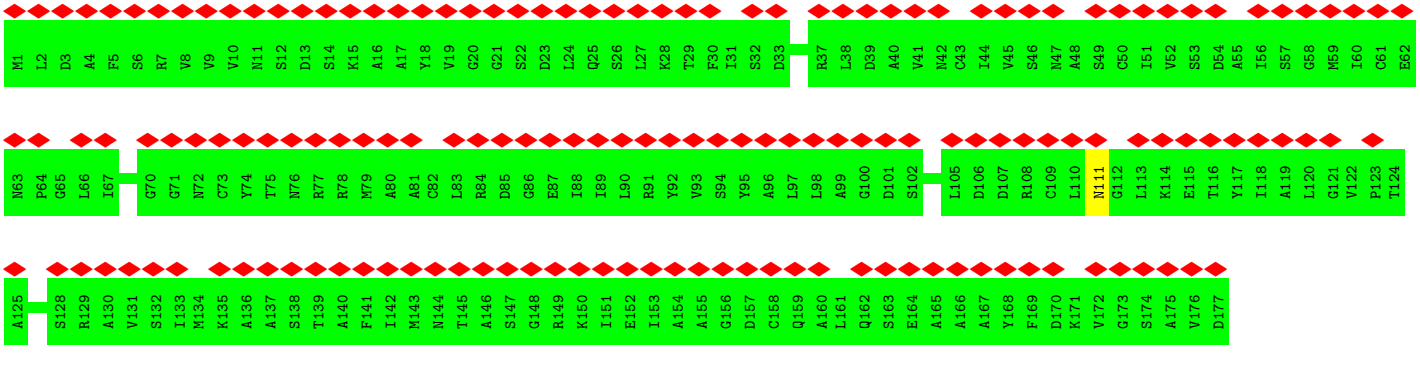

• Molecule 11: R-phycoerythrin beta chain

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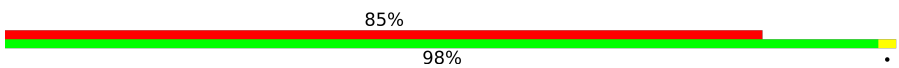

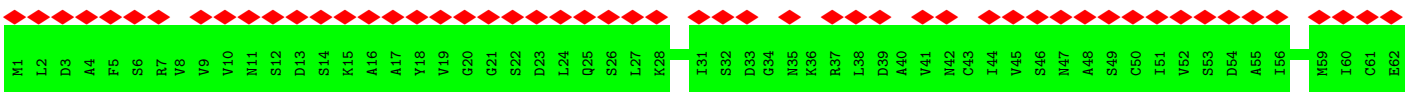

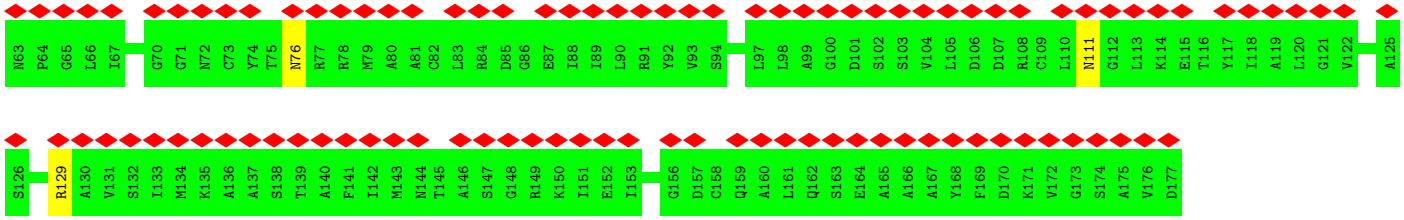

• Molecule 11: R-phycoerythrin beta chain

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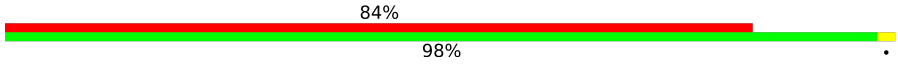

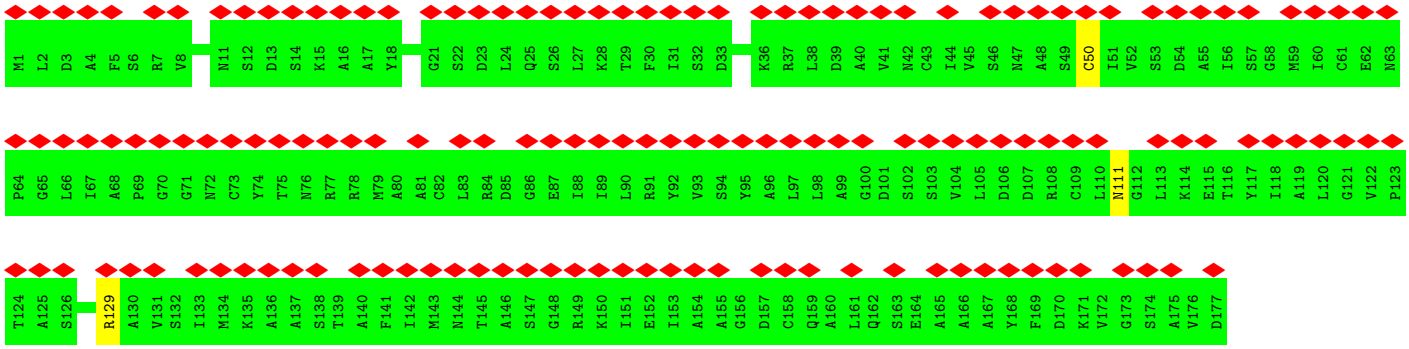

• Molecule 11: R-phycoerythrin beta chain

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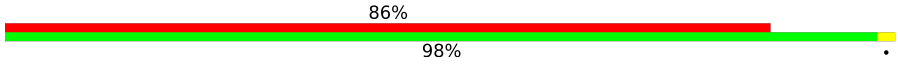

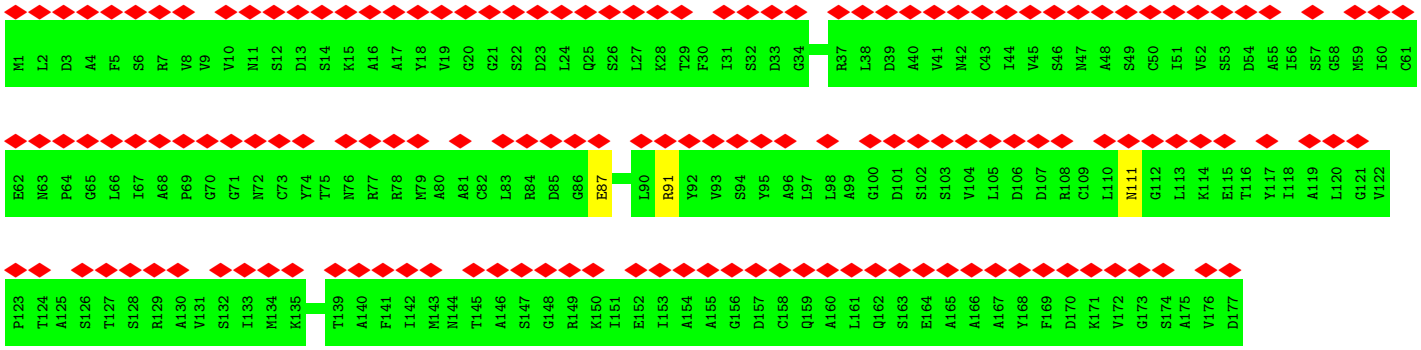

• Molecule 11: R-phycoerythrin beta chain

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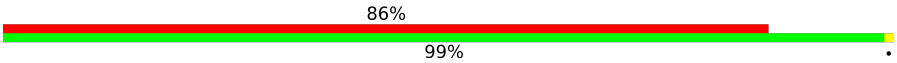
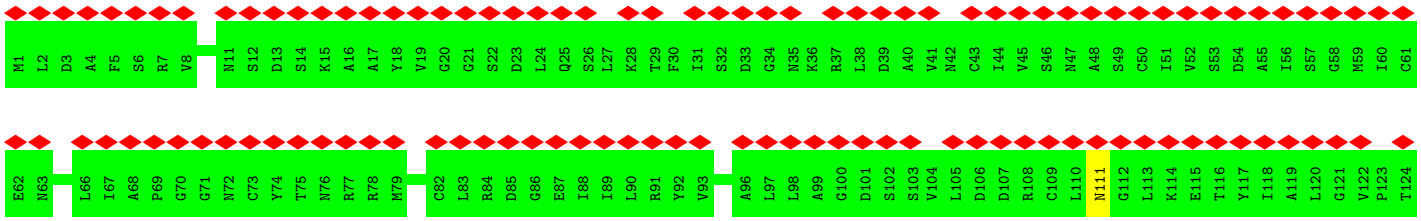
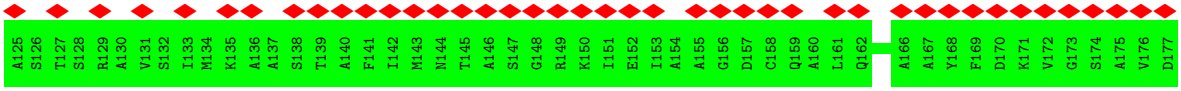
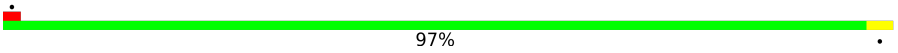


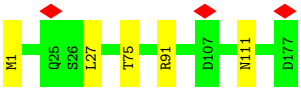




• Molecule 11: R-phycoerythrin beta chain

Chain bn:





• Molecule 11: R-phycoerythrin beta chain

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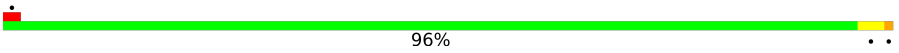
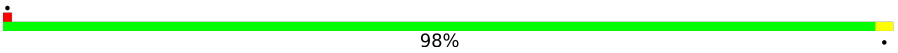
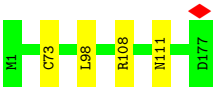


• Molecule 11: R-phycoerythrin beta chain

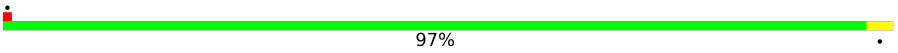
Chain bp:





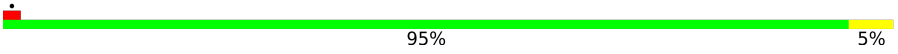
• Molecule 11: R-phycoerythrin beta chain

Chain bq:



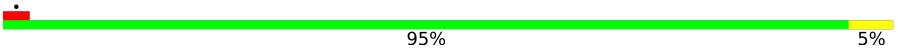
• Molecule 11: R-phycoerythrin beta chain

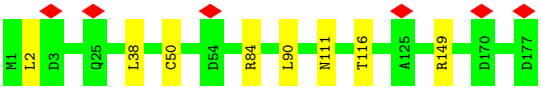
Chain br:



• Molecule 11: R-phycoerythrin beta chain

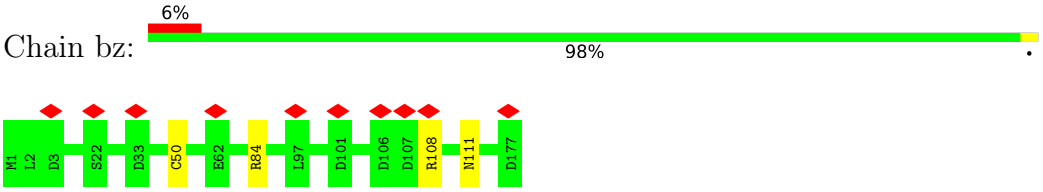
Chain bs:





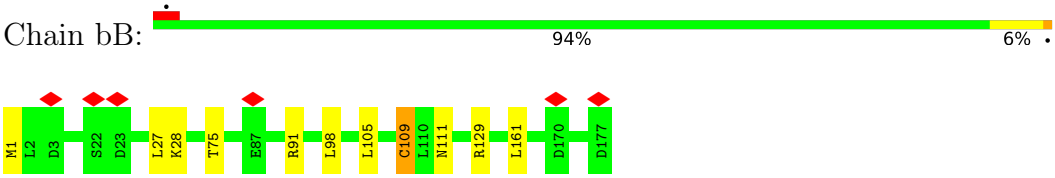
• Molecule 11: R-phycoerythrin beta chain

Chain bz:



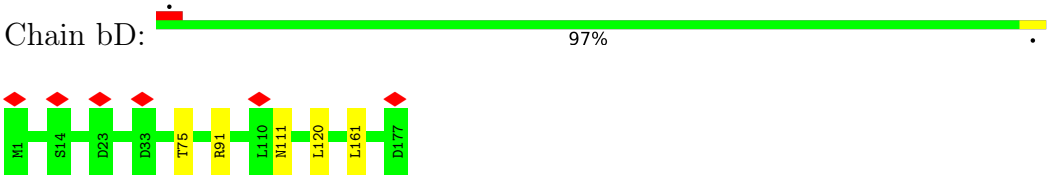
• Molecule 11: R-phycoerythrin beta chain

Chain bB:



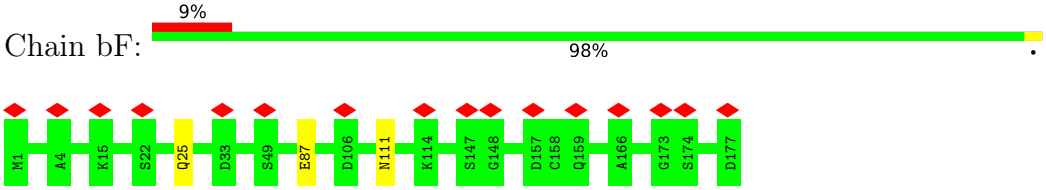
• Molecule 11: R-phycoerythrin beta chain

Chain bD:



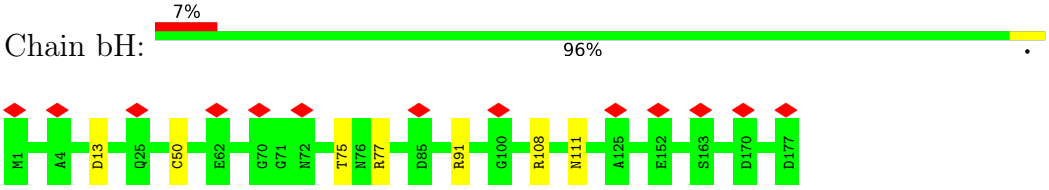
• Molecule 11: R-phycoerythrin beta chain

Chain bF:



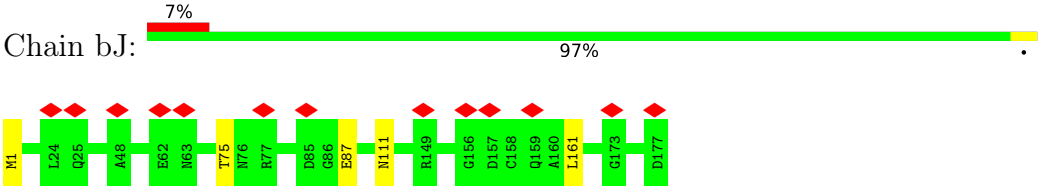
• Molecule 11: R-phycoerythrin beta chain

Chain bH:



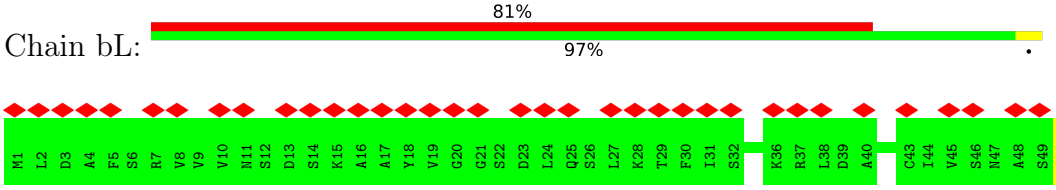
• Molecule 11: R-phycoerythrin beta chain

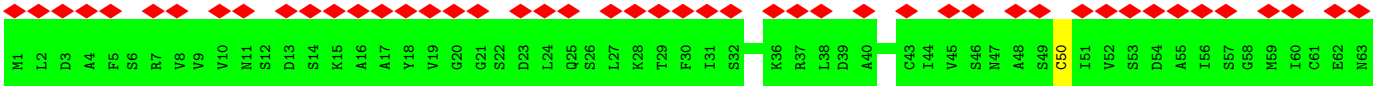
Chain bJ:

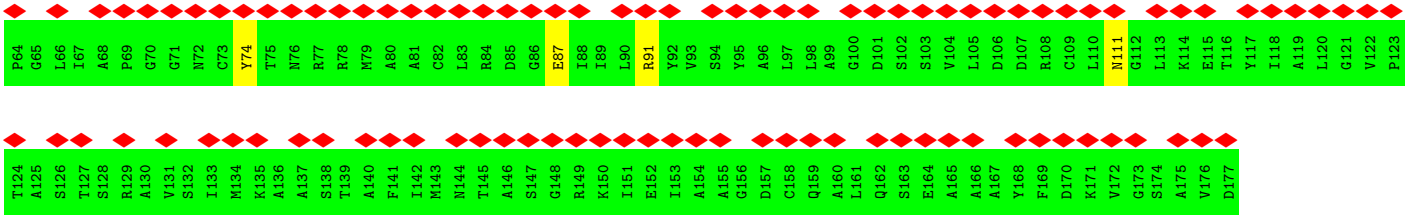


• Molecule 11: R-phycoerythrin beta chain

Chain bL:

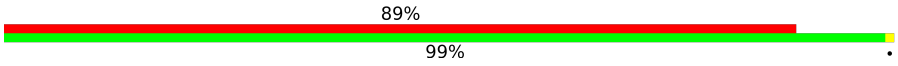


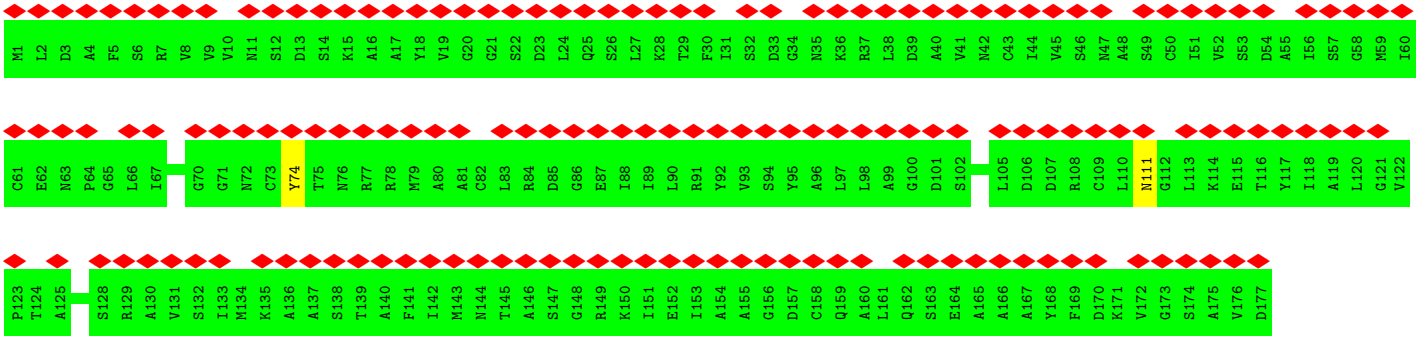




• Molecule 11: R-phycoerythrin beta chain

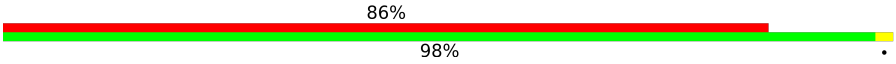
Chain bN:

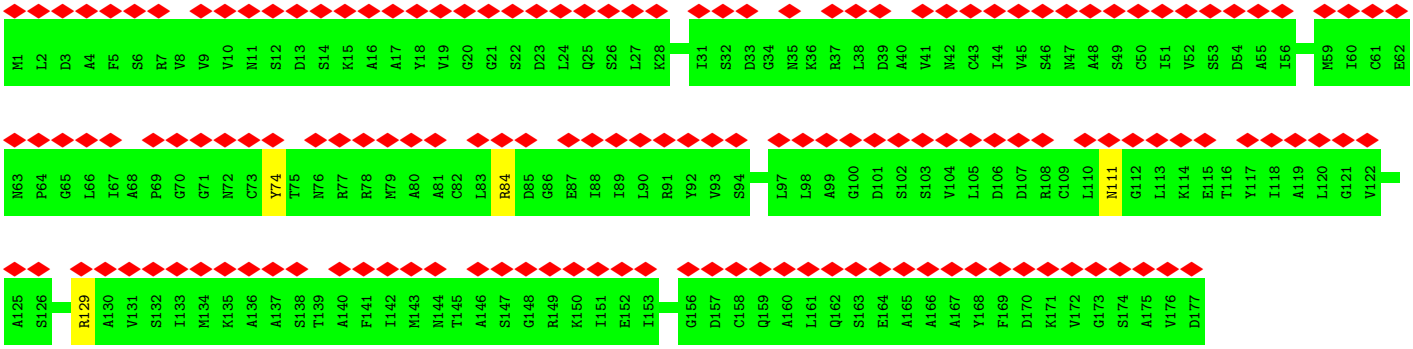




• Molecule 11: R-phycoerythrin beta chain

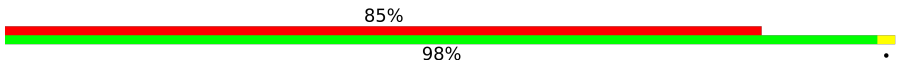
Chain bP:

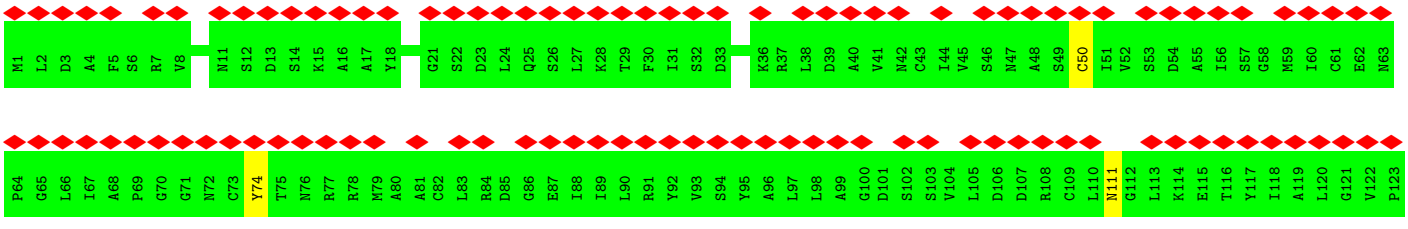


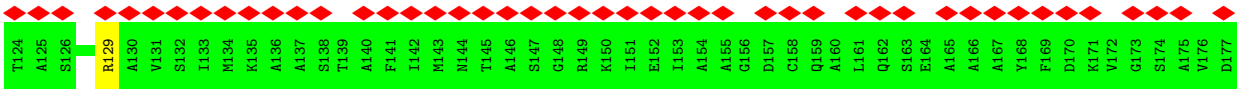


• Molecule 11: R-phycoerythrin beta chain

Chain bR:

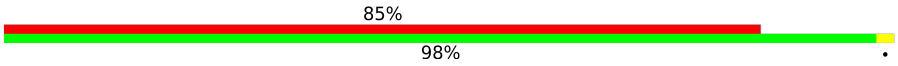


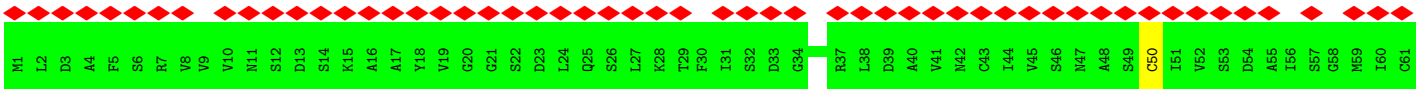




• Molecule 11: R-phycoerythrin beta chain

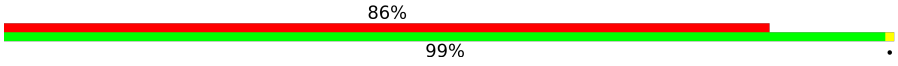
Chain bT:

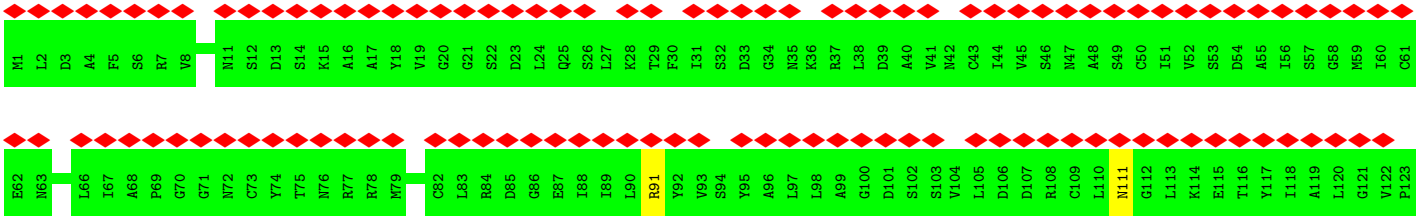




• Molecule 11: R-phycoerythrin beta chain

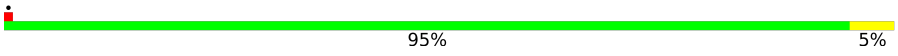
Chain bV:

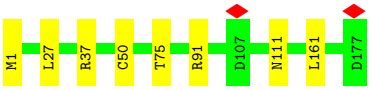




• Molecule 11: R-phycoerythrin beta chain

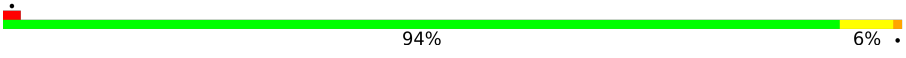
Chain cn:

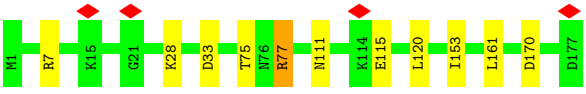




• Molecule 11: R-phycoerythrin beta chain

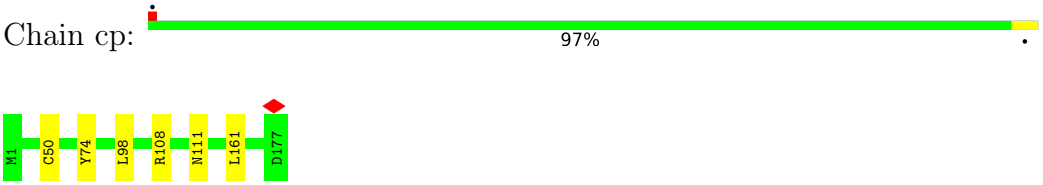
Chain co:





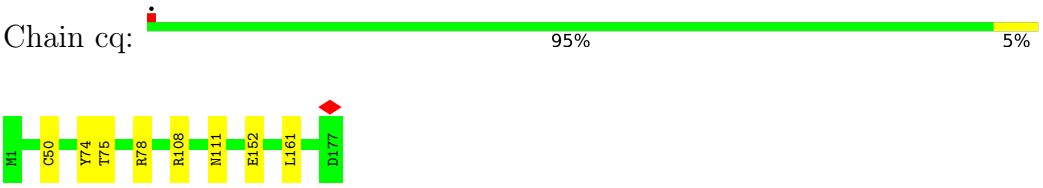
• Molecule 11: R-phycoerythrin beta chain

Chain cp:



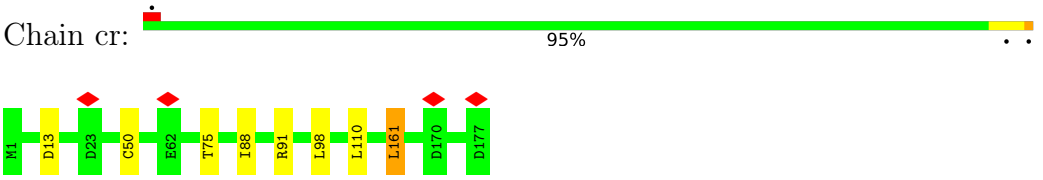
• Molecule 11: R-phycoerythrin beta chain

Chain cq:



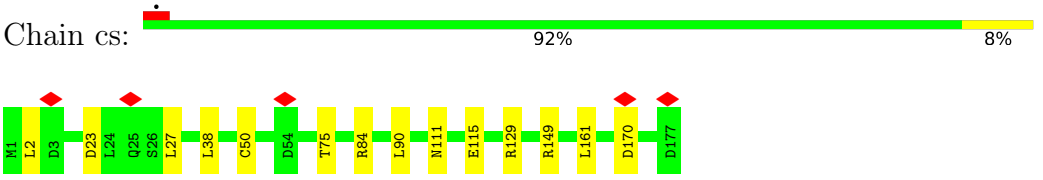
• Molecule 11: R-phycoerythrin beta chain

Chain cr:



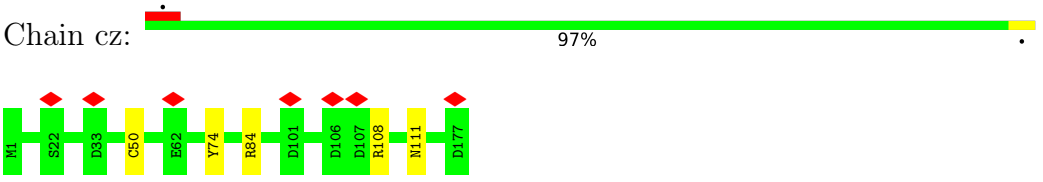
• Molecule 11: R-phycoerythrin beta chain

Chain cs:



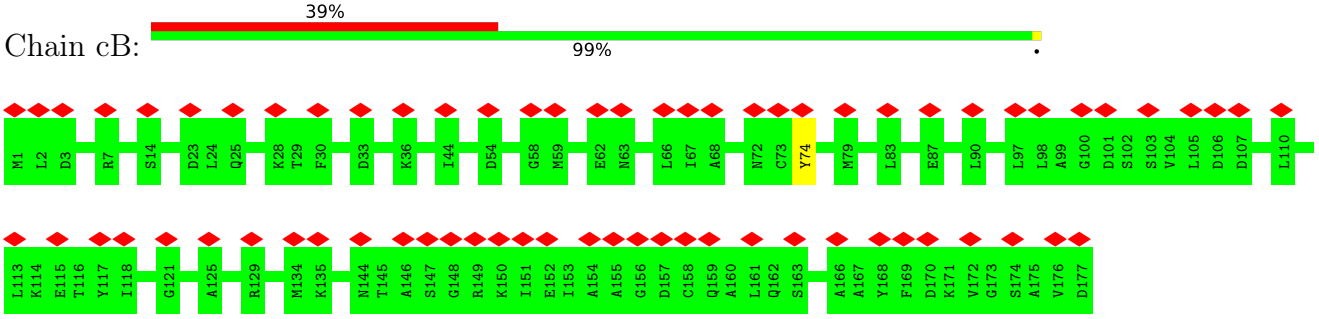
• Molecule 11: R-phycoerythrin beta chain

Chain cz:



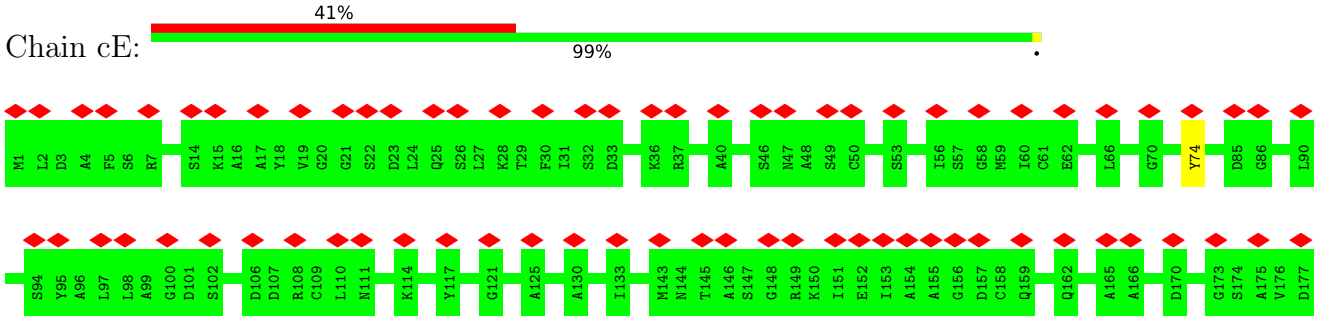
• Molecule 11: R-phycoerythrin beta chain

Chain cB:



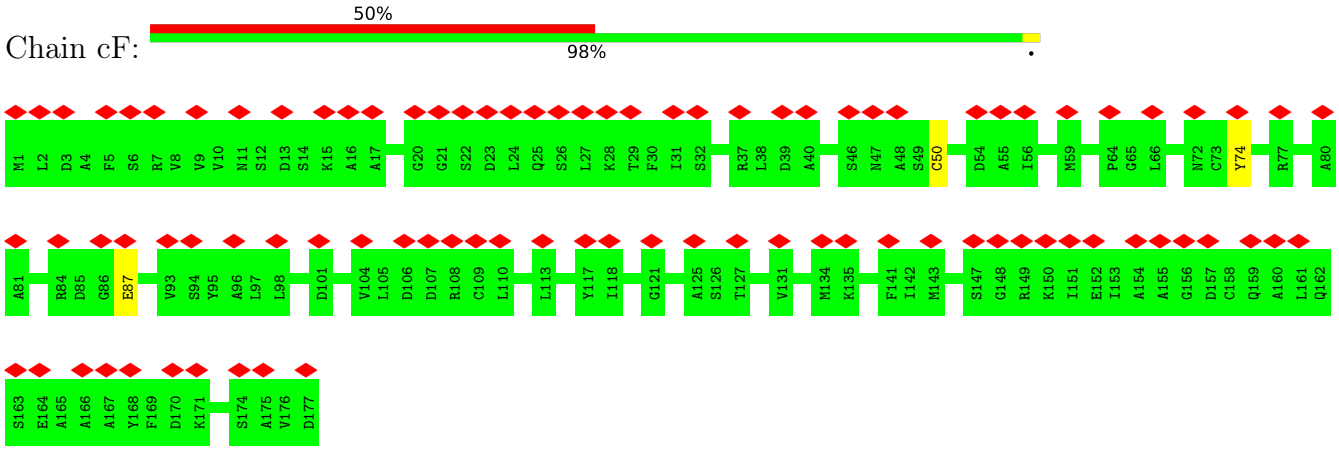
• Molecule 11: R-phycoerythrin beta chain

Chain cE:



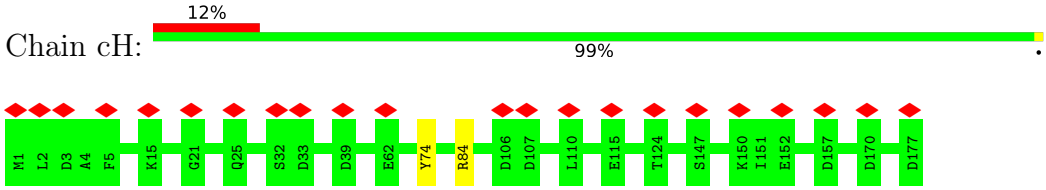
• Molecule 11: R-phycoerythrin beta chain

Chain cF:



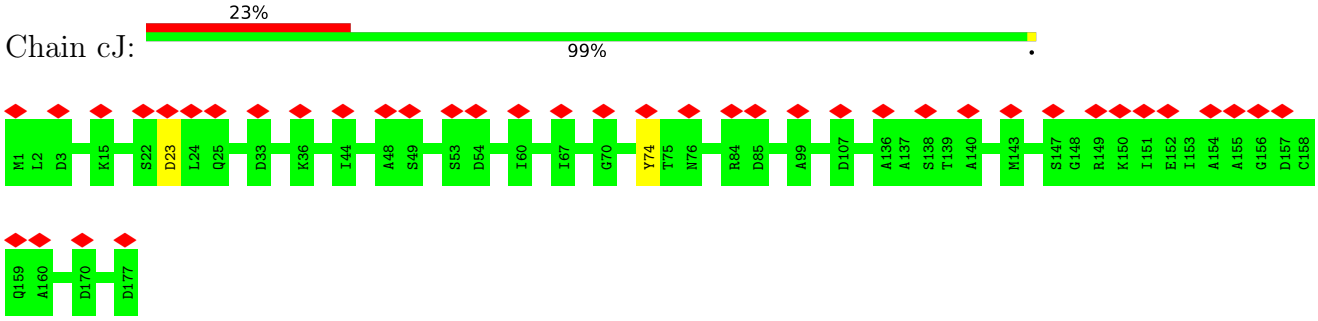
• Molecule 11: R-phycoerythrin beta chain

Chain cH:



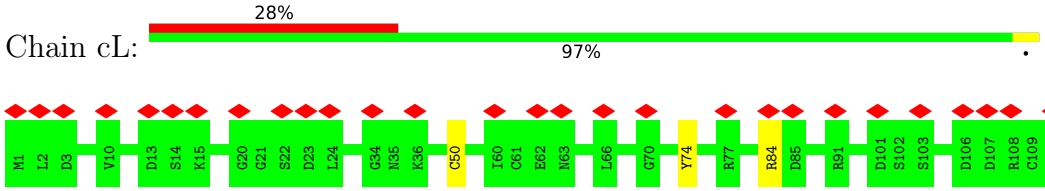
• Molecule 11: R-phycoerythrin beta chain

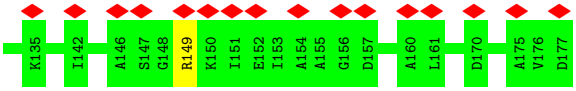
Chain cJ:



• Molecule 11: R-phycoerythrin beta chain

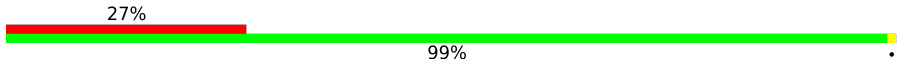
Chain cL:

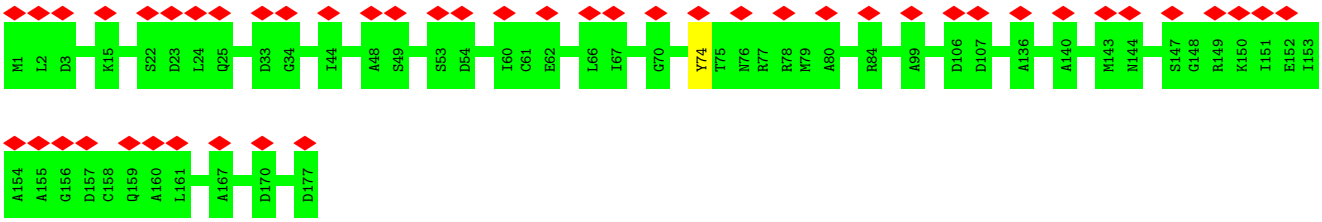




• Molecule 11: R-phycoerythrin beta chain

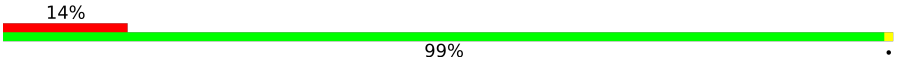
Chain cM:

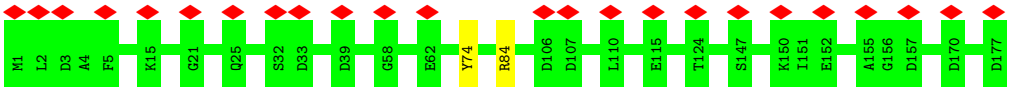




• Molecule 11: R-phycoerythrin beta chain

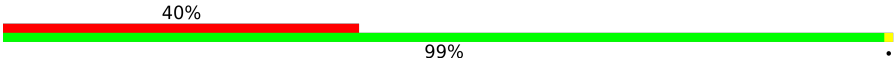
Chain cN:

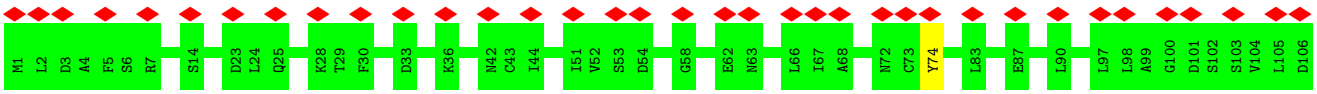


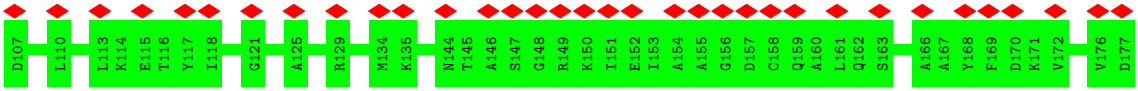


• Molecule 11: R-phycoerythrin beta chain

Chain cO:

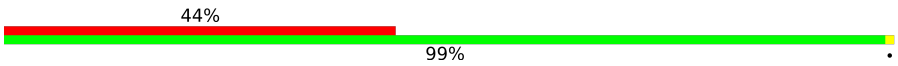


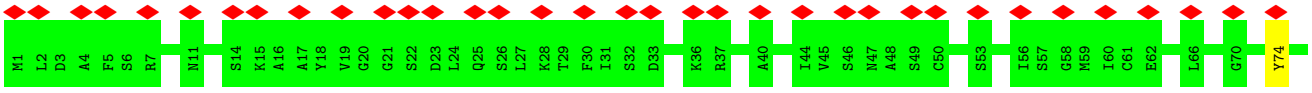


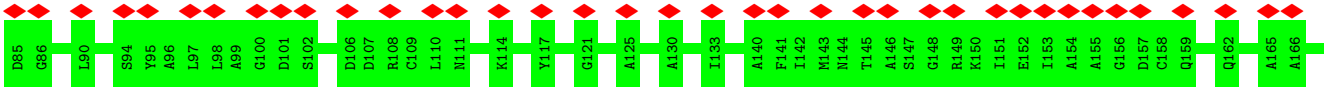


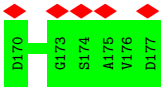
• Molecule 11: R-phycoerythrin beta chain

Chain cP:



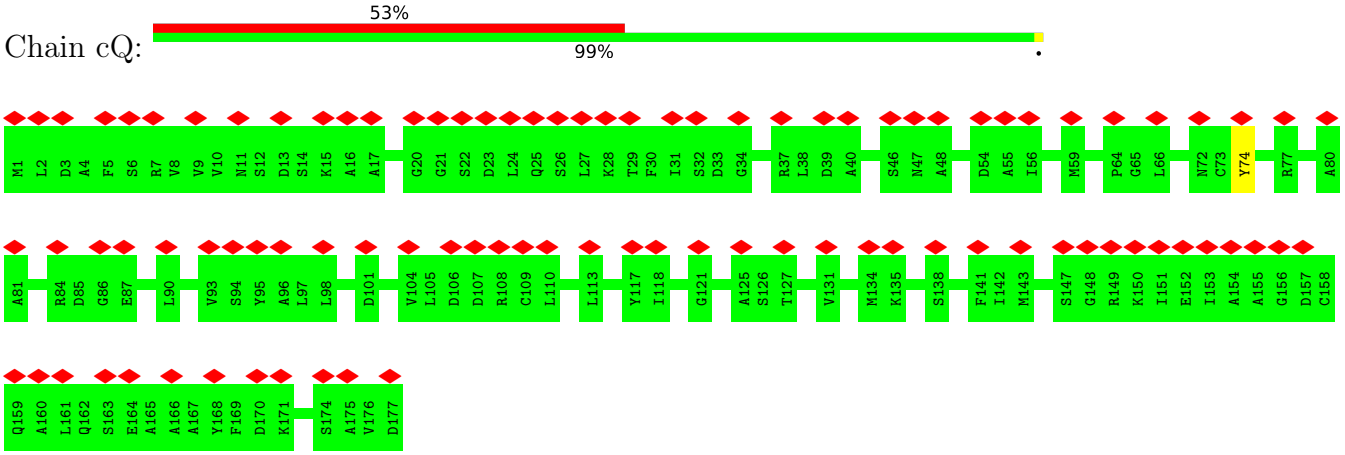






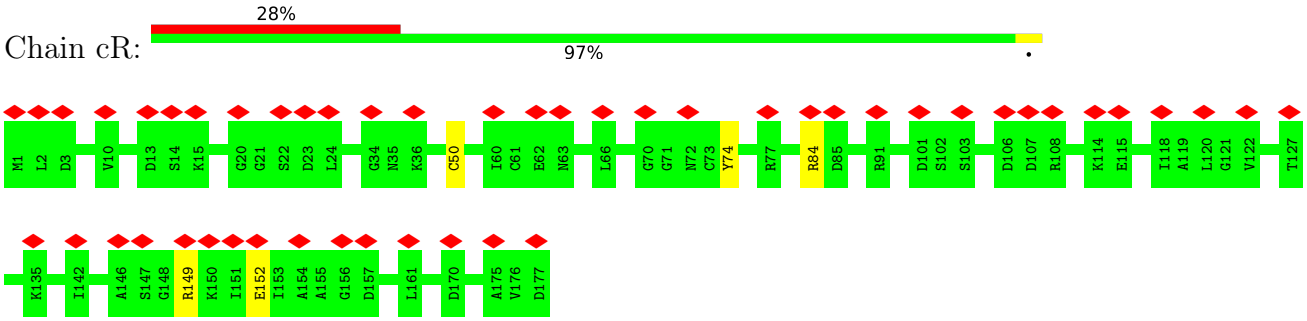
• Molecule 11: R-phycoerythrin beta chain

Chain cQ:



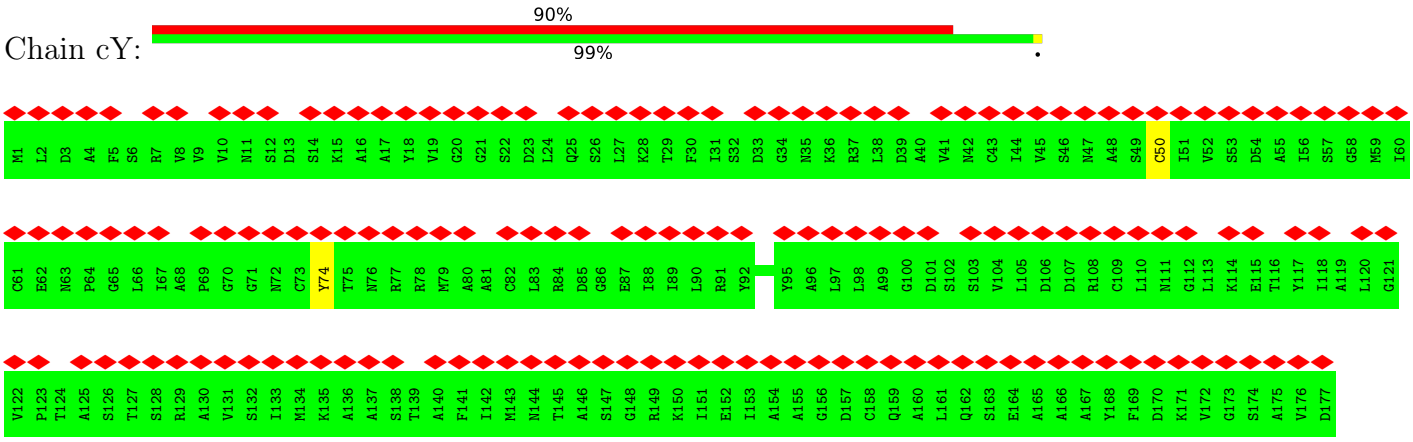
• Molecule 11: R-phycoerythrin beta chain

Chain cR:



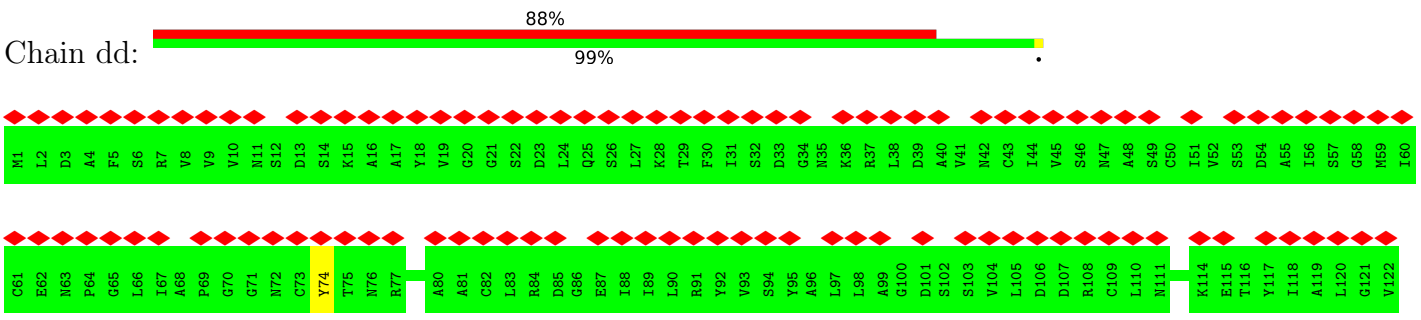
• Molecule 11: R-phycoerythrin beta chain

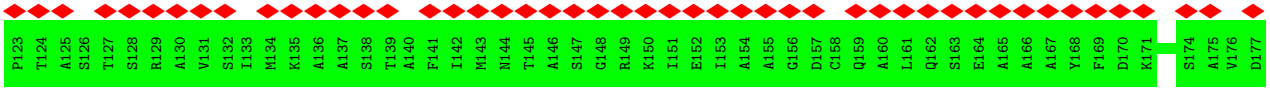
Chain cY:



• Molecule 11: R-phycoerythrin beta chain

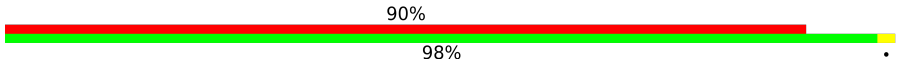
Chain dd:

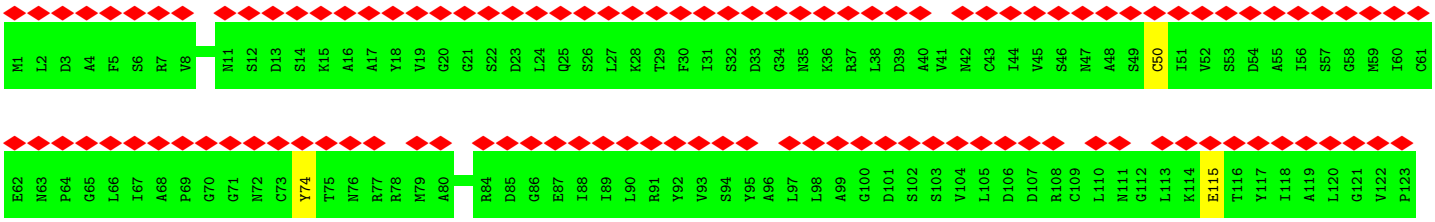




• Molecule 11: R-phycoerythrin beta chain

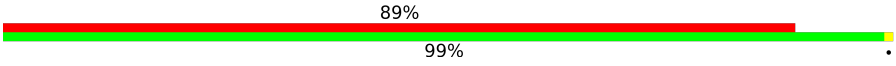
Chain df:

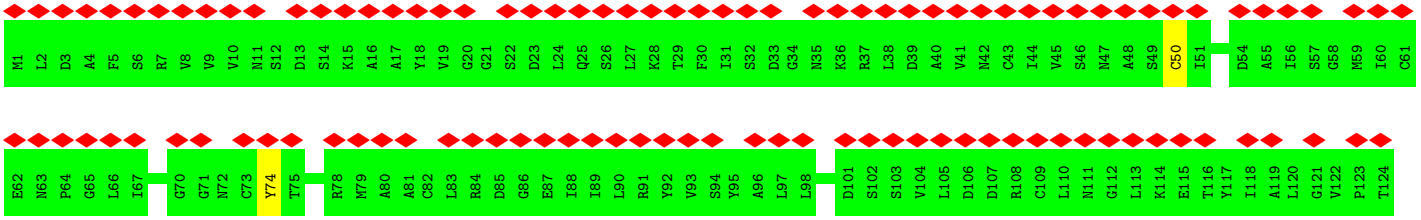




• Molecule 11: R-phycoerythrin beta chain

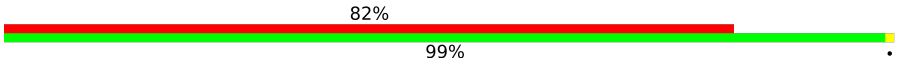
Chain dh:

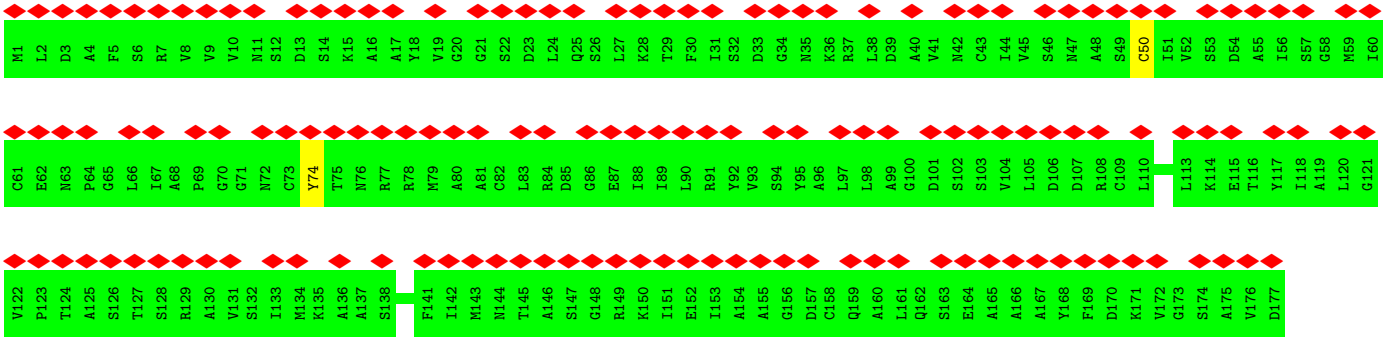




• Molecule 11: R-phycoerythrin beta chain

Chain di:





• Molecule 11: R-phycoerythrin beta chain

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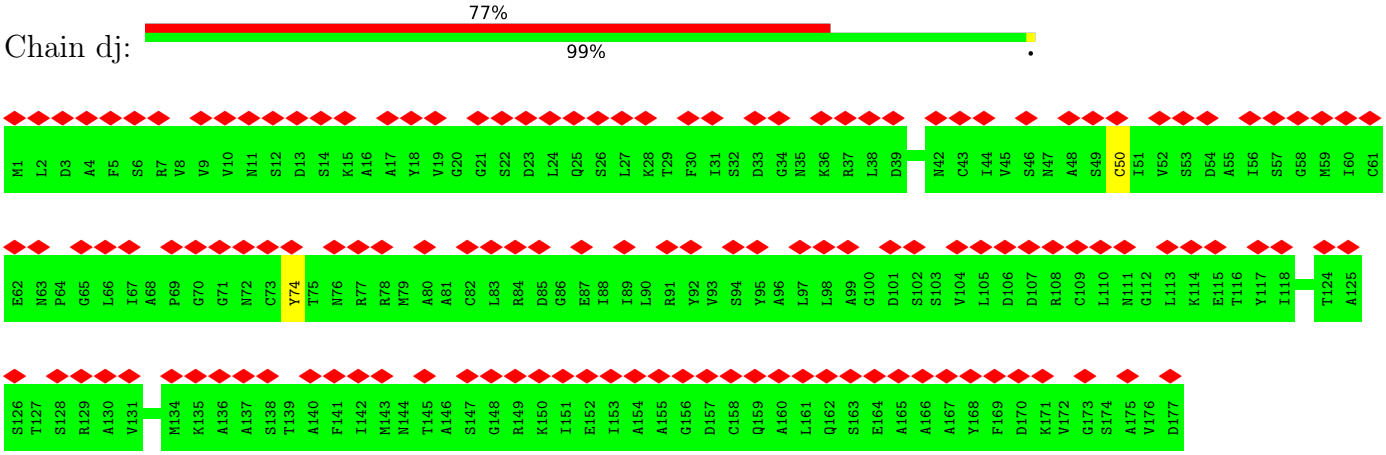
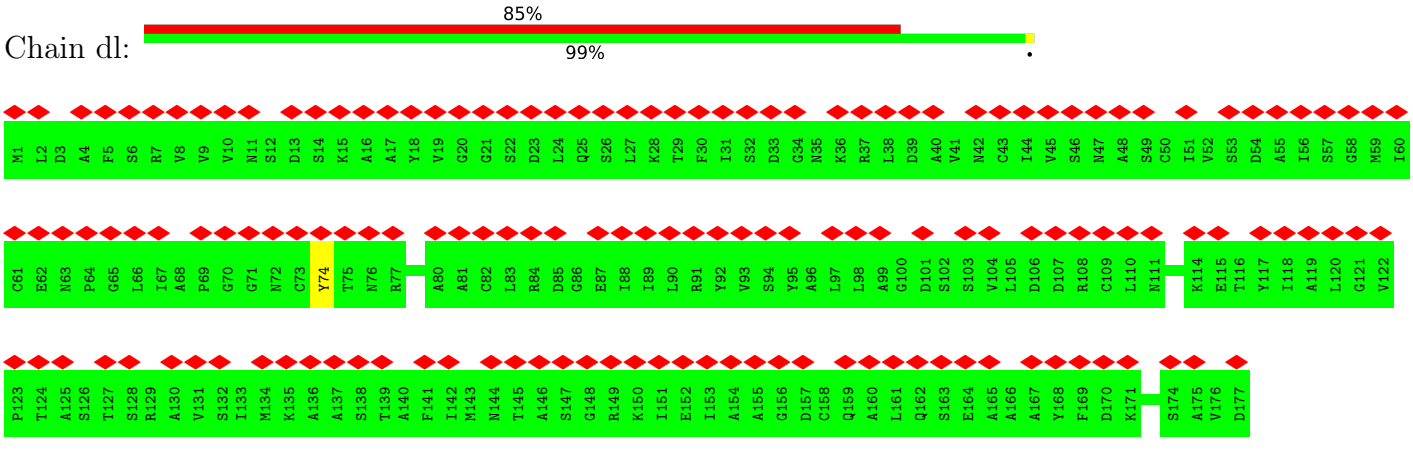


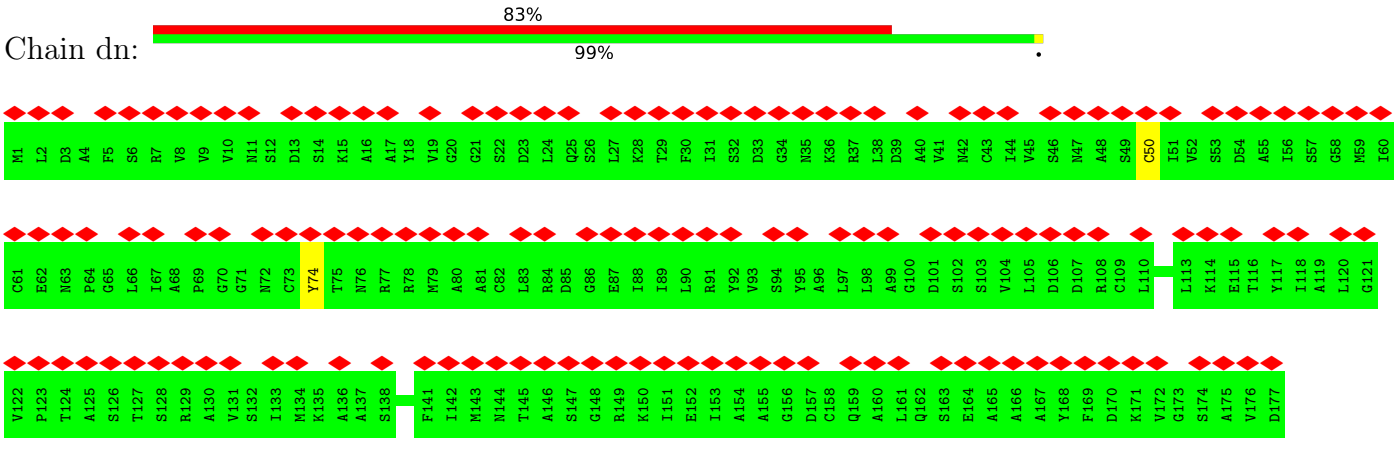
• Molecule 11: R-phycoerythrin beta chain

Chain dl:



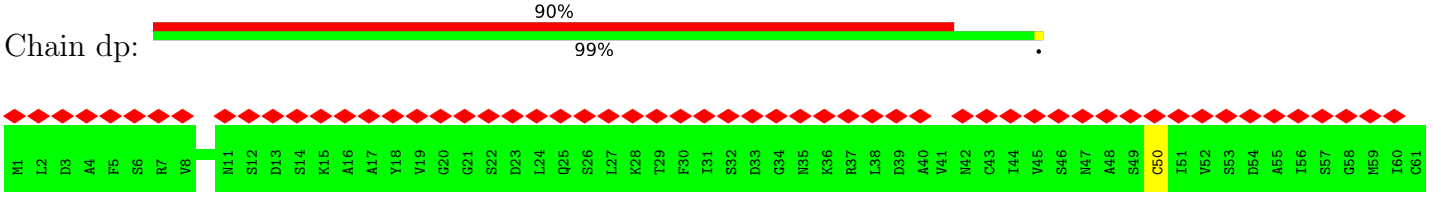
• Molecule 11: R-phycoerythrin beta chain

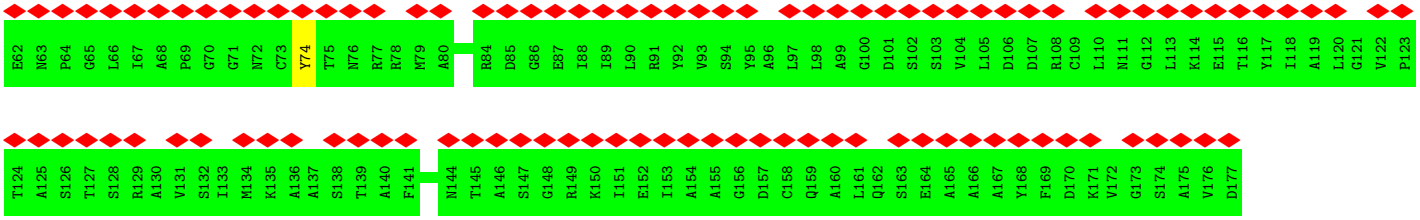
Chain dn:



• Molecule 11: R-phycoerythrin beta chain

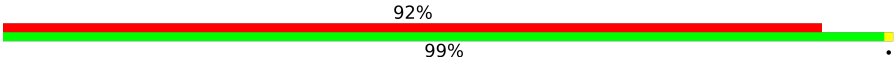
Chain dp:

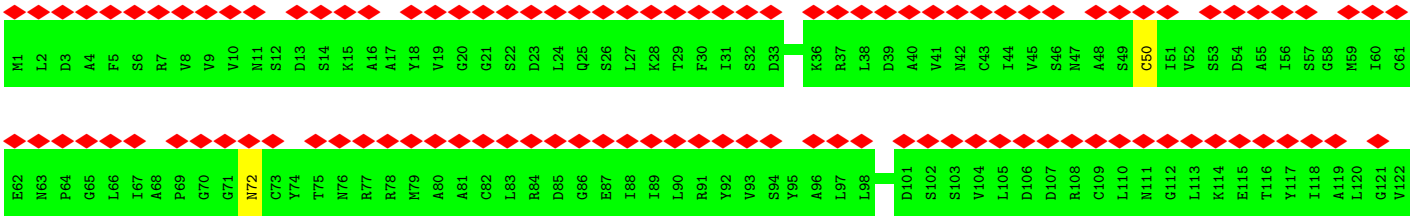




• Molecule 11: R-phycoerythrin beta chain

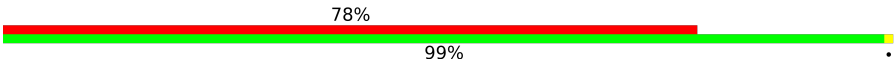
Chain dr:





• Molecule 11: R-phycoerythrin beta chain

Chain dt:



• Molecule 11: R-phycoerythrin beta chain

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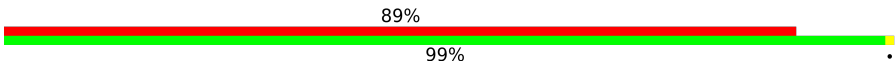
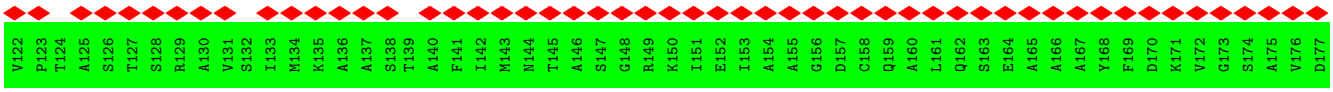
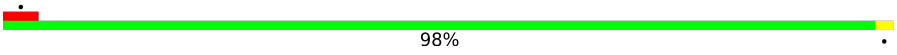
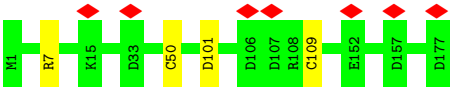




• Molecule 11: R-phycoerythrin beta chain

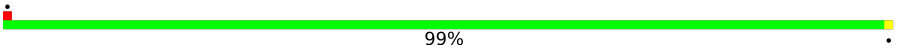
Chain dB:

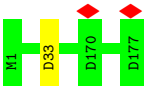




• Molecule 11: R-phycoerythrin beta chain

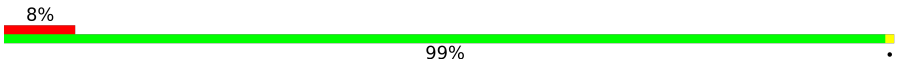
Chain dD:

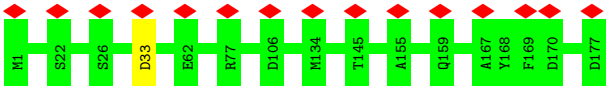




• Molecule 11: R-phycoerythrin beta chain

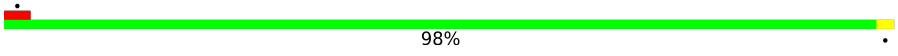
Chain dF:

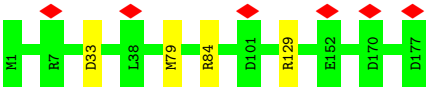




• Molecule 11: R-phycoerythrin beta chain

Chain dH:





• Molecule 11: R-phycoerythrin beta chain

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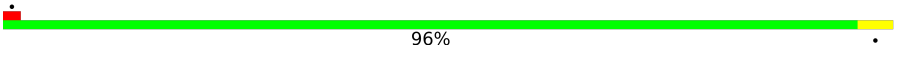
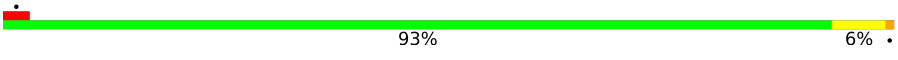


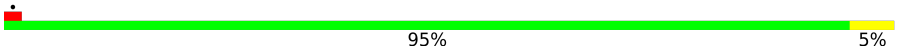
• Molecule 11: R-phycoerythrin beta chain

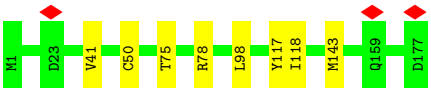
Chain dL:



• Molecule 11: R-phycoerythrin beta chain

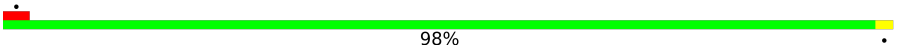
Chain dN:

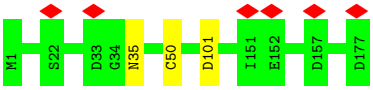




• Molecule 11: R-phycoerythrin beta chain

Chain dP:





• Molecule 11: R-phycoerythrin beta chain

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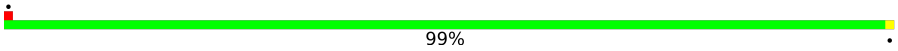
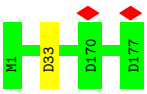
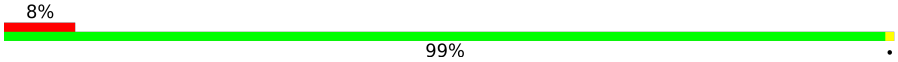
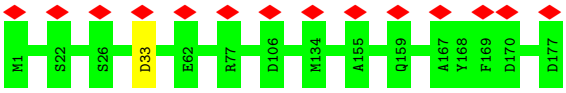




• Molecule 11: R-phycoerythrin beta chain

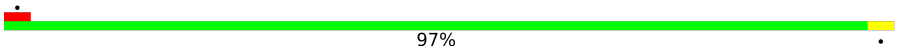
Chain dT:

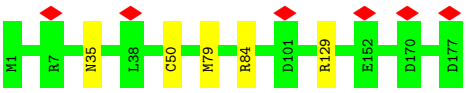




• Molecule 11: R-phycoerythrin beta chain

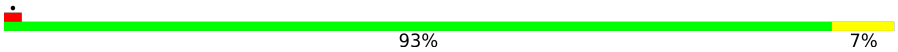
Chain dV:

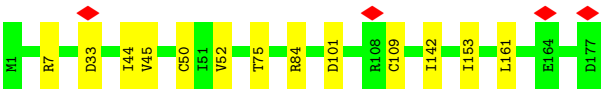




• Molecule 11: R-phycoerythrin beta chain

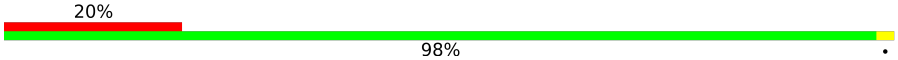
Chain dX:

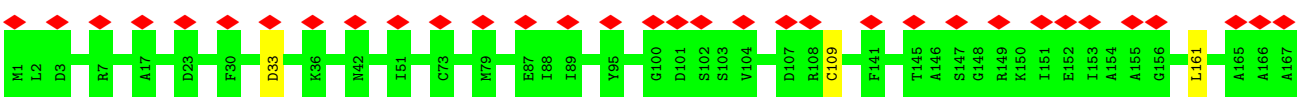


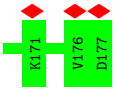


• Molecule 11: R-phycoerythrin beta chain

Chain dY:

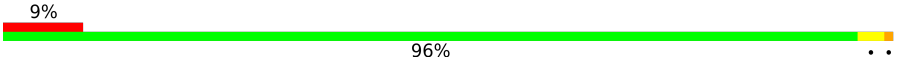


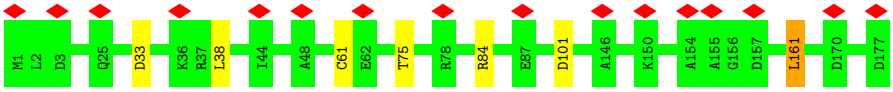




• Molecule 11: R-phycoerythrin beta chain

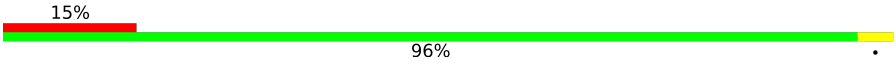
Chain eb:

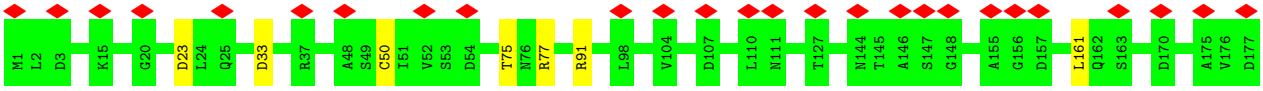




• Molecule 11: R-phycoerythrin beta chain

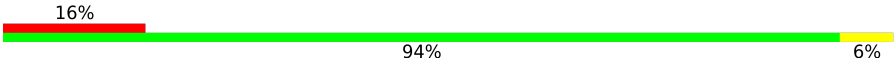
Chain ec:

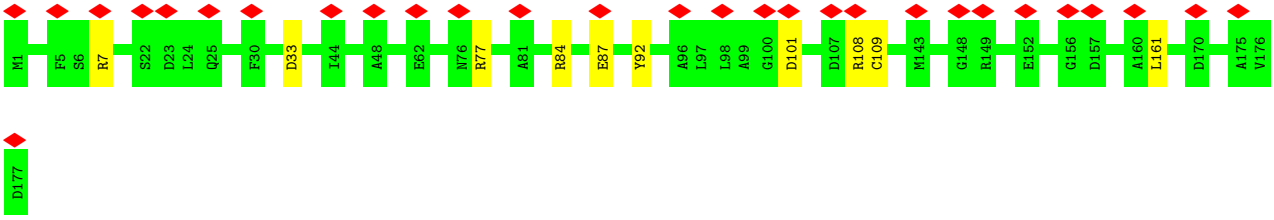




• Molecule 11: R-phycoerythrin beta chain

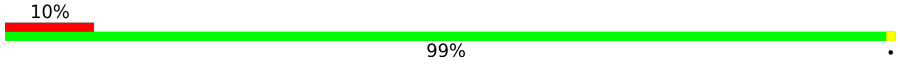
Chain ee:

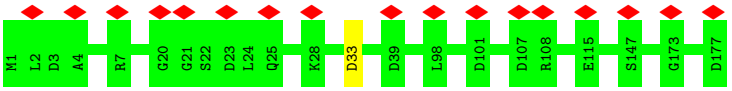




• Molecule 11: R-phycoerythrin beta chain

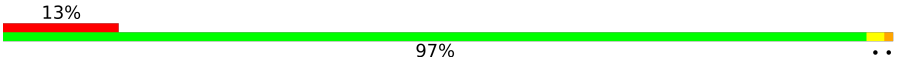
Chain eg:

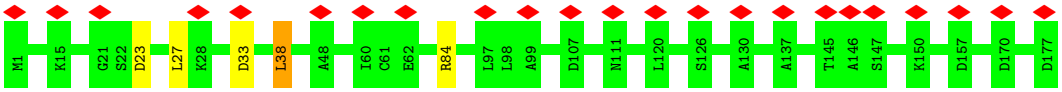




• Molecule 11: R-phycoerythrin beta chain

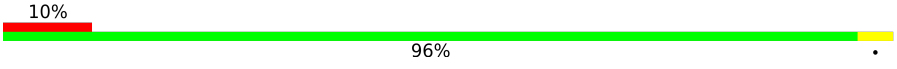
Chain ei:

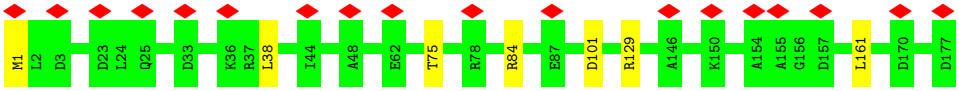




• Molecule 11: R-phycoerythrin beta chain

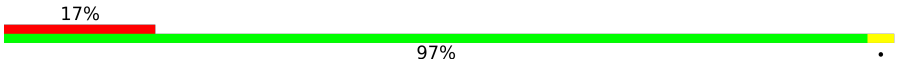
Chain el:

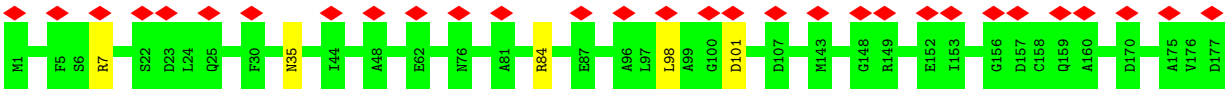




• Molecule 11: R-phycoerythrin beta chain

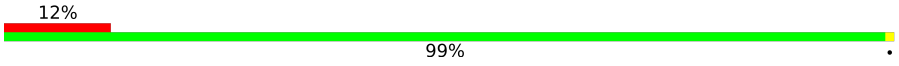
Chain en:

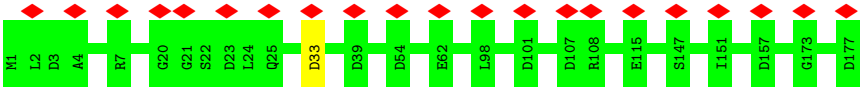




• Molecule 11: R-phycoerythrin beta chain

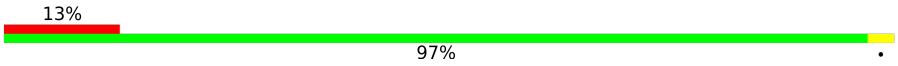
Chain ep:

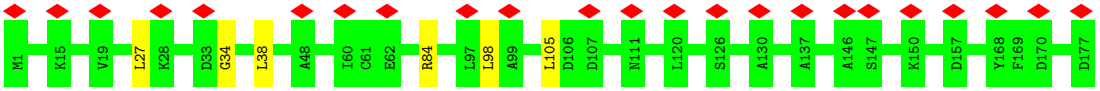




• Molecule 11: R-phycoerythrin beta chain

Chain er:





• Molecule 11: R-phycoerythrin beta chain

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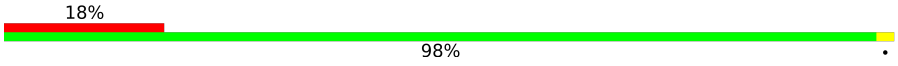
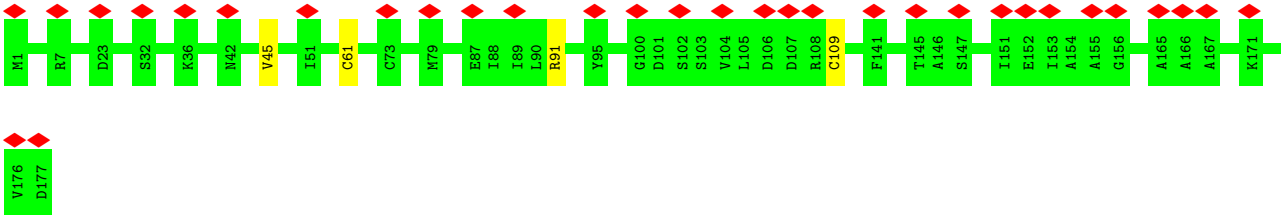
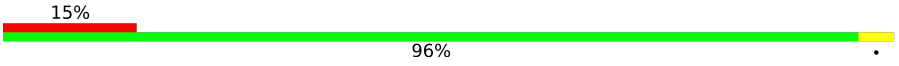
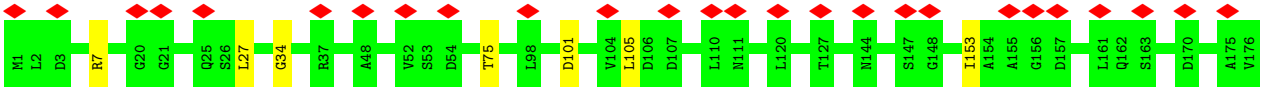




• Molecule 11: R-phycoerythrin beta chain

Chain ev:





• Molecule 11: R-phycoerythrin beta chain

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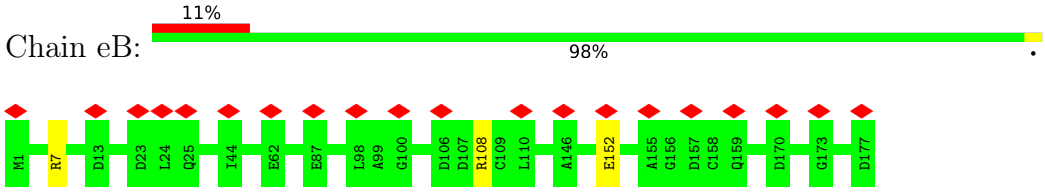

• Molecule 11: R-phycoerythrin beta chain

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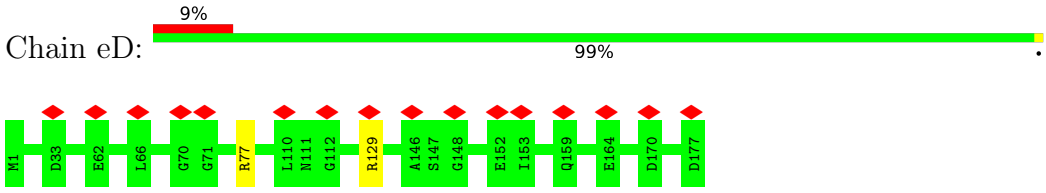
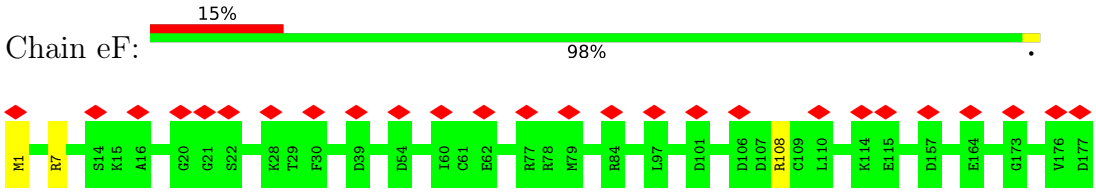


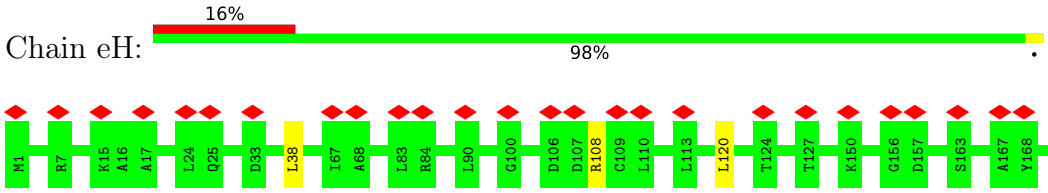
• Molecule 11: R-phycoerythrin beta chain

Chain eF:



• Molecule 11: R-phycoerythrin beta chain

Chain eH:



• Molecule 11: R-phycoerythrin beta chain

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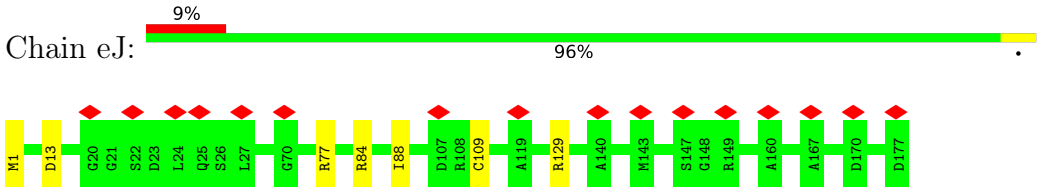

• Molecule 11: R-phycoerythrin beta chain

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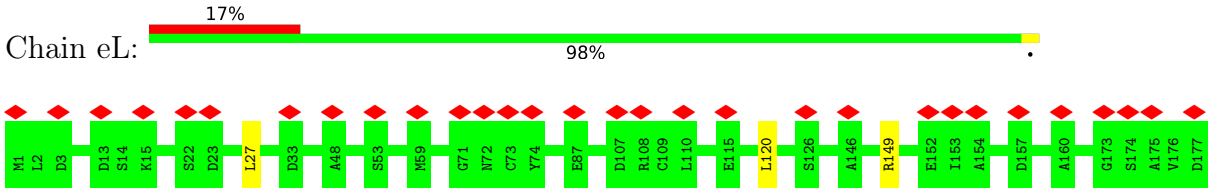

• Molecule 11: R-phycoerythrin beta chain

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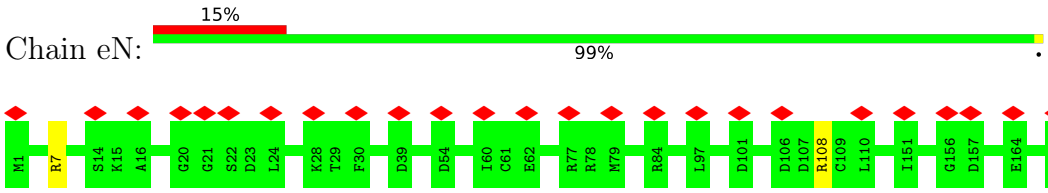

• Molecule 11: R-phycoerythrin beta chain

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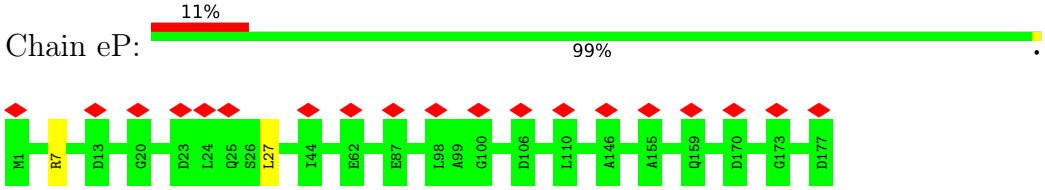

• Molecule 11: R-phycoerythrin beta chain

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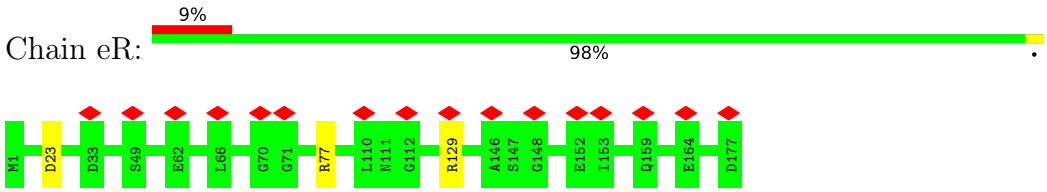

• Molecule 11: R-phycoerythrin beta chain

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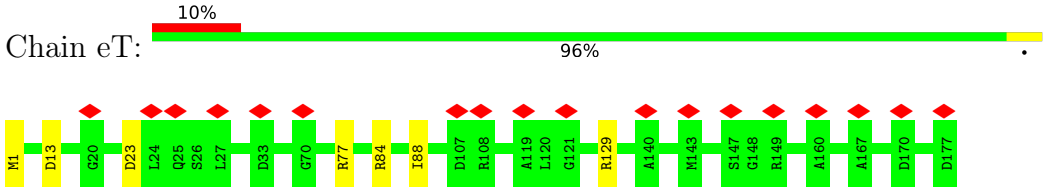
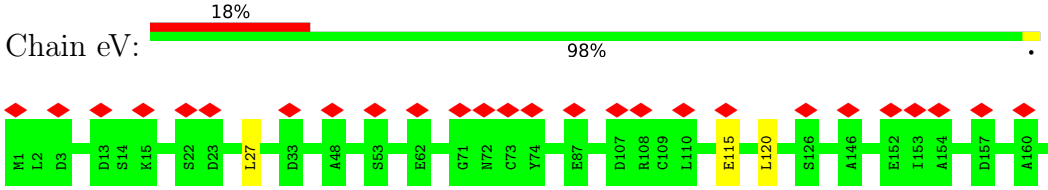


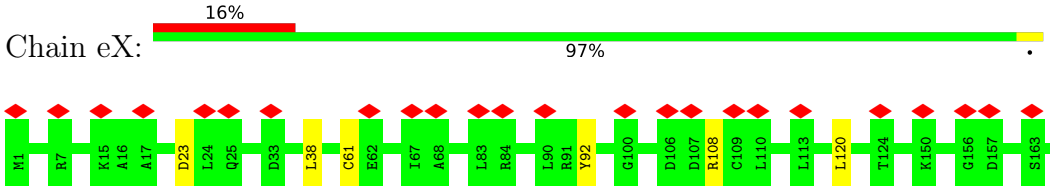
• Molecule 11: R-phycoerythrin beta chain

Chain eV:



• Molecule 11: R-phycoerythrin beta chain

Chain eX:



• Molecule 11: R-phycoerythrin beta chain

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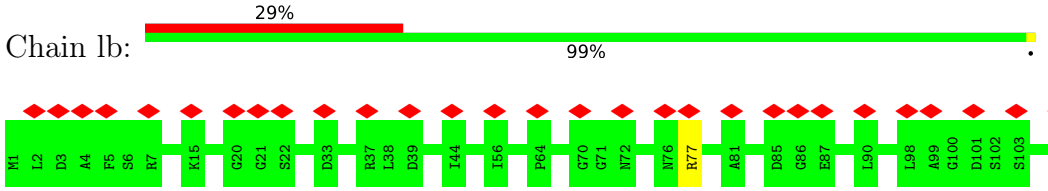

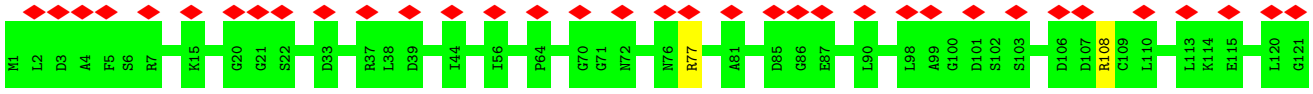

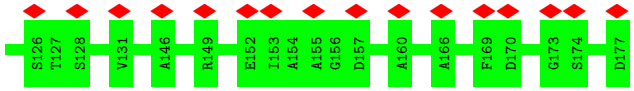

• Molecule 11: R-phycoerythrin beta chain

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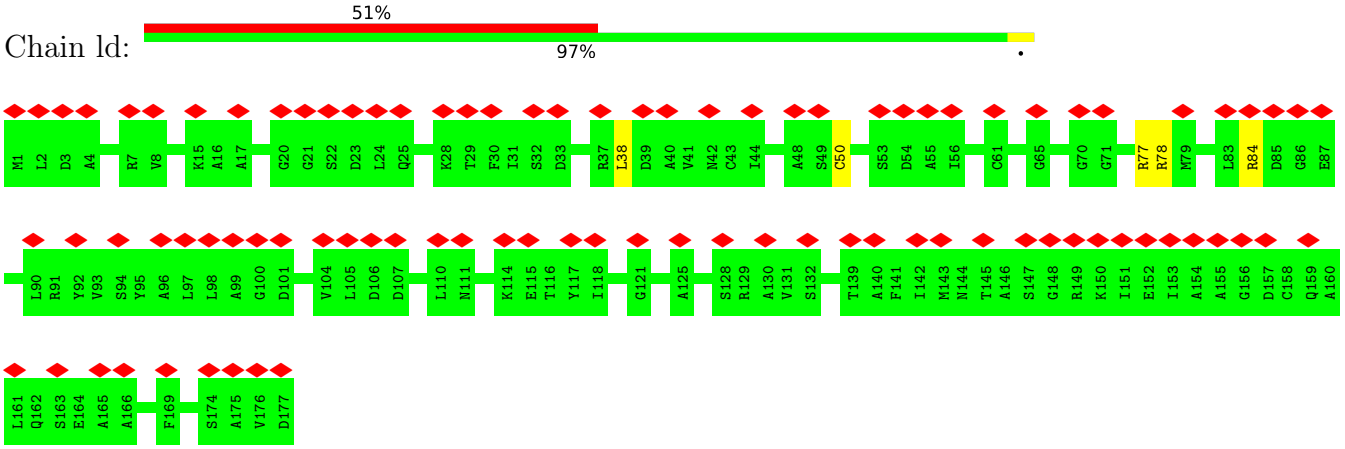
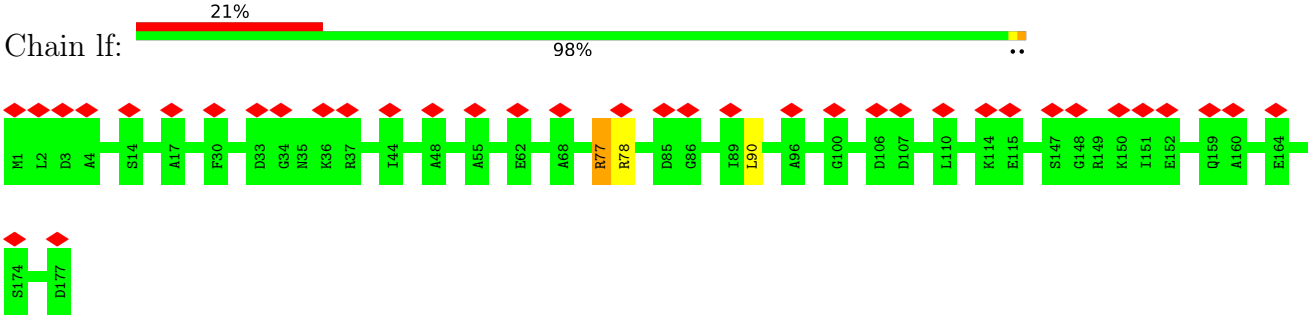


• Molecule 11: R-phycoerythrin beta chain

Chain lf:



• Molecule 11: R-phycoerythrin beta chain

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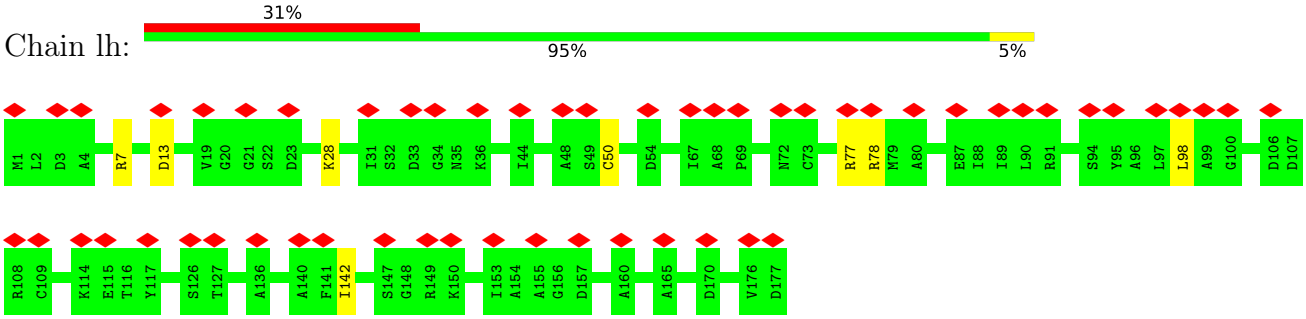
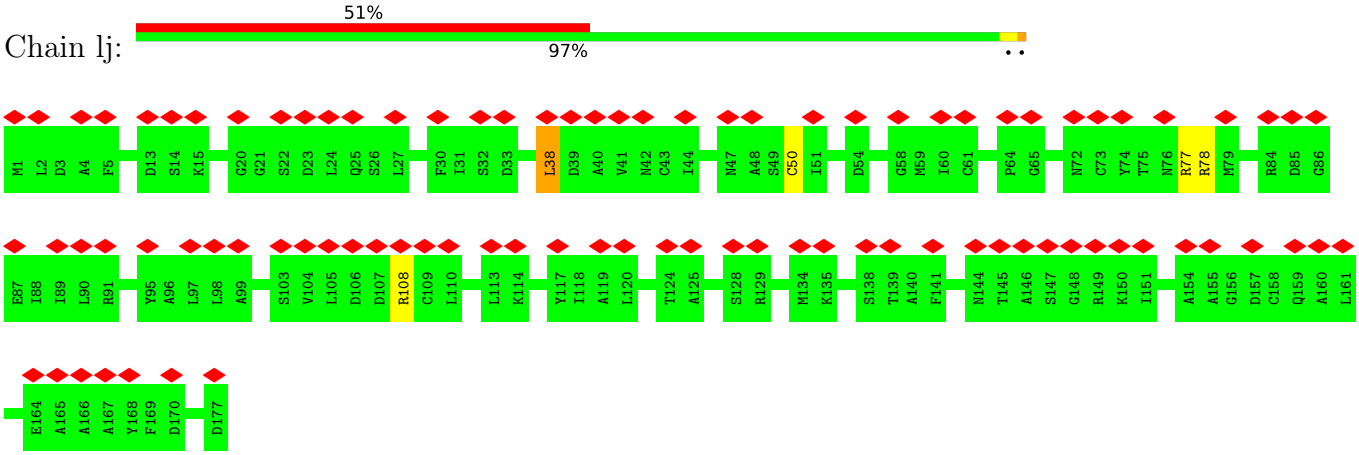


• Molecule 11: R-phycoerythrin beta chain

Chain lj:



• Molecule 11: R-phycoerythrin beta chain

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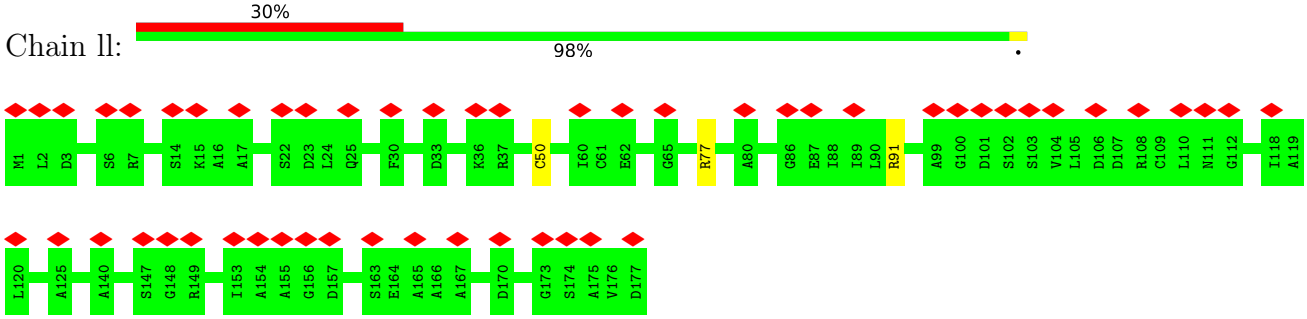

• Molecule 11: R-phycoerythrin beta chain

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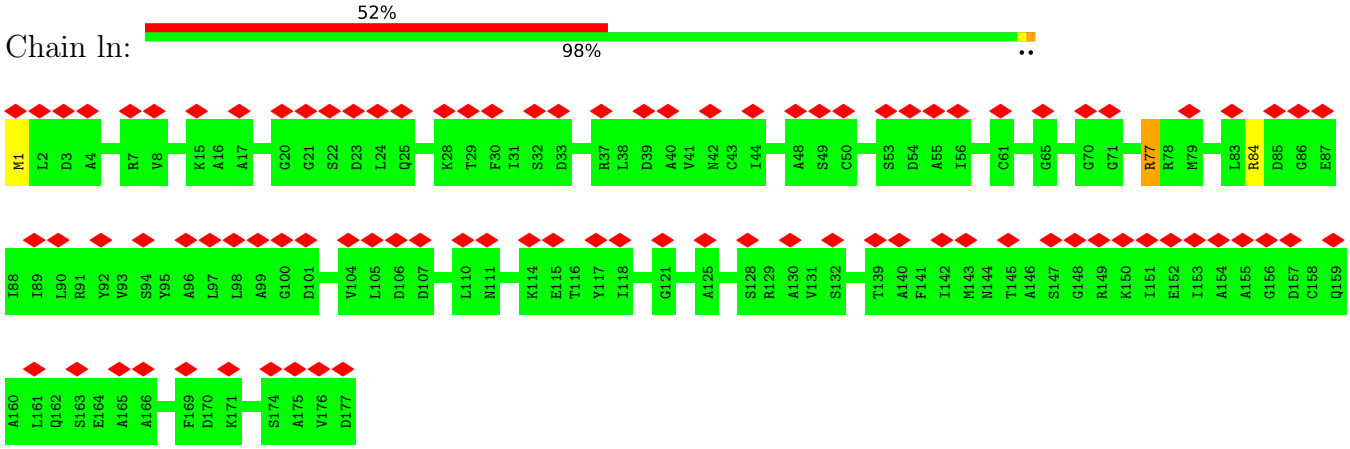

• Molecule 11: R-phycoerythrin beta chain

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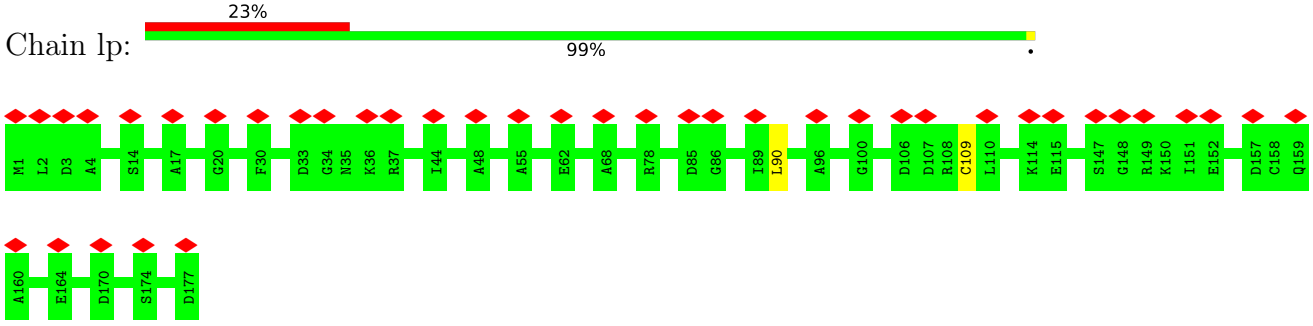

• Molecule 11: R-phycoerythrin beta chain

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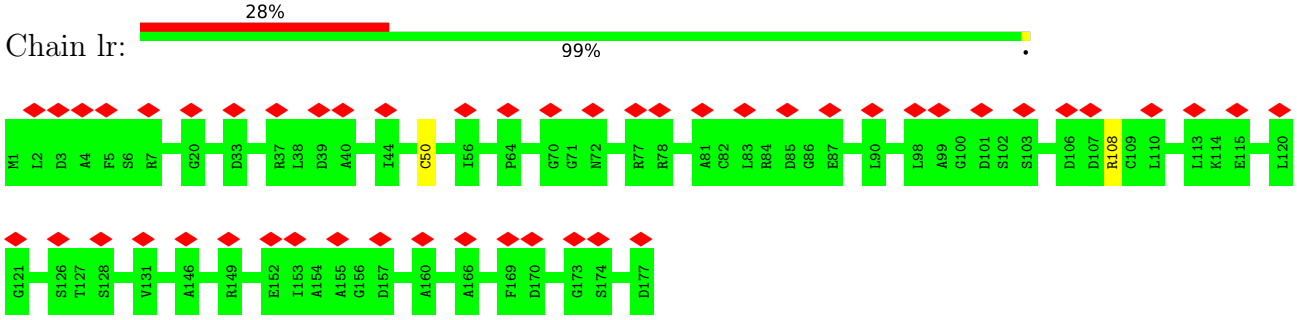

• Molecule 11: R-phycoerythrin beta chain

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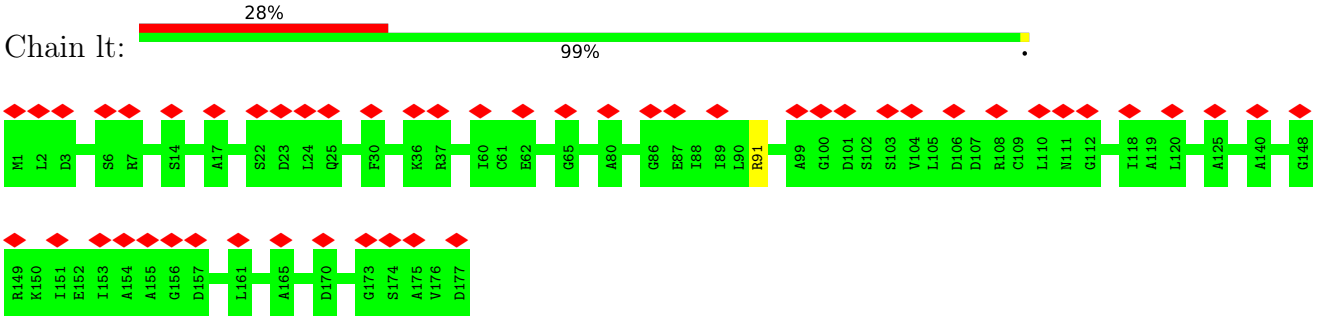

• Molecule 11: R-phycoerythrin beta chain

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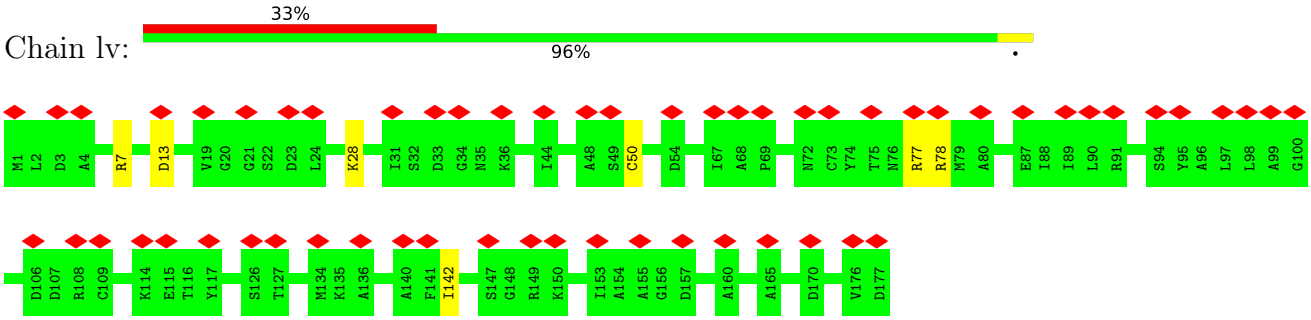
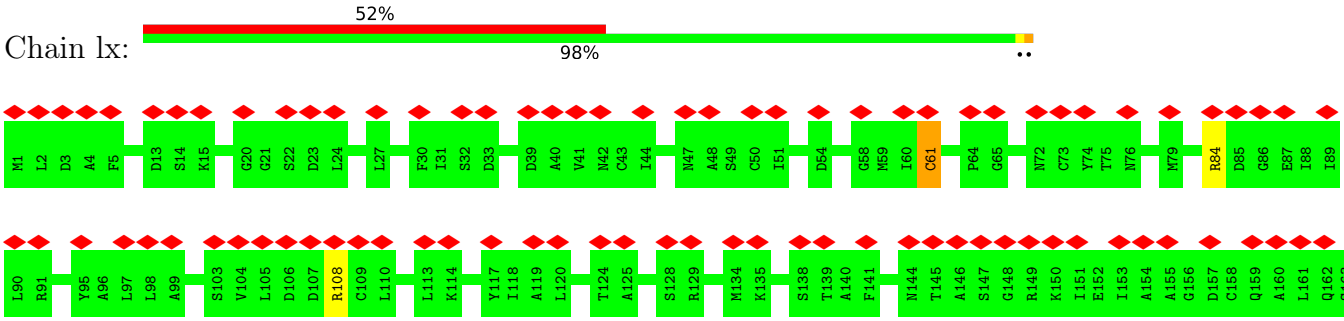


• Molecule 11: R-phycoerythrin beta chain

Chain lx:



• Molecule 11: R-phycoerythrin beta chain

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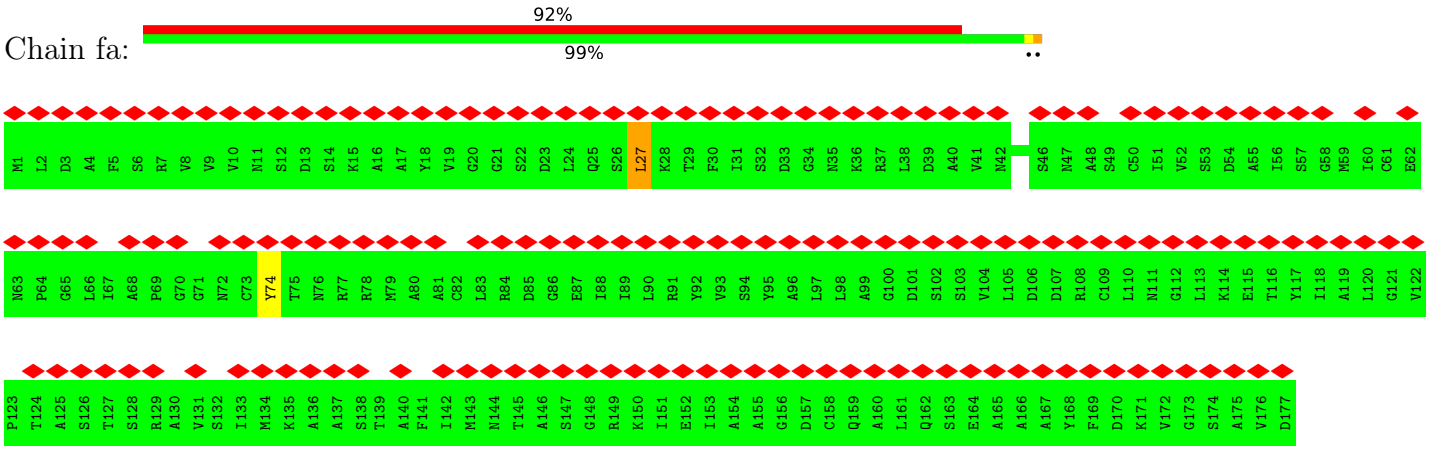
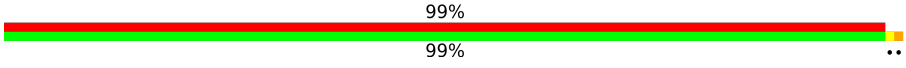
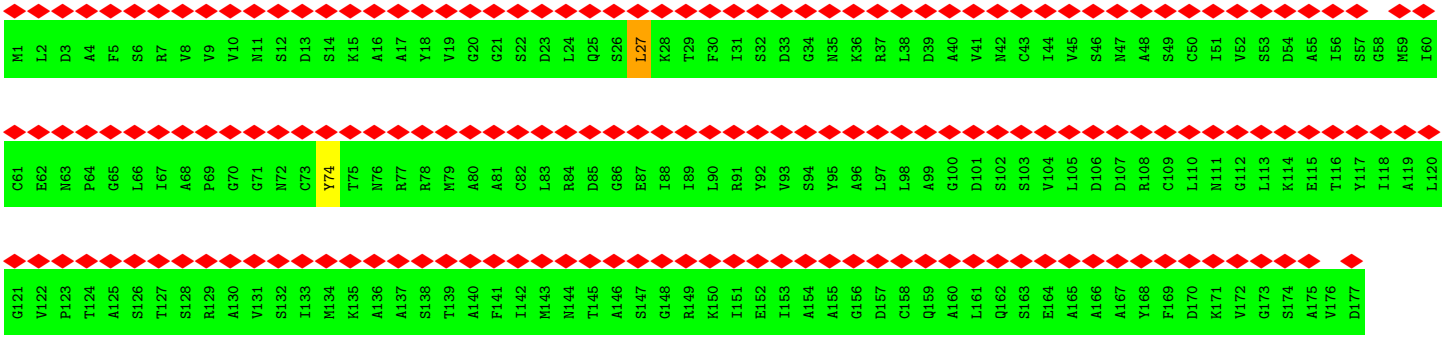


• Molecule 11: R-phycoerythrin beta chain

Chain fc:





• Molecule 11: R-phycoerythrin beta chain

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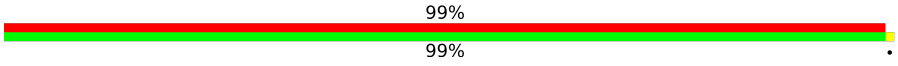

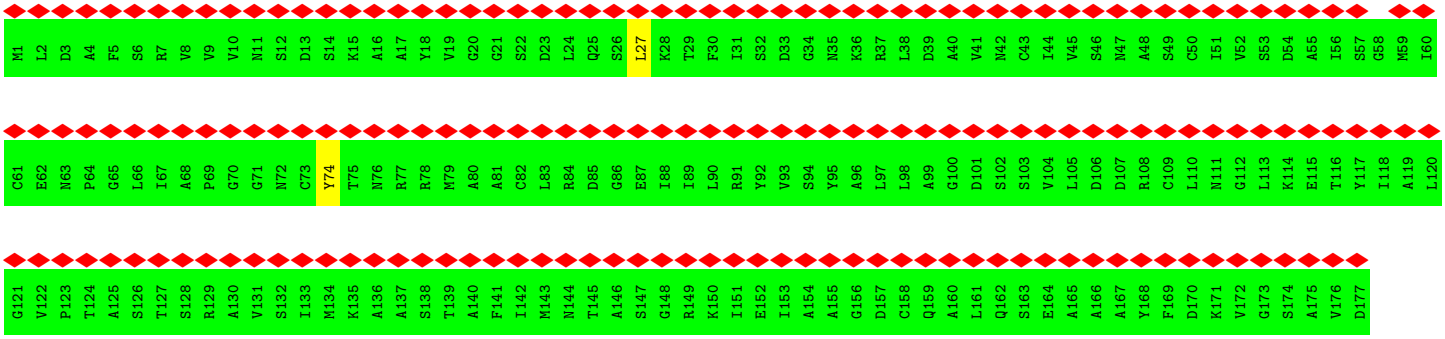

• Molecule 11: R-phycoerythrin beta chain

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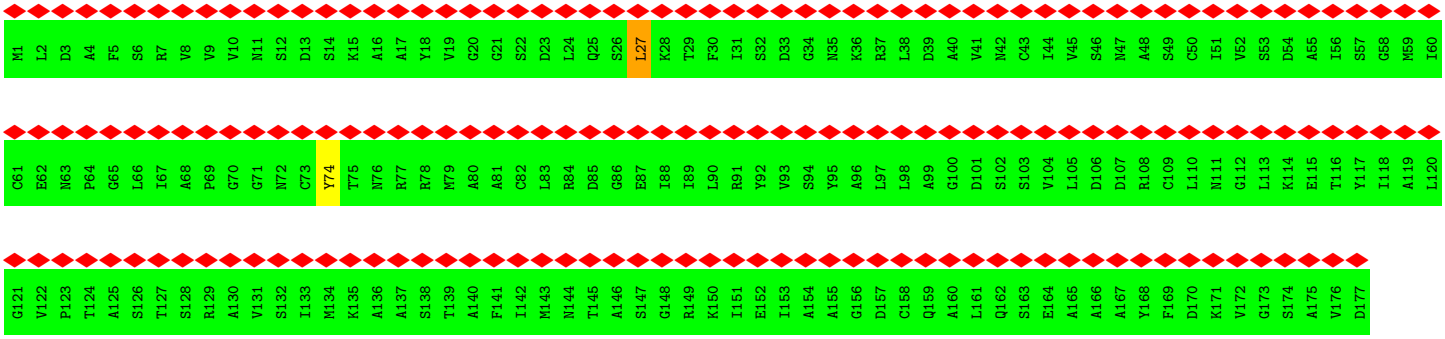

• Molecule 11: R-phycoerythrin beta chain

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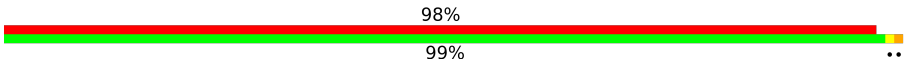

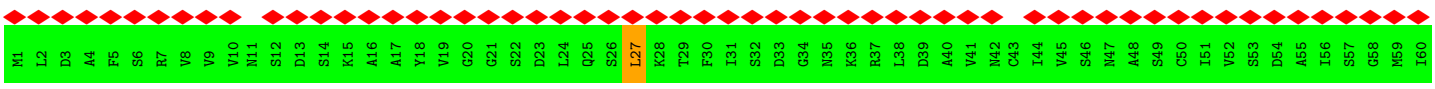

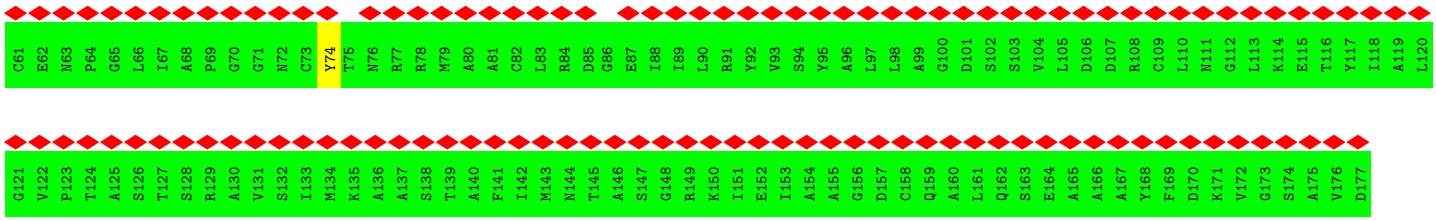

• Molecule 11: R-phycoerythrin beta chain

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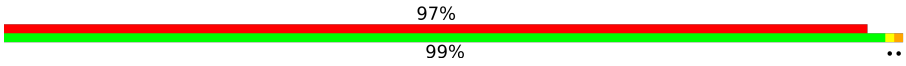
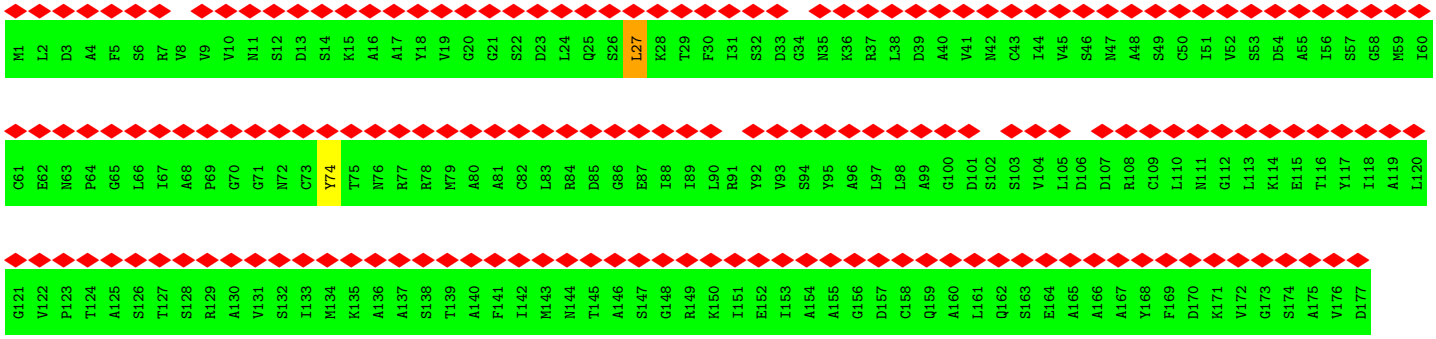
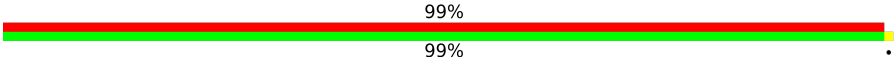
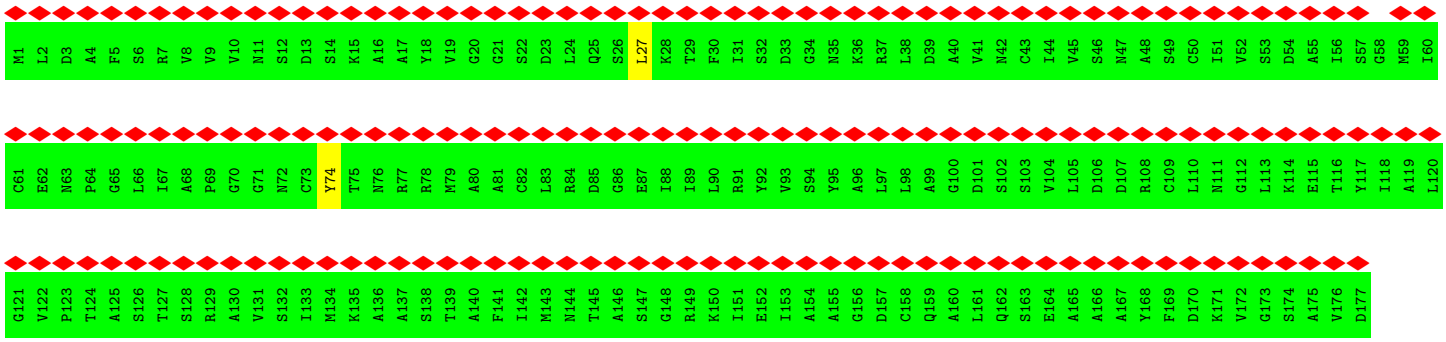




• Molecule 11: R-phycoerythrin beta chain

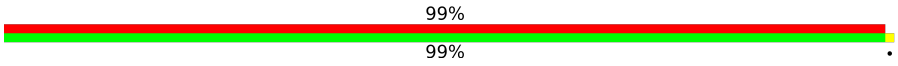
Chain fo:

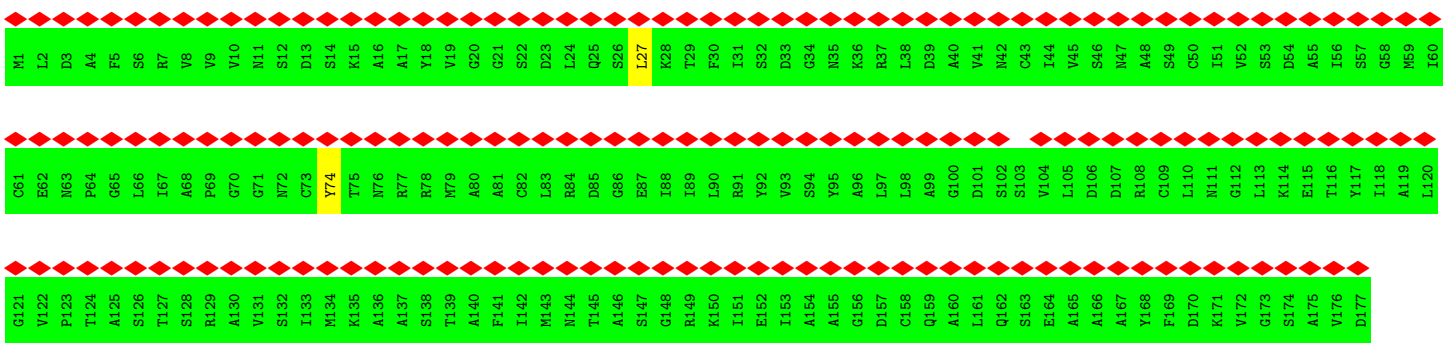




• Molecule 11: R-phycoerythrin beta chain

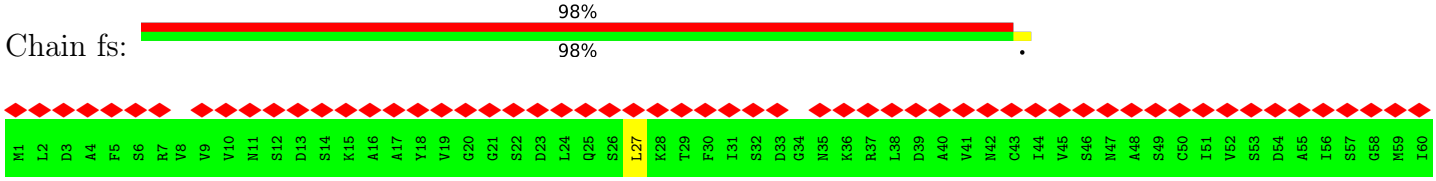
Chain fq:





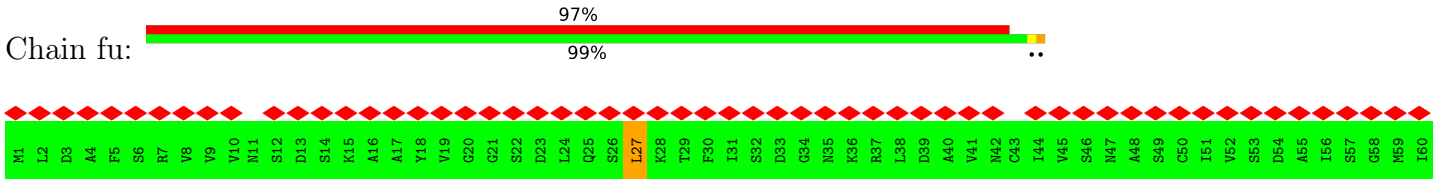
• Molecule 11: R-phycoerythrin beta chain

Chain fs:



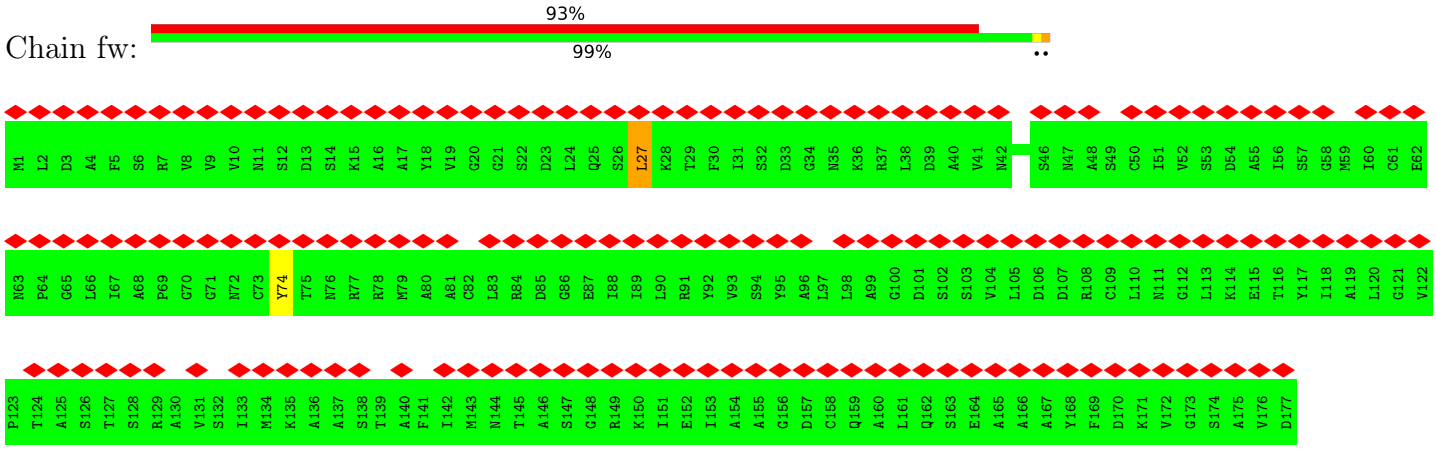
• Molecule 11: R-phycoerythrin beta chain

Chain fu:



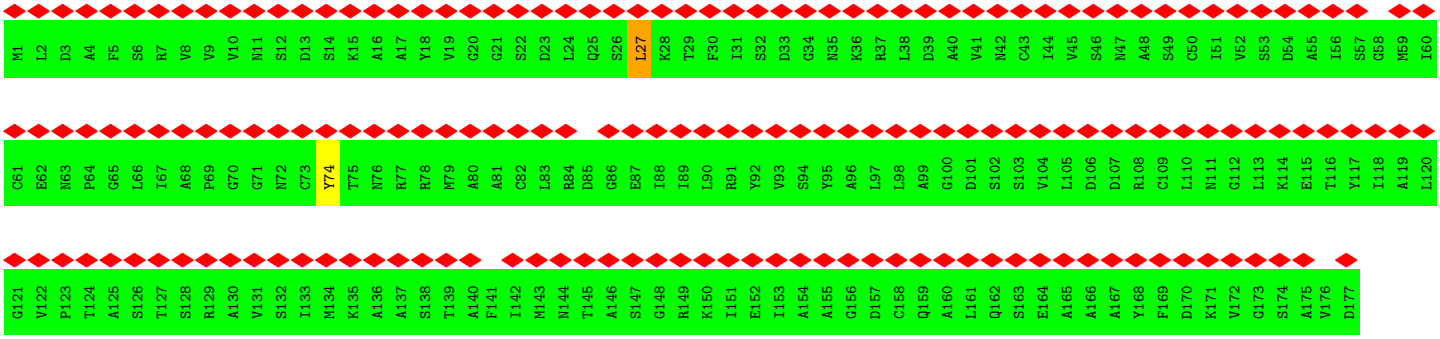
• Molecule 11: R-phycoerythrin beta chain

Chain fw:



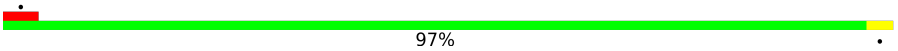
• Molecule 11: R-phycoerythrin beta chain

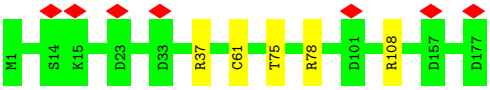
Chain fy:



• Molecule 11: R-phycoerythrin beta chain

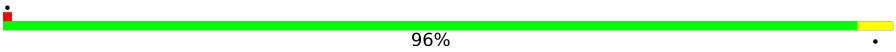
Chain ga:

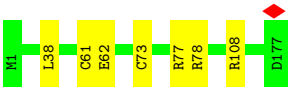




• Molecule 11: R-phycoerythrin beta chain

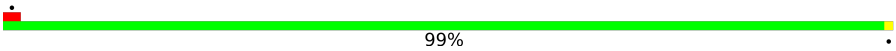
Chain gd:

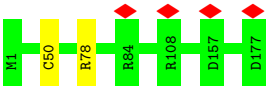




• Molecule 11: R-phycoerythrin beta chain

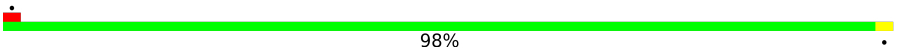
Chain ge:

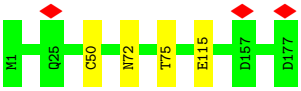




• Molecule 11: R-phycoerythrin beta chain

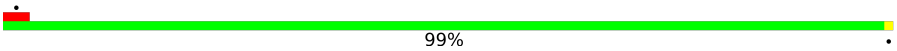
Chain gg:

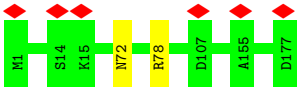




• Molecule 11: R-phycoerythrin beta chain

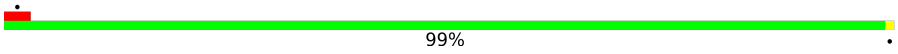
Chain gi:

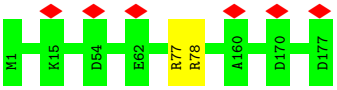




• Molecule 11: R-phycoerythrin beta chain

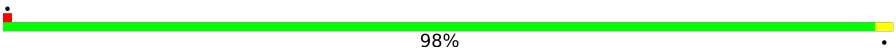
Chain gk:





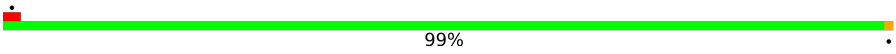
• Molecule 11: R-phycoerythrin beta chain

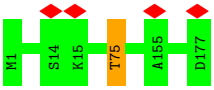
Chain gn:



• Molecule 11: R-phycoerythrin beta chain

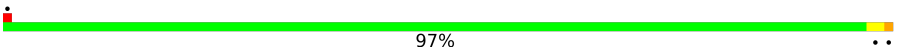
Chain gp:

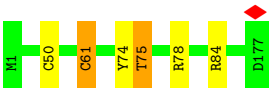




• Molecule 11: R-phycoerythrin beta chain

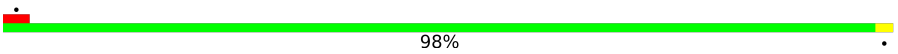
Chain gr:

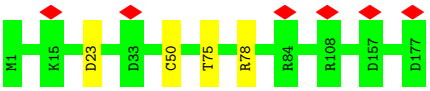




• Molecule 11: R-phycoerythrin beta chain

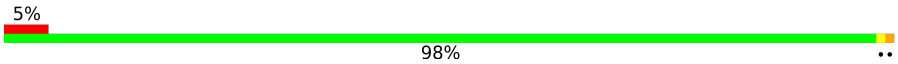
Chain gt:

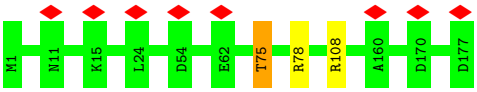




• Molecule 11: R-phycoerythrin beta chain

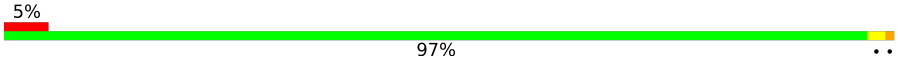
Chain gv:

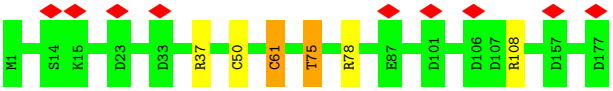




• Molecule 11: R-phycoerythrin beta chain

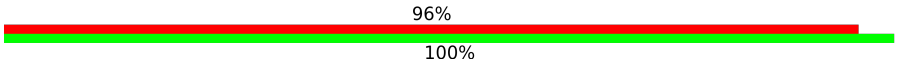
Chain gx:

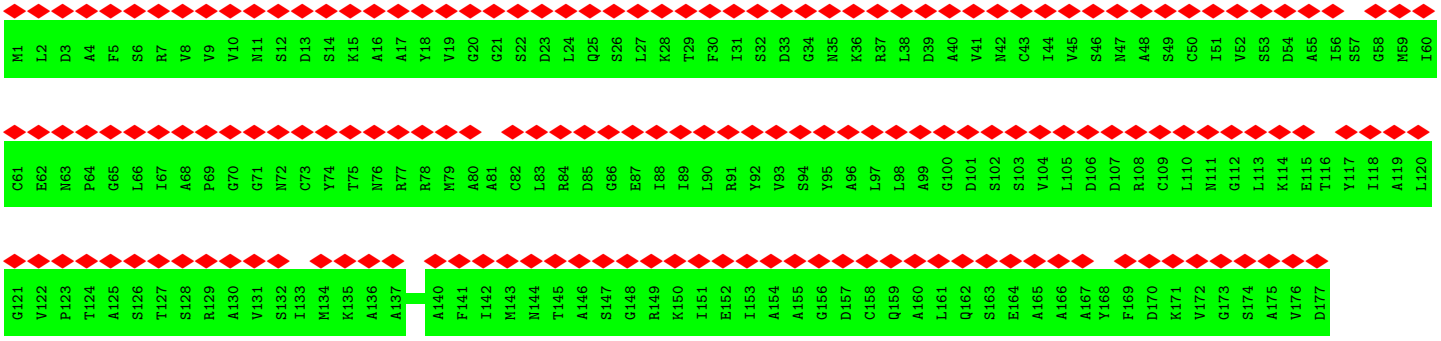




• Molecule 11: R-phycoerythrin beta chain

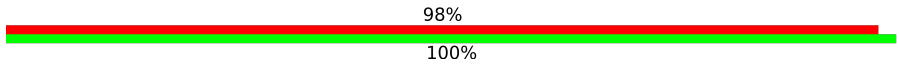
Chain hB:

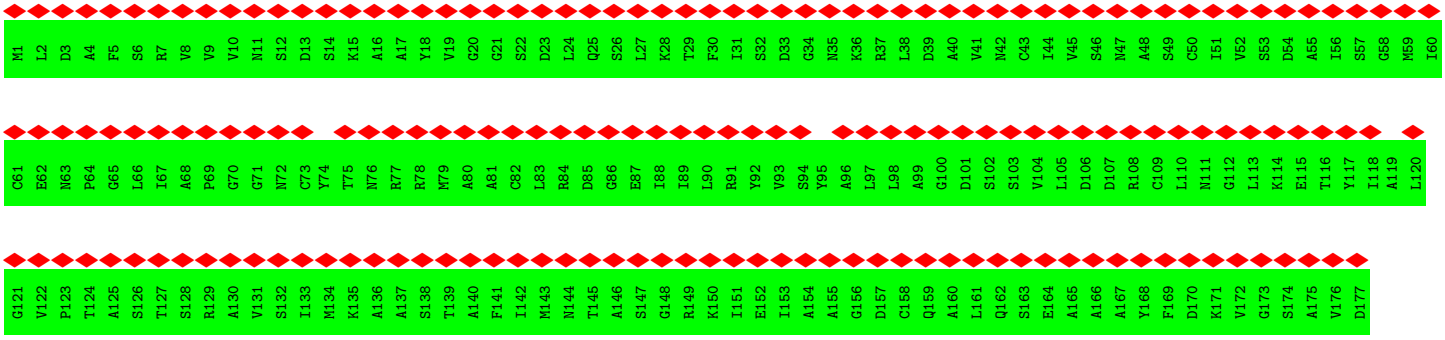




• Molecule 11: R-phycoerythrin beta chain

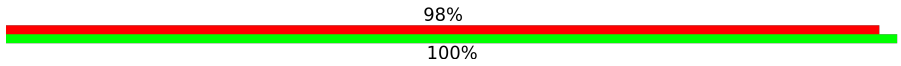
Chain hD:

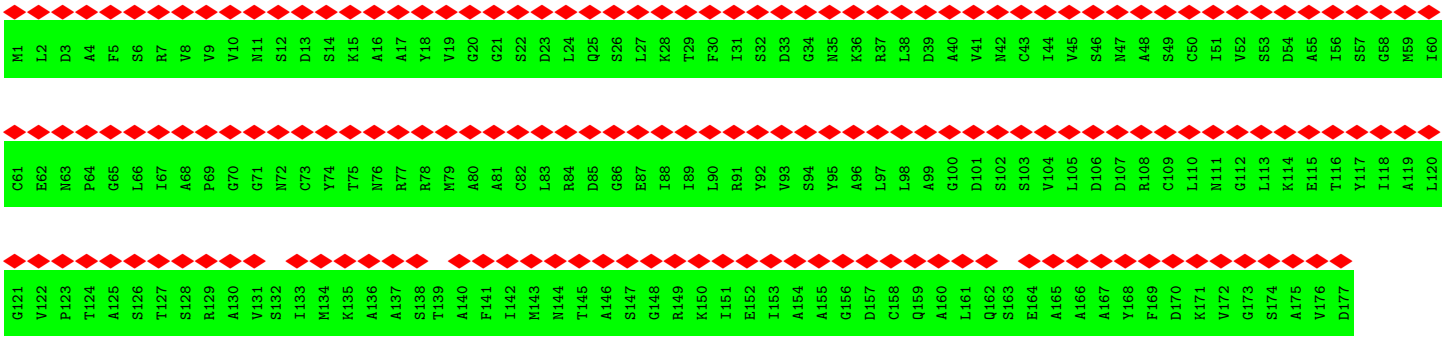




• Molecule 11: R-phycoerythrin beta chain

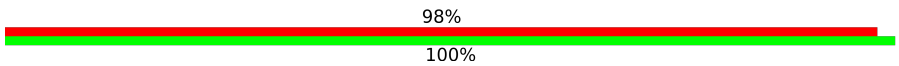
Chain hG:





• Molecule 11: R-phycoerythrin beta chain

Chain hH:



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C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain hJ: 97% 100%

M1 L2 D3 A4 F5 S6 R7 V8 V9 V10 N11 S12 D13 S14 K15 A16 A17 Y18 V19 G20 G21 S22 D23 L24 Q25 S26 L27 K28 T29 F30 I31 S32 D33 G34 N35 K36 R37 L38 D39 A40 V41 N42 C43 I44 V45 S46 N47 A48 S49 C50 I51 V52 S53 D54 A55 I56 S57 G58 M59 I60

C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain hL: 98% 100%

M1 L2 D3 A4 F5 S6 R7 V8 V9 V10 N11 S12 D13 S14 K15 A16 A17 Y18 V19 G20 G21 S22 D23 L24 Q25 S26 L27 K28 T29 F30 I31 S32 D33 G34 N35 K36 R37 L38 D39 A40 V41 N42 C43 I44 V45 S46 N47 A48 S49 C50 I51 V52 S53 D54 A55 I56 S57 G58 M59 I60

C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain hN: 98% 100%

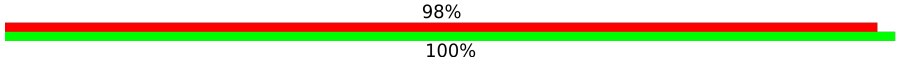
M1 L2 D3 A4 F5 S6 R7 V8 V9 V10 N11 S12 D13 S14 K15 A16 A17 Y18 V19 G20 G21 S22 D23 L24 Q25 S26 L27 K28 T29 F30 I31 S32 D33 G34 N35 K36 R37 L38 D39 A40 V41 N42 C43 I44 V45 S46 N47 A48 S49 C50 I51 V52 S53 D54 A55 I56 S57 G58 M59 I60

C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain hP:



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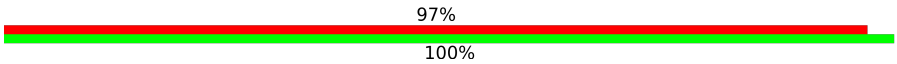
C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain hR:



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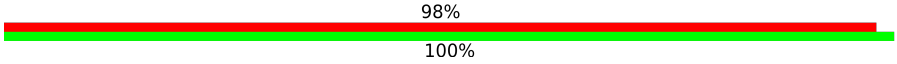
C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

Chain hT:



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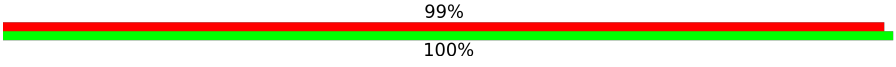
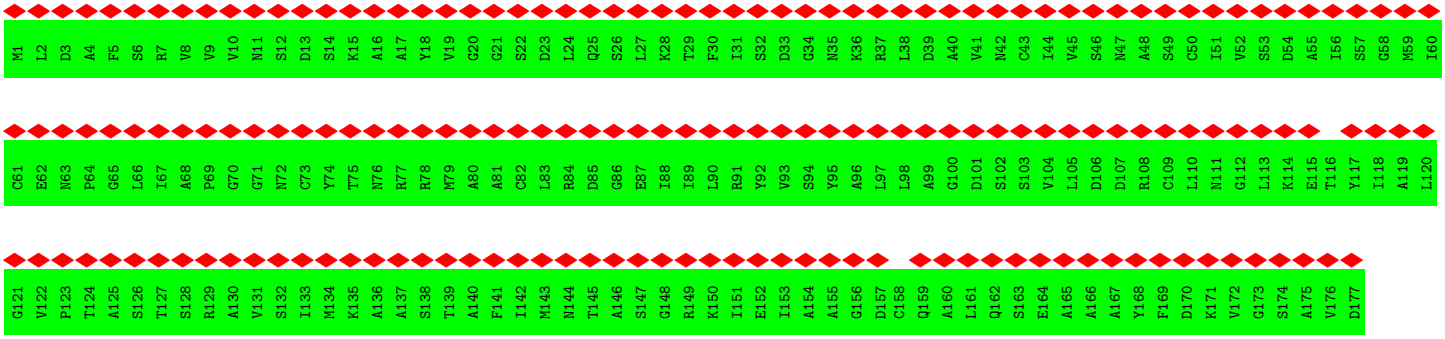
C61 E62 N63 P64 G65 L66 I67 A68 P69 G70 G71 N72 C73 Y74 T75 N76 R77 R78 M79 A80 A81 C82 L83 R84 D85 G86 E87 I88 I89 L90 R91 Y92 V93 S94 Y95 A96 L97 L98 A99 G100 D101 S102 S103 V104 L105 D106 D107 R108 C109 L110 N111 G112 L113 K114 E115 T116 Y117 I118 A119 L120

G121 V122 P123 T124 A125 S126 T127 S128 R129 A130 V131 S132 I133 M134 K135 A136 A137 S138 T139 A140 F141 I142 M143 N144 T145 A146 S147 G148 R149 K150 I151 E152 I153 A154 A155 G156 D157 C158 Q159 A160 L161 Q162 S163 E164 A165 A166 A167 Y168 F169 D170 K171 V172 G173 S174 A175 V176 D177

• Molecule 11: R-phycoerythrin beta chain

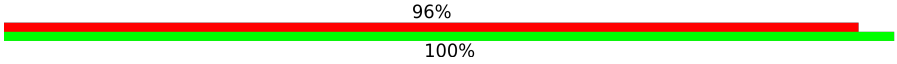
Chain hV:

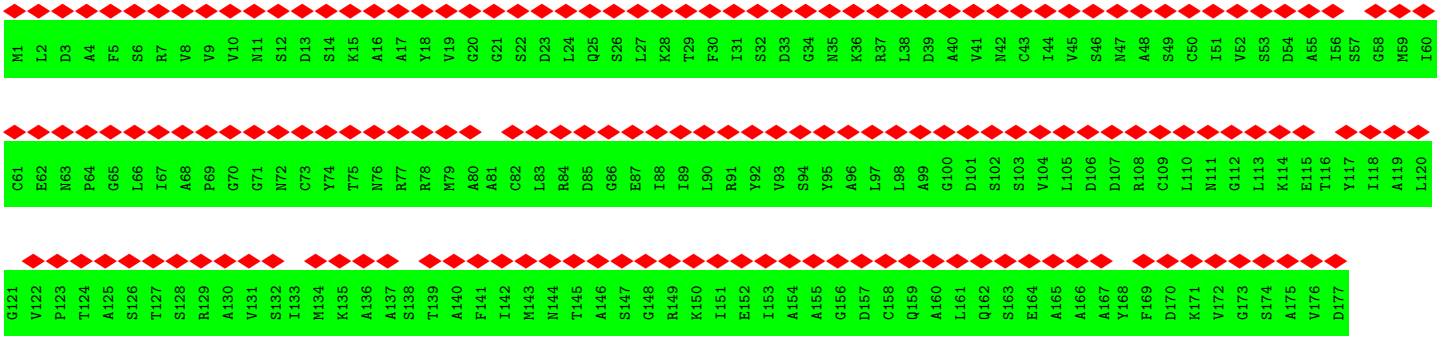




• Molecule 11: R-phycoerythrin beta chain

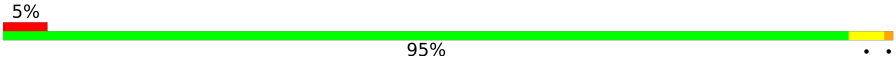
Chain hX:

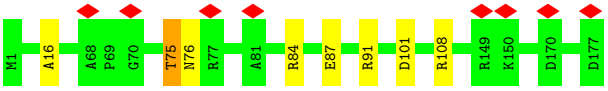




• Molecule 11: R-phycoerythrin beta chain

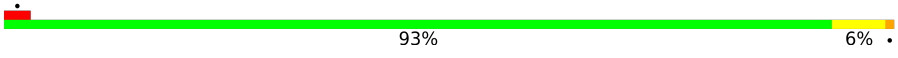
Chain iC:

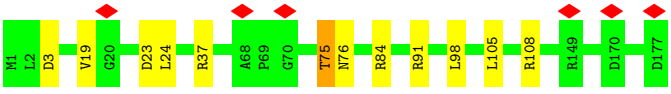




• Molecule 11: R-phycoerythrin beta chain

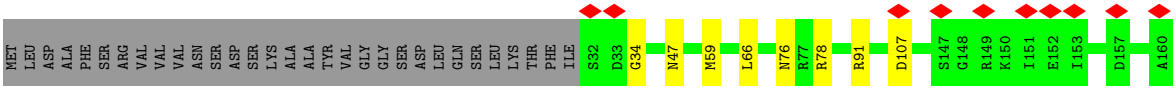
Chain iD:





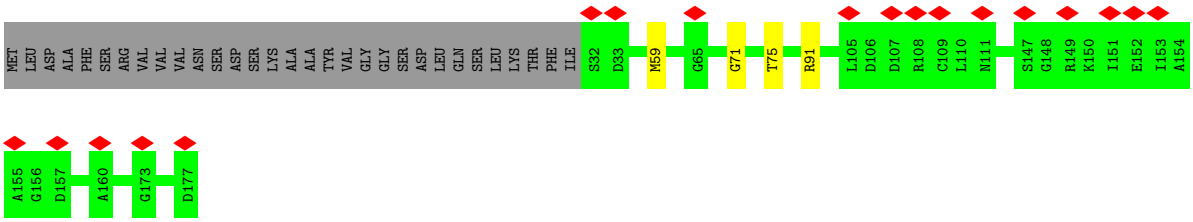
• Molecule 11: R-phycoerythrin beta chain

Chain iE:



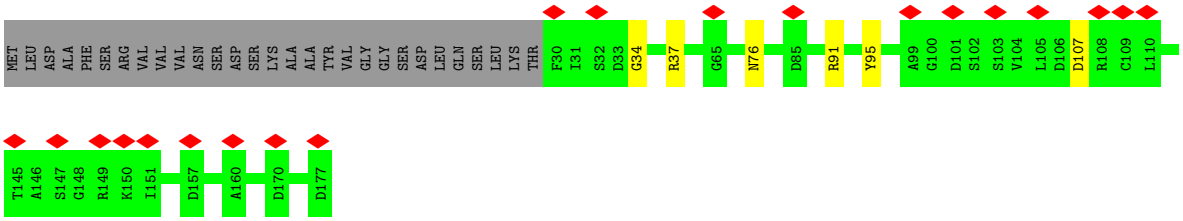
• Molecule 11: R-phycoerythrin beta chain

Chain iF:



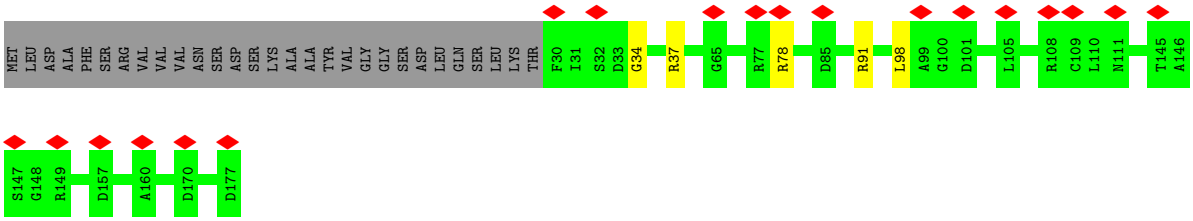
• Molecule 11: R-phycoerythrin beta chain

Chain iG:



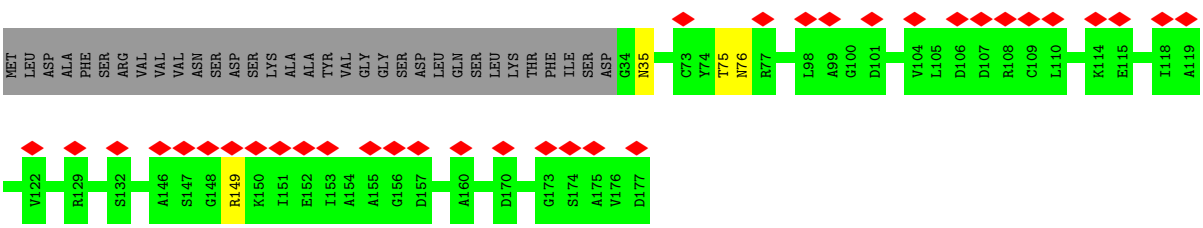
• Molecule 11: R-phycoerythrin beta chain

Chain iH:



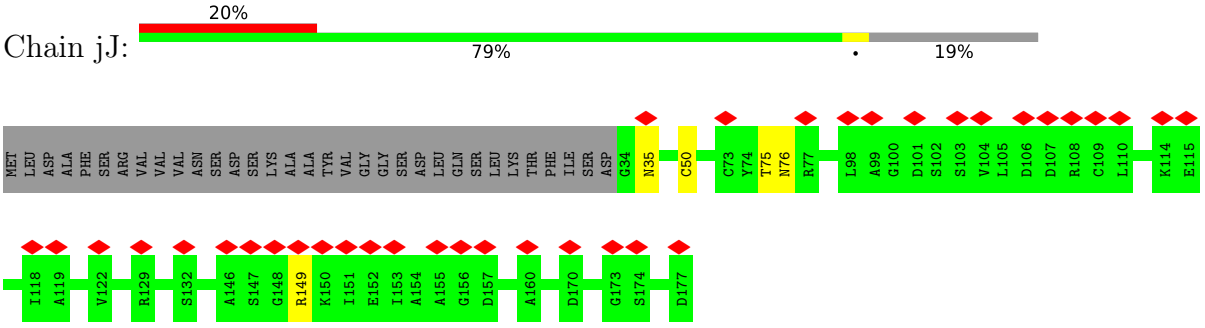
• Molecule 11: R-phycoerythrin beta chain

Chain jI:



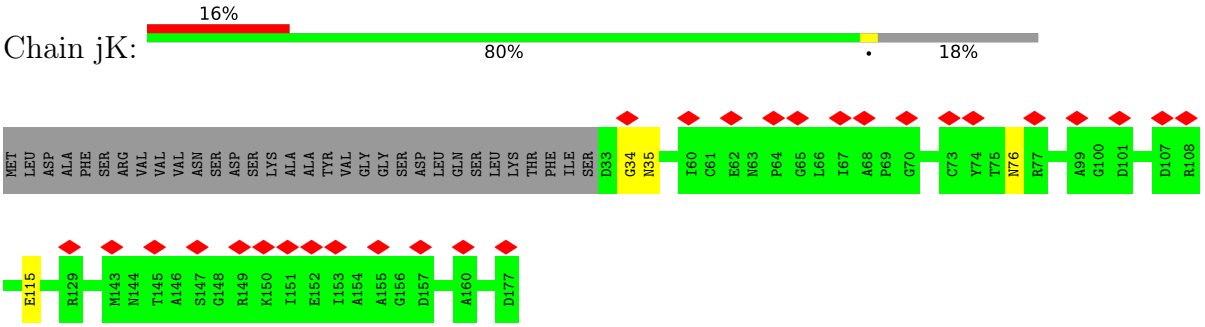
• Molecule 11: R-phycoerythrin beta chain

Chain jJ:



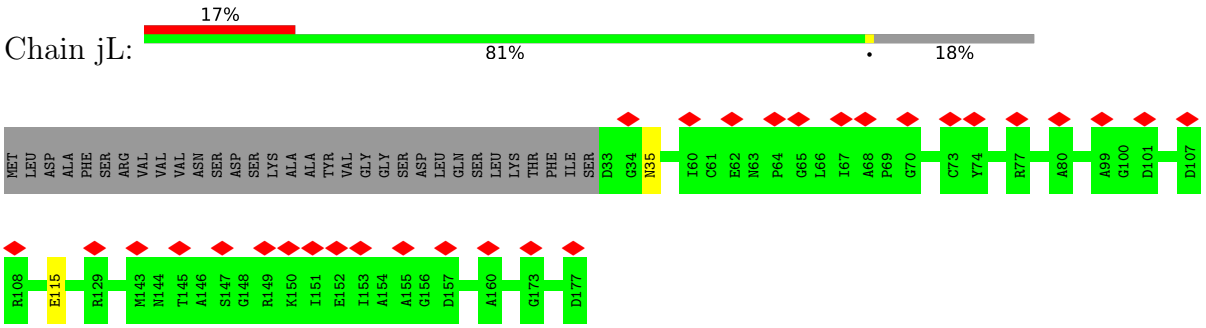
• Molecule 11: R-phycoerythrin beta chain

Chain jK:



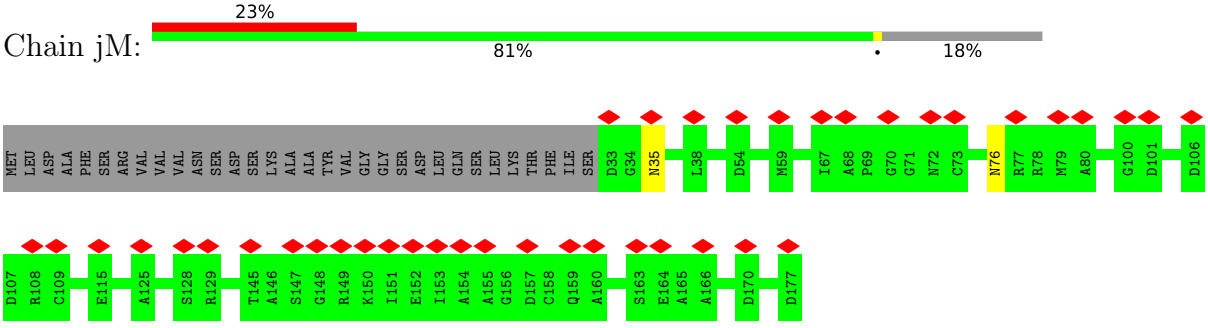
• Molecule 11: R-phycoerythrin beta chain

Chain jL:



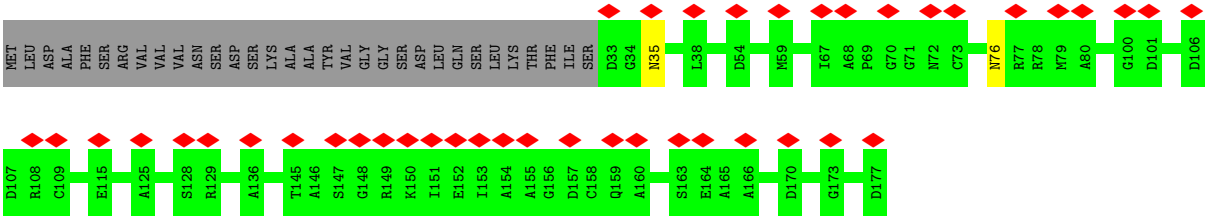
• Molecule 11: R-phycoerythrin beta chain

Chain jM:



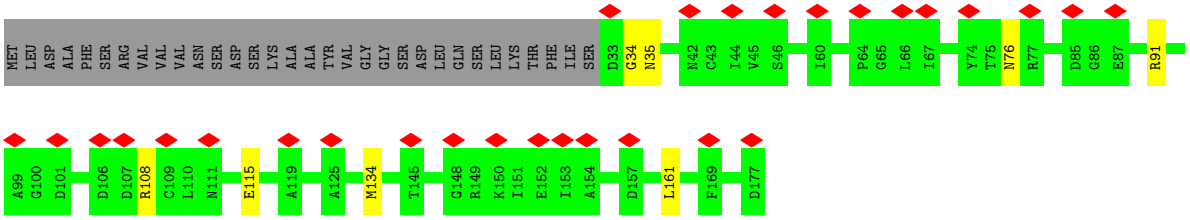
• Molecule 11: R-phycoerythrin beta chain

Chain jN:



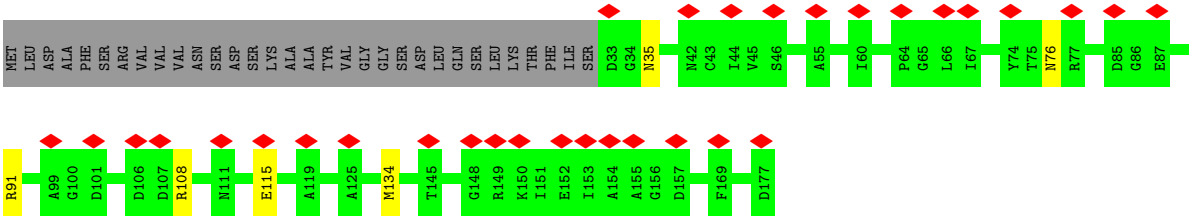
• Molecule 11: R-phycoerythrin beta chain

Chain jO:



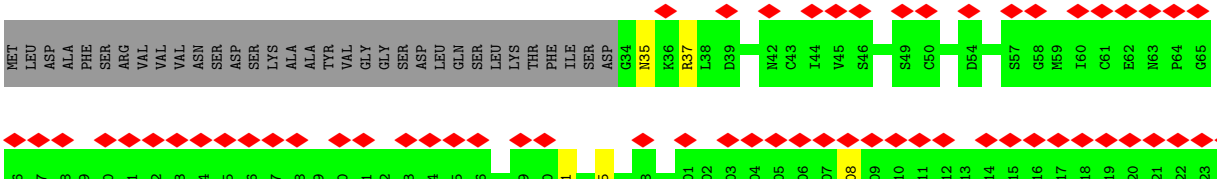
• Molecule 11: R-phycoerythrin beta chain

Chain jP:



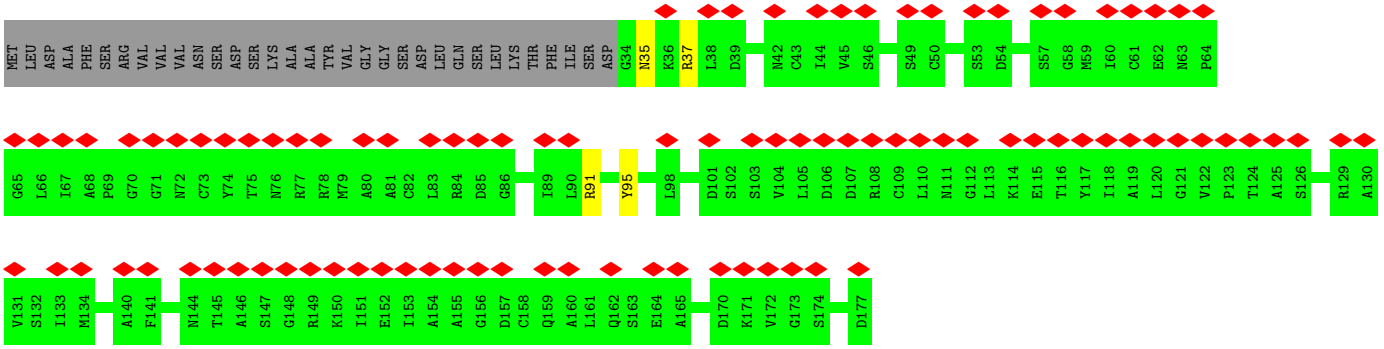
• Molecule 11: R-phycoerythrin beta chain

Chain kQ:



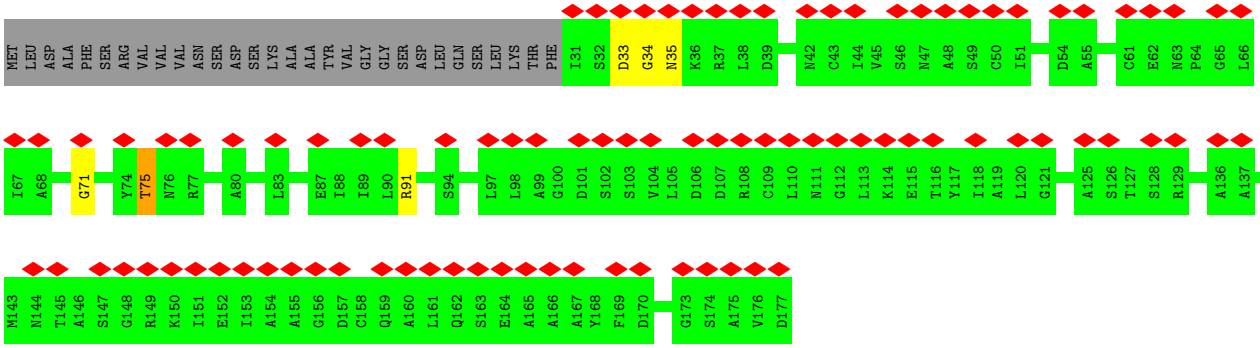
• Molecule 11: R-phycoerythrin beta chain

Chain kR:



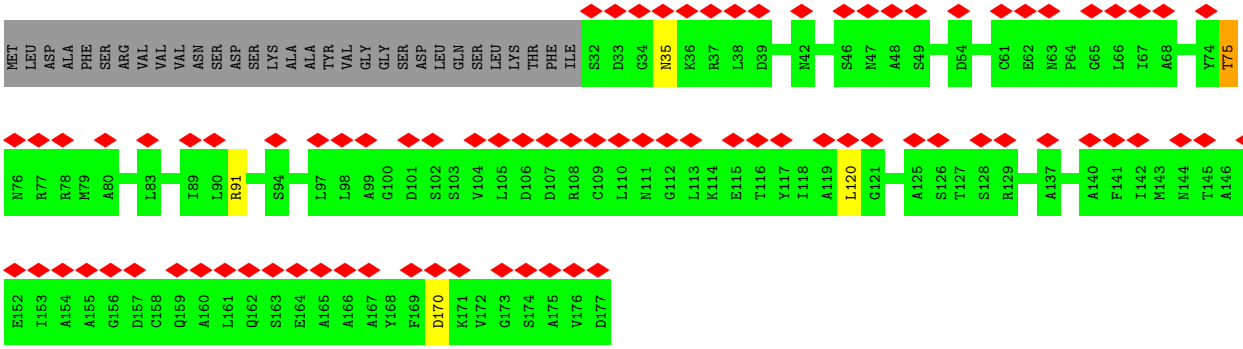
• Molecule 11: R-phycoerythrin beta chain

Chain kS:



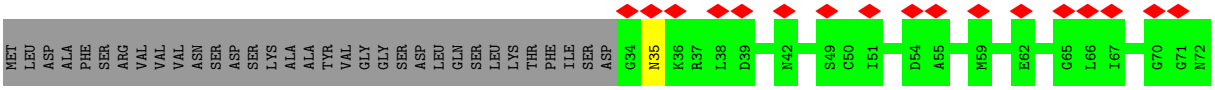
• Molecule 11: R-phycoerythrin beta chain

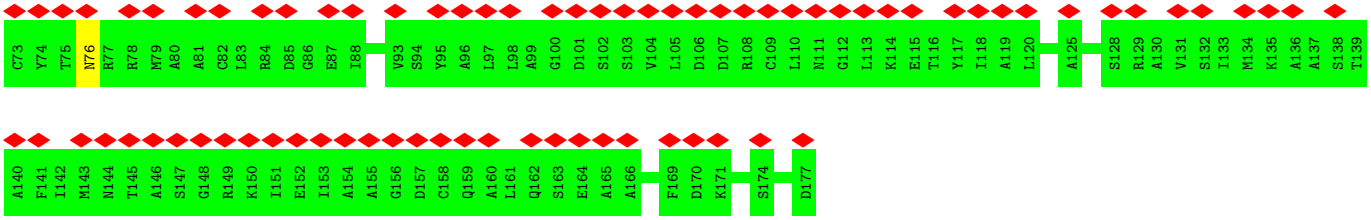
Chain kT:



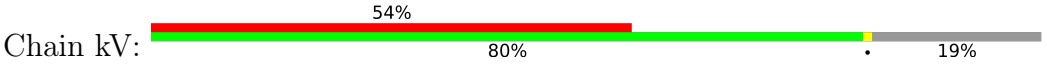
• Molecule 11: R-phycoerythrin beta chain

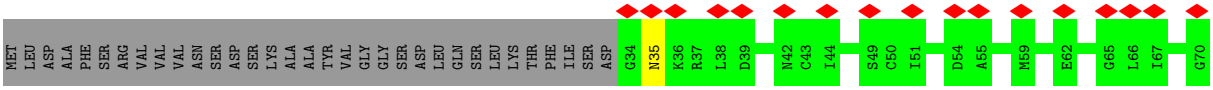
Chain kU:

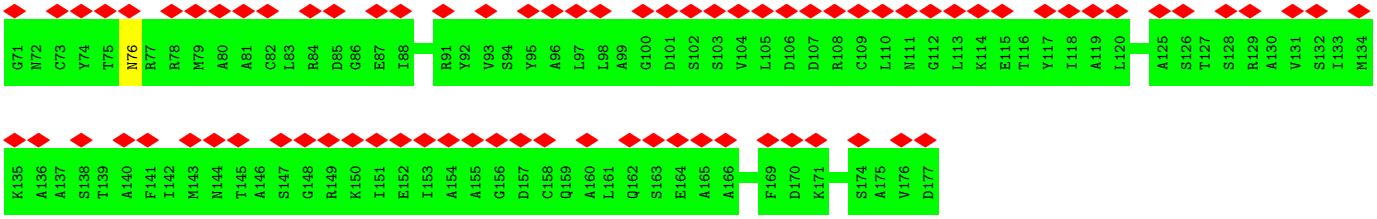




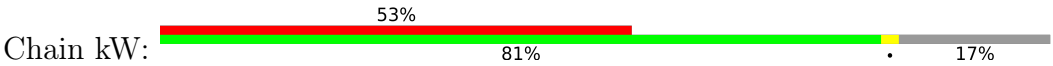
• Molecule 11: R-phycoerythrin beta chain

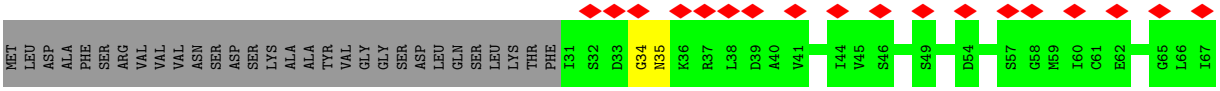


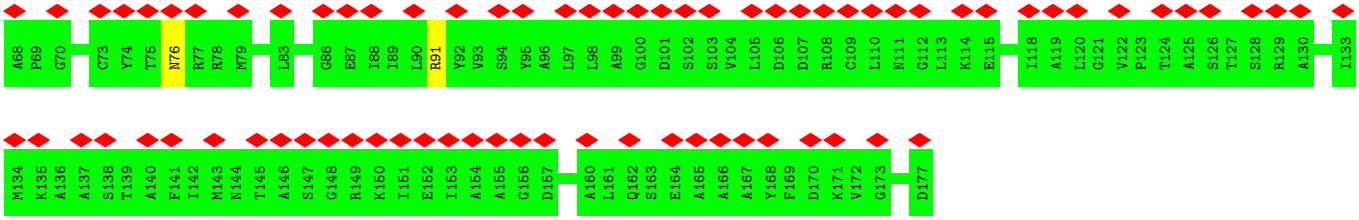




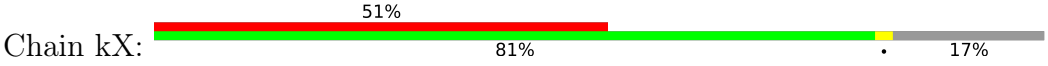
• Molecule 11: R-phycoerythrin beta chain

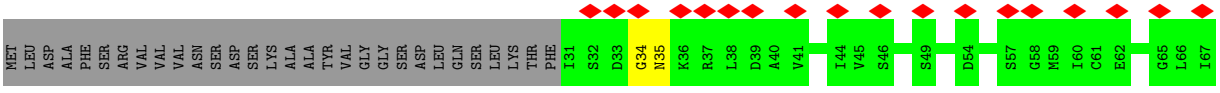


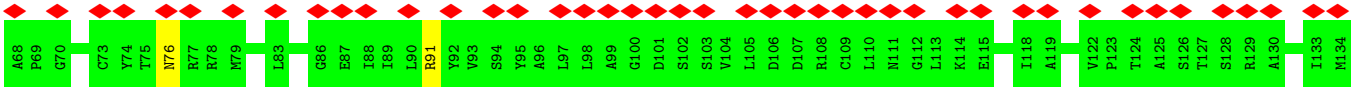


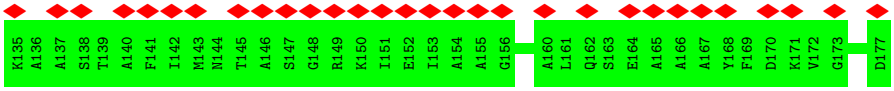


• Molecule 11: R-phycoerythrin beta chain



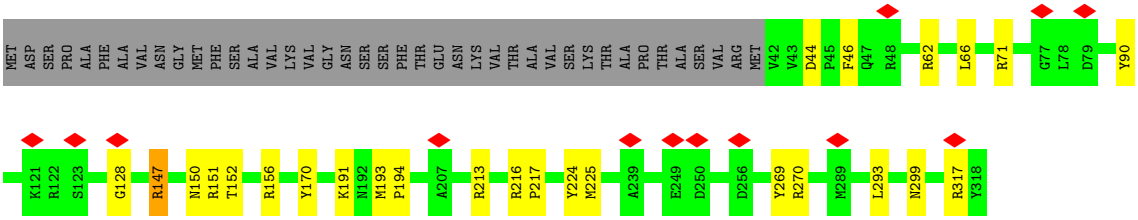






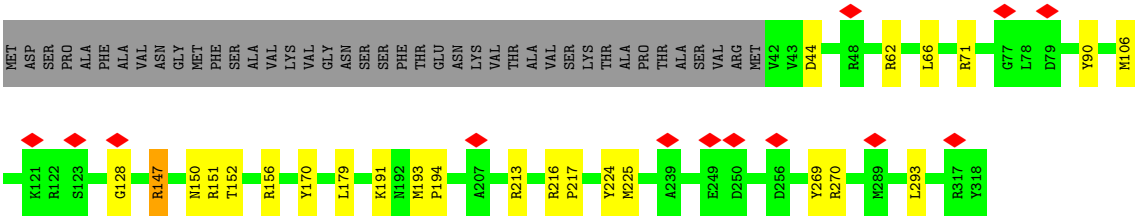
• Molecule 12: LR_gamma4

Chain A2:



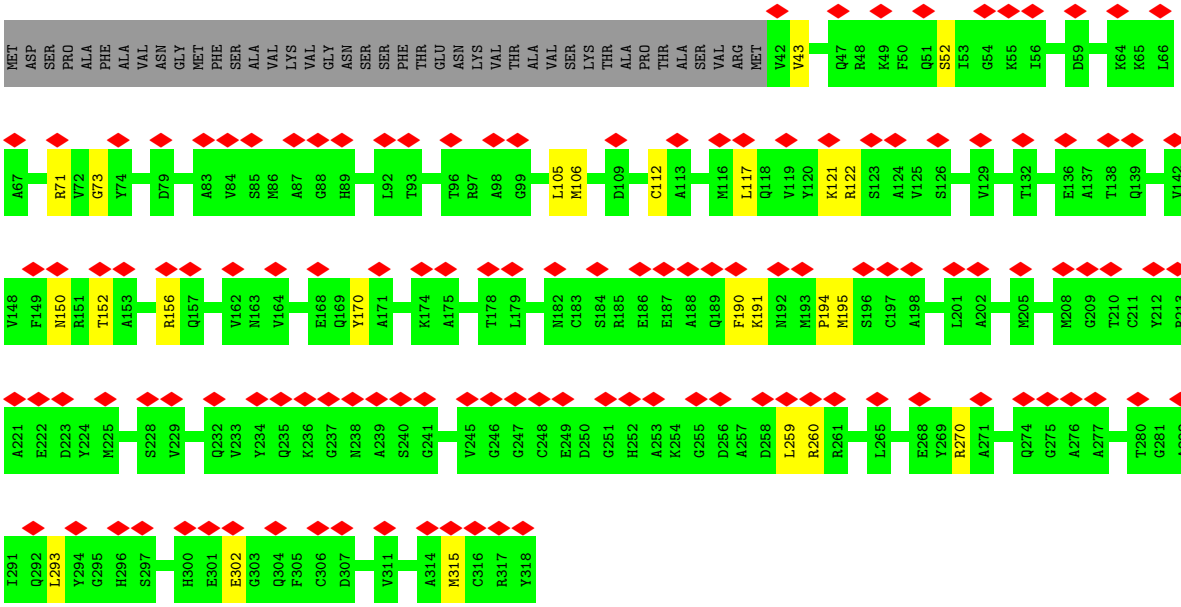
• Molecule 12: LR_gamma4

Chain a3:



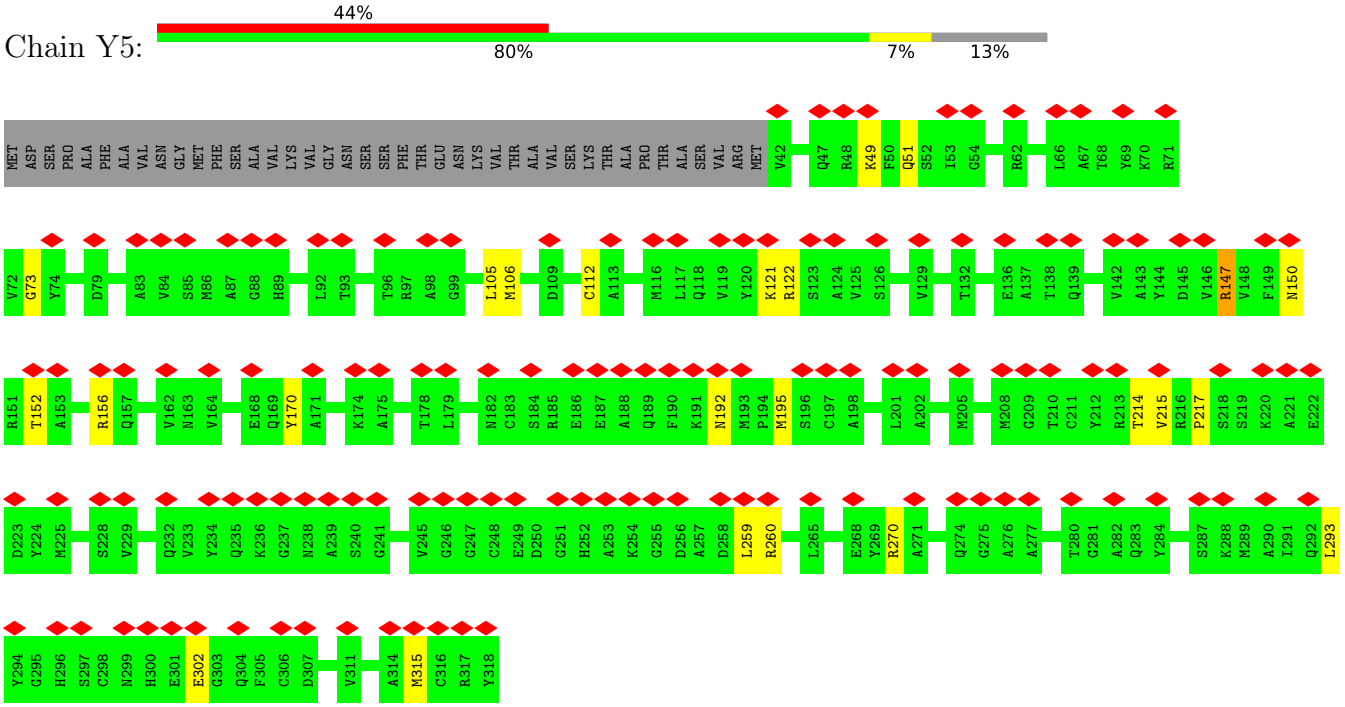
• Molecule 12: LR_gamma4

Chain 34:



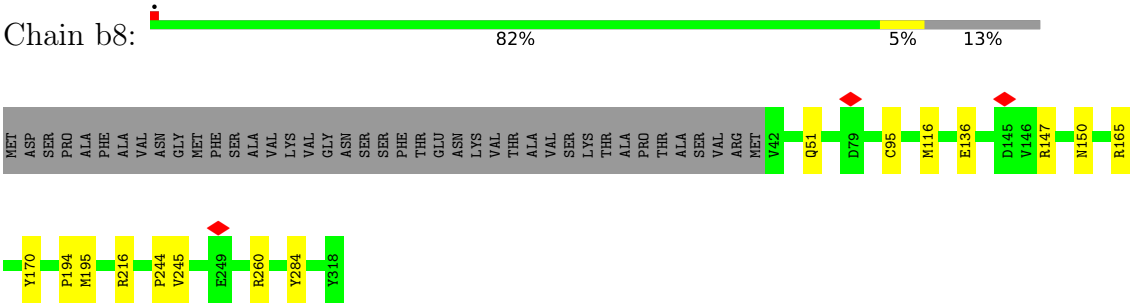
• Molecule 12: LR_gamma4

Chain Y5:



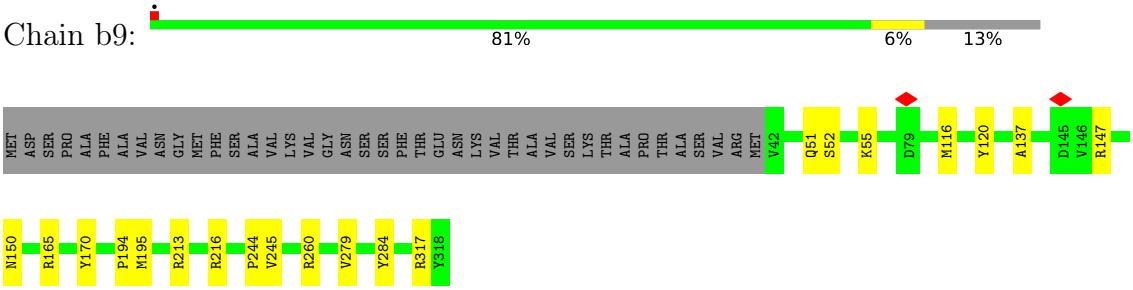
• Molecule 12: LR_gamma4

Chain b8:



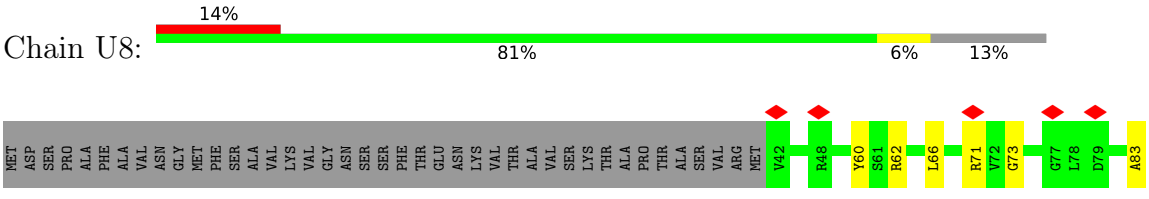
• Molecule 12: LR_gamma4

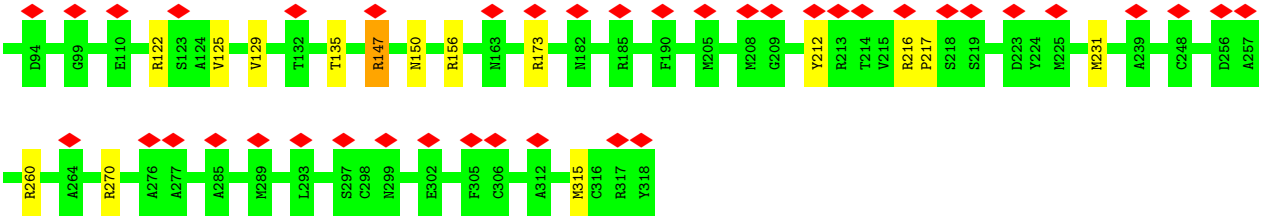
Chain b9:



• Molecule 12: LR_gamma4

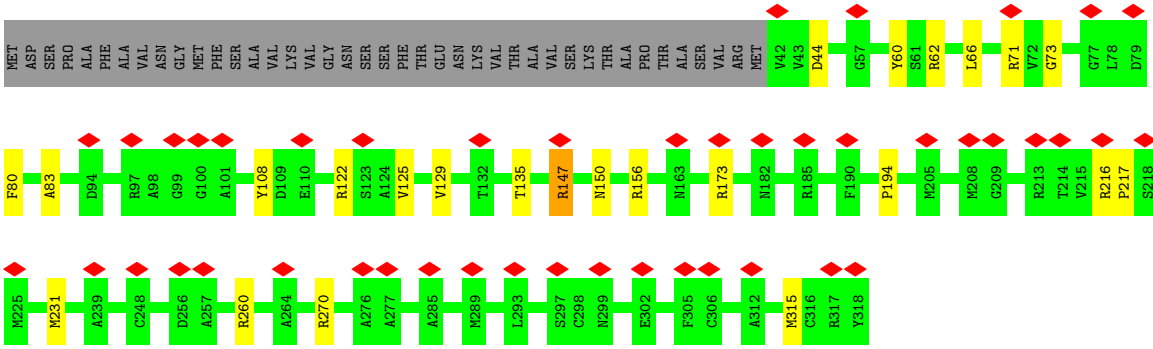
Chain U8:





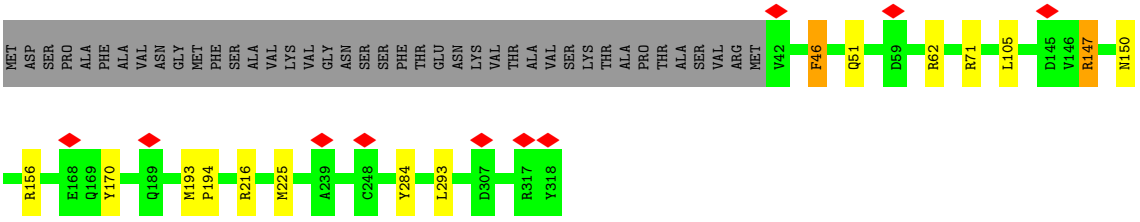
• Molecule 12: LR_gamma4

Chain Z9:



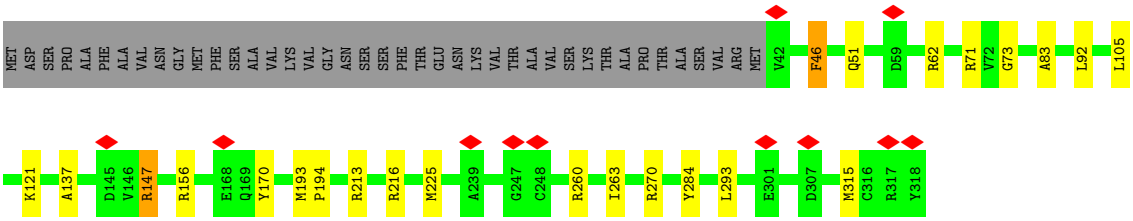
• Molecule 12: LR_gamma4

Chain aY:



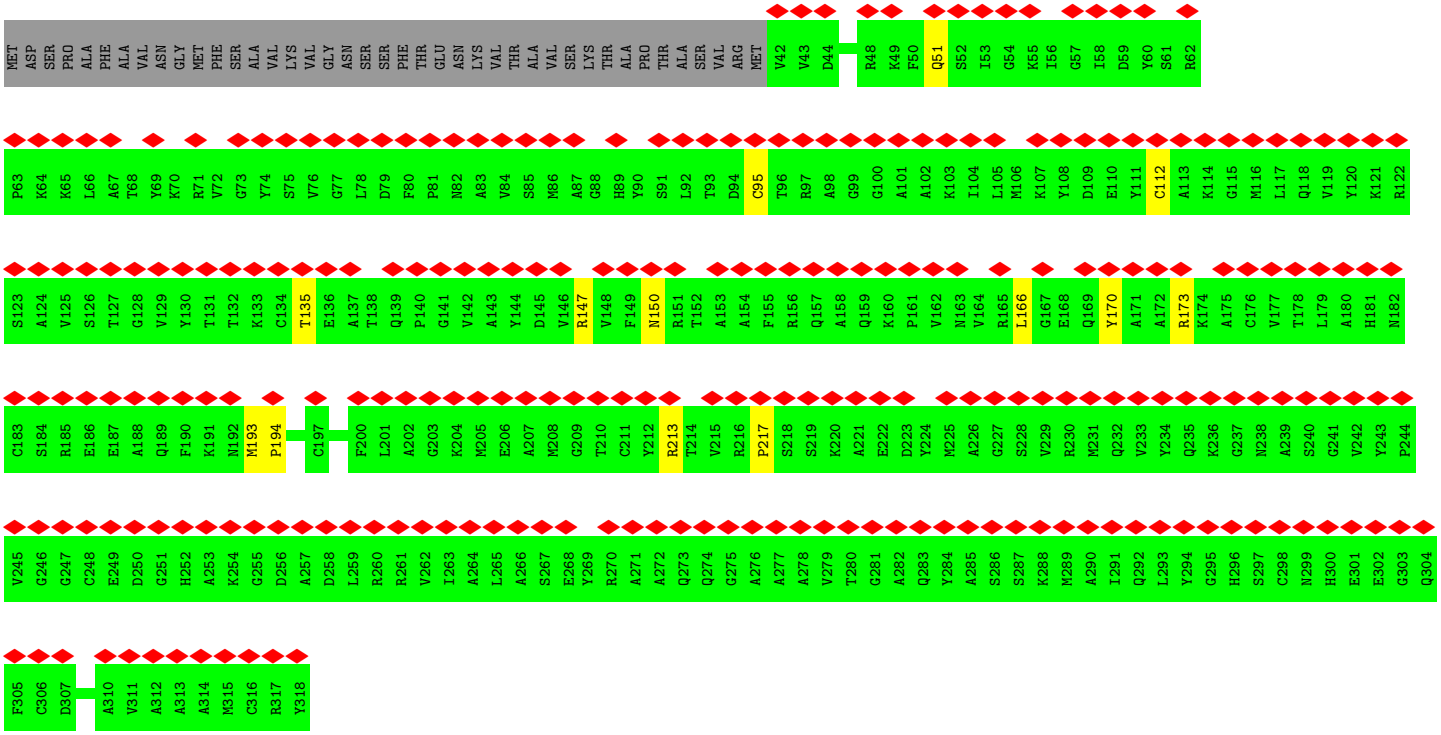
• Molecule 12: LR_gamma4

Chain bY:



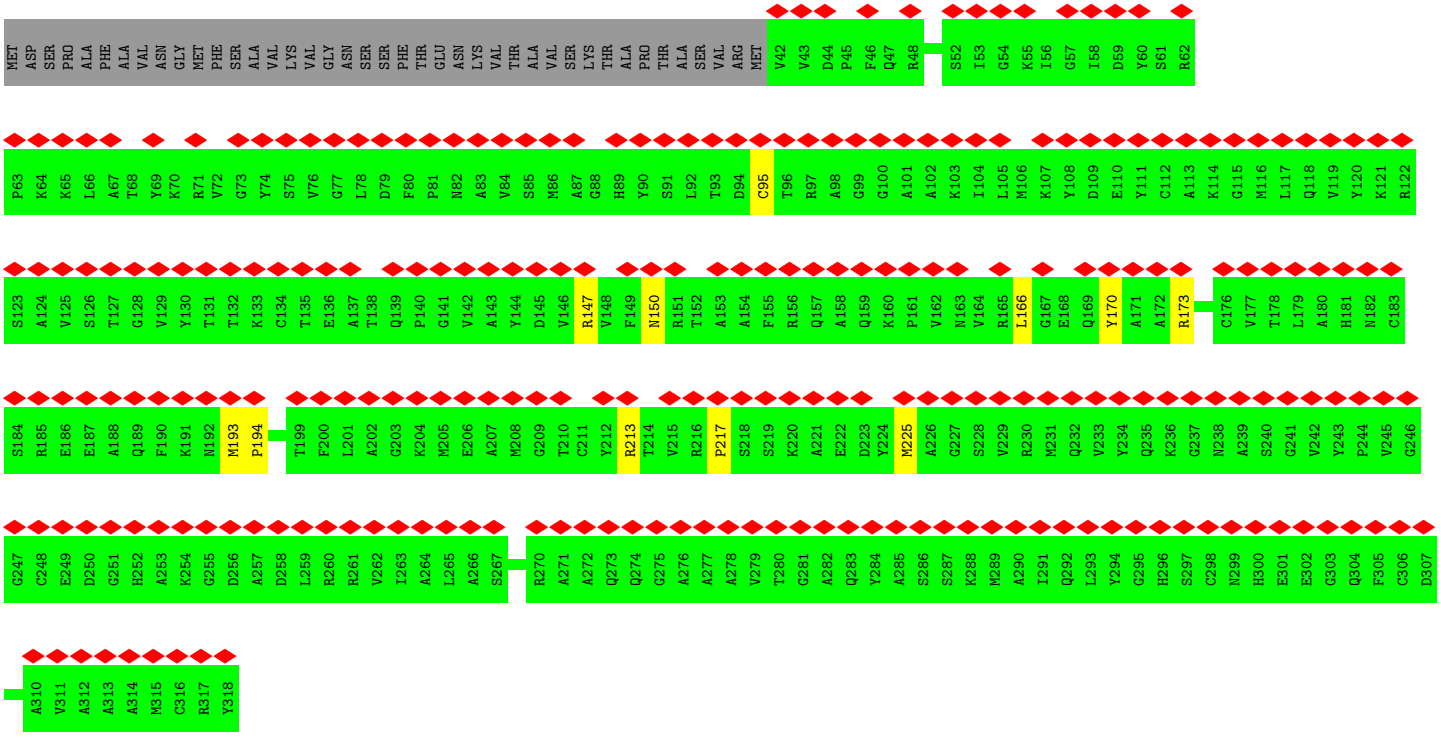
• Molecule 12: LR_gamma4

Chain dw:

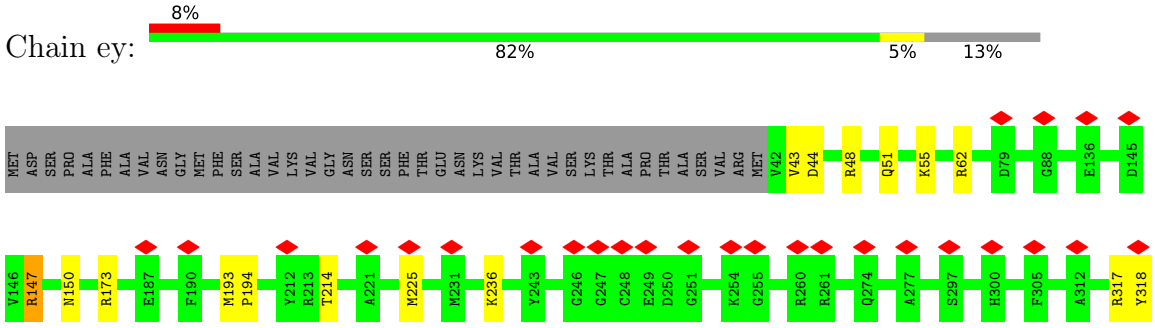


• Molecule 12: LR_gamma4

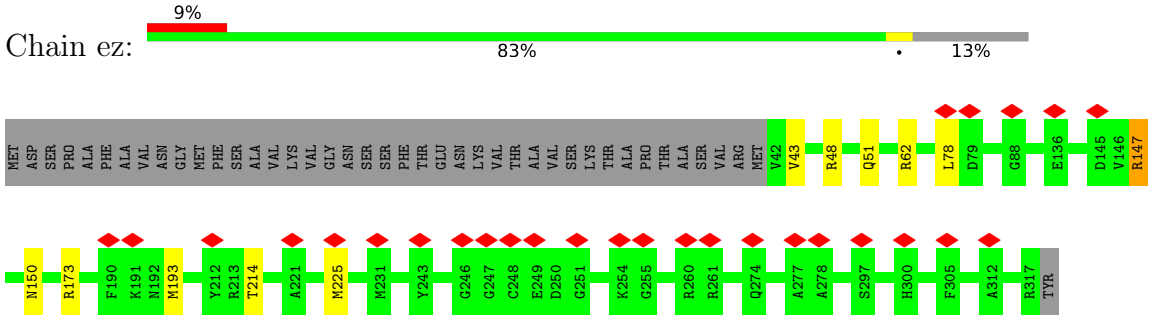
Chain dx:



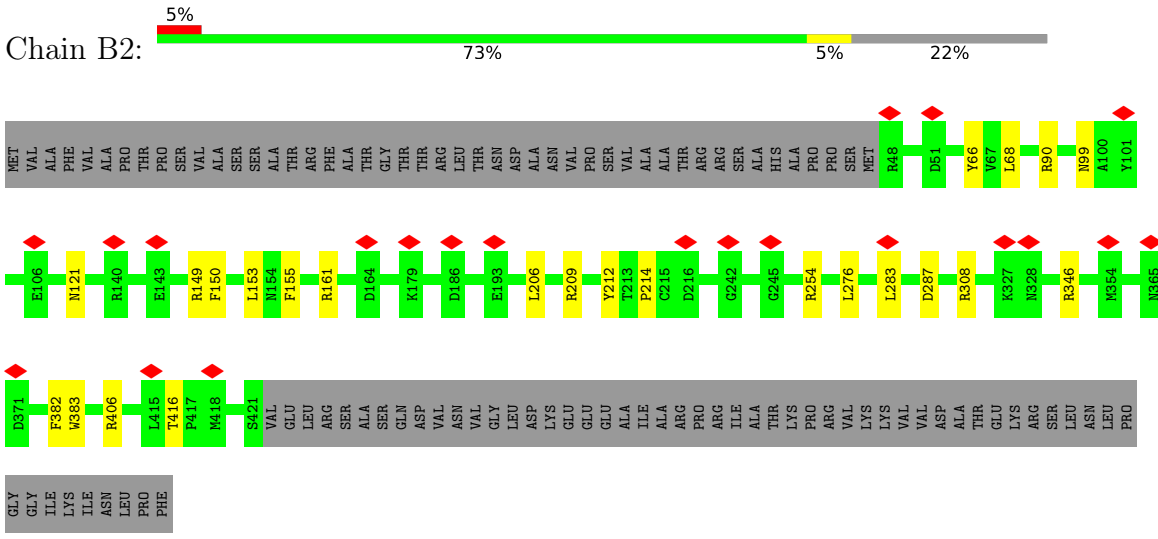
• Molecule 12: LR_gamma4



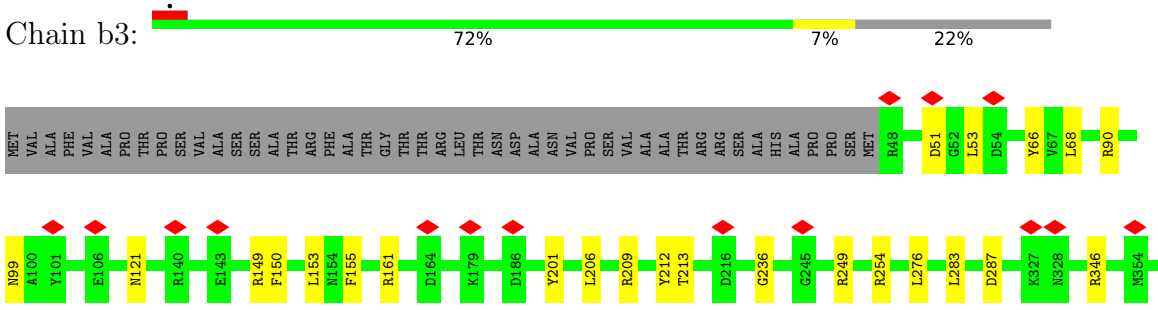
• Molecule 12: LR_gamma4

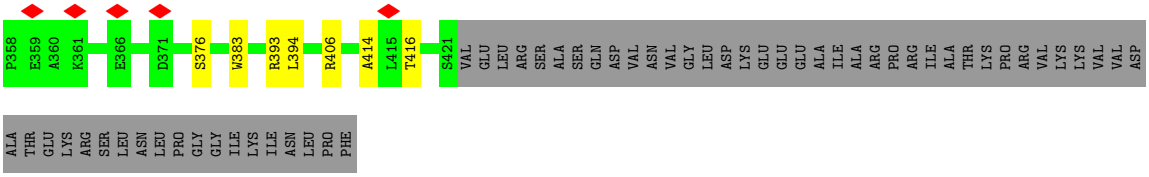


• Molecule 13: LRC2



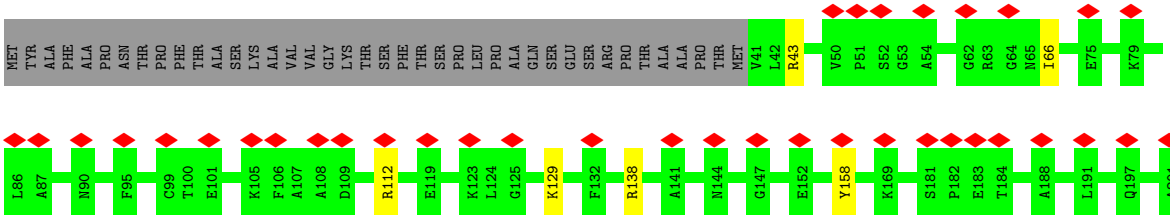
• Molecule 13: LRC2





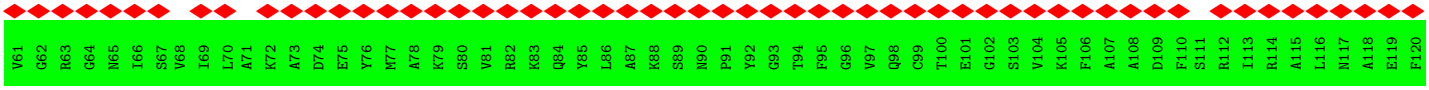
• Molecule 14: LR_gamma5

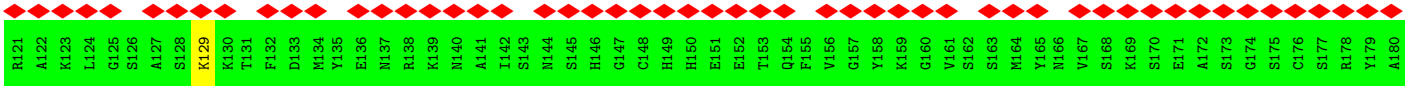
Chain C2:

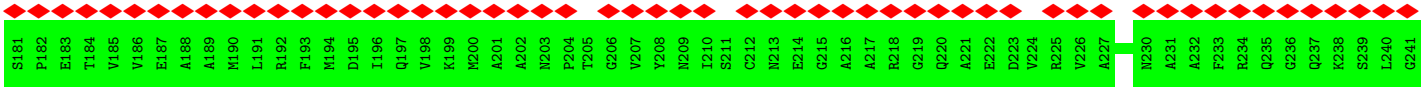


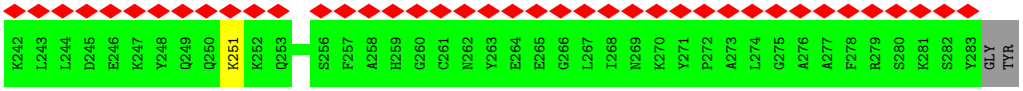
• Molecule 14: LR_gamma5

Chain D2:



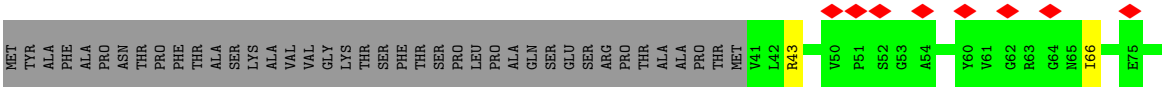


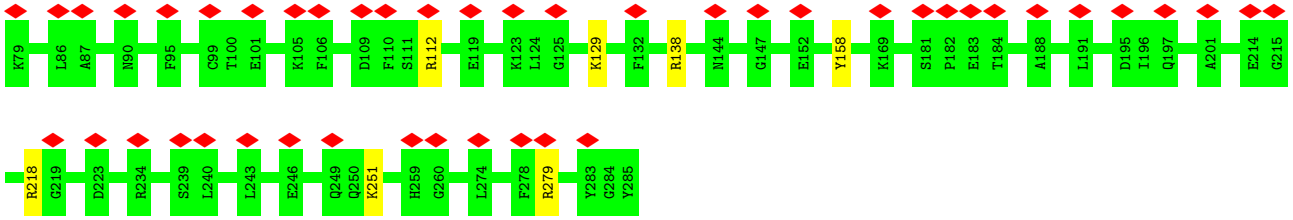




• Molecule 14: LR_gamma5

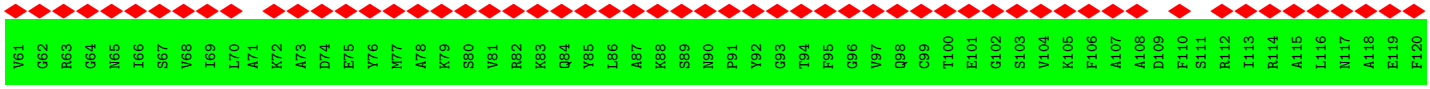
Chain c3:

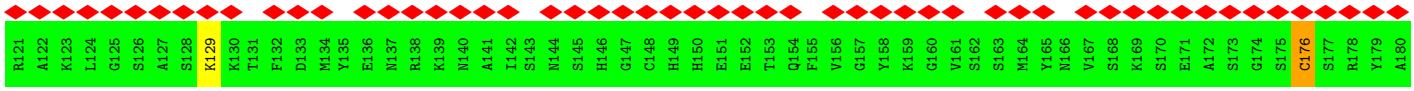


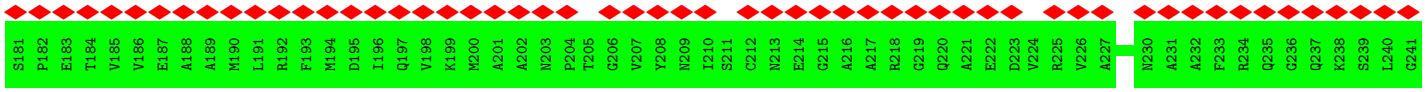


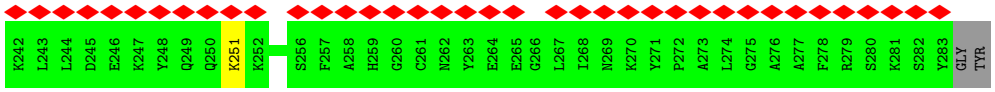
• Molecule 14: LR_gamma5

Chain d3:



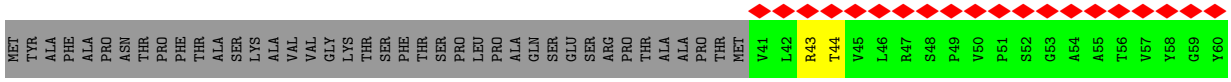


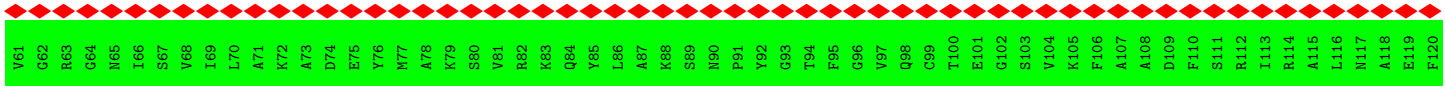


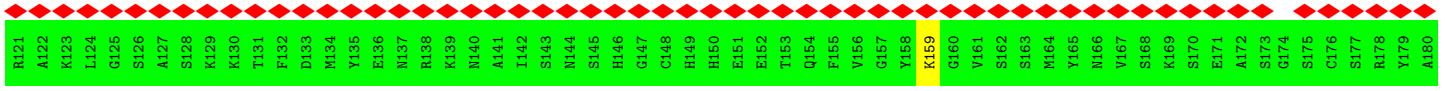


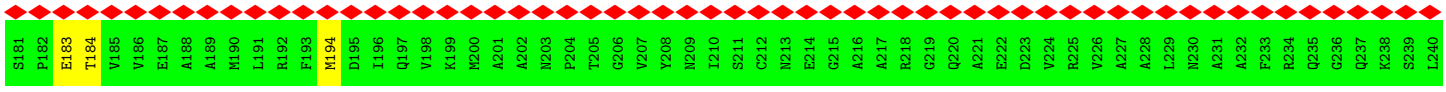
• Molecule 14: LR_gamma5

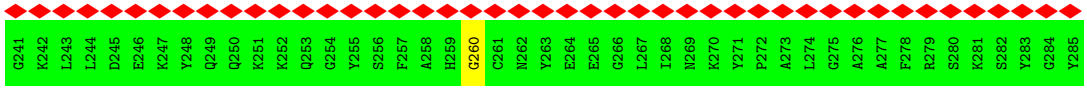
Chain 44:





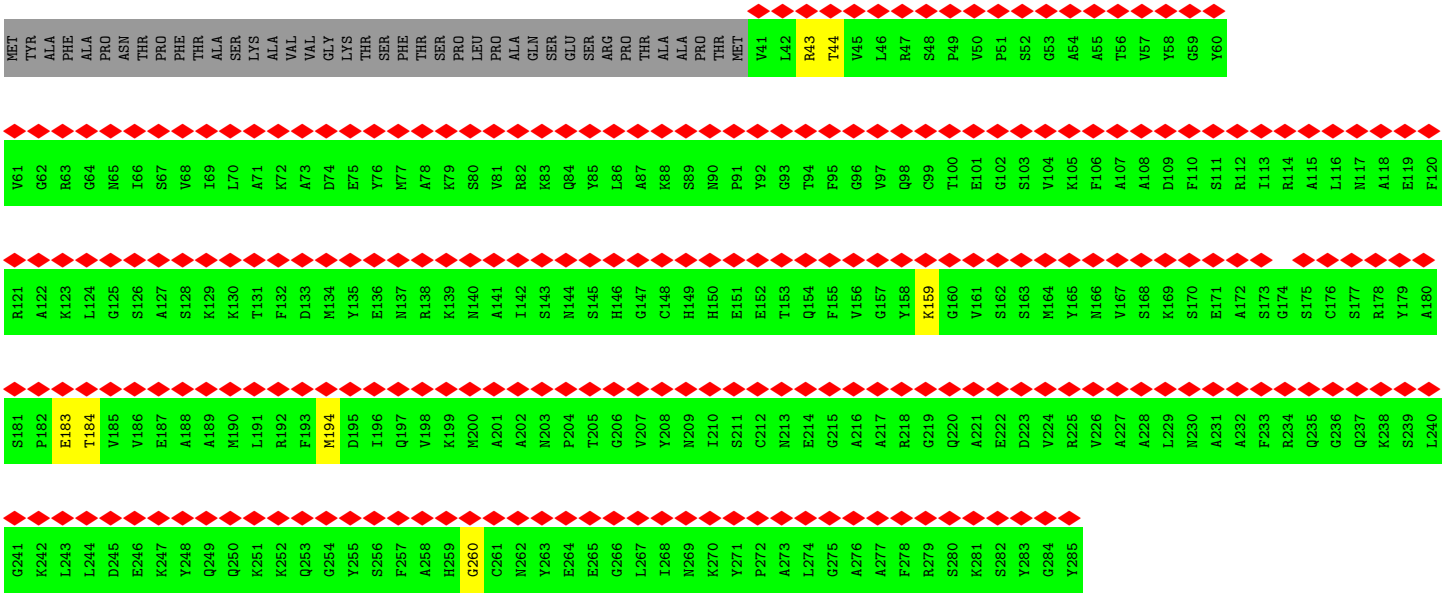






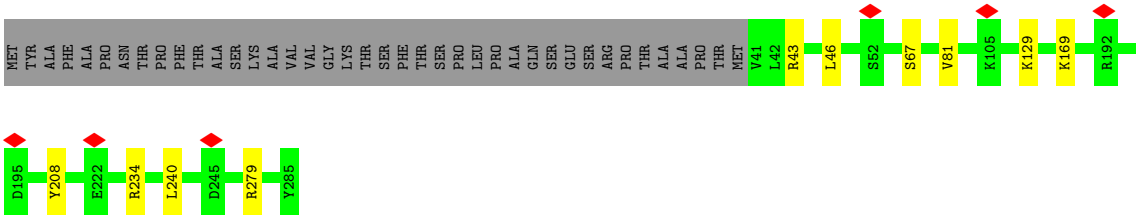
• Molecule 14: LR_gamma5

Chain Z5:



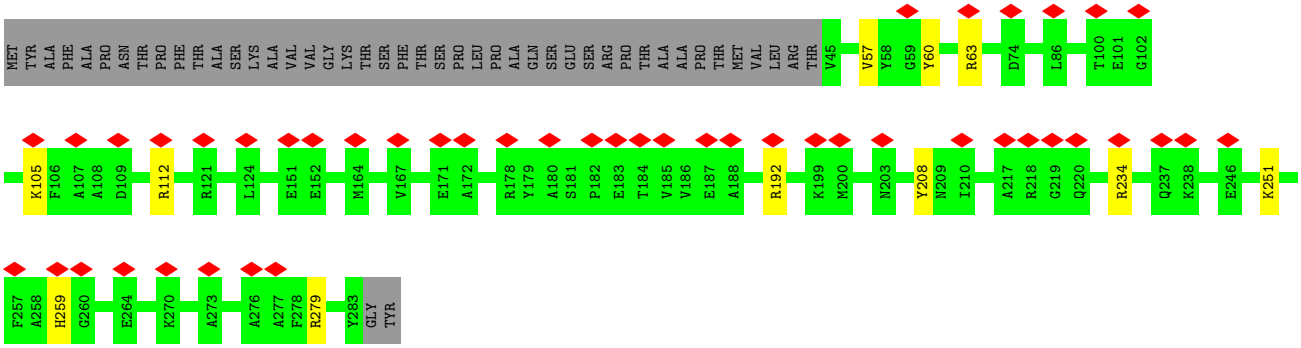
• Molecule 14: LR_gamma5

Chain c8:



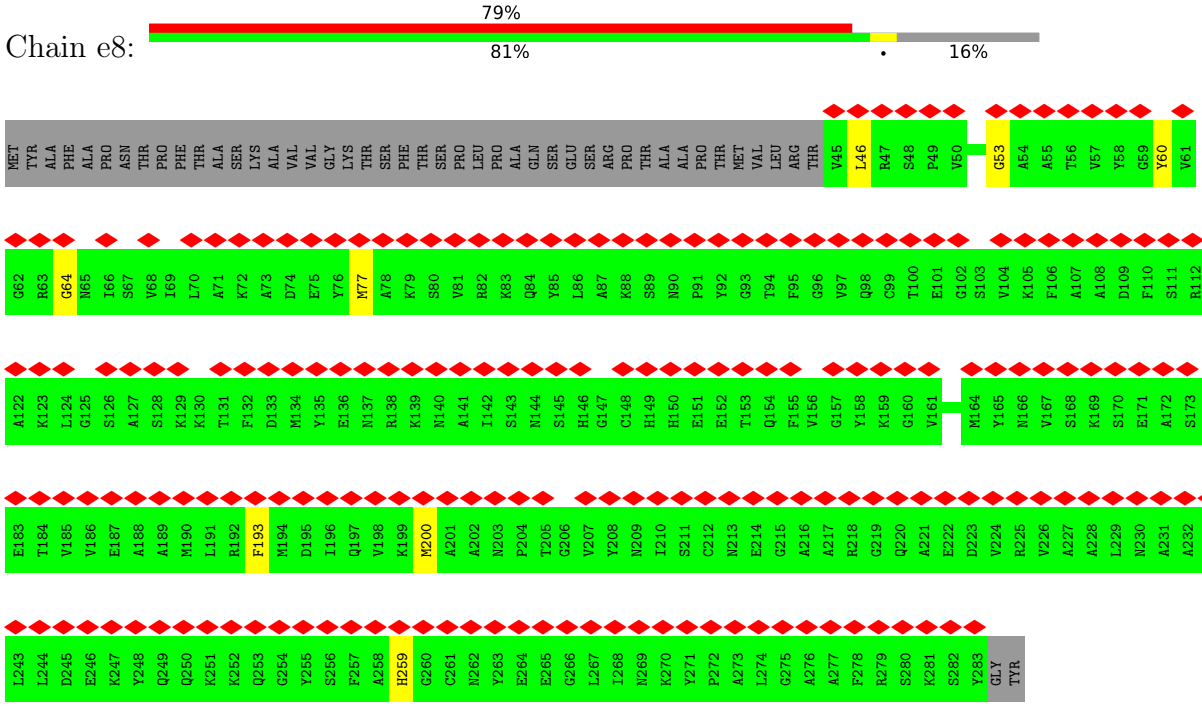
• Molecule 14: LR_gamma5

Chain d8:



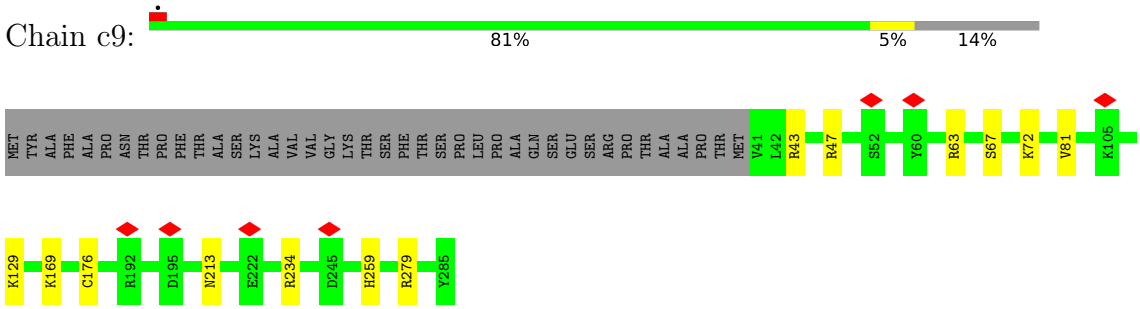
• Molecule 14: LR_gamma5

Chain e8:



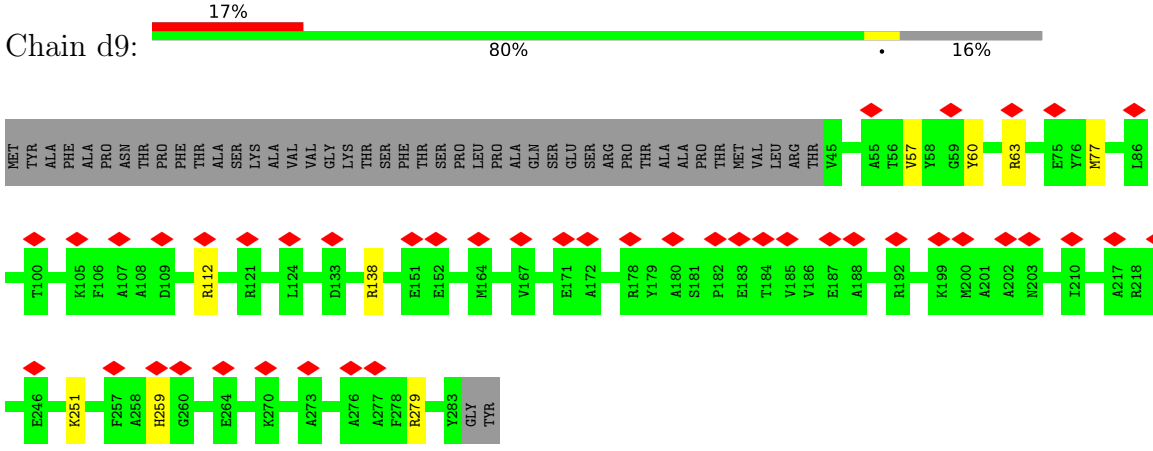
• Molecule 14: LR_gamma5

Chain c9:



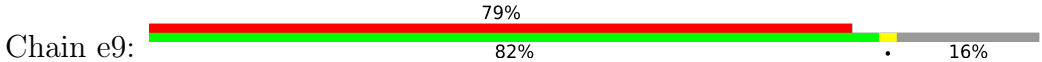
• Molecule 14: LR_gamma5

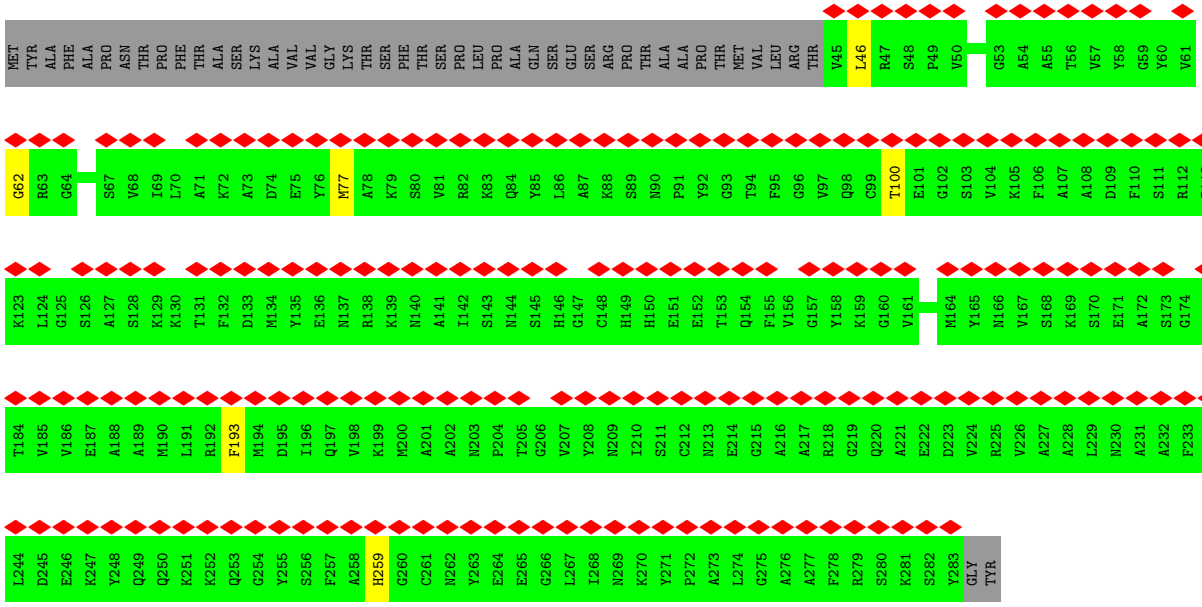
Chain d9:



• Molecule 14: LR_gamma5

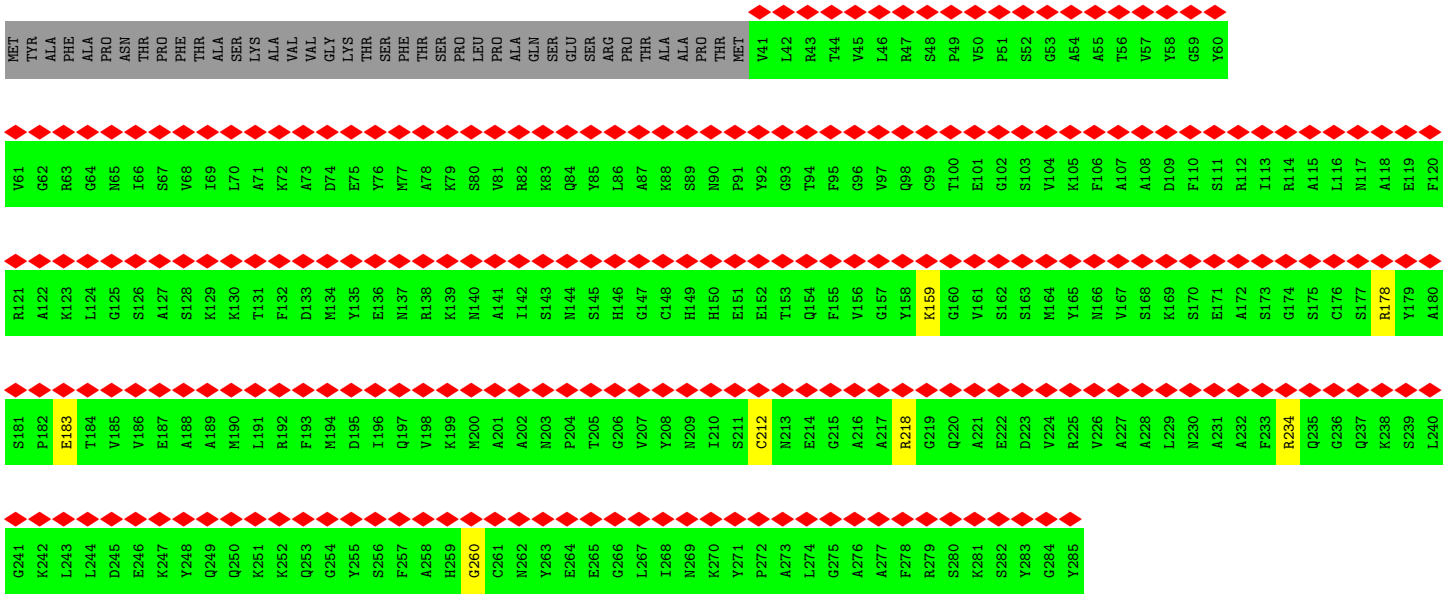
Chain e9:





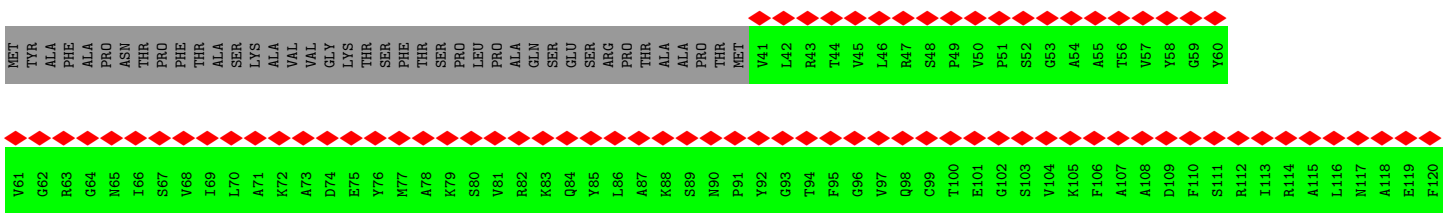
• Molecule 14: LR_gamma5

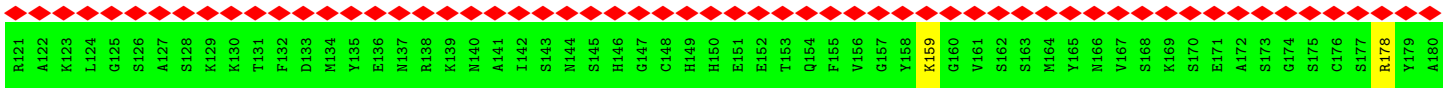
Chain T8:

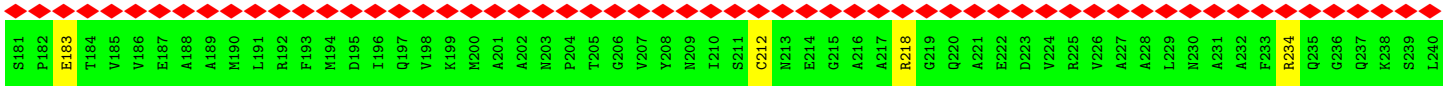


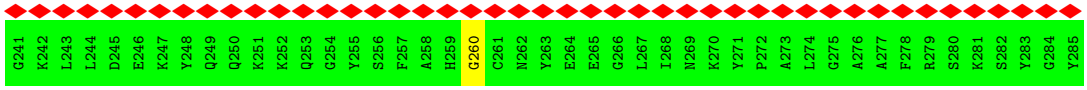
• Molecule 14: LR_gamma5

Chain Y9:



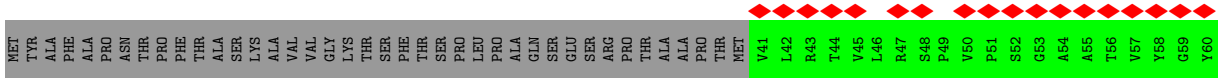


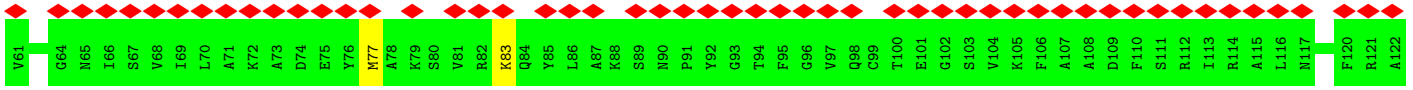


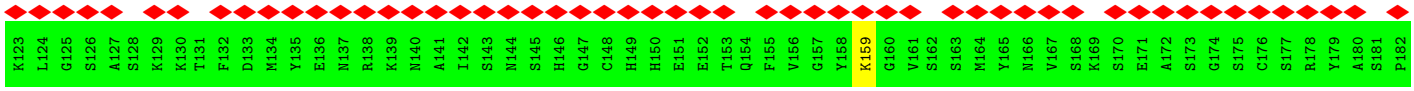


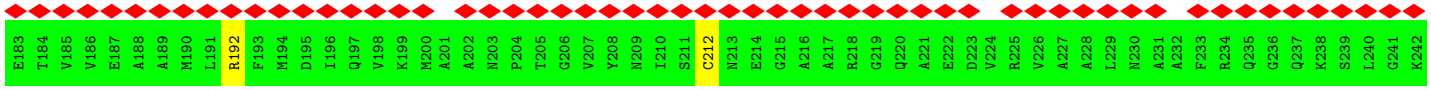
• Molecule 14: LR_gamma5

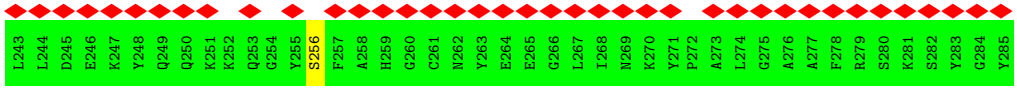
Chain aZ:





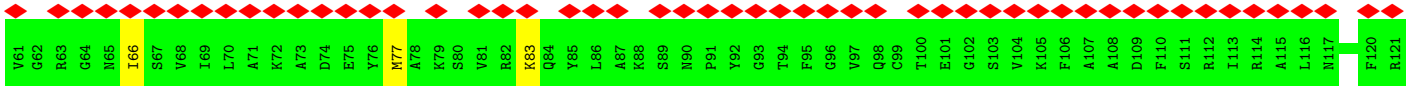


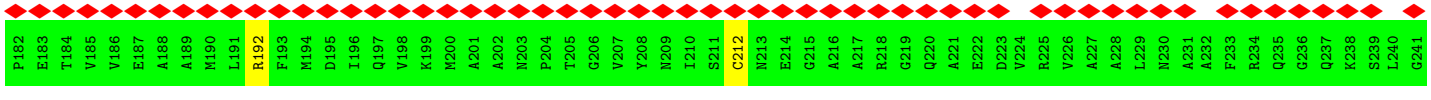


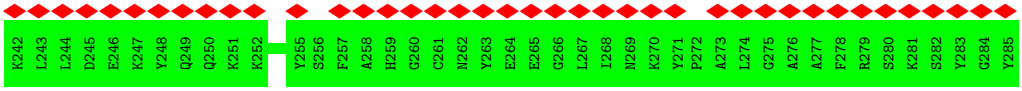


• Molecule 14: LR_gamma5

Chain bZ:

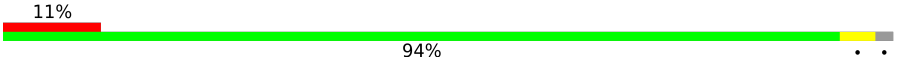


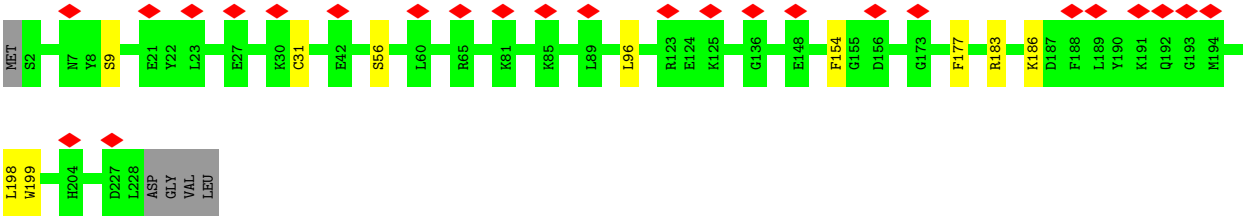




• Molecule 15: LRC1

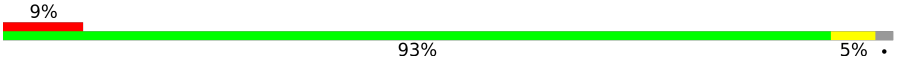
Chain 14:

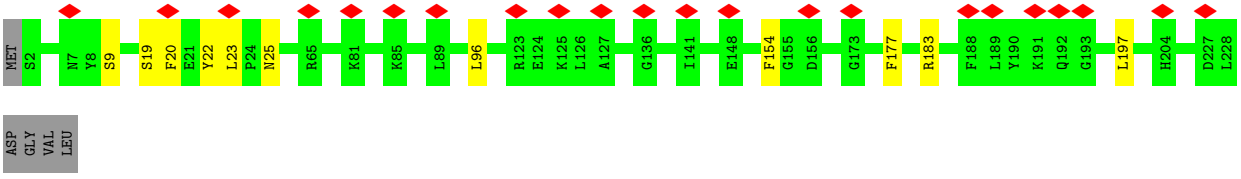




• Molecule 15: LRC1

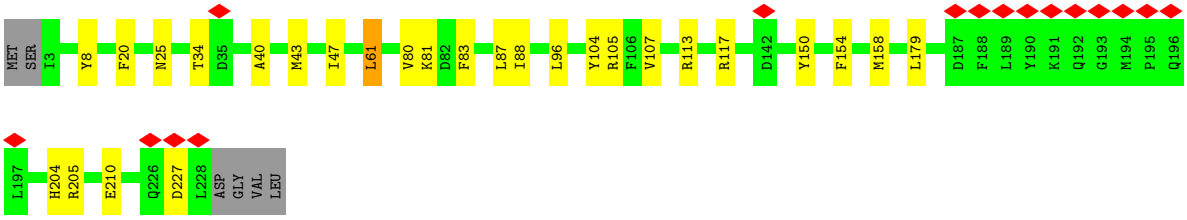
Chain W5:





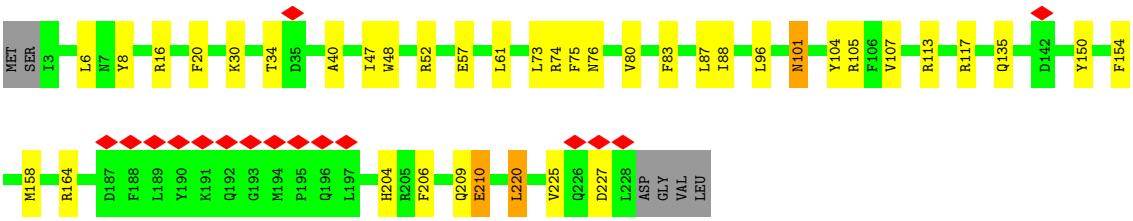
• Molecule 15: LRC1

Chain R8:



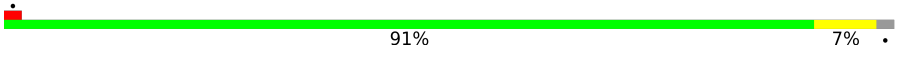
• Molecule 15: LRC1

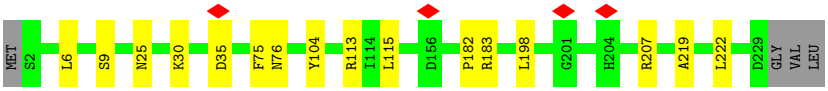
Chain W9:



• Molecule 15: LRC1

Chain aW:



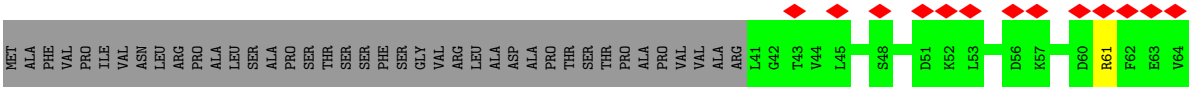


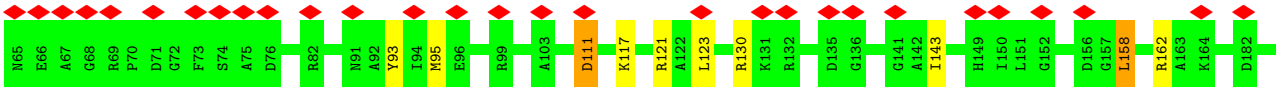
• Molecule 15: LRC1

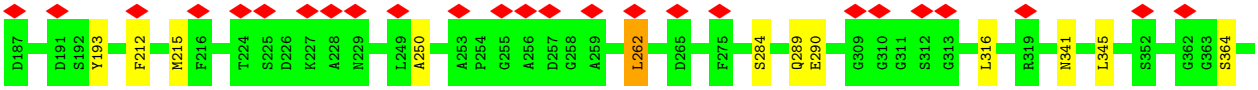
Chain bW:

• Molecule 16: LR1

Chain 24:

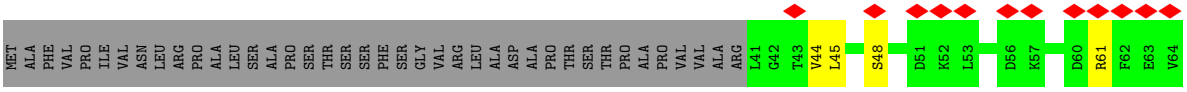


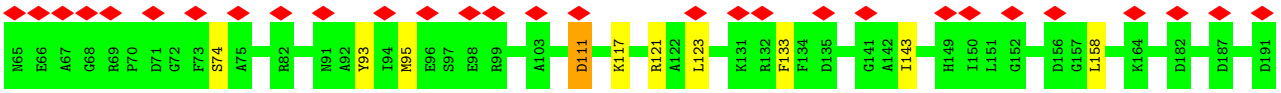


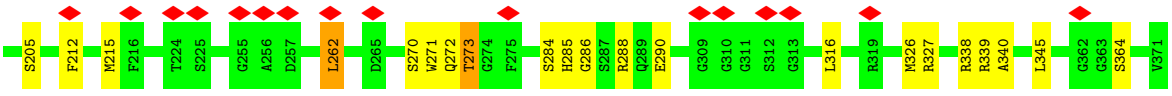


• Molecule 16: LR1

Chain X5:

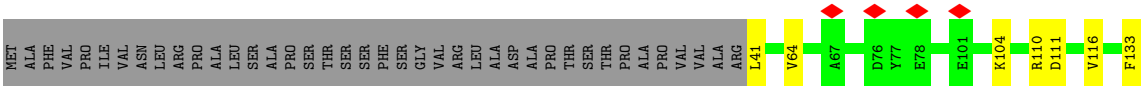






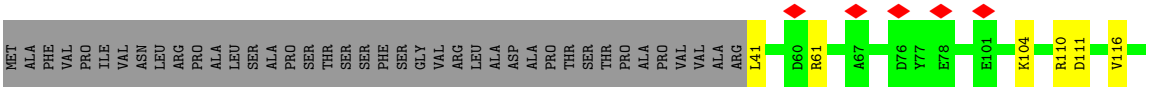
• Molecule 16: LR1

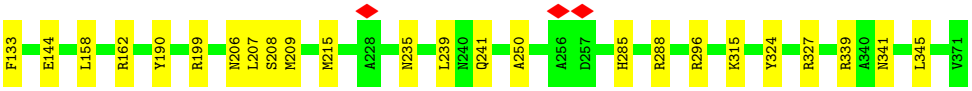
Chain S8:



• Molecule 16: LR1

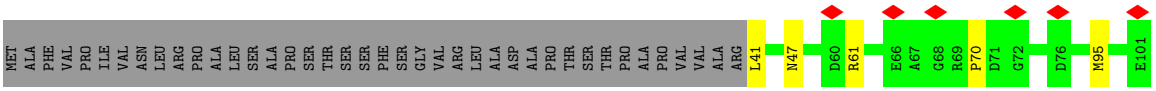
Chain X9:

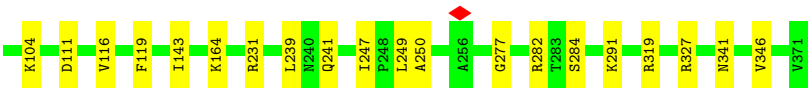




• Molecule 16: LR1

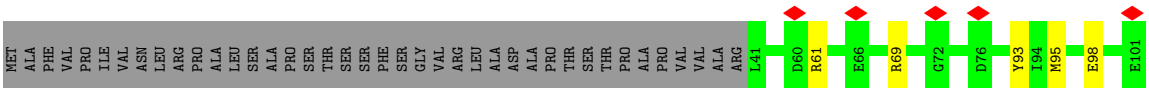
Chain aX:





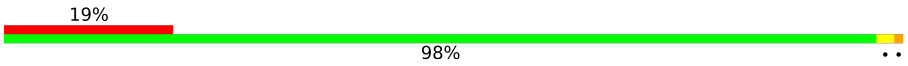
• Molecule 16: LR1

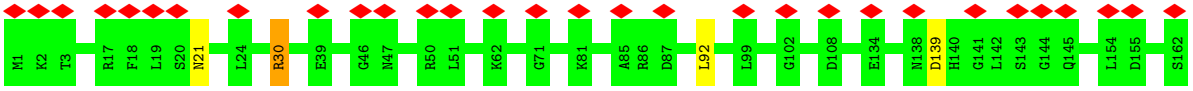
Chain bX:



• Molecule 17: alpha_PC

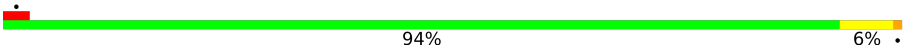
Chain a4:





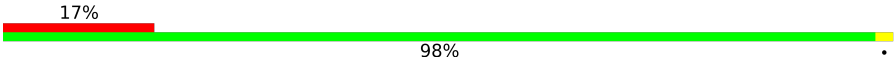
• Molecule 17: alpha_PC

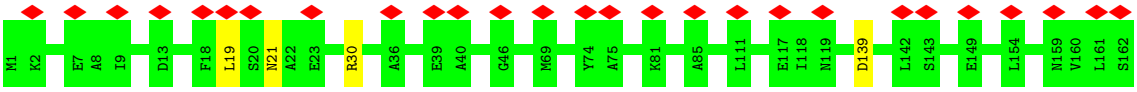
Chain b4:



• Molecule 17: alpha_PC

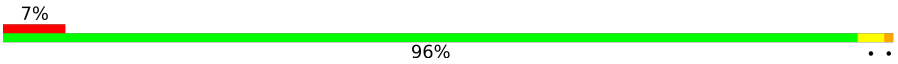
Chain d4:

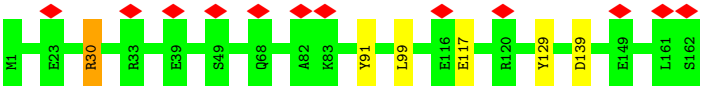




• Molecule 17: alpha_PC

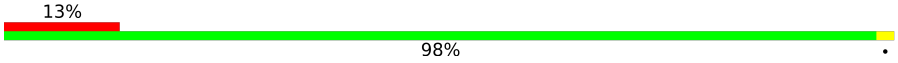
Chain f4:

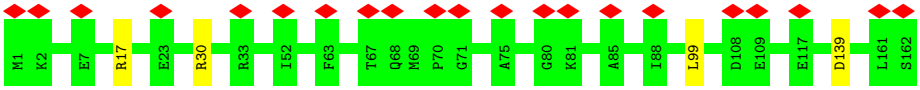




• Molecule 17: alpha_PC

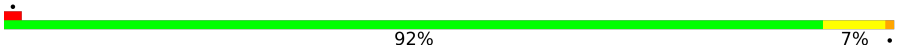
Chain i4:

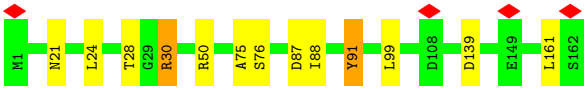




• Molecule 17: alpha_PC

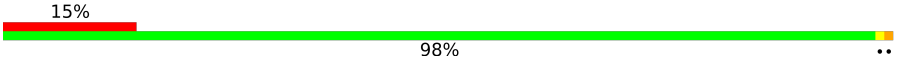
Chain k4:

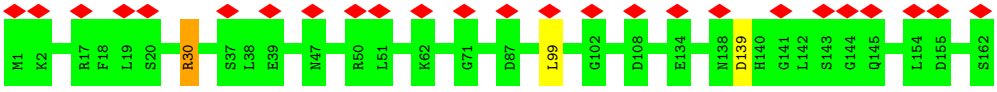




• Molecule 17: alpha_PC

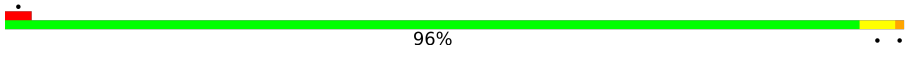
Chain a5:

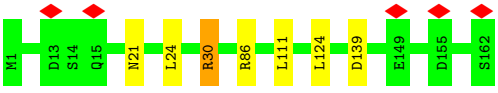




• Molecule 17: alpha_PC

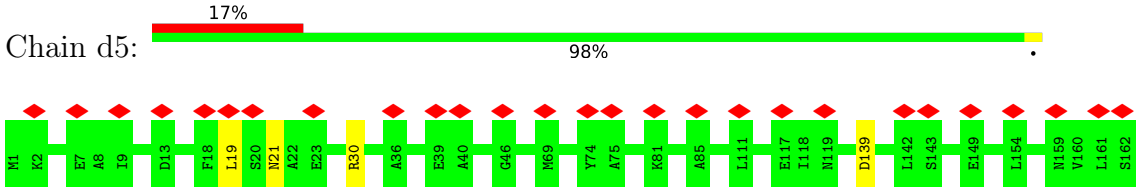
Chain b5:





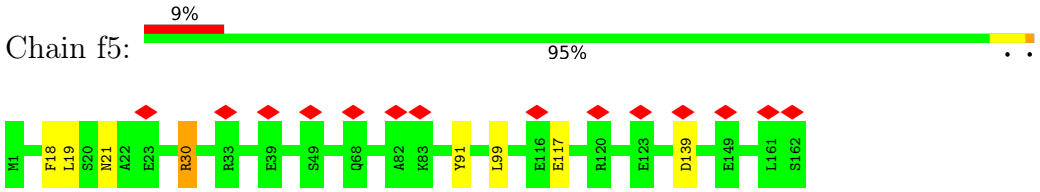
• Molecule 17: alpha_PC

Chain d5:



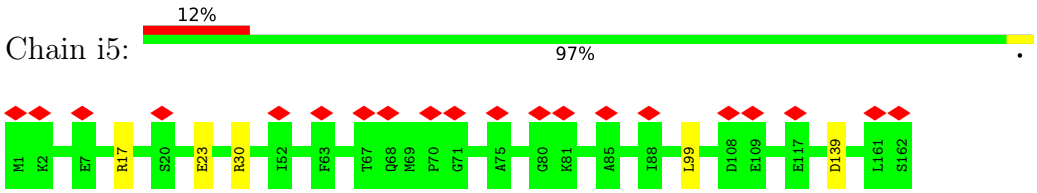
• Molecule 17: alpha_PC

Chain f5:



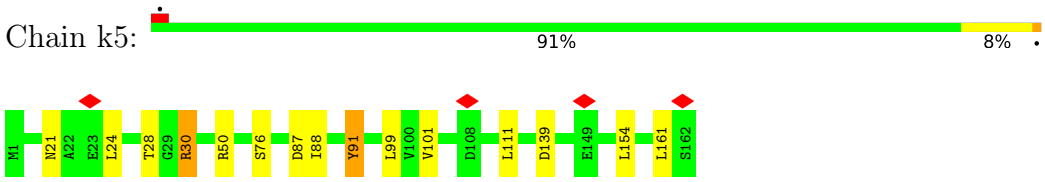
• Molecule 17: alpha_PC

Chain i5:



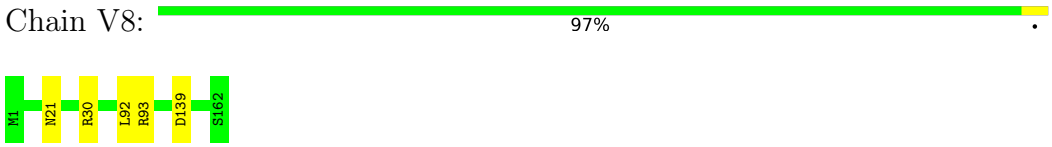
• Molecule 17: alpha_PC

Chain k5:



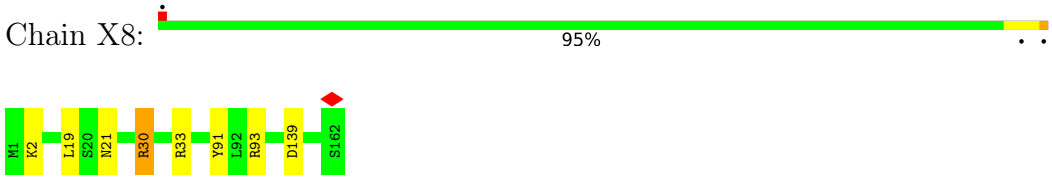
• Molecule 17: alpha_PC

Chain V8:



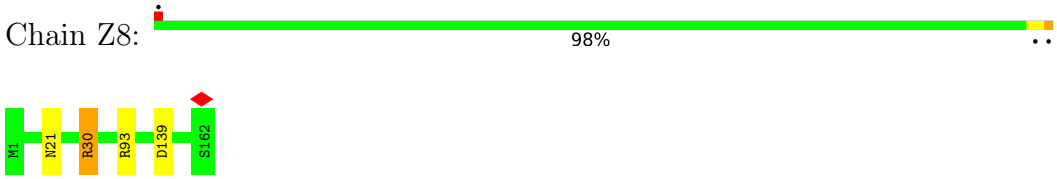
• Molecule 17: alpha_PC

Chain X8:



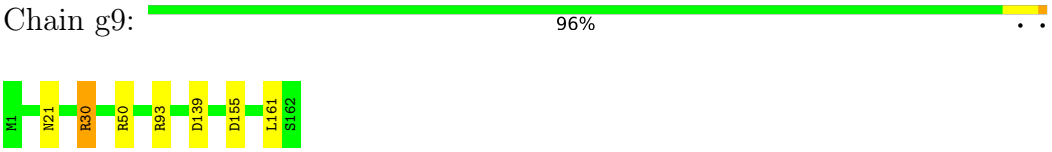
• Molecule 17: alpha_PC

Chain Z8:



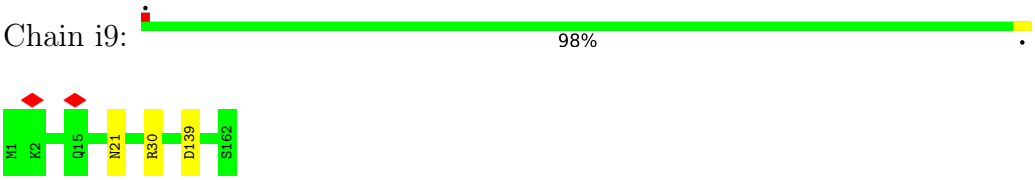
• Molecule 17: alpha_PC

Chain g9:



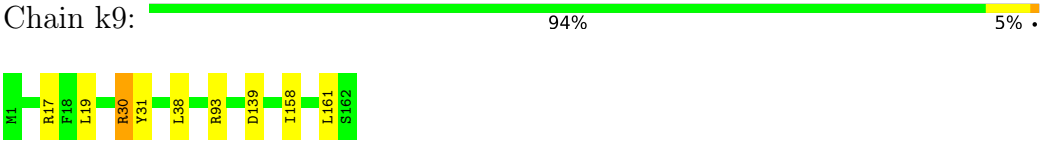
• Molecule 17: alpha_PC

Chain i9:



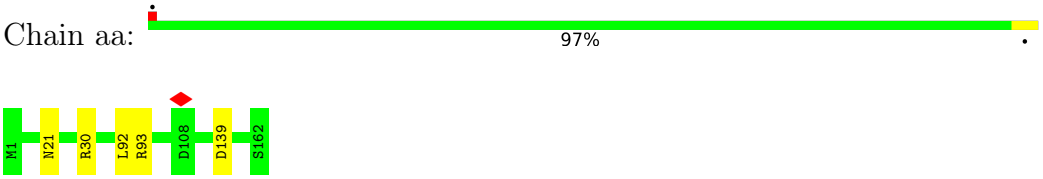
• Molecule 17: alpha_PC

Chain k9:



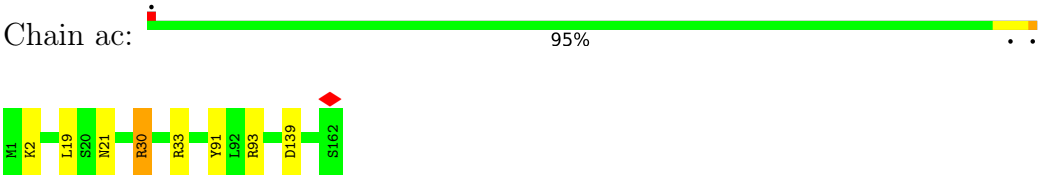
• Molecule 17: alpha_PC

Chain aa:



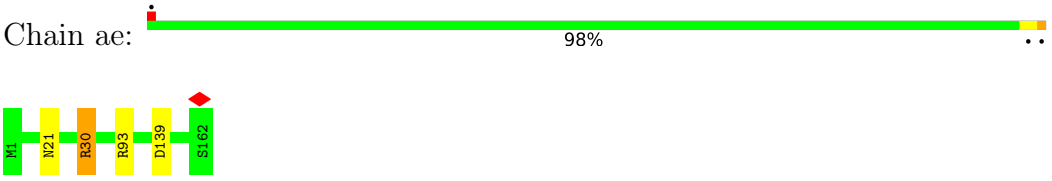
• Molecule 17: alpha_PC

Chain ac:



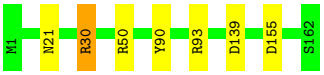
• Molecule 17: alpha_PC

Chain ae:



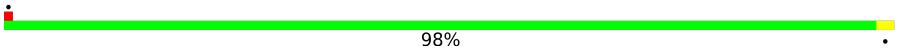
• Molecule 17: alpha_PC

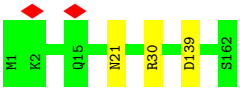
Chain ag:



• Molecule 17: alpha_PC

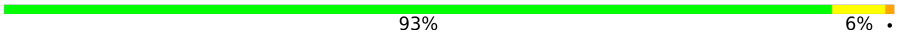
Chain ai:





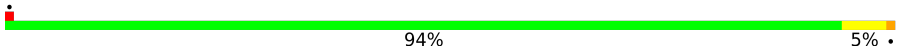
• Molecule 17: alpha_PC

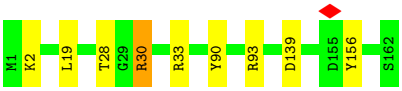
Chain ak:



• Molecule 17: alpha_PC

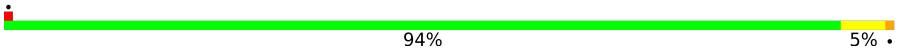
Chain ba:

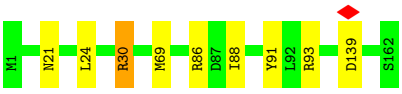




• Molecule 17: alpha_PC

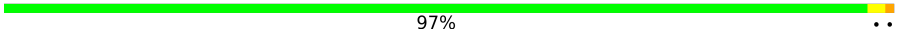
Chain bc:

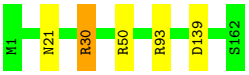




• Molecule 17: alpha_PC

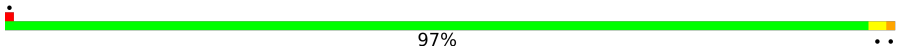
Chain be:

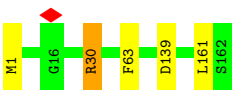




• Molecule 17: alpha_PC

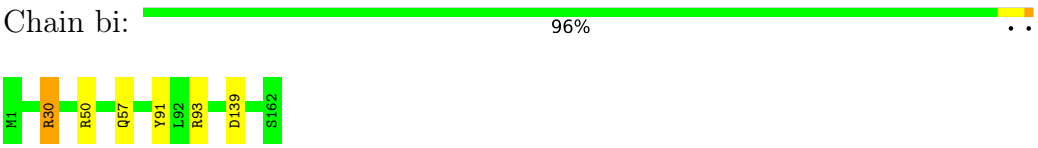
Chain bg:





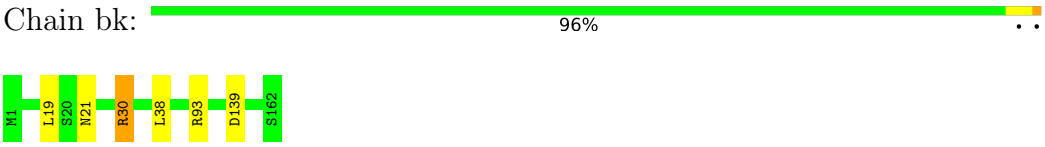
• Molecule 17: alpha_PC

Chain bi:



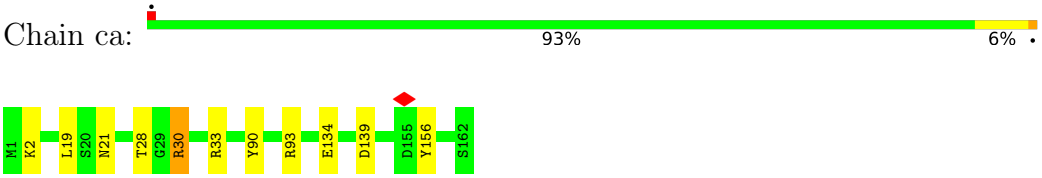
• Molecule 17: alpha_PC

Chain bk:



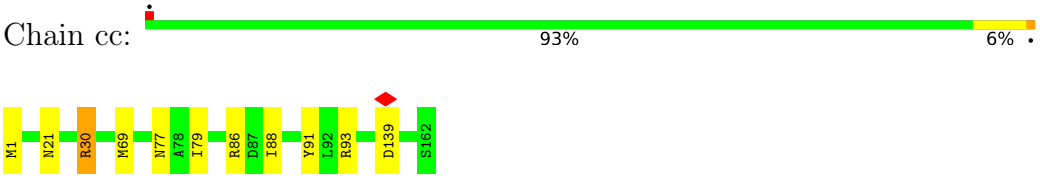
• Molecule 17: alpha_PC

Chain ca:



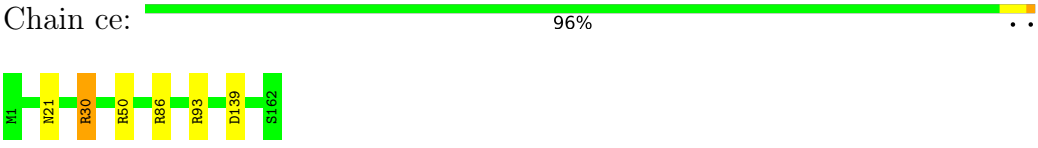
• Molecule 17: alpha_PC

Chain cc:



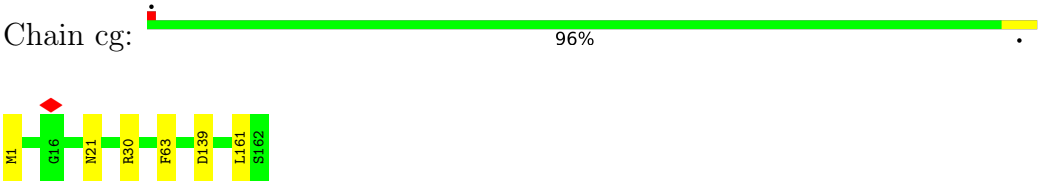
• Molecule 17: alpha_PC

Chain ce:



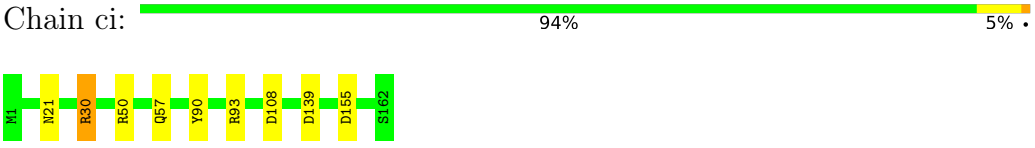
• Molecule 17: alpha_PC

Chain cg:



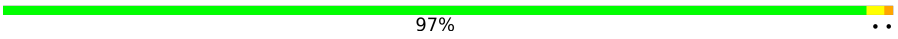
• Molecule 17: alpha_PC

Chain ci:



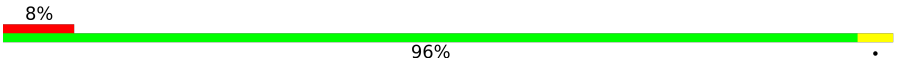
• Molecule 17: alpha_PC

Chain ck:



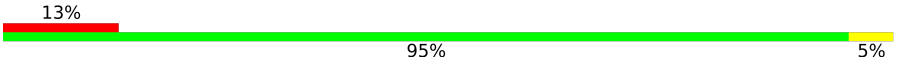
• Molecule 18: beta_PC

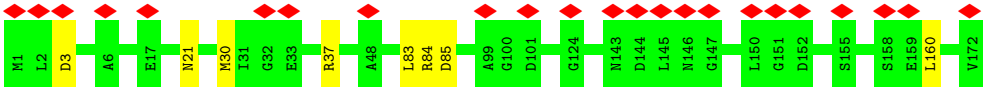
Chain c4:



• Molecule 18: beta_PC

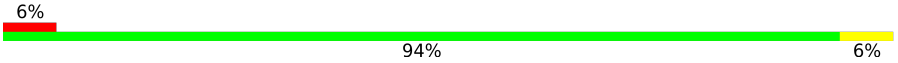
Chain e4:





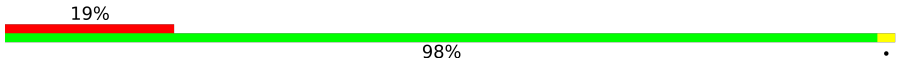
• Molecule 18: beta_PC

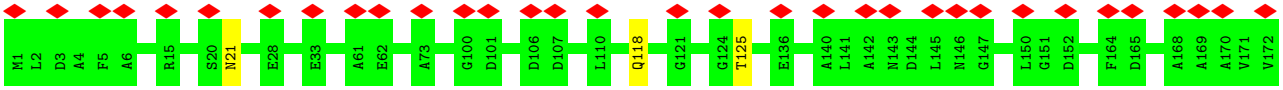
Chain g4:



• Molecule 18: beta_PC

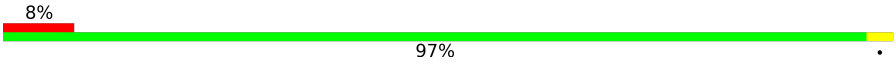
Chain h4:

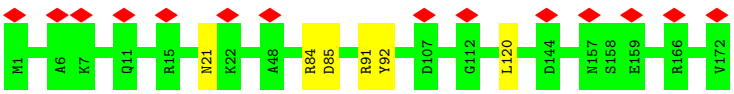




• Molecule 18: beta_PC

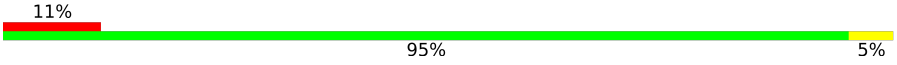
Chain j4:

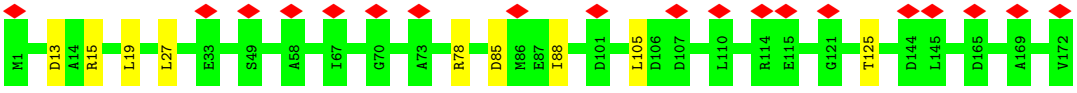




• Molecule 18: beta_PC

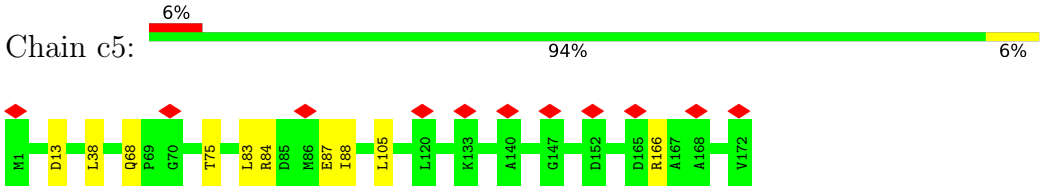
Chain l4:





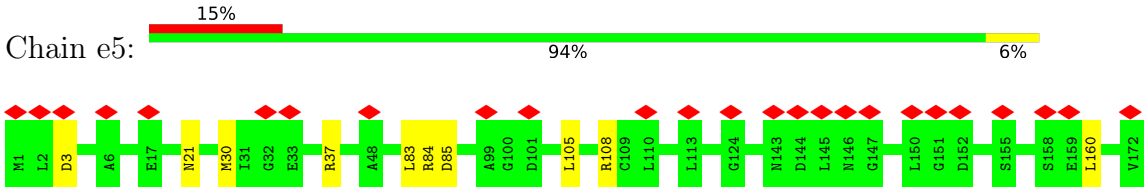
• Molecule 18: beta_PC

Chain c5:



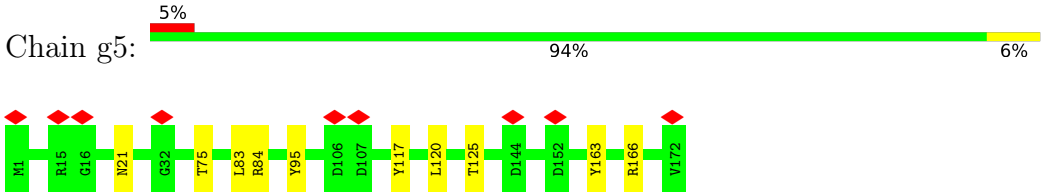
• Molecule 18: beta_PC

Chain e5:



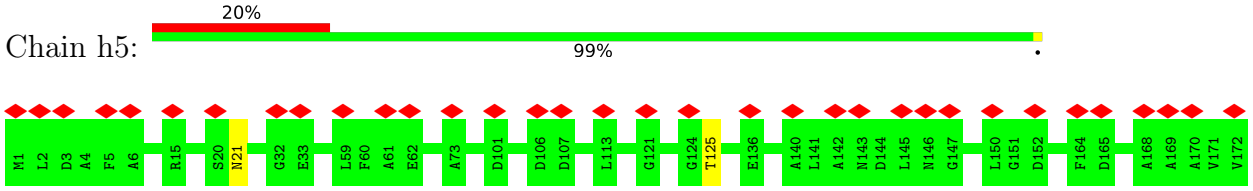
• Molecule 18: beta_PC

Chain g5:



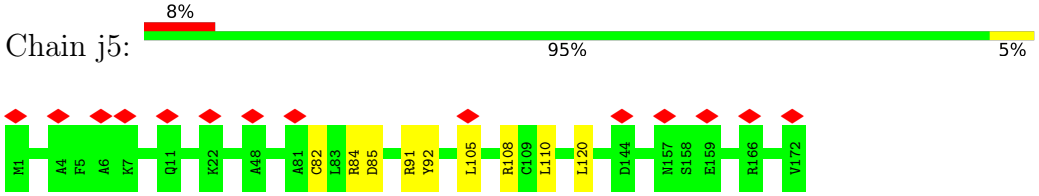
• Molecule 18: beta_PC

Chain h5:



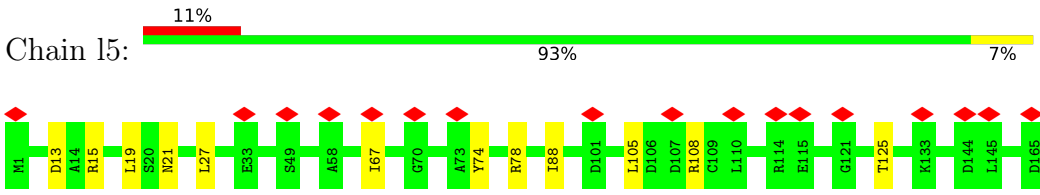
• Molecule 18: beta_PC

Chain j5:



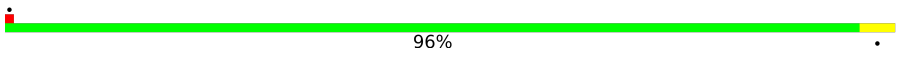
• Molecule 18: beta_PC

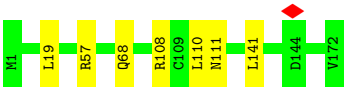
Chain l5:



• Molecule 18: beta_PC

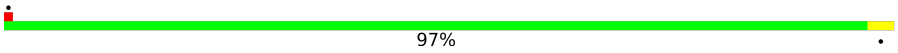
Chain W8:

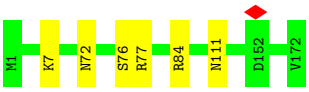




• Molecule 18: beta_PC

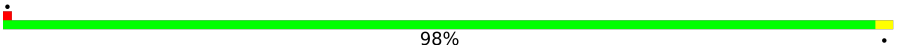
Chain Y8:

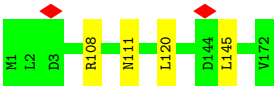




• Molecule 18: beta_PC

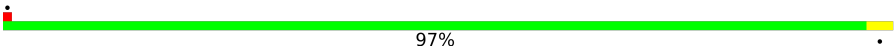
Chain f9:

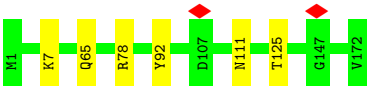




• Molecule 18: beta_PC

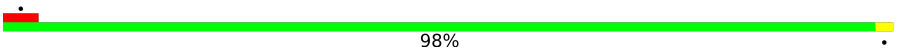
Chain h9:

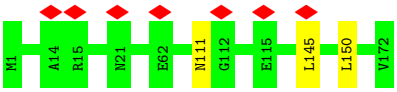




• Molecule 18: beta_PC

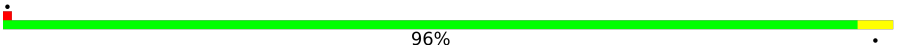
Chain j9:

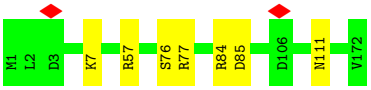




• Molecule 18: beta_PC

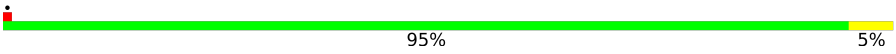
Chain l9:





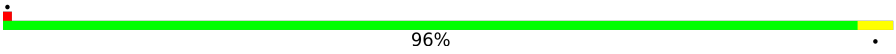
• Molecule 18: beta_PC

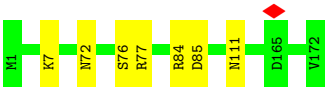
Chain ab:



• Molecule 18: beta_PC

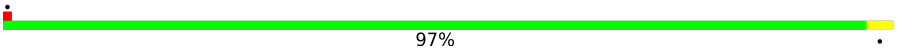
Chain ad:





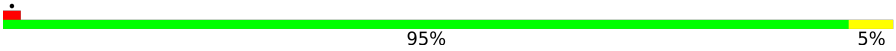
• Molecule 18: beta_PC

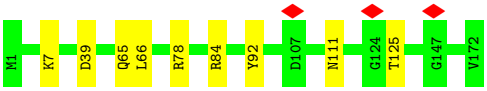
Chain af:



• Molecule 18: beta_PC

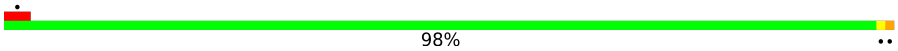
Chain ah:

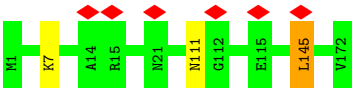




• Molecule 18: beta_PC

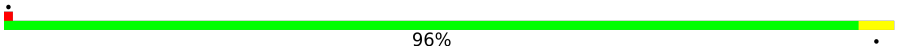
Chain aj:

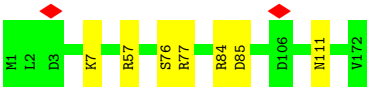




• Molecule 18: beta_PC

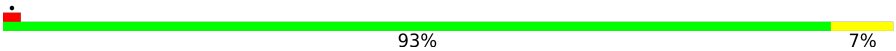
Chain al:

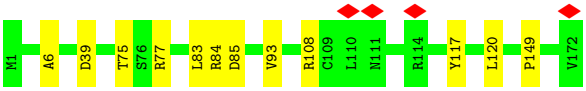




• Molecule 18: beta_PC

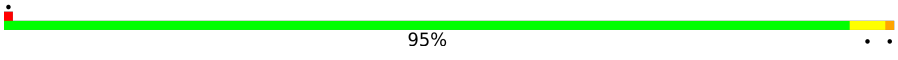
Chain bb:

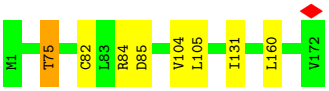




• Molecule 18: beta_PC

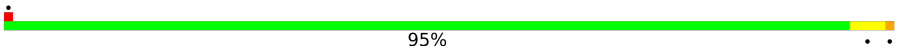
Chain bd:

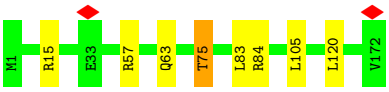




• Molecule 18: beta_PC

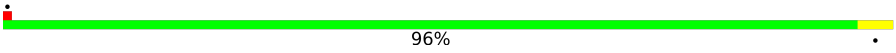
Chain bf:

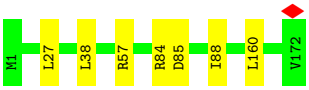




• Molecule 18: beta_PC

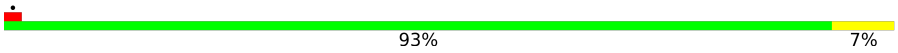
Chain bh:

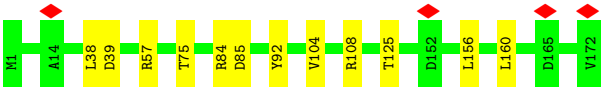




• Molecule 18: beta_PC

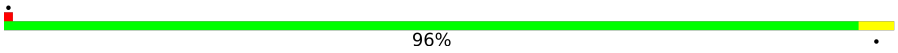
Chain bj:

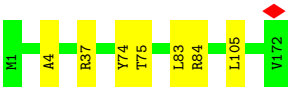




• Molecule 18: beta_PC

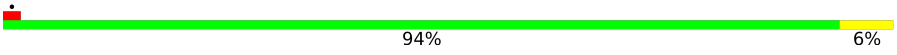
Chain bl:

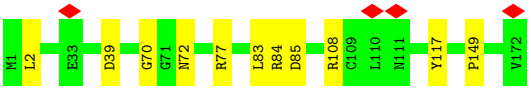




• Molecule 18: beta_PC

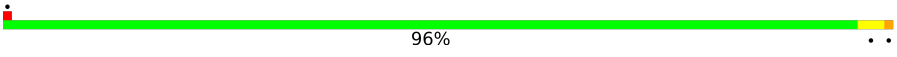
Chain cb:





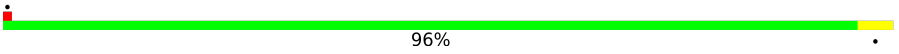
• Molecule 18: beta_PC

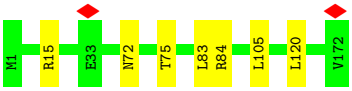
Chain cd:



• Molecule 18: beta_PC

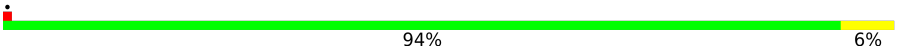
Chain cf:

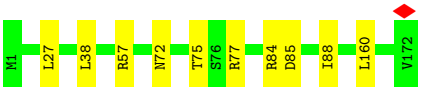




• Molecule 18: beta_PC

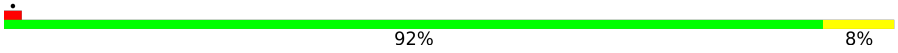
Chain ch:

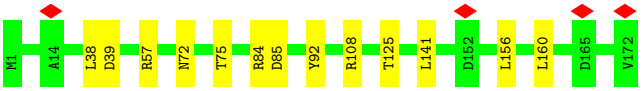




• Molecule 18: beta_PC

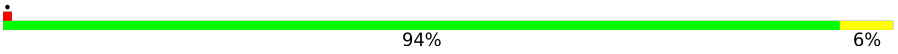
Chain cj:

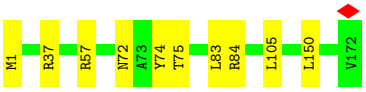




• Molecule 18: beta_PC

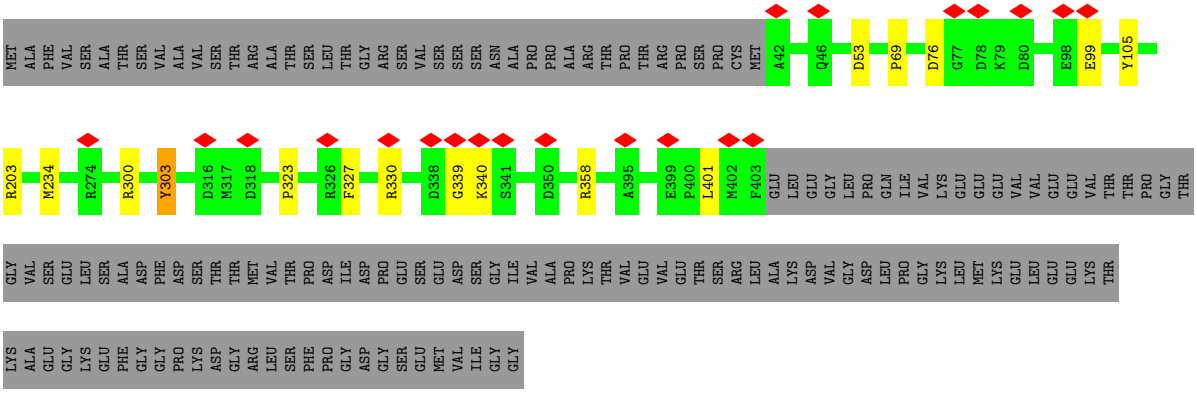
Chain cl:





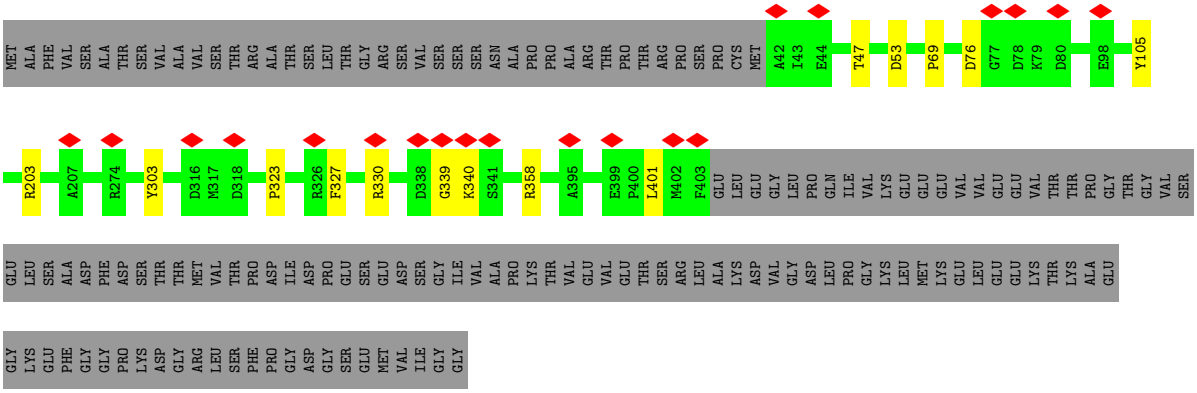
• Molecule 19: LRC3

Chain a8:



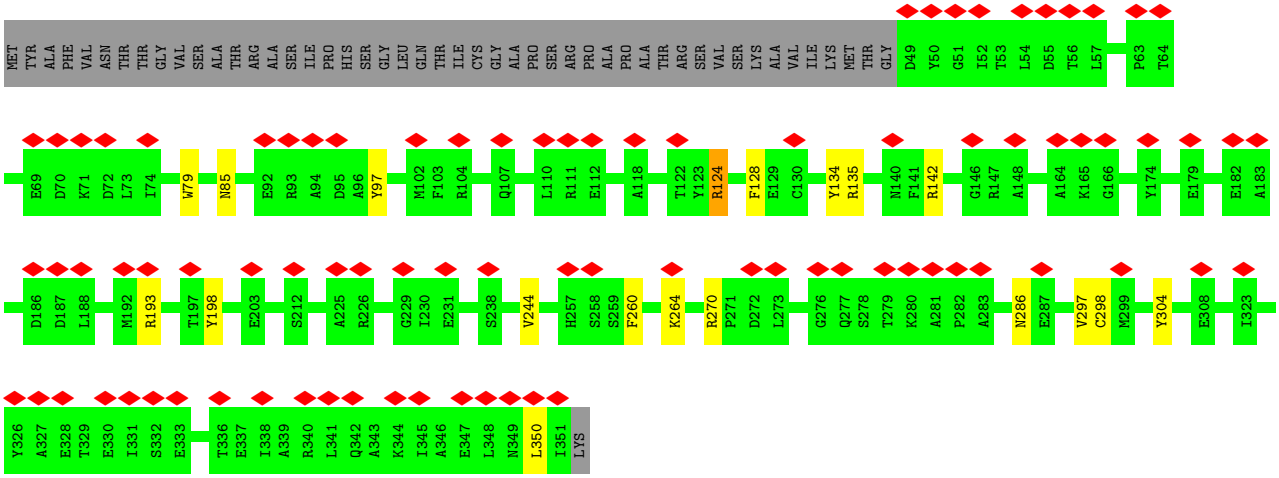
• Molecule 19: LRC3

Chain a9:



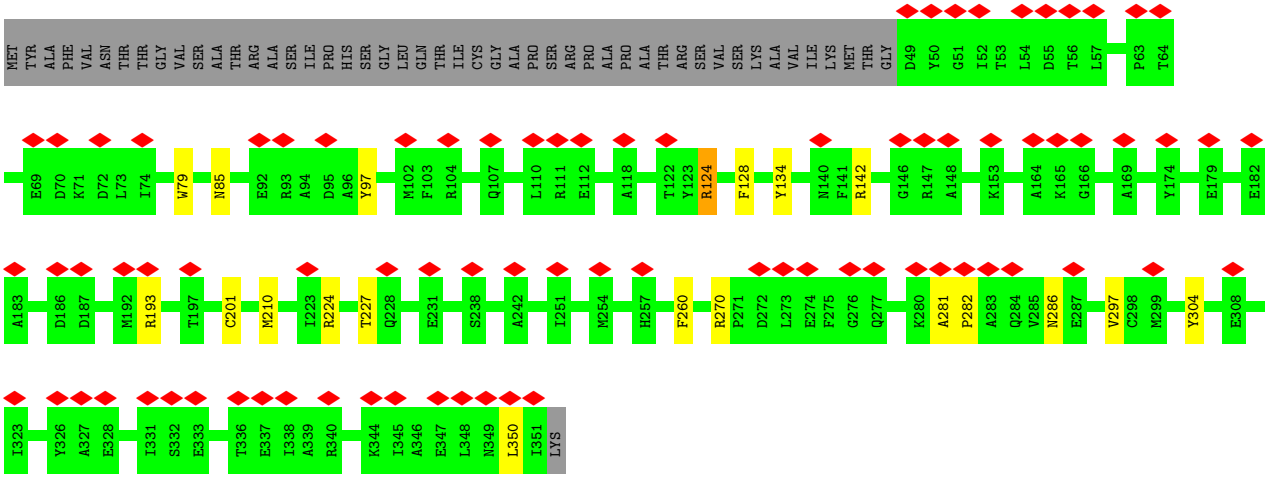
• Molecule 20: LR3

Chain dy:



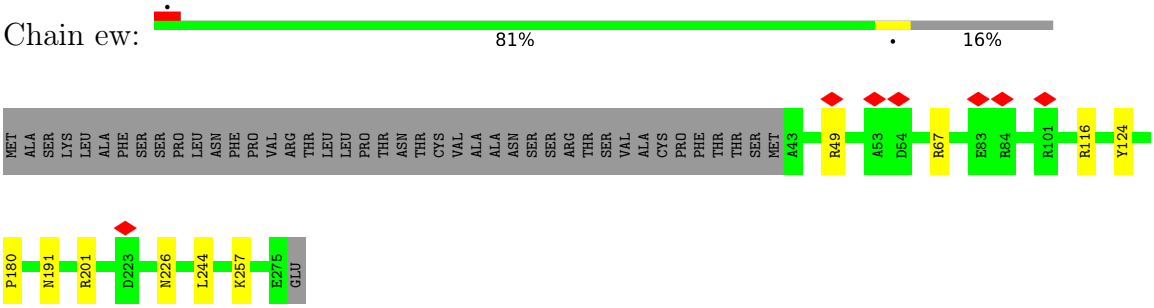
• Molecule 20: LR3

Chain dz:



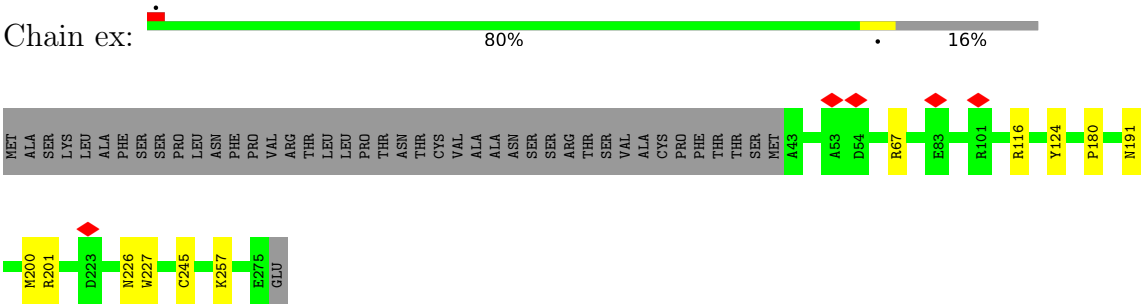
• Molecule 21: LR2

Chain ew:



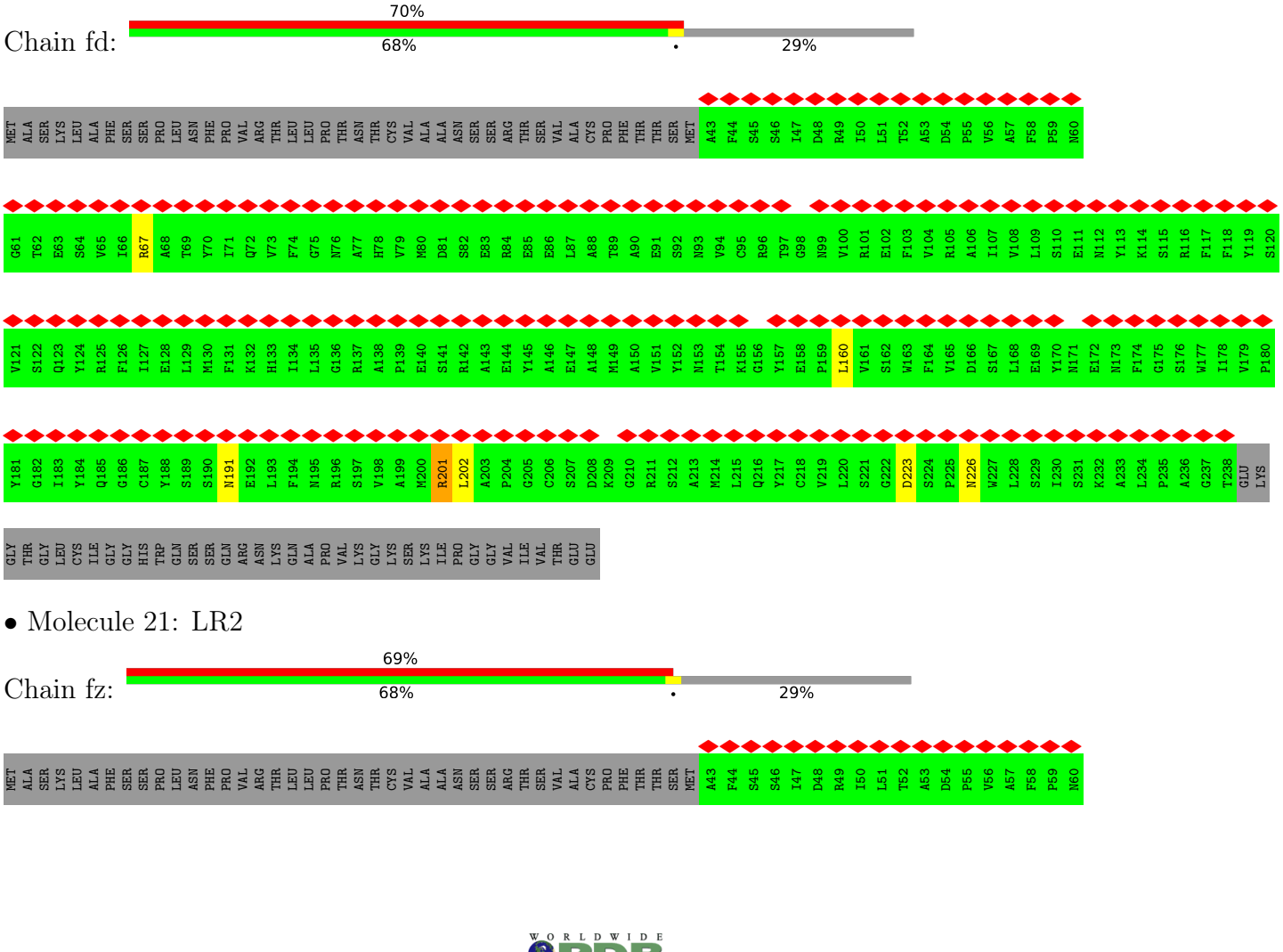
• Molecule 21: LR2

Chain ex:



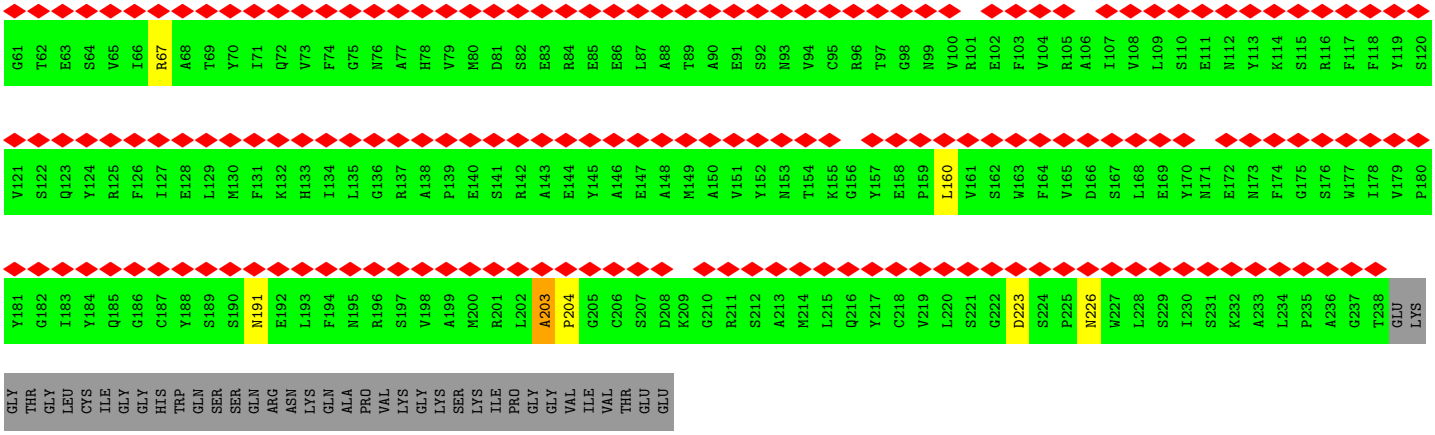
• Molecule 21: LR2

Chain fd:



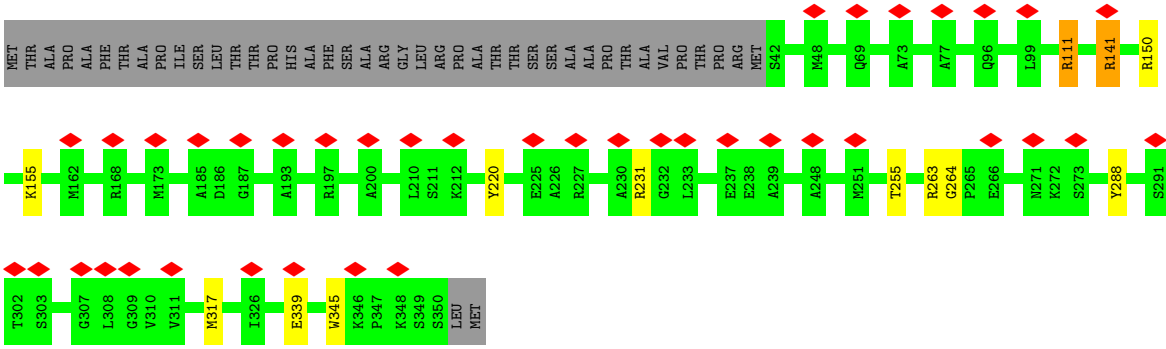
• Molecule 21: LR2

Chain fz:



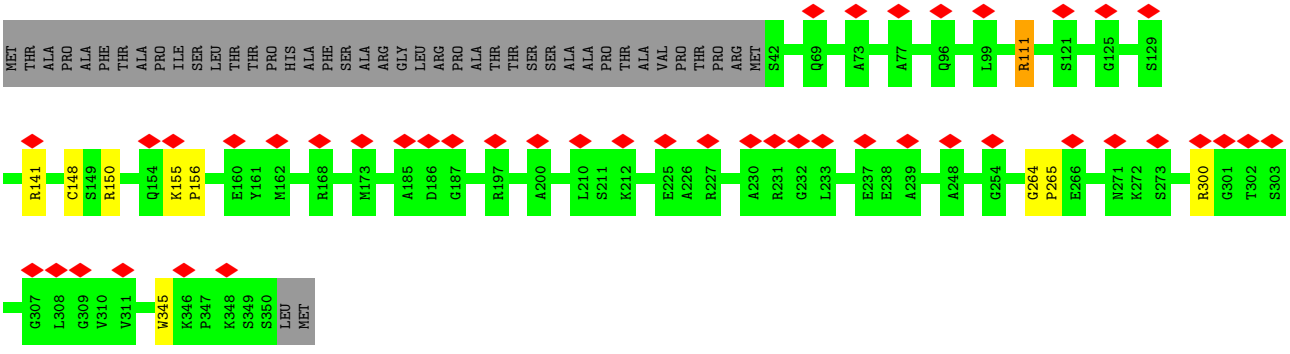
• Molecule 22: LR_gamma7

Chain eY:



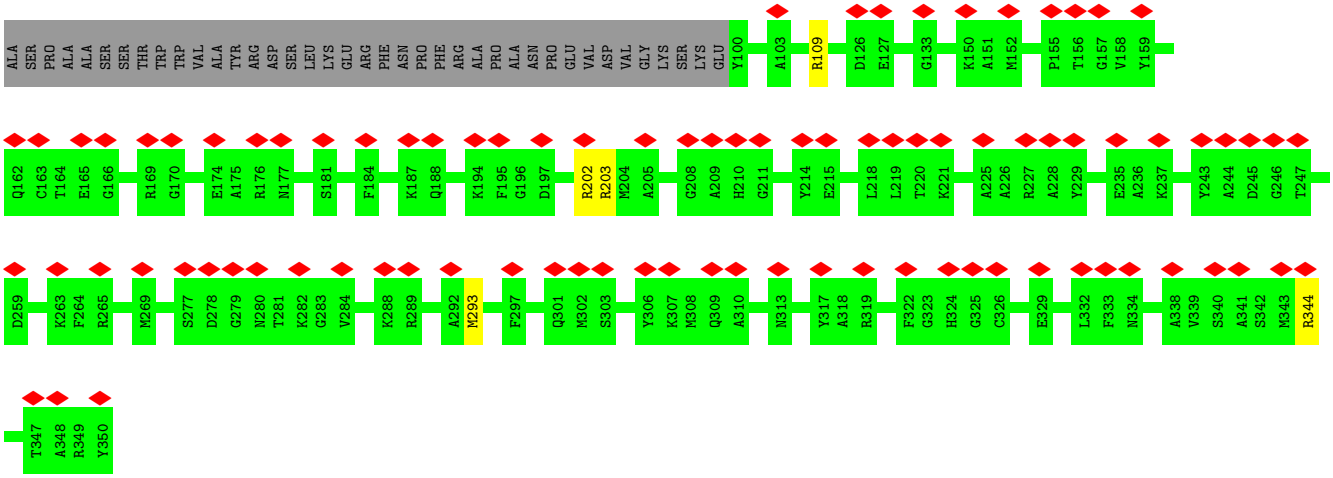
• Molecule 22: LR_gamma7

Chain eZ:



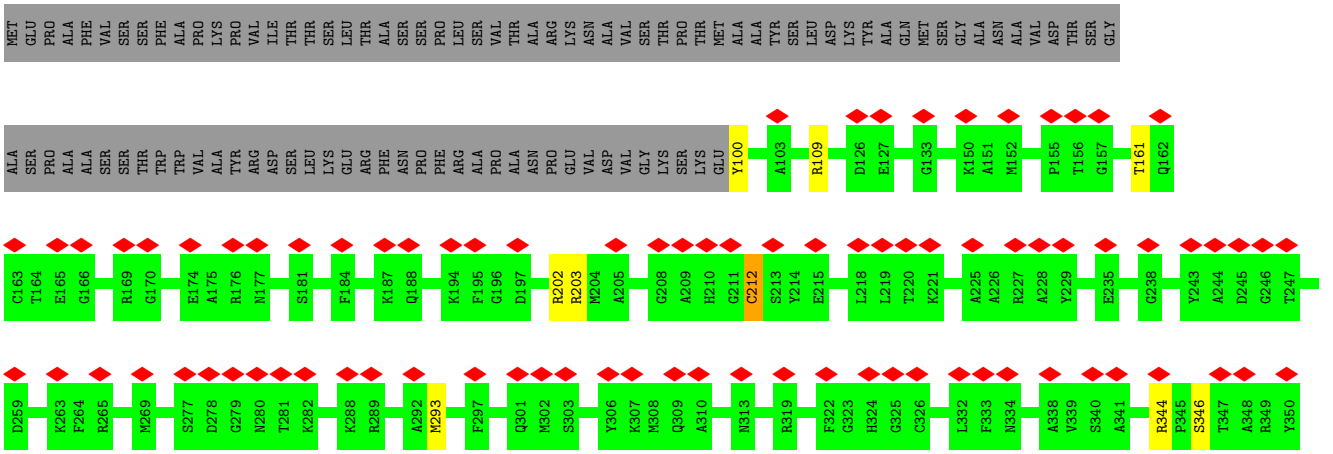
• Molecule 23: LR_gamma8

Chain ly:



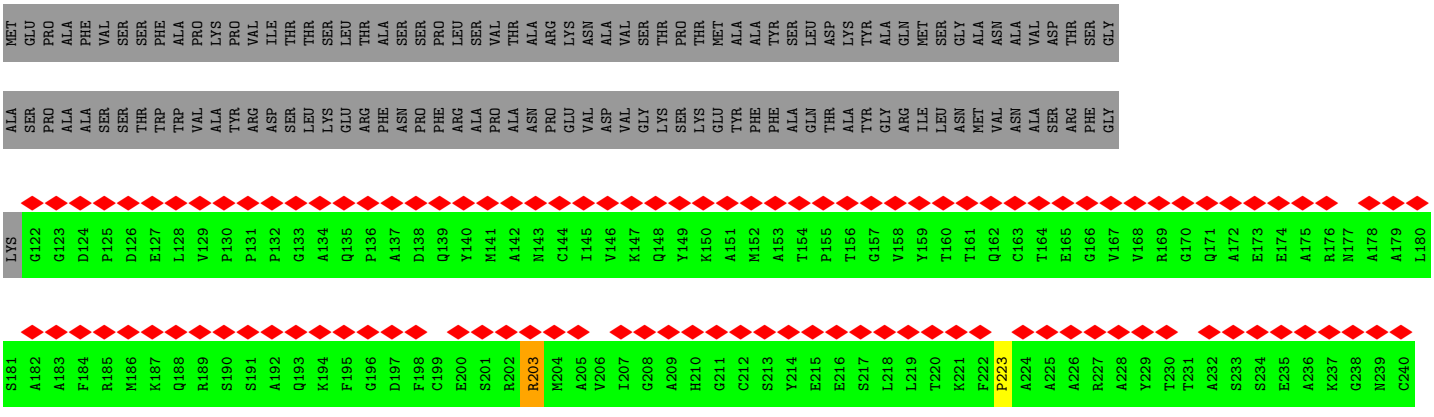
- Molecule 23: LR_gamma8

Chain lz:



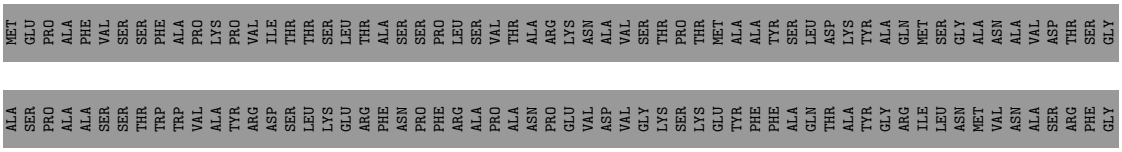
- Molecule 23: LR_gamma8

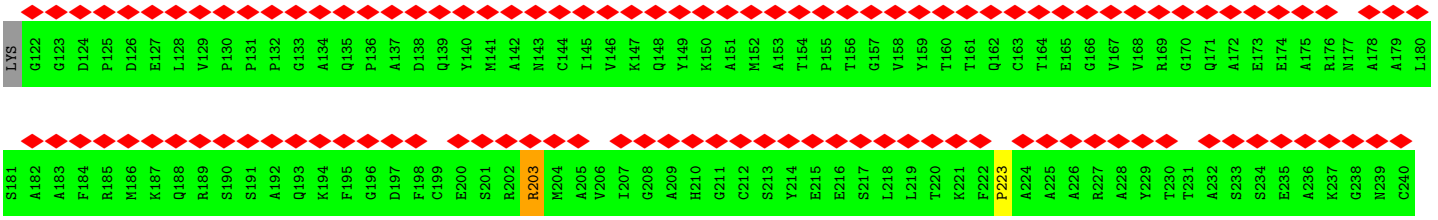
Chain hY:



• Molecule 23: LR_gamma8

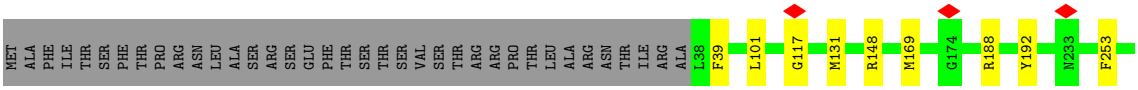
Chain hZ:





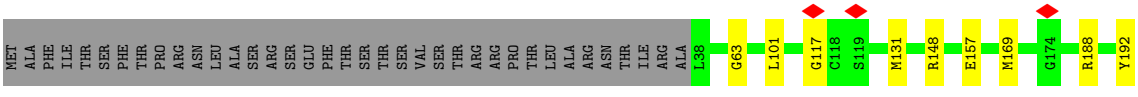
• Molecule 24: LR_gamma6

Chain gy:



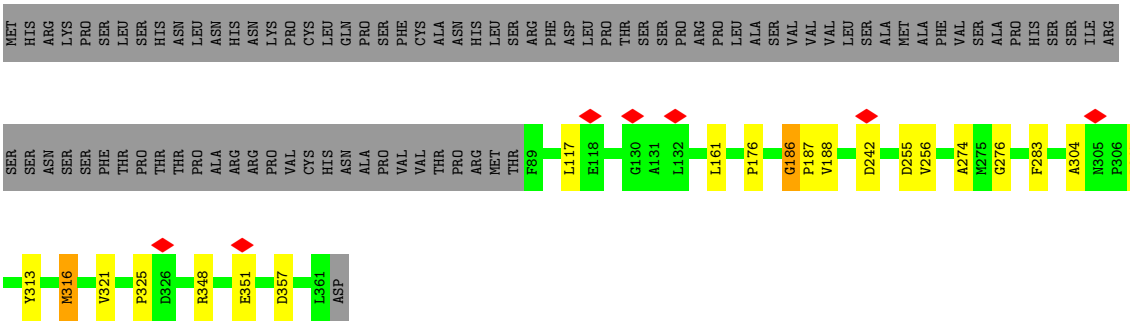
• Molecule 24: LR_gamma6

Chain gz:



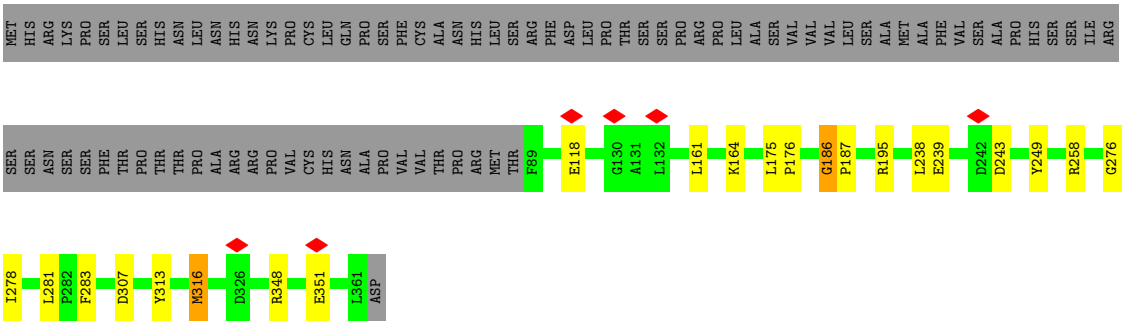
• Molecule 25: LR9

Chain ka:



• Molecule 25: LR9

Chain kb:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53403	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.130	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	739.2, 739.2, 739.2	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PVN, PEB, CYC, PUB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A1	0.89	4/1682 (0.2%)	1.00	5/2293 (0.2%)
1	B1	0.93	5/1687 (0.3%)	1.02	5/2300 (0.2%)
2	C1	0.95	3/1201 (0.2%)	1.08	11/1641 (0.7%)
2	D1	0.93	1/1192 (0.1%)	1.12	6/1629 (0.4%)
3	E1	0.85	1/2068 (0.0%)	1.00	13/2820 (0.5%)
3	F1	0.90	3/2068 (0.1%)	1.08	12/2820 (0.4%)
4	G1	1.46	10/1236 (0.8%)	1.39	23/1666 (1.4%)
4	I1	0.89	1/1236 (0.1%)	0.91	2/1666 (0.1%)
4	K1	0.89	2/1236 (0.2%)	0.93	6/1666 (0.4%)
4	N1	1.59	5/1236 (0.4%)	1.32	20/1666 (1.2%)
4	P1	1.30	6/1236 (0.5%)	1.29	15/1666 (0.9%)
4	R1	0.91	1/1236 (0.1%)	0.94	5/1666 (0.3%)
4	T1	1.00	1/1236 (0.1%)	1.13	9/1666 (0.5%)
4	X1	0.93	2/1236 (0.2%)	0.90	2/1666 (0.1%)
4	Z1	0.88	2/1236 (0.2%)	1.01	6/1666 (0.4%)
4	b1	1.42	8/1236 (0.6%)	1.41	23/1666 (1.4%)
4	d1	1.22	3/1236 (0.2%)	1.32	19/1666 (1.1%)
4	f1	1.21	4/1236 (0.3%)	1.20	13/1666 (0.8%)
4	i1	0.89	2/1236 (0.2%)	0.90	6/1666 (0.4%)
4	k1	1.02	2/1236 (0.2%)	1.17	13/1666 (0.8%)
4	o1	0.89	3/1236 (0.2%)	0.94	4/1666 (0.2%)
4	q1	1.24	5/1236 (0.4%)	1.21	19/1666 (1.1%)
4	s1	1.80	24/1236 (1.9%)	1.53	25/1666 (1.5%)
4	u1	0.89	2/1236 (0.2%)	0.96	5/1666 (0.3%)
4	w1	1.34	7/1236 (0.6%)	1.23	17/1666 (1.0%)
4	y1	2.03	25/1236 (2.0%)	1.66	34/1666 (2.0%)
5	H1	1.02	3/1240 (0.2%)	1.14	8/1680 (0.5%)
5	J1	0.89	0/1240	1.06	9/1680 (0.5%)
5	L1	1.02	1/1240 (0.1%)	1.15	10/1680 (0.6%)
5	M1	1.01	1/1240 (0.1%)	1.12	12/1680 (0.7%)
5	O1	1.30	3/1240 (0.2%)	1.47	20/1680 (1.2%)
5	S1	1.17	5/1240 (0.4%)	1.23	17/1680 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
5	U1	1.09	2/1240 (0.2%)	1.21	13/1680 (0.8%)
5	W1	1.30	5/1240 (0.4%)	1.25	12/1680 (0.7%)
5	Y1	0.91	1/1240 (0.1%)	1.10	10/1680 (0.6%)
5	a1	1.08	2/1240 (0.2%)	1.17	11/1680 (0.7%)
5	c1	1.05	3/1240 (0.2%)	1.17	11/1680 (0.7%)
5	e1	1.36	3/1233 (0.2%)	1.52	21/1672 (1.3%)
5	h1	1.03	1/1240 (0.1%)	1.14	13/1680 (0.8%)
5	j1	1.09	5/1240 (0.4%)	1.18	17/1680 (1.0%)
5	l1	1.02	1/1240 (0.1%)	1.16	12/1680 (0.7%)
5	n1	1.27	5/1240 (0.4%)	1.26	10/1680 (0.6%)
5	p1	1.17	6/1240 (0.5%)	1.17	13/1680 (0.8%)
5	r1	1.28	11/1240 (0.9%)	1.22	11/1680 (0.7%)
5	t1	1.17	4/1240 (0.3%)	1.23	14/1680 (0.8%)
5	v1	1.20	6/1240 (0.5%)	1.24	15/1680 (0.9%)
5	x1	1.28	11/1240 (0.9%)	1.20	10/1680 (0.6%)
5	z1	1.18	4/1240 (0.3%)	1.24	11/1680 (0.7%)
6	Q1	0.91	3/1419 (0.2%)	1.05	10/1924 (0.5%)
6	g1	0.98	2/1419 (0.1%)	1.12	12/1924 (0.6%)
7	V1	0.88	2/1281 (0.2%)	0.96	3/1731 (0.2%)
7	m1	0.87	1/1281 (0.1%)	1.00	5/1731 (0.3%)
8	a2	0.99	18/6626 (0.3%)	1.10	41/8939 (0.5%)
8	b2	0.96	13/6626 (0.2%)	1.04	35/8939 (0.4%)
9	c2	0.96	3/730 (0.4%)	1.24	8/976 (0.8%)
9	d2	0.90	0/730	1.18	5/976 (0.5%)
10	A3	0.70	0/1266	0.87	1/1709 (0.1%)
10	A4	0.74	0/1266	0.91	3/1709 (0.2%)
10	A5	0.84	0/1266	1.09	4/1709 (0.2%)
10	A6	1.01	3/1266 (0.2%)	1.11	7/1709 (0.4%)
10	A7	0.85	2/1266 (0.2%)	1.02	5/1709 (0.3%)
10	A9	0.74	0/1266	0.91	5/1709 (0.3%)
10	B8	0.44	0/1266	0.61	0/1709
10	C3	0.70	0/1266	0.83	2/1709 (0.1%)
10	C4	0.71	0/1266	0.83	2/1709 (0.1%)
10	C5	0.87	1/1266 (0.1%)	1.05	7/1709 (0.4%)
10	C6	0.89	1/1266 (0.1%)	1.13	7/1709 (0.4%)
10	C7	1.06	1/1266 (0.1%)	1.28	15/1709 (0.9%)
10	C9	0.58	0/1266	0.76	3/1709 (0.2%)
10	D8	0.77	0/1266	0.94	5/1709 (0.3%)
10	E2	0.70	0/1266	0.79	1/1709 (0.1%)
10	E3	0.66	1/1266 (0.1%)	0.85	1/1709 (0.1%)
10	E4	0.83	0/1266	1.05	4/1709 (0.2%)
10	E5	0.76	0/1266	1.00	5/1709 (0.3%)
10	E6	0.83	1/1266 (0.1%)	1.02	7/1709 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	E7	1.01	2/1266 (0.2%)	1.13	6/1709 (0.4%)
10	E9	0.82	0/1266	1.08	12/1709 (0.7%)
10	F8	0.42	0/1266	0.62	0/1709
10	G2	0.63	0/1266	0.77	0/1709
10	G3	0.66	0/1266	0.79	2/1709 (0.1%)
10	G4	0.90	1/1266 (0.1%)	1.06	6/1709 (0.4%)
10	G5	0.79	0/1266	0.98	2/1709 (0.1%)
10	G6	1.09	3/1266 (0.2%)	1.16	12/1709 (0.7%)
10	G7	0.85	1/1259 (0.1%)	1.05	6/1701 (0.4%)
10	G9	0.44	0/1266	0.63	0/1709
10	H8	0.42	0/1266	0.61	0/1709
10	I2	0.78	1/1266 (0.1%)	0.92	5/1709 (0.3%)
10	I3	0.70	0/1266	0.84	1/1709 (0.1%)
10	I4	0.75	0/1266	0.99	5/1709 (0.3%)
10	I5	0.85	0/1266	1.02	7/1709 (0.4%)
10	I6	0.85	1/1259 (0.1%)	1.03	7/1701 (0.4%)
10	I7	0.86	0/1266	1.05	4/1709 (0.2%)
10	I9	0.81	0/1266	1.00	4/1709 (0.2%)
10	J8	0.43	0/1266	0.64	1/1709 (0.1%)
10	K2	0.86	0/1266	1.06	6/1709 (0.4%)
10	K3	0.62	0/1266	0.75	1/1709 (0.1%)
10	K4	0.82	2/1266 (0.2%)	0.98	2/1709 (0.1%)
10	K5	0.43	0/1266	0.62	0/1709
10	K6	0.76	0/1266	0.95	3/1709 (0.2%)
10	K7	1.23	2/1266 (0.2%)	1.28	14/1709 (0.8%)
10	K9	0.43	0/1266	0.63	0/1709
10	L8	0.47	0/1266	0.66	0/1709
10	M2	0.73	0/1266	0.82	0/1709
10	M3	0.63	0/1266	0.78	2/1709 (0.1%)
10	M4	0.83	0/1266	0.98	7/1709 (0.4%)
10	M5	0.45	0/1266	0.63	0/1709
10	M6	0.61	1/1266 (0.1%)	0.79	4/1709 (0.2%)
10	M7	0.90	0/1266	1.10	9/1709 (0.5%)
10	M9	0.43	0/1266	0.61	0/1709
10	N8	0.45	0/1266	0.65	0/1709
10	O2	0.81	1/1266 (0.1%)	1.04	4/1709 (0.2%)
10	O3	0.48	0/1266	0.64	0/1709
10	O4	0.43	0/1266	0.62	0/1709
10	O5	0.41	0/1266	0.63	0/1709
10	O6	0.77	1/1266 (0.1%)	0.96	2/1709 (0.1%)
10	O7	0.67	0/1266	0.85	2/1709 (0.1%)
10	O9	0.43	0/1266	0.65	1/1709 (0.1%)
10	P8	0.44	0/1266	0.63	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	Q2	0.76	0/1266	0.85	4/1709 (0.2%)
10	Q3	0.46	0/1266	0.61	0/1709
10	Q4	0.45	0/1266	0.62	0/1709
10	Q5	0.40	0/1266	0.60	0/1709
10	Q6	0.83	0/1266	1.01	7/1709 (0.4%)
10	Q7	0.82	1/1266 (0.1%)	1.02	4/1709 (0.2%)
10	Q9	0.46	0/1266	0.66	0/1709
10	S2	0.58	0/1266	0.71	0/1709
10	S3	0.47	0/1266	0.63	0/1709
10	S4	0.41	0/1266	0.62	0/1709
10	S5	0.42	0/1266	0.63	0/1709
10	S6	0.96	2/1266 (0.2%)	1.07	7/1709 (0.4%)
10	S7	0.82	0/1266	0.97	3/1709 (0.2%)
10	S9	0.44	0/1266	0.65	0/1709
10	U2	0.74	0/1266	0.80	1/1709 (0.1%)
10	U3	0.53	0/1266	0.70	1/1709 (0.1%)
10	U4	0.40	0/1266	0.60	0/1709
10	U5	0.42	0/1266	0.61	0/1709
10	U6	0.76	0/1266	0.92	2/1709 (0.1%)
10	U7	0.86	0/1266	1.01	5/1709 (0.3%)
10	U9	0.44	0/1266	0.63	0/1709
10	W2	0.93	2/1266 (0.2%)	1.01	4/1709 (0.2%)
10	W3	0.48	0/1266	0.64	0/1709
10	W4	0.42	0/1266	0.63	0/1709
10	W6	0.83	0/1266	0.97	2/1709 (0.1%)
10	W7	1.05	4/1266 (0.3%)	1.16	8/1709 (0.5%)
10	Y2	0.61	0/1266	0.75	0/1709
10	Y3	0.48	0/1266	0.66	0/1709
10	Y4	0.41	0/1266	0.62	0/1709
10	Y6	0.51	0/1266	0.73	1/1709 (0.1%)
10	Y7	0.86	1/1266 (0.1%)	1.07	9/1709 (0.5%)
10	aA	0.71	1/1266 (0.1%)	0.82	3/1709 (0.2%)
10	aC	0.78	0/1266	0.99	4/1709 (0.2%)
10	aE	0.72	0/1266	0.91	4/1709 (0.2%)
10	aG	0.61	0/1266	0.77	3/1709 (0.2%)
10	aI	0.63	0/1266	0.77	4/1709 (0.2%)
10	aK	0.50	0/1266	0.67	3/1709 (0.2%)
10	aM	0.56	0/1266	0.74	1/1709 (0.1%)
10	aO	0.55	0/1266	0.71	1/1709 (0.1%)
10	aQ	0.47	0/1266	0.67	2/1709 (0.1%)
10	aS	0.48	0/1266	0.68	2/1709 (0.1%)
10	aU	0.49	0/1266	0.69	2/1709 (0.1%)
10	am	0.54	0/1266	0.75	2/1709 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	ao	0.72	0/1266	0.86	3/1709 (0.2%)
10	aq	0.61	0/1266	0.84	6/1709 (0.4%)
10	as	0.80	2/1266 (0.2%)	1.03	9/1709 (0.5%)
10	au	0.88	0/1266	1.04	5/1709 (0.3%)
10	aw	0.59	0/1266	0.79	3/1709 (0.2%)
10	ay	0.73	0/1266	0.86	4/1709 (0.2%)
10	bA	0.71	1/1266 (0.1%)	0.98	2/1709 (0.1%)
10	bC	0.81	0/1266	1.13	6/1709 (0.4%)
10	bE	0.77	0/1266	1.06	6/1709 (0.4%)
10	bG	0.64	0/1266	0.99	3/1709 (0.2%)
10	bI	0.64	0/1266	0.94	4/1709 (0.2%)
10	bK	0.53	0/1266	0.93	3/1709 (0.2%)
10	bM	0.59	1/1266 (0.1%)	1.19	3/1709 (0.2%)
10	bO	0.57	0/1266	0.71	1/1709 (0.1%)
10	bQ	0.48	0/1266	0.84	2/1709 (0.1%)
10	bS	0.51	0/1266	0.81	2/1709 (0.1%)
10	bU	0.52	0/1266	1.05	3/1709 (0.2%)
10	bm	0.95	2/1266 (0.2%)	1.14	11/1709 (0.6%)
10	bt	0.95	3/1266 (0.2%)	1.10	11/1709 (0.6%)
10	bu	0.83	0/1266	0.98	5/1709 (0.3%)
10	bv	1.00	2/1266 (0.2%)	1.10	8/1709 (0.5%)
10	bw	0.75	0/1266	0.91	6/1709 (0.4%)
10	bx	0.82	0/1266	0.93	3/1709 (0.2%)
10	by	0.82	3/1266 (0.2%)	0.94	6/1709 (0.4%)
10	cA	0.66	1/1266 (0.1%)	0.83	2/1709 (0.1%)
10	cC	0.62	0/1266	0.96	3/1709 (0.2%)
10	cD	0.56	0/1266	0.74	2/1709 (0.1%)
10	cG	0.55	0/1266	0.68	0/1709
10	cI	0.60	1/1266 (0.1%)	0.77	2/1709 (0.1%)
10	cK	0.58	0/1266	0.68	1/1709 (0.1%)
10	cS	0.55	0/1266	0.67	1/1709 (0.1%)
10	cT	0.55	0/1266	0.69	0/1709
10	cU	0.54	0/1266	0.70	0/1709
10	cV	0.47	0/1266	0.62	0/1709
10	cW	0.62	1/1266 (0.1%)	0.77	2/1709 (0.1%)
10	cX	0.55	0/1266	0.71	1/1709 (0.1%)
10	cZ	0.50	0/1266	0.66	1/1709 (0.1%)
10	cm	1.00	4/1266 (0.3%)	1.27	13/1709 (0.8%)
10	ct	0.96	3/1266 (0.2%)	1.21	12/1709 (0.7%)
10	cu	0.81	0/1266	0.98	7/1709 (0.4%)
10	cv	0.95	2/1266 (0.2%)	1.08	8/1709 (0.5%)
10	cw	0.75	0/1266	1.01	4/1709 (0.2%)
10	cx	0.84	0/1266	0.98	3/1709 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	cy	0.91	4/1266 (0.3%)	1.04	6/1709 (0.4%)
10	dA	1.29	5/1266 (0.4%)	1.40	18/1709 (1.1%)
10	dC	0.44	0/1266	0.61	0/1709
10	dE	0.52	0/1266	0.68	0/1709
10	dG	0.79	0/1266	0.98	2/1709 (0.1%)
10	dI	0.64	0/1266	0.75	1/1709 (0.1%)
10	dJ	1.06	4/1266 (0.3%)	1.15	8/1709 (0.5%)
10	dM	0.66	0/1266	0.76	1/1709 (0.1%)
10	dO	1.00	1/1266 (0.1%)	1.09	8/1709 (0.5%)
10	dQ	0.72	1/1266 (0.1%)	0.84	1/1709 (0.1%)
10	dS	0.51	0/1266	0.69	1/1709 (0.1%)
10	dU	0.74	0/1266	0.91	2/1709 (0.1%)
10	dW	1.07	3/1266 (0.2%)	1.18	8/1709 (0.5%)
10	dZ	0.66	0/1266	0.82	2/1709 (0.1%)
10	da	0.46	0/1266	0.64	0/1709
10	db	0.45	0/1266	0.77	6/1709 (0.4%)
10	dc	0.50	0/1266	0.93	1/1709 (0.1%)
10	de	0.49	0/1266	0.66	3/1709 (0.2%)
10	dg	0.50	0/1266	0.69	1/1709 (0.1%)
10	dk	0.43	0/1266	0.62	1/1709 (0.1%)
10	dm	0.46	0/1266	0.62	0/1709
10	do	0.45	0/1266	0.66	2/1709 (0.1%)
10	dq	0.45	0/1266	0.60	0/1709
10	ds	0.49	0/1266	0.66	0/1709
10	du	0.51	0/1266	0.68	2/1709 (0.1%)
10	e2	0.60	0/1266	0.76	2/1709 (0.1%)
10	e3	0.68	0/1266	0.78	1/1709 (0.1%)
10	eA	0.61	0/1266	0.81	4/1709 (0.2%)
10	eC	0.70	0/1266	0.89	4/1709 (0.2%)
10	eE	0.70	0/1266	0.88	3/1709 (0.2%)
10	eG	0.65	0/1266	0.84	5/1709 (0.3%)
10	eI	0.56	0/1266	0.74	1/1709 (0.1%)
10	eK	0.57	0/1266	0.72	2/1709 (0.1%)
10	eM	0.84	0/1266	0.96	6/1709 (0.4%)
10	eO	0.59	0/1266	0.73	1/1709 (0.1%)
10	eQ	0.68	0/1266	0.87	4/1709 (0.2%)
10	eS	0.54	0/1266	0.75	3/1709 (0.2%)
10	eU	0.62	0/1266	0.80	1/1709 (0.1%)
10	eW	0.70	0/1266	0.91	5/1709 (0.3%)
10	ea	0.63	0/1266	0.78	0/1709
10	ed	0.67	0/1266	0.84	1/1709 (0.1%)
10	ef	0.85	0/1266	0.97	5/1709 (0.3%)
10	eh	0.77	0/1266	0.90	1/1709 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	ej	0.72	0/1266	0.89	1/1709 (0.1%)
10	ek	0.66	0/1266	0.81	3/1709 (0.2%)
10	em	0.69	0/1266	0.87	1/1709 (0.1%)
10	eo	0.80	0/1266	0.94	1/1709 (0.1%)
10	eq	0.73	0/1266	0.86	2/1709 (0.1%)
10	es	0.73	0/1266	0.91	1/1709 (0.1%)
10	eu	0.65	0/1266	0.80	1/1709 (0.1%)
10	f6	0.77	0/1266	1.01	6/1709 (0.4%)
10	f7	0.71	2/1266 (0.2%)	0.87	4/1709 (0.2%)
10	fb	0.37	0/1266	0.59	0/1709
10	fe	0.39	0/1266	0.60	0/1709
10	fg	0.32	0/1266	0.57	0/1709
10	fh	0.43	0/1266	0.65	0/1709
10	fk	0.41	0/1266	0.64	0/1709
10	fl	0.34	0/1266	0.59	0/1709
10	fn	0.54	0/1266	0.70	1/1709 (0.1%)
10	fp	0.43	0/1266	0.68	2/1709 (0.1%)
10	fr	0.42	0/1266	0.67	0/1709
10	ft	0.31	0/1266	0.55	1/1709 (0.1%)
10	fv	0.49	0/1266	0.67	0/1709
10	fx	0.38	0/1266	0.63	1/1709 (0.1%)
10	g2	0.67	1/1266 (0.1%)	0.80	2/1709 (0.1%)
10	g3	0.57	0/1266	0.69	0/1709
10	g6	0.83	0/1266	0.99	3/1709 (0.2%)
10	g7	0.77	0/1266	1.01	5/1709 (0.3%)
10	gb	0.71	0/1266	0.88	5/1709 (0.3%)
10	gc	0.83	1/1266 (0.1%)	0.90	2/1709 (0.1%)
10	gf	0.58	0/1266	0.74	1/1709 (0.1%)
10	gh	0.53	0/1266	0.86	8/1709 (0.5%)
10	gj	0.53	0/1266	0.73	3/1709 (0.2%)
10	gl	0.49	0/1266	0.69	1/1709 (0.1%)
10	gm	1.18	6/1266 (0.5%)	1.16	8/1709 (0.5%)
10	go	0.50	0/1266	0.83	5/1709 (0.3%)
10	gq	0.70	0/1266	0.97	6/1709 (0.4%)
10	gs	0.84	1/1266 (0.1%)	0.93	3/1709 (0.2%)
10	gu	0.53	0/1266	0.71	1/1709 (0.1%)
10	gw	0.49	0/1266	0.84	1/1709 (0.1%)
10	h6	0.68	0/1266	0.87	5/1709 (0.3%)
10	h7	0.82	1/1266 (0.1%)	0.99	4/1709 (0.2%)
10	hA	0.42	0/1266	0.58	1/1709 (0.1%)
10	hC	0.40	0/1266	0.59	1/1709 (0.1%)
10	hE	0.34	0/1266	0.53	0/1709
10	hF	0.39	0/1266	0.57	0/1709

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	hI	0.37	0/1266	0.55	0/1709
10	hK	0.35	0/1266	0.55	0/1709
10	hM	0.36	0/1266	0.55	0/1709
10	hO	0.34	0/1266	0.53	0/1709
10	hQ	0.36	0/1266	0.55	0/1709
10	hS	0.37	0/1266	0.57	1/1709 (0.1%)
10	hU	0.36	0/1266	0.56	0/1709
10	hW	0.38	0/1266	0.56	0/1709
10	i2	0.70	0/1266	0.85	1/1709 (0.1%)
10	i3	0.79	1/1266 (0.1%)	0.93	6/1709 (0.4%)
10	i6	0.53	0/1266	0.71	1/1709 (0.1%)
10	i7	0.84	0/1266	1.14	12/1709 (0.7%)
10	i8	0.45	0/1266	0.64	1/1709 (0.1%)
10	iA	1.02	4/1266 (0.3%)	1.07	9/1709 (0.5%)
10	iB	1.00	4/1266 (0.3%)	1.06	9/1709 (0.5%)
10	j6	0.83	0/1266	1.10	9/1709 (0.5%)
10	j7	0.83	0/1266	1.01	6/1709 (0.4%)
10	j8	0.39	0/1266	0.63	2/1709 (0.1%)
10	k2	0.60	0/1266	0.74	1/1709 (0.1%)
10	k3	0.89	0/1266	1.06	6/1709 (0.4%)
10	k6	0.87	1/1266 (0.1%)	1.10	5/1709 (0.3%)
10	k7	0.86	1/1266 (0.1%)	1.09	9/1709 (0.5%)
10	k8	0.62	1/1266 (0.1%)	0.81	3/1709 (0.2%)
10	l8	0.46	0/1266	0.67	1/1709 (0.1%)
10	la	1.10	4/1266 (0.3%)	1.21	13/1709 (0.8%)
10	lc	0.54	0/1266	0.72	1/1709 (0.1%)
10	le	0.73	0/1266	0.87	2/1709 (0.1%)
10	lg	0.62	1/1266 (0.1%)	0.81	2/1709 (0.1%)
10	li	0.72	0/1266	1.00	5/1709 (0.3%)
10	lk	0.59	0/1266	0.77	0/1709
10	lm	0.59	0/1266	0.78	2/1709 (0.1%)
10	lo	0.75	1/1266 (0.1%)	0.87	1/1709 (0.1%)
10	lq	0.96	3/1266 (0.2%)	1.06	6/1709 (0.4%)
10	ls	0.60	0/1266	0.79	1/1709 (0.1%)
10	lu	0.61	1/1266 (0.1%)	0.80	3/1709 (0.2%)
10	lw	0.66	0/1266	0.93	7/1709 (0.4%)
10	m2	0.62	0/1266	0.75	1/1709 (0.1%)
10	m3	0.81	0/1266	0.95	3/1709 (0.2%)
10	m4	0.89	3/1266 (0.2%)	1.08	6/1709 (0.4%)
10	m5	0.96	3/1266 (0.2%)	1.14	7/1709 (0.4%)
10	m6	0.72	0/1266	0.89	1/1709 (0.1%)
10	m7	0.85	1/1266 (0.1%)	1.08	5/1709 (0.3%)
10	m8	0.49	0/1266	0.72	1/1709 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	m9	0.55	0/1266	0.75	2/1709 (0.1%)
10	o2	0.48	0/1266	0.65	1/1709 (0.1%)
10	o3	0.79	0/1266	0.93	3/1709 (0.2%)
10	o4	0.67	0/1266	0.85	0/1709
10	o5	0.68	0/1266	0.87	1/1709 (0.1%)
10	o6	0.86	1/1266 (0.1%)	1.09	9/1709 (0.5%)
10	o7	0.76	0/1266	0.94	3/1709 (0.2%)
10	o9	0.69	0/1266	0.85	3/1709 (0.2%)
10	q2	0.45	0/1266	0.61	0/1709
10	q3	0.78	1/1266 (0.1%)	0.87	3/1709 (0.2%)
10	q4	0.88	0/1266	1.15	11/1709 (0.6%)
10	q5	0.89	0/1266	1.18	12/1709 (0.7%)
10	q6	0.51	0/1266	0.71	1/1709 (0.1%)
10	q7	0.81	0/1266	1.02	4/1709 (0.2%)
10	q8	0.60	0/1266	0.79	3/1709 (0.2%)
10	q9	0.63	0/1266	0.86	6/1709 (0.4%)
10	r8	0.56	0/1266	0.79	1/1709 (0.1%)
10	s2	0.46	0/1266	0.61	0/1709
10	s3	0.59	0/1266	0.73	0/1709
10	s4	0.86	1/1266 (0.1%)	1.07	8/1709 (0.5%)
10	s5	0.90	2/1266 (0.2%)	1.12	8/1709 (0.5%)
10	s6	0.81	0/1266	1.04	6/1709 (0.4%)
10	s7	0.77	0/1266	0.99	5/1709 (0.3%)
10	s8	0.44	0/1266	0.66	1/1709 (0.1%)
10	s9	0.79	2/1266 (0.2%)	1.00	9/1709 (0.5%)
10	t8	0.60	0/1266	0.85	2/1709 (0.1%)
10	u2	0.53	0/1266	0.68	1/1709 (0.1%)
10	u3	0.80	1/1266 (0.1%)	0.84	2/1709 (0.1%)
10	u4	0.80	2/1266 (0.2%)	0.98	2/1709 (0.1%)
10	u5	0.81	2/1266 (0.2%)	1.01	2/1709 (0.1%)
10	u6	0.75	0/1266	0.97	4/1709 (0.2%)
10	u7	0.54	0/1266	0.74	2/1709 (0.1%)
10	u8	0.51	0/1266	0.70	1/1709 (0.1%)
10	u9	0.87	0/1266	1.05	6/1709 (0.4%)
10	v8	0.73	0/1266	0.90	3/1709 (0.2%)
10	w2	0.51	0/1266	0.65	0/1709
10	w3	0.95	2/1266 (0.2%)	1.03	5/1709 (0.3%)
10	w4	0.80	1/1266 (0.1%)	0.93	3/1709 (0.2%)
10	w5	0.78	1/1266 (0.1%)	0.91	1/1709 (0.1%)
10	w6	0.40	0/1266	0.59	1/1709 (0.1%)
10	w7	0.46	0/1266	0.68	1/1709 (0.1%)
10	w9	0.59	0/1266	0.79	3/1709 (0.2%)
10	x8	0.57	0/1266	0.74	2/1709 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
10	y2	0.48	0/1266	0.65	0/1709
10	y3	0.65	0/1266	0.78	0/1709
10	y4	0.91	0/1266	1.11	6/1709 (0.4%)
10	y5	0.93	1/1266 (0.1%)	1.14	8/1709 (0.5%)
10	y9	0.72	0/1266	0.84	5/1709 (0.3%)
10	z8	0.74	0/1266	0.96	8/1709 (0.5%)
11	A8	0.57	0/1298	0.80	4/1754 (0.2%)
11	B3	0.74	0/1298	0.88	5/1754 (0.3%)
11	B4	0.74	0/1298	0.90	4/1754 (0.2%)
11	B5	0.82	0/1298	1.07	8/1754 (0.5%)
11	B6	0.83	0/1298	1.06	7/1754 (0.4%)
11	B7	1.01	1/1298 (0.1%)	1.03	8/1754 (0.5%)
11	B9	0.61	0/1298	0.74	1/1754 (0.1%)
11	C8	0.67	0/1298	0.90	2/1754 (0.1%)
11	D3	0.71	0/1298	0.90	2/1754 (0.1%)
11	D4	0.69	0/1298	0.89	4/1754 (0.2%)
11	D5	0.84	0/1298	1.13	8/1754 (0.5%)
11	D6	0.71	0/1298	0.92	3/1754 (0.2%)
11	D7	0.81	0/1298	1.09	7/1754 (0.4%)
11	D9	0.84	0/1298	1.00	2/1754 (0.1%)
11	E8	0.72	0/1298	0.89	3/1754 (0.2%)
11	F2	0.60	0/1298	0.80	2/1754 (0.1%)
11	F3	0.63	0/1298	0.88	3/1754 (0.2%)
11	F4	0.82	0/1298	1.08	8/1754 (0.5%)
11	F5	0.73	0/1298	0.96	4/1754 (0.2%)
11	F6	0.98	0/1298	1.13	12/1754 (0.7%)
11	F7	0.74	0/1298	0.93	3/1754 (0.2%)
11	F9	0.58	0/1298	0.81	4/1754 (0.2%)
11	G8	0.42	0/1298	0.65	0/1754
11	H2	0.76	0/1298	1.08	8/1754 (0.5%)
11	H3	0.66	0/1298	0.83	2/1754 (0.1%)
11	H4	0.86	0/1298	1.13	9/1754 (0.5%)
11	H5	0.75	1/1298 (0.1%)	1.02	5/1754 (0.3%)
11	H6	0.81	0/1298	1.02	6/1754 (0.3%)
11	H7	0.78	0/1298	1.03	7/1754 (0.4%)
11	H9	0.73	0/1298	0.97	5/1754 (0.3%)
11	I8	0.45	0/1298	0.65	0/1754
11	J2	0.62	0/1298	0.86	3/1754 (0.2%)
11	J3	0.57	0/1298	0.75	2/1754 (0.1%)
11	J4	0.73	0/1298	0.95	5/1754 (0.3%)
11	J5	0.83	0/1298	1.08	8/1754 (0.5%)
11	J6	0.76	0/1298	1.02	5/1754 (0.3%)
11	J7	0.90	3/1298 (0.2%)	1.04	9/1754 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	J9	0.69	0/1298	0.86	4/1754 (0.2%)
11	K8	0.41	0/1298	0.63	0/1754
11	L2	0.91	0/1298	1.16	12/1754 (0.7%)
11	L3	0.60	0/1298	0.81	3/1754 (0.2%)
11	L4	0.74	1/1298 (0.1%)	1.02	5/1754 (0.3%)
11	L5	0.42	0/1298	0.63	1/1754 (0.1%)
11	L6	1.04	5/1298 (0.4%)	1.20	15/1754 (0.9%)
11	L7	0.82	0/1298	1.05	3/1754 (0.2%)
11	L9	0.42	0/1298	0.66	0/1754
11	M8	0.43	0/1298	0.63	0/1754
11	N2	0.71	0/1298	0.91	3/1754 (0.2%)
11	N3	0.65	0/1298	0.81	1/1754 (0.1%)
11	N4	0.83	0/1298	1.08	9/1754 (0.5%)
11	N5	0.39	0/1298	0.61	0/1754
11	N6	0.89	0/1298	1.11	7/1754 (0.4%)
11	N7	1.03	1/1298 (0.1%)	1.19	9/1754 (0.5%)
11	N9	0.45	0/1298	0.65	0/1754
11	O8	0.40	0/1298	0.62	0/1754
11	P2	0.54	0/1298	0.74	2/1754 (0.1%)
11	P3	0.45	0/1298	0.63	0/1754
11	P4	0.42	0/1298	0.62	1/1754 (0.1%)
11	P5	0.41	0/1298	0.65	2/1754 (0.1%)
11	P6	0.89	1/1298 (0.1%)	1.05	9/1754 (0.5%)
11	P7	0.89	0/1298	1.11	6/1754 (0.3%)
11	P9	0.41	0/1298	0.63	0/1754
11	Q8	0.40	0/1298	0.61	0/1754
11	R2	0.63	0/1298	0.78	2/1754 (0.1%)
11	R3	0.45	0/1298	0.67	2/1754 (0.1%)
11	R4	0.38	0/1298	0.60	0/1754
11	R5	0.41	0/1298	0.61	0/1754
11	R6	0.98	1/1298 (0.1%)	1.16	8/1754 (0.5%)
11	R7	0.86	1/1298 (0.1%)	1.10	8/1754 (0.5%)
11	R9	0.44	0/1298	0.64	0/1754
11	T2	0.78	0/1298	1.01	6/1754 (0.3%)
11	T3	0.48	0/1298	0.65	1/1754 (0.1%)
11	T4	0.41	0/1298	0.65	1/1754 (0.1%)
11	T5	0.41	0/1298	0.61	0/1754
11	T6	0.99	1/1298 (0.1%)	1.10	9/1754 (0.5%)
11	T7	0.79	0/1298	1.01	5/1754 (0.3%)
11	T9	0.41	0/1298	0.62	0/1754
11	V2	0.94	0/1298	1.07	5/1754 (0.3%)
11	V3	0.51	0/1298	0.71	0/1754
11	V4	0.41	0/1298	0.61	0/1754

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	V5	0.44	1/1298 (0.1%)	0.62	1/1754 (0.1%)
11	V6	0.77	0/1298	0.99	5/1754 (0.3%)
11	V7	0.95	1/1298 (0.1%)	1.13	10/1754 (0.6%)
11	V9	0.40	0/1298	0.61	0/1754
11	X2	0.74	0/1298	0.91	2/1754 (0.1%)
11	X3	0.48	0/1298	0.65	0/1754
11	X4	0.41	0/1298	0.61	0/1754
11	X6	0.96	2/1298 (0.2%)	1.14	10/1754 (0.6%)
11	X7	1.02	3/1298 (0.2%)	1.10	12/1754 (0.7%)
11	Z2	0.64	0/1298	0.84	3/1754 (0.2%)
11	Z3	0.45	0/1298	0.66	1/1754 (0.1%)
11	Z4	0.44	1/1298 (0.1%)	0.63	1/1754 (0.1%)
11	Z6	0.83	1/1298 (0.1%)	1.02	6/1754 (0.3%)
11	Z7	0.95	2/1298 (0.2%)	1.15	6/1754 (0.3%)
11	a6	0.88	2/1298 (0.2%)	1.08	6/1754 (0.3%)
11	a7	0.92	0/1298	1.15	12/1754 (0.7%)
11	aB	0.78	0/1298	0.99	5/1754 (0.3%)
11	aD	0.68	0/1298	0.91	3/1754 (0.2%)
11	aF	0.58	1/1298 (0.1%)	0.74	0/1754
11	aH	0.83	0/1298	1.01	4/1754 (0.2%)
11	aJ	0.69	1/1298 (0.1%)	0.87	1/1754 (0.1%)
11	aL	0.50	0/1298	0.70	1/1754 (0.1%)
11	aN	0.50	0/1298	0.70	0/1754
11	aP	0.47	0/1298	0.68	1/1754 (0.1%)
11	aR	0.49	0/1298	0.69	1/1754 (0.1%)
11	aT	0.52	1/1298 (0.1%)	0.76	1/1754 (0.1%)
11	aV	0.48	0/1298	0.67	0/1754
11	an	0.67	0/1298	0.94	8/1754 (0.5%)
11	ap	0.86	0/1298	1.08	8/1754 (0.5%)
11	ar	0.82	0/1298	0.98	6/1754 (0.3%)
11	at	0.91	0/1298	1.14	10/1754 (0.6%)
11	av	0.84	0/1298	1.05	7/1754 (0.4%)
11	ax	0.78	0/1298	0.97	5/1754 (0.3%)
11	az	0.79	0/1298	1.07	9/1754 (0.5%)
11	b6	0.71	0/1298	0.87	4/1754 (0.2%)
11	b7	0.66	0/1298	0.89	5/1754 (0.3%)
11	bB	0.80	0/1298	1.01	6/1754 (0.3%)
11	bD	0.67	0/1298	0.92	3/1754 (0.2%)
11	bF	0.61	1/1298 (0.1%)	0.76	0/1754
11	bH	0.78	0/1298	0.97	5/1754 (0.3%)
11	bJ	0.71	1/1298 (0.1%)	0.88	1/1754 (0.1%)
11	bL	0.52	1/1298 (0.1%)	0.69	1/1754 (0.1%)
11	bN	0.51	0/1298	0.70	0/1754

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	bP	0.49	0/1298	0.71	2/1754 (0.1%)
11	bR	0.51	0/1298	0.71	1/1754 (0.1%)
11	bT	0.52	0/1298	0.76	1/1754 (0.1%)
11	bV	0.50	0/1298	0.69	1/1754 (0.1%)
11	bn	0.65	0/1298	0.84	4/1754 (0.2%)
11	bo	0.71	0/1298	0.99	7/1754 (0.4%)
11	bp	0.74	0/1298	0.90	2/1754 (0.1%)
11	bq	0.90	1/1298 (0.1%)	1.06	7/1754 (0.4%)
11	br	0.85	0/1298	1.11	8/1754 (0.5%)
11	bs	0.82	0/1298	0.99	6/1754 (0.3%)
11	bz	0.59	0/1298	0.76	2/1754 (0.1%)
11	c6	0.92	0/1298	1.15	11/1754 (0.6%)
11	c7	0.87	2/1298 (0.2%)	1.01	6/1754 (0.3%)
11	cB	0.50	0/1298	0.67	0/1754
11	cE	0.55	0/1298	0.74	0/1754
11	cF	0.52	1/1298 (0.1%)	0.64	0/1754
11	cH	0.57	0/1298	0.74	1/1754 (0.1%)
11	cJ	0.50	0/1298	0.68	0/1754
11	cL	0.60	0/1298	0.75	3/1754 (0.2%)
11	cM	0.51	0/1298	0.70	0/1754
11	cN	0.54	0/1298	0.72	1/1754 (0.1%)
11	cO	0.47	0/1298	0.64	0/1754
11	cP	0.53	0/1298	0.70	0/1754
11	cQ	0.51	0/1298	0.63	0/1754
11	cR	0.54	1/1298 (0.1%)	0.71	2/1754 (0.1%)
11	cY	0.44	0/1298	0.60	0/1754
11	cn	0.69	0/1298	0.88	5/1754 (0.3%)
11	co	0.81	0/1298	1.06	9/1754 (0.5%)
11	cp	0.78	0/1298	0.92	2/1754 (0.1%)
11	cq	0.89	1/1298 (0.1%)	1.04	6/1754 (0.3%)
11	cr	0.80	0/1298	1.03	6/1754 (0.3%)
11	cs	0.87	0/1298	1.08	9/1754 (0.5%)
11	cz	0.60	0/1298	0.77	2/1754 (0.1%)
11	d6	0.72	0/1298	0.97	4/1754 (0.2%)
11	d7	0.77	0/1298	0.99	4/1754 (0.2%)
11	dB	0.68	0/1298	0.84	2/1754 (0.1%)
11	dD	0.46	0/1298	0.68	0/1754
11	dF	0.42	0/1298	0.63	0/1754
11	dH	0.78	0/1298	0.92	3/1754 (0.2%)
11	dK	0.81	1/1298 (0.1%)	0.95	3/1754 (0.2%)
11	dL	0.87	0/1298	1.17	9/1754 (0.5%)
11	dN	0.91	1/1298 (0.1%)	1.02	5/1754 (0.3%)
11	dP	0.68	0/1298	0.89	2/1754 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	dR	0.47	0/1298	0.68	0/1754
11	dT	0.43	0/1298	0.64	0/1754
11	dV	0.77	0/1298	0.94	4/1754 (0.2%)
11	dX	0.93	0/1298	1.26	13/1754 (0.7%)
11	dY	0.67	0/1298	0.85	1/1754 (0.1%)
11	dd	0.43	0/1298	0.59	0/1754
11	df	0.44	0/1298	0.62	0/1754
11	dh	0.44	0/1298	0.61	0/1754
11	di	0.44	0/1298	0.61	0/1754
11	dj	0.46	0/1298	0.64	0/1754
11	dl	0.41	0/1298	0.59	0/1754
11	dn	0.43	0/1298	0.61	0/1754
11	dp	0.43	0/1298	0.60	0/1754
11	dr	0.40	0/1298	0.57	0/1754
11	dt	0.47	0/1298	0.64	0/1754
11	dv	0.45	0/1298	0.63	0/1754
11	e6	0.80	0/1298	1.01	3/1754 (0.2%)
11	e7	0.70	0/1298	0.89	2/1754 (0.1%)
11	eB	0.56	0/1298	0.80	3/1754 (0.2%)
11	eD	0.64	0/1298	0.81	2/1754 (0.1%)
11	eF	0.55	0/1298	0.76	3/1754 (0.2%)
11	eH	0.66	0/1298	0.86	3/1754 (0.2%)
11	eJ	0.71	2/1298 (0.2%)	0.89	6/1754 (0.3%)
11	eL	0.56	0/1298	0.82	3/1754 (0.2%)
11	eN	0.56	0/1298	0.78	2/1754 (0.1%)
11	eP	0.56	0/1298	0.79	2/1754 (0.1%)
11	eR	0.62	0/1298	0.81	2/1754 (0.1%)
11	eT	0.73	2/1298 (0.2%)	0.91	6/1754 (0.3%)
11	eV	0.56	0/1298	0.81	2/1754 (0.1%)
11	eX	0.69	1/1298 (0.1%)	0.89	4/1754 (0.2%)
11	eb	0.76	0/1298	0.95	4/1754 (0.2%)
11	ec	0.74	0/1298	0.93	2/1754 (0.1%)
11	ee	0.80	3/1298 (0.2%)	0.96	4/1754 (0.2%)
11	eg	0.68	0/1298	0.84	0/1754
11	ei	0.71	0/1298	1.01	6/1754 (0.3%)
11	el	0.76	0/1298	0.96	6/1754 (0.3%)
11	en	0.73	0/1298	0.93	3/1754 (0.2%)
11	ep	0.67	0/1298	0.83	0/1754
11	er	0.75	0/1298	1.06	8/1754 (0.5%)
11	et	0.71	0/1298	0.90	2/1754 (0.1%)
11	ev	0.79	0/1298	0.99	5/1754 (0.3%)
11	f2	0.63	0/1298	0.90	3/1754 (0.2%)
11	f3	0.59	0/1298	0.78	3/1754 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	f8	0.39	0/1298	0.59	0/1754
11	fa	0.34	0/1298	0.53	1/1754 (0.1%)
11	fc	0.34	0/1298	0.55	1/1754 (0.1%)
11	ff	0.46	0/1298	0.67	0/1754
11	fi	0.30	0/1298	0.55	1/1754 (0.1%)
11	fj	0.28	0/1298	0.52	1/1754 (0.1%)
11	fm	0.35	0/1298	0.59	1/1754 (0.1%)
11	fo	0.45	0/1298	0.64	0/1754
11	fq	0.44	0/1298	0.63	0/1754
11	fs	0.36	0/1298	0.63	1/1754 (0.1%)
11	fu	0.28	0/1298	0.52	1/1754 (0.1%)
11	fw	0.29	0/1298	0.52	1/1754 (0.1%)
11	fy	0.34	0/1298	0.55	1/1754 (0.1%)
11	g8	0.48	0/1298	0.63	0/1754
11	ga	0.74	0/1298	0.85	2/1754 (0.1%)
11	gd	0.71	0/1298	0.83	2/1754 (0.1%)
11	ge	0.54	0/1298	0.70	0/1754
11	gg	0.59	1/1298 (0.1%)	0.70	0/1754
11	gi	0.50	0/1298	0.67	0/1754
11	gk	0.58	0/1298	0.74	0/1754
11	gn	0.58	1/1298 (0.1%)	0.72	0/1754
11	gp	0.53	0/1298	0.66	0/1754
11	gr	0.75	0/1298	0.85	2/1754 (0.1%)
11	gt	0.53	0/1298	0.71	0/1754
11	gv	0.62	0/1298	0.80	2/1754 (0.1%)
11	gx	0.77	1/1298 (0.1%)	0.88	3/1754 (0.2%)
11	h2	0.66	0/1298	0.83	3/1754 (0.2%)
11	h3	0.76	0/1298	1.09	7/1754 (0.4%)
11	h8	0.50	0/1298	0.77	2/1754 (0.1%)
11	hB	0.29	0/1298	0.49	0/1754
11	hD	0.33	0/1298	0.54	0/1754
11	hG	0.31	0/1298	0.51	0/1754
11	hH	0.31	0/1298	0.51	0/1754
11	hJ	0.32	0/1298	0.53	0/1754
11	hL	0.33	0/1298	0.53	0/1754
11	hN	0.31	0/1298	0.52	0/1754
11	hP	0.32	0/1298	0.52	0/1754
11	hR	0.31	0/1298	0.53	0/1754
11	hT	0.33	0/1298	0.53	0/1754
11	hV	0.31	0/1298	0.51	0/1754
11	hX	0.30	0/1298	0.50	0/1754
11	iC	0.82	1/1298 (0.1%)	0.98	4/1754 (0.2%)
11	iD	0.81	0/1298	0.96	6/1754 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	iE	0.66	0/1063	0.87	3/1437 (0.2%)
11	iF	0.74	0/1063	0.90	2/1437 (0.1%)
11	iG	0.59	0/1083	0.76	2/1464 (0.1%)
11	iH	0.59	0/1083	0.80	4/1464 (0.3%)
11	j2	0.56	0/1298	0.75	2/1754 (0.1%)
11	j3	0.57	0/1298	0.80	2/1754 (0.1%)
11	jI	0.54	0/1049	0.77	1/1418 (0.1%)
11	jJ	0.56	0/1049	0.78	2/1418 (0.1%)
11	jK	0.55	0/1057	0.78	1/1429 (0.1%)
11	jL	0.56	0/1057	0.78	1/1429 (0.1%)
11	jM	0.34	0/1057	0.58	0/1429
11	jN	0.34	0/1057	0.57	0/1429
11	jO	0.83	1/1057 (0.1%)	1.25	7/1429 (0.5%)
11	jP	0.76	1/1057 (0.1%)	1.15	7/1429 (0.5%)
11	kQ	0.55	0/1049	0.80	5/1418 (0.4%)
11	kR	0.57	0/1049	0.79	3/1418 (0.2%)
11	kS	0.62	0/1071	0.78	1/1448 (0.1%)
11	kT	0.81	0/1063	1.08	4/1437 (0.3%)
11	kU	0.39	0/1049	0.59	0/1418
11	kV	0.42	0/1049	0.60	0/1418
11	kW	0.45	0/1071	0.67	1/1448 (0.1%)
11	kX	0.45	0/1071	0.67	1/1448 (0.1%)
11	l2	0.58	0/1298	0.78	3/1754 (0.2%)
11	l3	0.84	0/1298	1.08	10/1754 (0.6%)
11	l6	0.75	0/1298	0.91	3/1754 (0.2%)
11	l7	0.90	2/1298 (0.2%)	1.06	5/1754 (0.3%)
11	lb	0.62	0/1298	0.76	1/1754 (0.1%)
11	ld	0.55	0/1298	0.80	4/1754 (0.2%)
11	lf	0.67	0/1298	0.87	3/1754 (0.2%)
11	lh	0.76	0/1298	1.03	7/1754 (0.4%)
11	lj	0.73	0/1298	0.96	4/1754 (0.2%)
11	ll	0.51	0/1298	0.75	2/1754 (0.1%)
11	ln	0.56	0/1298	0.84	6/1754 (0.3%)
11	lp	0.73	0/1298	0.92	2/1754 (0.1%)
11	lr	0.62	0/1298	0.80	2/1754 (0.1%)
11	lt	0.50	0/1298	0.74	1/1754 (0.1%)
11	lv	0.74	0/1298	0.99	6/1754 (0.3%)
11	lx	0.71	0/1298	0.93	5/1754 (0.3%)
11	n2	0.63	0/1298	0.78	0/1754
11	n3	0.71	0/1298	0.90	2/1754 (0.1%)
11	n4	0.76	0/1298	1.00	5/1754 (0.3%)
11	n5	0.70	0/1298	0.89	3/1754 (0.2%)
11	n6	0.84	1/1298 (0.1%)	1.04	6/1754 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	n7	0.81	0/1298	0.97	6/1754 (0.3%)
11	n8	0.67	0/1298	0.86	0/1754
11	n9	0.66	0/1298	0.92	7/1754 (0.4%)
11	o8	0.55	0/1298	0.78	2/1754 (0.1%)
11	p2	0.46	0/1298	0.63	0/1754
11	p3	0.54	0/1298	0.74	1/1754 (0.1%)
11	p4	0.63	0/1298	0.82	1/1754 (0.1%)
11	p5	0.64	0/1298	0.83	1/1754 (0.1%)
11	p6	0.79	1/1298 (0.1%)	1.01	4/1754 (0.2%)
11	p7	0.85	0/1298	1.06	6/1754 (0.3%)
11	p8	0.58	0/1298	0.73	0/1754
11	p9	0.93	0/1298	1.16	11/1754 (0.6%)
11	r2	0.46	0/1298	0.68	2/1754 (0.1%)
11	r3	0.62	0/1298	0.78	3/1754 (0.2%)
11	r4	0.81	0/1298	1.06	6/1754 (0.3%)
11	r5	0.78	0/1298	1.03	5/1754 (0.3%)
11	r6	0.87	0/1298	1.08	4/1754 (0.2%)
11	r7	0.77	0/1298	1.07	8/1754 (0.5%)
11	r9	0.86	0/1298	1.03	6/1754 (0.3%)
11	t2	0.48	0/1298	0.64	0/1754
11	t3	0.70	0/1298	0.93	3/1754 (0.2%)
11	t4	0.80	1/1298 (0.1%)	1.10	7/1754 (0.4%)
11	t5	0.78	1/1298 (0.1%)	1.12	9/1754 (0.5%)
11	t6	0.80	0/1298	1.12	10/1754 (0.6%)
11	t7	0.65	0/1298	0.82	1/1754 (0.1%)
11	t9	0.92	0/1298	1.10	9/1754 (0.5%)
11	v2	0.52	0/1298	0.70	1/1754 (0.1%)
11	v3	0.90	0/1298	1.07	5/1754 (0.3%)
11	v4	0.79	0/1298	1.06	9/1754 (0.5%)
11	v5	0.80	0/1298	1.07	10/1754 (0.6%)
11	v6	0.63	0/1298	0.76	2/1754 (0.1%)
11	v7	0.93	0/1298	1.14	7/1754 (0.4%)
11	v9	0.87	0/1298	1.11	6/1754 (0.3%)
11	w8	0.60	0/1298	0.73	1/1754 (0.1%)
11	x2	0.48	0/1298	0.66	1/1754 (0.1%)
11	x3	0.68	0/1298	0.87	2/1754 (0.1%)
11	x4	0.99	1/1298 (0.1%)	1.22	14/1754 (0.8%)
11	x5	0.91	0/1298	1.20	12/1754 (0.7%)
11	x6	0.43	0/1298	0.70	2/1754 (0.1%)
11	x7	0.55	0/1298	0.80	0/1754
11	x9	0.79	0/1298	0.99	7/1754 (0.4%)
11	y6	0.38	0/1298	0.59	0/1754
11	y7	0.66	0/1298	0.91	5/1754 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
11	y8	0.79	0/1298	0.95	2/1754 (0.1%)
11	z2	0.46	0/1298	0.66	1/1754 (0.1%)
11	z3	0.66	0/1298	0.86	3/1754 (0.2%)
11	z4	0.73	0/1298	1.02	8/1754 (0.5%)
11	z5	0.70	0/1298	0.97	6/1754 (0.3%)
11	z6	0.50	0/1298	0.76	3/1754 (0.2%)
11	z7	0.63	0/1298	0.86	0/1754
11	z9	0.76	0/1298	1.02	7/1754 (0.4%)
12	34	1.01	1/2147 (0.0%)	1.21	22/2891 (0.8%)
12	A2	1.04	3/2147 (0.1%)	1.27	20/2891 (0.7%)
12	U8	1.01	3/2147 (0.1%)	1.20	16/2891 (0.6%)
12	Y5	1.23	2/2147 (0.1%)	1.17	18/2891 (0.6%)
12	Z9	1.02	5/2147 (0.2%)	1.18	15/2891 (0.5%)
12	a3	1.07	3/2147 (0.1%)	1.31	21/2891 (0.7%)
12	aY	0.91	2/2147 (0.1%)	1.07	11/2891 (0.4%)
12	b8	0.98	1/2147 (0.0%)	1.09	5/2891 (0.2%)
12	b9	1.03	2/2147 (0.1%)	1.16	9/2891 (0.3%)
12	bY	0.99	2/2147 (0.1%)	1.19	18/2891 (0.6%)
12	dw	0.61	0/2147	0.81	4/2891 (0.1%)
12	dx	0.59	0/2147	0.79	4/2891 (0.1%)
12	ey	0.78	0/2147	1.01	9/2891 (0.3%)
12	ez	0.76	0/2134	0.96	7/2873 (0.2%)
13	B2	0.85	5/2998 (0.2%)	1.10	21/4060 (0.5%)
13	b3	0.87	6/2998 (0.2%)	1.15	27/4060 (0.7%)
14	44	0.57	0/1914	0.79	1/2571 (0.0%)
14	C2	0.84	2/1914 (0.1%)	1.00	7/2571 (0.3%)
14	D2	0.53	0/1864	0.71	1/2503 (0.0%)
14	T8	0.52	0/1914	0.76	3/2571 (0.1%)
14	Y9	0.52	0/1914	0.78	3/2571 (0.1%)
14	Z5	0.56	0/1914	0.79	1/2571 (0.0%)
14	aZ	0.63	2/1914 (0.1%)	0.81	4/2571 (0.2%)
14	bZ	0.66	2/1914 (0.1%)	0.84	4/2571 (0.2%)
14	c3	0.81	2/1914 (0.1%)	0.98	6/2571 (0.2%)
14	c8	0.89	0/1914	1.10	9/2571 (0.4%)
14	c9	0.95	0/1914	1.14	7/2571 (0.3%)
14	d3	0.54	0/1864	0.71	1/2503 (0.0%)
14	d8	0.85	0/1864	1.08	11/2503 (0.4%)
14	d9	0.83	0/1864	1.07	13/2503 (0.5%)
14	e8	0.51	0/1864	0.77	7/2503 (0.3%)
14	e9	0.63	1/1864 (0.1%)	0.84	5/2503 (0.2%)
15	14	0.66	0/1924	0.94	3/2603 (0.1%)
15	R8	1.14	12/1915 (0.6%)	1.21	18/2591 (0.7%)
15	W5	0.72	0/1924	1.02	7/2603 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
15	W9	1.28	17/1915 (0.9%)	1.33	23/2591 (0.9%)
15	aW	0.79	3/1932 (0.2%)	1.01	6/2614 (0.2%)
15	bW	0.83	4/1932 (0.2%)	1.03	9/2614 (0.3%)
16	24	1.01	3/2633 (0.1%)	1.19	16/3548 (0.5%)
16	S8	1.00	2/2639 (0.1%)	1.16	17/3555 (0.5%)
16	X5	1.09	4/2639 (0.2%)	1.25	21/3555 (0.6%)
16	X9	1.04	3/2639 (0.1%)	1.27	19/3555 (0.5%)
16	aX	0.96	1/2639 (0.0%)	1.12	10/3555 (0.3%)
16	bX	0.96	2/2639 (0.1%)	1.15	10/3555 (0.3%)
17	V8	0.66	0/1248	0.79	3/1693 (0.2%)
17	X8	0.88	1/1248 (0.1%)	0.94	6/1693 (0.4%)
17	Z8	0.65	0/1248	0.79	3/1693 (0.2%)
17	a4	0.69	0/1248	0.88	4/1693 (0.2%)
17	a5	0.78	0/1248	0.99	4/1693 (0.2%)
17	aa	0.67	0/1248	0.78	3/1693 (0.2%)
17	ac	0.84	1/1248 (0.1%)	0.91	6/1693 (0.4%)
17	ae	0.66	0/1257	0.80	3/1705 (0.2%)
17	ag	0.82	1/1248 (0.1%)	0.93	6/1693 (0.4%)
17	ai	0.51	0/1248	0.60	1/1693 (0.1%)
17	ak	0.94	1/1248 (0.1%)	1.16	11/1693 (0.6%)
17	b4	0.93	2/1248 (0.2%)	0.98	7/1693 (0.4%)
17	b5	0.83	0/1248	0.94	5/1693 (0.3%)
17	ba	0.94	2/1248 (0.2%)	1.14	8/1693 (0.5%)
17	bc	0.92	2/1248 (0.2%)	0.99	8/1693 (0.5%)
17	be	0.80	0/1257	0.96	5/1705 (0.3%)
17	bg	0.96	0/1248	1.09	5/1693 (0.3%)
17	bi	0.82	1/1248 (0.1%)	0.97	5/1693 (0.3%)
17	bk	0.80	0/1248	0.97	6/1693 (0.4%)
17	ca	0.98	4/1248 (0.3%)	1.18	10/1693 (0.6%)
17	cc	0.99	3/1248 (0.2%)	1.04	8/1693 (0.5%)
17	ce	0.78	0/1257	0.94	6/1705 (0.4%)
17	cg	0.96	0/1248	1.09	4/1693 (0.2%)
17	ci	0.93	1/1248 (0.1%)	1.07	8/1693 (0.5%)
17	ck	0.84	0/1248	1.00	4/1693 (0.2%)
17	d4	0.64	0/1248	0.81	3/1693 (0.2%)
17	d5	0.65	0/1248	0.82	3/1693 (0.2%)
17	f4	0.94	3/1248 (0.2%)	1.06	4/1693 (0.2%)
17	f5	0.89	2/1248 (0.2%)	1.04	5/1693 (0.3%)
17	g9	0.78	0/1248	0.89	6/1693 (0.4%)
17	i4	0.73	0/1248	0.88	4/1693 (0.2%)
17	i5	0.71	0/1248	0.86	4/1693 (0.2%)
17	i9	0.51	0/1248	0.60	1/1693 (0.1%)
17	k4	0.97	2/1248 (0.2%)	1.17	11/1693 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
17	k5	1.05	2/1248 (0.2%)	1.24	15/1693 (0.9%)
17	k9	0.95	1/1248 (0.1%)	1.17	10/1693 (0.6%)
18	W8	0.77	0/1293	0.92	5/1749 (0.3%)
18	Y8	0.61	0/1293	0.75	1/1749 (0.1%)
18	ab	0.78	1/1293 (0.1%)	0.93	4/1749 (0.2%)
18	ad	0.65	0/1293	0.82	3/1749 (0.2%)
18	af	0.84	0/1293	1.00	2/1749 (0.1%)
18	ah	0.83	2/1293 (0.2%)	0.87	4/1749 (0.2%)
18	aj	0.61	0/1293	0.75	1/1749 (0.1%)
18	al	0.70	1/1293 (0.1%)	0.93	7/1749 (0.4%)
18	bb	1.17	1/1293 (0.1%)	1.16	15/1749 (0.9%)
18	bd	0.88	0/1293	1.03	5/1749 (0.3%)
18	bf	0.98	1/1293 (0.1%)	1.04	8/1749 (0.5%)
18	bh	0.76	0/1293	1.05	8/1749 (0.5%)
18	bj	0.96	1/1299 (0.1%)	1.11	9/1757 (0.5%)
18	bl	1.01	1/1293 (0.1%)	1.16	6/1749 (0.3%)
18	c4	0.76	1/1293 (0.1%)	0.93	5/1749 (0.3%)
18	c5	0.80	1/1293 (0.1%)	0.97	7/1749 (0.4%)
18	cb	1.05	1/1293 (0.1%)	1.20	12/1749 (0.7%)
18	cd	0.83	0/1293	0.95	6/1749 (0.3%)
18	cf	0.97	0/1293	1.02	6/1749 (0.3%)
18	ch	0.81	0/1293	1.07	8/1749 (0.5%)
18	cj	0.96	1/1299 (0.1%)	1.10	10/1757 (0.6%)
18	cl	1.02	1/1293 (0.1%)	1.18	8/1749 (0.5%)
18	e4	0.74	0/1293	1.02	6/1749 (0.3%)
18	e5	0.75	0/1293	1.04	8/1749 (0.5%)
18	f9	0.80	0/1293	0.96	3/1749 (0.2%)
18	g4	0.97	1/1293 (0.1%)	1.09	8/1749 (0.5%)
18	g5	1.01	2/1293 (0.2%)	1.13	8/1749 (0.5%)
18	h4	0.71	0/1293	0.90	1/1749 (0.1%)
18	h5	0.71	0/1293	0.90	1/1749 (0.1%)
18	h9	0.81	1/1293 (0.1%)	0.87	2/1749 (0.1%)
18	j4	0.83	1/1299 (0.1%)	1.00	4/1757 (0.2%)
18	j5	0.97	3/1299 (0.2%)	1.14	8/1757 (0.5%)
18	j9	0.58	0/1293	0.76	2/1749 (0.1%)
18	l4	0.83	0/1293	1.13	9/1749 (0.5%)
18	l5	0.93	2/1293 (0.2%)	1.14	9/1749 (0.5%)
18	l9	0.70	1/1293 (0.1%)	0.91	5/1749 (0.3%)
19	a8	0.61	3/2987 (0.1%)	0.83	12/4033 (0.3%)
19	a9	0.59	3/2987 (0.1%)	0.81	8/4033 (0.2%)
20	dy	0.79	4/2426 (0.2%)	0.98	13/3288 (0.4%)
20	dz	0.78	4/2426 (0.2%)	0.98	12/3288 (0.4%)
21	ew	1.00	2/1864 (0.1%)	1.04	5/2523 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
21	ex	1.00	3/1864 (0.2%)	1.00	5/2523 (0.2%)
21	fd	0.49	0/1588	0.72	1/2153 (0.0%)
21	fz	0.46	0/1588	0.65	2/2153 (0.1%)
22	eY	0.73	2/2375 (0.1%)	0.91	7/3209 (0.2%)
22	eZ	0.67	0/2375	0.94	2/3209 (0.1%)
23	hY	0.40	0/1784	0.60	1/2406 (0.0%)
23	hZ	0.42	0/1784	0.61	1/2406 (0.0%)
23	ly	0.62	0/1969	0.80	3/2654 (0.1%)
23	lz	0.64	0/1969	0.83	5/2654 (0.2%)
24	gy	0.66	0/2052	0.89	5/2777 (0.2%)
24	gz	0.67	0/2052	0.91	6/2777 (0.2%)
25	ka	0.94	3/2086 (0.1%)	1.05	7/2845 (0.2%)
25	kb	0.95	3/2086 (0.1%)	1.13	13/2845 (0.5%)
All	All	0.74	635/1162581 (0.1%)	0.91	3857/1570501 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	M1	0	1
5	O1	0	1
5	U1	0	1
5	W1	0	1
5	c1	0	1
5	e1	0	1
5	h1	0	1
5	l1	0	1
5	n1	0	1
5	r1	0	1
6	Q1	0	1
6	g1	0	1
8	a2	0	3
8	b2	0	4
10	A5	0	1
10	A7	0	1
10	C3	0	1
10	C4	0	1
10	C5	0	2
10	C6	0	1
10	C7	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	E3	0	1
10	E4	0	1
10	E5	0	1
10	E6	0	1
10	E7	0	1
10	G2	0	1
10	G3	0	1
10	G4	0	2
10	G5	0	1
10	G7	0	1
10	I3	0	1
10	I4	0	1
10	I5	0	1
10	I6	0	1
10	I7	0	1
10	K3	0	1
10	K4	0	1
10	K5	0	1
10	K6	0	1
10	K7	0	2
10	M3	0	1
10	M4	0	1
10	M5	0	1
10	M7	0	1
10	O3	0	1
10	O4	0	1
10	O5	0	1
10	O6	0	1
10	O7	0	1
10	Q2	0	1
10	Q3	0	1
10	Q4	0	1
10	Q5	0	1
10	Q6	0	1
10	Q7	0	1
10	S3	0	1
10	S4	0	1
10	S5	0	1
10	S6	0	1
10	S7	0	1
10	U2	0	1
10	U3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	U4	0	1
10	U5	0	1
10	U6	0	1
10	U7	0	1
10	W2	0	1
10	W3	0	1
10	W4	0	1
10	W7	0	1
10	Y3	0	1
10	Y4	0	1
10	Y6	0	1
10	Y7	0	1
10	aA	0	1
10	aC	0	1
10	aE	0	1
10	aG	0	1
10	aI	0	1
10	aK	0	1
10	aO	0	1
10	aQ	0	1
10	aS	0	1
10	aU	0	1
10	bA	0	1
10	bC	0	1
10	bE	0	1
10	bG	0	1
10	bI	0	1
10	bK	0	1
10	bM	0	1
10	bO	0	1
10	bQ	0	1
10	bS	0	1
10	bU	0	1
10	bt	0	1
10	cA	0	1
10	cC	0	1
10	cD	0	1
10	cG	0	1
10	cI	0	2
10	cK	0	2
10	cS	0	1
10	cT	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	cV	0	1
10	cW	0	1
10	cX	0	1
10	cZ	0	1
10	cm	0	1
10	ct	0	1
10	dA	0	1
10	dC	0	1
10	dE	0	1
10	dG	0	1
10	dI	0	1
10	dJ	0	1
10	dM	0	1
10	dO	0	1
10	dQ	0	1
10	dS	0	1
10	dU	0	1
10	dW	0	1
10	dZ	0	1
10	da	0	1
10	db	0	1
10	dc	0	1
10	de	0	1
10	dk	0	1
10	dm	0	1
10	dq	0	1
10	e2	0	1
10	eA	0	1
10	eC	0	1
10	eE	0	1
10	eG	0	1
10	eI	0	1
10	eK	0	1
10	eM	0	1
10	eO	0	1
10	eQ	0	1
10	eS	0	1
10	ea	0	1
10	ed	0	2
10	ef	0	1
10	eh	0	1
10	ej	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	ek	0	1
10	em	0	2
10	eo	0	1
10	eq	0	1
10	es	0	2
10	f6	0	1
10	f7	0	1
10	fb	0	3
10	fe	0	3
10	fg	0	5
10	fh	0	3
10	fk	0	3
10	fl	0	5
10	fn	0	2
10	fp	0	3
10	fr	0	3
10	ft	0	2
10	fv	0	2
10	fx	0	2
10	g2	0	1
10	g3	0	1
10	g6	0	1
10	g7	0	1
10	gb	0	1
10	gc	0	1
10	gh	0	1
10	gj	0	1
10	gl	0	1
10	gm	0	2
10	go	0	1
10	gq	0	1
10	gs	0	1
10	gu	0	1
10	gw	0	1
10	h7	0	1
10	hA	0	1
10	hC	0	1
10	hE	0	1
10	hF	0	1
10	hI	0	1
10	hK	0	1
10	hM	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	hO	0	1
10	hQ	0	1
10	hS	0	1
10	hU	0	1
10	hW	0	1
10	i2	0	1
10	i6	0	1
10	i7	0	1
10	i8	0	1
10	j6	0	1
10	j7	0	1
10	j8	0	1
10	k2	0	1
10	k6	0	1
10	k7	0	1
10	k8	0	1
10	l8	0	1
10	la	0	2
10	lc	0	3
10	le	0	2
10	lg	0	2
10	li	0	1
10	lk	0	2
10	lm	0	2
10	lo	0	2
10	lq	0	2
10	ls	0	2
10	lu	0	2
10	m2	0	1
10	m3	0	1
10	m4	0	1
10	m5	0	1
10	m6	0	1
10	m7	0	1
10	m8	0	1
10	o4	0	1
10	o5	0	1
10	o6	0	1
10	o7	0	1
10	q2	0	1
10	q3	0	1
10	q4	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	q5	0	1
10	q6	0	1
10	q7	0	1
10	q8	0	1
10	r8	0	1
10	s2	0	1
10	s3	0	1
10	s4	0	1
10	s5	0	2
10	s6	0	1
10	s7	0	1
10	s8	0	1
10	t8	0	1
10	u2	0	1
10	u3	0	1
10	u4	0	1
10	u5	0	1
10	u6	0	1
10	u7	0	1
10	u8	0	1
10	w2	0	1
10	w3	0	1
10	w4	0	1
10	w5	0	1
10	w6	0	1
10	w7	0	1
10	y2	0	1
10	y5	0	2
11	A8	0	3
11	B3	0	1
11	B9	0	3
11	D3	0	1
11	D4	0	1
11	D9	0	2
11	E8	0	1
11	F2	0	1
11	F9	0	3
11	G8	0	3
11	H9	0	1
11	I8	0	3
11	J9	0	1
11	K8	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	L2	0	1
11	L3	0	1
11	L9	0	3
11	M8	0	3
11	N2	0	1
11	N9	0	3
11	O8	0	2
11	P2	0	1
11	P3	0	1
11	P9	0	1
11	Q8	0	1
11	R3	0	1
11	R9	0	3
11	T3	0	1
11	T9	0	2
11	V3	0	1
11	V9	0	2
11	X2	0	1
11	X3	0	1
11	Z2	0	1
11	an	0	3
11	ar	0	2
11	ax	0	1
11	az	0	1
11	b7	0	1
11	bL	0	1
11	bN	0	1
11	bP	0	1
11	bR	0	1
11	bT	0	1
11	cB	0	1
11	cE	0	1
11	cF	0	1
11	cH	0	1
11	cJ	0	1
11	cL	0	1
11	cM	0	1
11	cN	0	1
11	cO	0	1
11	cP	0	1
11	cQ	0	1
11	cR	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	cY	0	1
11	cp	0	1
11	cq	0	1
11	cz	0	1
11	dD	0	1
11	dF	0	1
11	dH	0	1
11	dK	0	1
11	dL	0	1
11	dR	0	1
11	dT	0	1
11	dY	0	1
11	dd	0	1
11	df	0	1
11	dh	0	1
11	di	0	1
11	dj	0	1
11	dl	0	1
11	dn	0	1
11	dp	0	1
11	dt	0	1
11	dv	0	1
11	eb	0	1
11	ec	0	1
11	ee	0	1
11	eg	0	1
11	ei	0	1
11	ep	0	1
11	fa	0	1
11	fc	0	1
11	ff	0	1
11	fi	0	1
11	fj	0	1
11	fm	0	1
11	fo	0	1
11	fq	0	1
11	fs	0	1
11	fu	0	1
11	fw	0	1
11	fy	0	1
11	gr	0	1
11	h2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
11	iC	0	1
11	iD	0	1
11	j2	0	1
11	kS	0	1
11	kT	0	1
11	n2	0	1
11	n3	0	1
11	n9	0	3
11	p2	0	1
11	r2	0	1
11	r9	0	1
11	t2	0	1
11	v2	0	1
11	w8	0	3
11	x2	0	1
11	x9	0	1
11	z2	0	1
11	z3	0	1
11	z9	0	1
12	ey	0	1
12	ez	0	1
14	44	0	1
14	T8	0	2
14	Y9	0	2
14	Z5	0	1
14	aZ	0	1
14	bZ	0	2
14	c9	0	1
14	d3	0	1
15	W9	0	1
16	S8	0	1
16	X5	0	2
16	X9	0	2
16	aX	0	1
16	bX	0	3
17	k4	0	1
17	k5	0	1
18	c5	0	1
19	a8	0	1
20	dy	0	1
20	dz	0	1
21	fd	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	gy	0	1
24	gz	0	2
25	kb	0	1
All	All	0	493

All (635) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	Y5	302	GLU	CD-OE2	31.42	1.60	1.25
4	y1	103	PRO	N-CD	-29.12	1.07	1.47
4	N1	103	PRO	N-CD	-26.83	1.10	1.47
4	N1	20	PRO	N-CD	-23.31	1.15	1.47
18	bb	149	PRO	N-CD	-20.54	1.19	1.47
8	b2	394	PRO	N-CD	-20.34	1.19	1.47
21	ex	180	PRO	N-CD	-18.77	1.21	1.47
21	ew	180	PRO	N-CD	-17.84	1.22	1.47
10	E7	19	PRO	N-CD	16.93	1.71	1.47
12	Y5	302	GLU	CD-OE1	16.17	1.43	1.25
4	G1	103	PRO	N-CD	-14.16	1.28	1.47
10	A6	142	ARG	CZ-NH1	13.73	1.50	1.33
16	X5	93	TYR	CE1-CZ	13.69	1.56	1.38
4	s1	151	PHE	CG-CD2	12.61	1.57	1.38
17	b4	4	PRO	N-CD	-12.23	1.30	1.47
16	X5	93	TYR	CG-CD2	12.04	1.54	1.39
4	y1	151	PHE	CG-CD2	11.90	1.56	1.38
12	34	302	GLU	CD-OE2	11.85	1.38	1.25
4	s1	87	TYR	CE1-CZ	11.48	1.53	1.38
5	e1	83	ARG	CZ-NH1	11.39	1.47	1.33
4	y1	87	TYR	CE1-CZ	10.80	1.52	1.38
4	y1	59	PHE	CE2-CZ	10.77	1.57	1.37
8	a2	605	ARG	CZ-NH1	10.65	1.46	1.33
4	y1	151	PHE	CG-CD1	10.64	1.54	1.38
4	s1	151	PHE	CG-CD1	10.44	1.54	1.38
11	L6	95	TYR	CE1-CZ	10.41	1.52	1.38
4	s1	87	TYR	CG-CD2	10.24	1.52	1.39
10	iB	108	TRP	CZ3-CH2	-10.12	1.23	1.40
10	la	111	ALA	C-O	10.06	1.42	1.23
18	l5	74	TYR	CG-CD1	-10.05	1.26	1.39
4	y1	87	TYR	CG-CD2	9.58	1.51	1.39
4	w1	17	TYR	CE2-CZ	9.50	1.50	1.38
15	W9	150	TYR	CE1-CZ	-9.42	1.26	1.38
15	R8	150	TYR	CE1-CZ	-9.41	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	z1	18	TYR	CG-CD2	9.35	1.51	1.39
4	s1	59	PHE	CE2-CZ	9.32	1.55	1.37
14	bZ	192	ARG	CZ-NH2	9.15	1.45	1.33
4	b1	151	PHE	CG-CD2	9.15	1.52	1.38
3	F1	50	TYR	CG-CD1	-9.10	1.27	1.39
5	O1	83	ARG	CZ-NH1	9.10	1.44	1.33
13	B2	383	TRP	CE3-CZ3	-9.03	1.23	1.38
13	b3	383	TRP	CB-CG	-8.97	1.34	1.50
5	S1	83	ARG	CZ-NH1	8.94	1.44	1.33
13	b3	383	TRP	CE3-CZ3	-8.86	1.23	1.38
5	t1	18	TYR	CG-CD2	8.83	1.50	1.39
13	B2	383	TRP	CB-CG	-8.82	1.34	1.50
10	iA	108	TRP	CZ3-CH2	-8.80	1.25	1.40
11	B7	87	GLU	CG-CD	8.77	1.65	1.51
4	w1	151	PHE	CG-CD2	8.55	1.51	1.38
10	dA	111	ALA	C-O	8.54	1.39	1.23
4	b1	151	PHE	CG-CD1	8.54	1.51	1.38
4	s1	73	TYR	CE1-CZ	-8.54	1.27	1.38
15	bW	104	TYR	CE1-CZ	8.50	1.49	1.38
15	aW	104	TYR	CE1-CZ	8.46	1.49	1.38
3	F1	248	GLU	CD-OE2	8.45	1.34	1.25
4	s1	111	GLY	C-O	-8.43	1.10	1.23
5	c1	18	TYR	CG-CD2	8.37	1.50	1.39
10	G4	83	TYR	CE1-CZ	8.36	1.49	1.38
4	G1	151	PHE	CG-CD2	8.29	1.51	1.38
4	s1	15	ALA	C-O	-8.24	1.07	1.23
4	q1	151	PHE	CG-CD2	8.22	1.51	1.38
11	bq	78	ARG	CZ-NH1	8.11	1.43	1.33
8	b2	363	PHE	CE1-CZ	8.08	1.52	1.37
5	H1	18	TYR	CG-CD2	8.02	1.49	1.39
10	C5	83	TYR	CE1-CZ	8.01	1.49	1.38
8	a2	156	TRP	CB-CG	-7.99	1.35	1.50
5	v1	78	TYR	CE1-CZ	7.98	1.49	1.38
2	C1	59	ARG	CZ-NH2	7.96	1.43	1.33
8	b2	156	TRP	CB-CG	-7.96	1.35	1.50
8	a2	363	PHE	CE1-CZ	7.95	1.52	1.37
4	y1	59	PHE	CB-CG	-7.93	1.37	1.51
10	f7	142	ARG	CZ-NH1	7.93	1.43	1.33
4	y1	94	TYR	CB-CG	-7.92	1.39	1.51
14	aZ	192	ARG	CZ-NH2	7.92	1.43	1.33
11	cq	78	ARG	CZ-NH1	7.90	1.43	1.33
4	G1	151	PHE	CG-CD1	7.88	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	X9	61	ARG	NE-CZ	-7.78	1.23	1.33
6	g1	18	TYR	CG-CD2	7.75	1.49	1.39
4	y1	15	ALA	C-O	-7.72	1.08	1.23
4	y1	73	TYR	CE1-CZ	-7.70	1.28	1.38
11	ee	87	GLU	CG-CD	7.66	1.63	1.51
5	p1	63	SER	CA-CB	-7.64	1.41	1.52
5	W1	106	GLU	CD-OE1	7.58	1.33	1.25
14	bZ	192	ARG	CD-NE	7.58	1.59	1.46
15	R8	104	TYR	CE1-CZ	-7.56	1.28	1.38
4	y1	111	GLY	C-O	-7.56	1.11	1.23
15	W9	104	TYR	CE1-CZ	-7.55	1.28	1.38
17	X8	91	TYR	CE1-CZ	-7.49	1.28	1.38
16	24	93	TYR	CE1-CZ	7.46	1.48	1.38
10	iB	91	ARG	CZ-NH1	-7.43	1.23	1.33
10	w4	13	ASP	CB-CG	7.43	1.67	1.51
10	K7	89	TYR	CE2-CZ	7.39	1.48	1.38
8	b2	834	TYR	CE1-CZ	-7.38	1.28	1.38
5	x1	106	GLU	CD-OE1	7.37	1.33	1.25
10	W7	89	TYR	CE2-CZ	7.37	1.48	1.38
5	r1	106	GLU	CD-OE1	7.34	1.33	1.25
10	W7	127	TYR	CE2-CZ	7.34	1.48	1.38
15	R8	150	TYR	CG-CD2	-7.33	1.29	1.39
15	W9	150	TYR	CG-CD2	-7.33	1.29	1.39
17	bc	91	TYR	CE1-CZ	-7.33	1.29	1.38
6	Q1	18	TYR	CG-CD2	7.31	1.48	1.39
20	dy	79	TRP	CB-CG	-7.26	1.37	1.50
5	x1	90	ARG	CZ-NH2	7.25	1.42	1.33
11	aJ	87	GLU	CG-CD	7.23	1.62	1.51
4	P1	90	ARG	CZ-NH1	7.23	1.42	1.33
17	k5	76	SER	CB-OG	-7.21	1.32	1.42
5	x1	87	TYR	CG-CD1	7.20	1.48	1.39
8	a2	834	TYR	CE1-CZ	-7.20	1.29	1.38
17	ca	90	TYR	CE1-CZ	7.19	1.48	1.38
18	g4	95	TYR	CE2-CZ	-7.19	1.29	1.38
20	dz	79	TRP	CB-CG	-7.18	1.37	1.50
17	ac	91	TYR	CE1-CZ	-7.16	1.29	1.38
18	bl	74	TYR	CE1-CZ	7.14	1.47	1.38
5	p1	78	TYR	CE1-CZ	7.13	1.47	1.38
4	y1	59	PHE	CG-CD2	7.12	1.49	1.38
5	r1	87	TYR	CG-CD1	7.12	1.48	1.39
18	g5	95	TYR	CE2-CZ	-7.10	1.29	1.38
14	aZ	192	ARG	CD-NE	7.10	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	v1	63	SER	CA-CB	-7.08	1.42	1.52
11	bJ	87	GLU	CG-CD	7.07	1.62	1.51
8	a2	405	GLU	CD-OE1	7.04	1.33	1.25
15	W9	48	TRP	CZ3-CH2	7.04	1.51	1.40
10	cy	89	TYR	CG-CD1	7.01	1.48	1.39
21	ew	124	TYR	CE1-CZ	6.99	1.47	1.38
10	gm	63	TYR	CG-CD2	-6.99	1.30	1.39
18	cl	74	TYR	CE1-CZ	6.98	1.47	1.38
4	P1	81	CYS	CB-SG	-6.97	1.70	1.82
4	s1	59	PHE	CB-CG	-6.94	1.39	1.51
5	W1	153	PHE	CG-CD1	6.93	1.49	1.38
5	j1	18	TYR	CG-CD2	6.92	1.48	1.39
10	dJ	83	TYR	CE1-CZ	-6.92	1.29	1.38
4	b1	75	GLU	CG-CD	6.91	1.62	1.51
5	U1	83	ARG	CZ-NH1	6.90	1.42	1.33
17	f4	91	TYR	CE1-CZ	-6.86	1.29	1.38
5	n1	106	GLU	CD-OE1	6.84	1.33	1.25
10	iA	91	ARG	CZ-NH1	-6.84	1.24	1.33
11	a6	92	TYR	CG-CD1	-6.83	1.30	1.39
5	z1	91	TYR	CE2-CZ	6.83	1.47	1.38
5	S1	18	TYR	CG-CD2	6.79	1.48	1.39
17	f4	117	GLU	CD-OE1	6.76	1.33	1.25
21	ex	124	TYR	CE1-CZ	6.75	1.47	1.38
5	e1	83	ARG	NE-CZ	6.75	1.41	1.33
19	a9	105	TYR	CG-CD2	-6.73	1.30	1.39
5	n1	153	PHE	CG-CD1	6.72	1.48	1.38
4	f1	81	CYS	CB-SG	-6.70	1.70	1.82
17	cc	91	TYR	CE1-CZ	-6.70	1.29	1.38
4	N1	19	SER	CB-OG	6.69	1.50	1.42
5	c1	18	TYR	CE1-CZ	6.69	1.47	1.38
8	b2	405	GLU	CD-OE1	6.67	1.32	1.25
11	Z7	92	TYR	CG-CD1	-6.67	1.30	1.39
5	e1	77	ARG	CZ-NH1	6.67	1.41	1.33
20	dz	304	TYR	CG-CD1	-6.65	1.30	1.39
10	by	89	TYR	CG-CD1	6.64	1.47	1.39
8	a2	592	TYR	CG-CD2	6.63	1.47	1.39
12	a3	170	TYR	CE2-CZ	6.57	1.47	1.38
4	y1	91	LEU	CB-CG	6.57	1.71	1.52
12	A2	170	TYR	CE2-CZ	6.55	1.47	1.38
10	A6	142	ARG	CD-NE	6.55	1.57	1.46
11	J7	95	TYR	CE1-CZ	6.53	1.47	1.38
10	w5	13	ASP	CB-CG	6.52	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	iC	87	GLU	CG-CD	6.52	1.61	1.51
10	S6	127	TYR	CE2-CZ	6.51	1.47	1.38
5	r1	90	ARG	CZ-NH2	6.50	1.41	1.33
10	lu	142	ARG	CZ-NH1	6.50	1.41	1.33
4	b1	87	TYR	CE1-CZ	6.50	1.47	1.38
10	gm	83	TYR	CE1-CZ	-6.49	1.30	1.38
10	gs	83	TYR	CE1-CZ	-6.49	1.30	1.38
15	R8	210	GLU	CG-CD	6.48	1.61	1.51
4	y1	148	GLU	CD-OE2	-6.47	1.18	1.25
17	k5	91	TYR	CG-CD1	-6.46	1.30	1.39
10	dA	89	TYR	CE1-CZ	6.46	1.47	1.38
15	R8	158	MET	C-O	6.46	1.35	1.23
5	n1	94	TYR	CB-CG	-6.45	1.42	1.51
13	b3	383	TRP	CE2-CZ2	-6.45	1.28	1.39
20	dz	97	TYR	CD2-CE2	-6.44	1.29	1.39
4	u1	151	PHE	CG-CD2	6.43	1.48	1.38
13	B2	383	TRP	CE2-CZ2	-6.43	1.28	1.39
17	f5	91	TYR	CE1-CZ	-6.42	1.30	1.38
10	gm	63	TYR	CE1-CZ	-6.42	1.30	1.38
10	gm	70	GLY	C-O	6.42	1.33	1.23
10	dW	83	TYR	CE1-CZ	-6.41	1.30	1.38
10	s4	83	TYR	CE1-CZ	6.40	1.46	1.38
4	P1	20	PRO	N-CD	6.40	1.56	1.47
10	cI	33	ARG	CZ-NH2	-6.39	1.24	1.33
9	c2	63	TYR	CD2-CE2	-6.38	1.29	1.39
11	eT	77	ARG	CZ-NH1	6.38	1.41	1.33
4	y1	73	TYR	C-O	6.36	1.35	1.23
11	N7	82	CYS	CB-SG	6.36	1.93	1.82
4	s1	73	TYR	C-O	6.35	1.35	1.23
10	bt	137	ARG	CZ-NH1	6.34	1.41	1.33
11	l7	95	TYR	CE1-CZ	6.34	1.46	1.38
11	L6	91	ARG	NE-CZ	6.34	1.41	1.33
10	dO	111	ALA	C-O	6.34	1.35	1.23
10	gc	83	TYR	CE1-CZ	-6.33	1.30	1.38
5	H1	35	GLU	CG-CD	6.32	1.61	1.51
5	h1	94	TYR	CE1-CZ	6.31	1.46	1.38
10	la	18	PHE	CG-CD2	6.30	1.48	1.38
15	W9	135	GLN	CG-CD	-6.30	1.36	1.51
5	O1	83	ARG	NE-CZ	6.30	1.41	1.33
8	a2	592	TYR	CE1-CZ	6.30	1.46	1.38
8	b2	592	TYR	CG-CD2	6.30	1.47	1.39
20	dy	97	TYR	CD2-CE2	-6.29	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W9	150	TYR	CD1-CE1	-6.27	1.29	1.39
12	bY	284	TYR	CE2-CZ	6.26	1.46	1.38
4	G1	75	GLU	CG-CD	6.26	1.61	1.51
10	lq	111	ALA	C-O	6.25	1.35	1.23
15	R8	150	TYR	CD1-CE1	-6.25	1.29	1.39
5	t1	91	TYR	CE2-CZ	6.25	1.46	1.38
5	z1	10	ASN	CG-ND2	6.24	1.48	1.32
4	P1	75	GLU	CG-CD	6.23	1.61	1.51
8	b2	580	TYR	CG-CD1	6.22	1.47	1.39
15	W9	210	GLU	CG-CD	6.22	1.61	1.51
17	k9	31	TYR	CE1-CZ	6.22	1.46	1.38
11	eJ	77	ARG	CZ-NH1	6.21	1.41	1.33
4	K1	17	TYR	CE2-CZ	6.21	1.46	1.38
4	o1	151	PHE	CG-CD2	6.20	1.48	1.38
10	dA	83	TYR	CE1-CZ	-6.20	1.30	1.38
5	t1	10	ASN	CG-ND2	6.20	1.48	1.32
15	W9	158	MET	C-O	6.20	1.35	1.23
5	M1	94	TYR	CE1-CZ	6.19	1.46	1.38
17	ak	31	TYR	CE1-CZ	6.18	1.46	1.38
10	ct	54	GLU	CD-OE2	6.17	1.32	1.25
17	k4	76	SER	CB-OG	-6.17	1.34	1.42
12	a3	90	TYR	CG-CD2	6.17	1.47	1.39
10	s5	83	TYR	CE1-CZ	6.16	1.46	1.38
10	lq	83	TYR	CG-CD1	6.15	1.47	1.39
8	a2	834	TYR	CE2-CZ	-6.15	1.30	1.38
17	f5	117	GLU	CD-OE1	6.15	1.32	1.25
18	l5	74	TYR	CE2-CZ	-6.15	1.30	1.38
10	K7	60	PHE	CE2-CZ	6.14	1.49	1.37
5	x1	77	ARG	CZ-NH2	6.14	1.41	1.33
10	m5	83	TYR	CE1-CZ	6.14	1.46	1.38
10	iA	89	TYR	CE1-CZ	6.13	1.46	1.38
4	s1	151	PHE	CE1-CZ	6.12	1.49	1.37
5	v1	78	TYR	CG-CD2	6.12	1.47	1.39
11	L6	30	PHE	CG-CD1	6.12	1.48	1.38
12	Z9	135	THR	CB-CG2	-6.11	1.32	1.52
10	la	152	PHE	CG-CD1	-6.11	1.29	1.38
8	a2	372	TYR	CE2-CZ	6.08	1.46	1.38
4	s1	73	TYR	CG-CD1	-6.07	1.31	1.39
12	U8	135	THR	CB-CG2	-6.07	1.32	1.52
5	S1	94	TYR	CG-CD1	-6.06	1.31	1.39
15	R8	83	PHE	CG-CD2	-6.06	1.29	1.38
5	W1	94	TYR	CB-CG	-6.05	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	cA	33	ARG	CZ-NH2	-6.05	1.25	1.33
5	c1	35	GLU	CG-CD	6.05	1.61	1.51
15	R8	117	ARG	CZ-NH1	6.04	1.41	1.33
5	a1	124	GLY	C-O	6.04	1.33	1.23
5	l1	83	ARG	CZ-NH1	6.03	1.40	1.33
1	A1	234	TYR	CE1-CZ	-6.03	1.30	1.38
1	B1	109	PHE	CB-CG	-6.02	1.41	1.51
17	ba	90	TYR	CE1-CZ	6.01	1.46	1.38
11	V5	87	GLU	CG-CD	6.01	1.60	1.51
10	k7	18	PHE	CG-CD2	6.01	1.47	1.38
11	Z4	87	GLU	CG-CD	6.01	1.60	1.51
4	G1	116	TYR	CB-CG	-6.00	1.42	1.51
10	s9	65	TYR	CE1-CZ	6.00	1.46	1.38
13	b3	383	TRP	CG-CD2	-6.00	1.33	1.43
5	W1	76	ARG	CZ-NH1	6.00	1.40	1.33
15	bW	104	TYR	CG-CD1	5.99	1.47	1.39
18	j5	82	CYS	C-O	5.99	1.34	1.23
11	X7	95	TYR	CE1-CZ	5.99	1.46	1.38
12	U8	60	TYR	CE2-CZ	-5.99	1.30	1.38
11	eT	77	ARG	CD-NE	5.98	1.56	1.46
15	aW	104	TYR	CG-CD1	5.98	1.47	1.39
10	E6	95	TYR	CG-CD2	-5.97	1.31	1.39
4	R1	87	TYR	CE1-CZ	5.97	1.46	1.38
4	G1	87	TYR	CE1-CZ	5.97	1.46	1.38
10	M6	142	ARG	CD-NE	5.96	1.56	1.46
10	cy	54	GLU	CD-OE1	-5.95	1.19	1.25
4	Z1	90	ARG	CZ-NH2	-5.94	1.25	1.33
10	w3	95	TYR	CE1-CZ	5.93	1.46	1.38
19	a9	303	TYR	CE1-CZ	5.93	1.46	1.38
10	dA	130	SER	CB-OG	-5.93	1.34	1.42
25	kb	239	GLU	CD-OE2	5.93	1.32	1.25
10	cm	91	ARG	CZ-NH1	-5.91	1.25	1.33
4	s1	59	PHE	CG-CD2	5.90	1.47	1.38
20	dy	304	TYR	CG-CD1	-5.90	1.31	1.39
7	V1	17	TYR	CG-CD1	-5.90	1.31	1.39
5	j1	18	TYR	CE1-CZ	5.90	1.46	1.38
12	A2	90	TYR	CG-CD2	5.89	1.46	1.39
8	a2	335	PHE	CB-CG	-5.88	1.41	1.51
8	b2	707	ARG	CZ-NH1	5.88	1.40	1.33
4	b1	116	TYR	CB-CG	-5.88	1.42	1.51
8	a2	342	GLU	CD-OE2	5.88	1.32	1.25
17	k4	91	TYR	CG-CD1	-5.87	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G6	96	SER	CB-OG	-5.87	1.34	1.42
18	j4	92	TYR	CG-CD1	-5.86	1.31	1.39
18	j5	92	TYR	CG-CD1	-5.86	1.31	1.39
11	J7	91	ARG	NE-CZ	5.86	1.40	1.33
1	B1	45	TYR	CE1-CZ	5.86	1.46	1.38
18	h9	92	TYR	CE1-CZ	-5.86	1.30	1.38
11	p6	95	TYR	CE1-CZ	5.86	1.46	1.38
4	i1	87	TYR	CE1-CZ	5.85	1.46	1.38
5	r1	77	ARG	CZ-NH2	5.85	1.40	1.33
11	gg	115	GLU	CD-OE2	5.85	1.32	1.25
10	A7	95	TYR	CG-CD2	-5.84	1.31	1.39
5	H1	18	TYR	CE1-CZ	5.83	1.46	1.38
10	S6	89	TYR	CE2-CZ	5.83	1.46	1.38
4	s1	139	SER	CB-OG	5.82	1.49	1.42
8	b2	834	TYR	CE2-CZ	-5.82	1.30	1.38
11	X7	5	PHE	CG-CD1	-5.82	1.30	1.38
15	W9	117	ARG	CZ-NH1	5.82	1.40	1.33
10	G6	127	TYR	CE2-CZ	5.80	1.46	1.38
12	Z9	108	TYR	CB-CG	-5.80	1.43	1.51
19	a8	105	TYR	CE2-CZ	5.80	1.46	1.38
2	C1	128	GLU	CD-OE2	5.80	1.32	1.25
4	y1	151	PHE	CE1-CZ	5.80	1.48	1.37
10	K4	17	ARG	NE-CZ	5.80	1.40	1.33
10	dA	111	ALA	C-N	5.79	1.43	1.33
5	x1	78	TYR	C-O	5.79	1.34	1.23
11	a6	52	VAL	C-O	5.78	1.34	1.23
11	V7	92	TYR	CE2-CZ	-5.78	1.31	1.38
4	o1	38	ARG	CZ-NH1	5.78	1.40	1.33
3	F1	167	TRP	CE3-CZ3	-5.77	1.28	1.38
10	W7	91	ARG	CZ-NH2	5.77	1.40	1.33
10	bt	83	TYR	CE1-CZ	5.77	1.46	1.38
4	y1	73	TYR	CG-CD1	-5.77	1.31	1.39
13	B2	383	TRP	CG-CD2	-5.77	1.33	1.43
16	aX	119	PHE	CG-CD1	5.77	1.47	1.38
10	u4	89	TYR	CE2-CZ	5.76	1.46	1.38
10	by	54	GLU	CD-OE1	-5.76	1.19	1.25
11	gn	115	GLU	CD-OE2	5.75	1.31	1.25
4	y1	94	TYR	CD1-CE1	5.75	1.48	1.39
4	s1	89	LEU	C-O	5.74	1.34	1.23
11	R7	74	TYR	CE1-CZ	5.73	1.46	1.38
11	R6	82	CYS	CB-SG	5.72	1.92	1.82
10	bv	83	TYR	CE1-CZ	5.72	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B1	84	PHE	CE2-CZ	5.72	1.48	1.37
8	a2	344	SER	CB-OG	5.71	1.49	1.42
10	aA	65	TYR	CE1-CZ	5.70	1.46	1.38
10	iB	89	TYR	CE1-CZ	5.70	1.46	1.38
10	u5	89	TYR	CE2-CZ	5.69	1.46	1.38
20	dy	134	TYR	CB-CG	-5.68	1.43	1.51
10	u5	89	TYR	CE1-CZ	5.68	1.46	1.38
15	R8	80	VAL	CB-CG2	-5.68	1.41	1.52
10	o6	18	PHE	CG-CD2	5.68	1.47	1.38
9	c2	63	TYR	CB-CG	-5.68	1.43	1.51
11	eJ	77	ARG	CD-NE	5.68	1.56	1.46
5	x1	87	TYR	CB-CG	-5.67	1.43	1.51
5	O1	77	ARG	CZ-NH1	5.67	1.40	1.33
4	T1	111	GLY	C-O	-5.66	1.14	1.23
5	t1	18	TYR	CE2-CZ	-5.66	1.31	1.38
4	s1	81	CYS	CB-SG	-5.66	1.72	1.81
16	bX	119	PHE	CG-CD1	5.66	1.47	1.38
10	cm	117	TYR	CE1-CZ	-5.65	1.31	1.38
10	lg	142	ARG	CZ-NH1	5.65	1.40	1.33
4	G1	59	PHE	CE2-CZ	5.65	1.48	1.37
13	B2	150	PHE	CB-CG	-5.65	1.41	1.51
11	x4	92	TYR	CG-CD1	-5.64	1.31	1.39
10	i3	130	SER	CB-OG	-5.64	1.34	1.42
5	x1	91	TYR	CE1-CZ	5.64	1.45	1.38
10	I6	127	TYR	CG-CD2	5.63	1.46	1.39
16	24	290	GLU	CG-CD	5.63	1.60	1.51
10	bm	91	ARG	CZ-NH1	-5.63	1.25	1.33
5	v1	91	TYR	CG-CD1	-5.62	1.31	1.39
4	y1	89	LEU	C-O	5.61	1.34	1.23
12	Z9	156	ARG	CZ-NH1	5.61	1.40	1.33
19	a8	303	TYR	CE1-CZ	5.60	1.45	1.38
4	s1	148	GLU	CD-OE2	-5.60	1.19	1.25
4	y1	139	SER	CB-OG	5.60	1.49	1.42
10	m5	111	ALA	C-O	5.59	1.33	1.23
15	R8	150	TYR	CE2-CZ	-5.59	1.31	1.38
10	u4	89	TYR	CE1-CZ	5.59	1.45	1.38
10	E7	127	TYR	CE1-CZ	5.58	1.45	1.38
11	c7	74	TYR	CE1-CZ	5.58	1.45	1.38
7	V1	116	TYR	CE2-CZ	5.57	1.45	1.38
18	al	77	ARG	CZ-NH2	-5.57	1.25	1.33
11	gx	61	CYS	CB-SG	5.57	1.91	1.82
11	L4	82	CYS	CB-SG	5.57	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U8	156	ARG	CZ-NH1	5.56	1.40	1.33
11	t4	92	TYR	CG-CD1	-5.55	1.31	1.39
18	ah	84	ARG	NE-CZ	5.55	1.40	1.33
13	b3	150	PHE	CB-CG	-5.55	1.42	1.51
10	as	65	TYR	CE1-CZ	5.55	1.45	1.38
4	w1	155	TYR	CE2-CZ	5.54	1.45	1.38
18	j5	82	CYS	CB-SG	-5.54	1.72	1.81
10	W2	95	TYR	CE1-CZ	5.54	1.45	1.38
15	W9	83	PHE	CG-CD2	-5.54	1.30	1.38
10	ct	137	ARG	CZ-NH1	5.54	1.40	1.33
15	bW	75	PHE	CG-CD1	5.53	1.47	1.38
5	r1	116	TYR	CG-CD1	-5.53	1.31	1.39
18	cj	92	TYR	CG-CD1	-5.52	1.31	1.39
11	dK	117	TYR	CE1-CZ	5.52	1.45	1.38
11	eX	92	TYR	CE1-CZ	-5.52	1.31	1.38
5	x1	83	ARG	CZ-NH1	-5.51	1.25	1.33
12	Z9	60	TYR	CE2-CZ	-5.51	1.31	1.38
4	u1	38	ARG	CZ-NH1	5.50	1.40	1.33
8	a2	580	TYR	CG-CD1	5.50	1.46	1.39
8	a2	363	PHE	CG-CD2	5.50	1.47	1.38
4	y1	75	GLU	CD-OE2	5.50	1.31	1.25
10	W7	130	SER	CB-OG	-5.49	1.35	1.42
5	z1	18	TYR	CE2-CZ	-5.49	1.31	1.38
11	H5	82	CYS	CB-SG	5.49	1.91	1.82
5	S1	18	TYR	CE1-CZ	5.49	1.45	1.38
11	jO	91	ARG	CZ-NH1	-5.49	1.25	1.33
4	d1	87	TYR	CE1-CZ	5.48	1.45	1.38
11	T6	87	GLU	CG-CD	5.48	1.60	1.51
18	c4	87	GLU	CD-OE1	5.47	1.31	1.25
11	Z6	95	TYR	CE1-CZ	5.47	1.45	1.38
18	l9	77	ARG	CZ-NH2	-5.47	1.25	1.33
11	bL	87	GLU	CG-CD	5.47	1.60	1.51
5	j1	94	TYR	CG-CD1	-5.47	1.32	1.39
15	bW	56	SER	CB-OG	-5.47	1.35	1.42
4	i1	73	TYR	CE1-CZ	-5.46	1.31	1.38
5	p1	78	TYR	CG-CD2	5.46	1.46	1.39
11	bF	87	GLU	CG-CD	5.46	1.60	1.51
18	cb	70	GLY	C-O	-5.46	1.15	1.23
10	I2	130	SER	CB-OG	-5.45	1.35	1.42
15	W9	154	PHE	CG-CD2	-5.45	1.30	1.38
5	r1	78	TYR	C-O	5.45	1.33	1.23
4	q1	27	LYS	CD-CE	5.44	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	k6	95	TYR	CE1-CZ	5.44	1.45	1.38
4	s1	88	TYR	CE1-CZ	5.44	1.45	1.38
5	x1	18	TYR	CG-CD2	5.44	1.46	1.39
11	c7	95	TYR	CE1-CZ	5.44	1.45	1.38
4	G1	94	TYR	CG-CD2	5.43	1.46	1.39
5	L1	124	GLY	C-O	5.43	1.32	1.23
16	S8	144	GLU	CD-OE1	-5.43	1.19	1.25
22	eY	255	THR	CB-CG2	-5.43	1.34	1.52
16	X9	144	GLU	CD-OE1	-5.42	1.19	1.25
10	gm	83	TYR	CD1-CE1	-5.42	1.31	1.39
10	h7	130	SER	CB-OG	-5.42	1.35	1.42
15	R8	154	PHE	CG-CD2	-5.42	1.30	1.38
4	G1	116	TYR	CE2-CZ	5.42	1.45	1.38
8	a2	316	GLU	CD-OE1	5.42	1.31	1.25
3	E1	167	TRP	CE3-CZ3	-5.42	1.29	1.38
5	j1	78	TYR	CE1-CZ	5.42	1.45	1.38
12	b9	120	TYR	CE1-CZ	-5.42	1.31	1.38
17	bc	91	TYR	CG-CD1	-5.42	1.32	1.39
5	j1	91	TYR	CE1-CZ	5.42	1.45	1.38
1	A1	109	PHE	CE1-CZ	5.41	1.47	1.37
11	Z7	52	VAL	C-O	5.41	1.33	1.23
14	C2	158	TYR	CG-CD1	5.41	1.46	1.39
16	X5	290	GLU	CG-CD	5.41	1.60	1.51
17	f4	129	TYR	CG-CD1	5.41	1.46	1.39
4	s1	88	TYR	N-CA	-5.40	1.35	1.46
4	y1	59	PHE	CD1-CE1	5.40	1.50	1.39
5	W1	78	TYR	CG-CD2	5.40	1.46	1.39
16	S8	324	TYR	CE1-CZ	-5.40	1.31	1.38
10	cy	54	GLU	CD-OE2	-5.39	1.19	1.25
9	c2	63	TYR	CD1-CE1	-5.39	1.31	1.39
4	N1	12	ASP	CG-OD1	5.39	1.37	1.25
4	f1	94	TYR	CB-CG	-5.39	1.43	1.51
4	y1	59	PHE	CE1-CZ	5.39	1.47	1.37
17	ba	156	TYR	CD2-CE2	-5.38	1.31	1.39
18	bf	63	GLN	CD-OE1	5.38	1.35	1.24
10	bm	117	TYR	CE1-CZ	-5.38	1.31	1.38
10	iB	95	TYR	CE1-CZ	5.38	1.45	1.38
4	b1	59	PHE	CE2-CZ	5.38	1.47	1.37
8	a2	473	PHE	C-O	-5.37	1.13	1.23
10	u3	95	TYR	CE1-CZ	5.37	1.45	1.38
5	Y1	83	ARG	NE-CZ	5.37	1.40	1.33
6	Q1	81	ALA	C-O	5.37	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	n1	76	ARG	CZ-NH1	5.36	1.40	1.33
4	f1	94	TYR	CG-CD2	5.36	1.46	1.39
10	dW	111	ALA	C-O	5.36	1.33	1.23
4	w1	47	ARG	CZ-NH1	5.36	1.40	1.33
10	cv	89	TYR	CE2-CZ	5.35	1.45	1.38
5	a1	107	ARG	CZ-NH1	5.35	1.40	1.33
15	W9	107	VAL	CA-CB	-5.34	1.43	1.54
10	ct	83	TYR	CE1-CZ	5.34	1.45	1.38
20	dz	134	TYR	CB-CG	-5.34	1.43	1.51
4	b1	88	TYR	CG-CD1	5.33	1.46	1.39
4	d1	94	TYR	CG-CD2	5.33	1.46	1.39
4	d1	12	ASP	CG-OD1	5.33	1.37	1.25
5	r1	91	TYR	CE1-CZ	5.33	1.45	1.38
2	D1	83	GLU	CG-CD	5.32	1.59	1.51
4	f1	116	TYR	CG-CD1	5.32	1.46	1.39
16	24	212	PHE	CG-CD1	5.32	1.46	1.38
10	dJ	111	ALA	C-O	5.32	1.33	1.23
18	ah	92	TYR	CE1-CZ	-5.31	1.31	1.38
4	q1	47	ARG	CZ-NH1	5.31	1.40	1.33
10	m4	83	TYR	CE1-CZ	5.31	1.45	1.38
10	bt	83	TYR	CE2-CZ	-5.31	1.31	1.38
17	ci	90	TYR	CG-CD1	5.30	1.46	1.39
1	A1	109	PHE	CB-CG	-5.30	1.42	1.51
10	A6	95	TYR	CE1-CZ	5.30	1.45	1.38
11	dN	117	TYR	CG-CD1	5.29	1.46	1.39
14	C2	158	TYR	CE1-CZ	5.29	1.45	1.38
10	cm	67	LYS	CD-CE	5.29	1.64	1.51
4	y1	91	LEU	CG-CD1	5.28	1.71	1.51
18	g5	75	THR	CB-CG2	-5.28	1.34	1.52
15	W9	76	ASN	C-O	-5.28	1.13	1.23
10	lq	18	PHE	CG-CD2	5.28	1.46	1.38
4	Z1	29	PHE	CG-CD1	-5.28	1.30	1.38
4	P1	94	TYR	CB-CG	-5.28	1.43	1.51
14	c3	158	TYR	CE1-CZ	5.27	1.45	1.38
5	x1	116	TYR	CG-CD1	-5.27	1.32	1.39
18	c5	87	GLU	CD-OE1	5.26	1.31	1.25
12	b9	170	TYR	CE1-CZ	-5.26	1.31	1.38
5	p1	91	TYR	CG-CD1	-5.26	1.32	1.39
10	by	54	GLU	CD-OE2	-5.26	1.19	1.25
11	aT	87	GLU	CG-CD	5.26	1.59	1.51
17	b4	39	GLU	CG-CD	5.25	1.59	1.51
10	dW	89	TYR	CE1-CZ	5.25	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	g1	81	ALA	C-O	5.25	1.33	1.23
6	Q1	92	TYR	CE1-CZ	-5.25	1.31	1.38
10	Q7	127	TYR	CE1-CZ	5.25	1.45	1.38
5	r1	90	ARG	NE-CZ	5.25	1.39	1.33
22	eY	288	TYR	CG-CD2	5.24	1.46	1.39
15	aW	75	PHE	CG-CD1	5.24	1.46	1.38
10	k8	89	TYR	CG-CD1	5.24	1.46	1.39
18	bj	92	TYR	CG-CD1	-5.23	1.32	1.39
25	kb	313	TYR	CA-CB	-5.23	1.42	1.53
12	A2	224	TYR	CB-CG	-5.23	1.43	1.51
11	ee	87	GLU	CD-OE2	5.23	1.31	1.25
17	cc	91	TYR	CG-CD1	-5.22	1.32	1.39
10	m4	111	ALA	C-O	5.22	1.33	1.23
11	jP	91	ARG	CZ-NH1	-5.22	1.26	1.33
11	L6	95	TYR	CG-CD2	5.21	1.46	1.39
12	a3	224	TYR	CB-CG	-5.21	1.43	1.51
15	W9	47	ILE	C-O	5.21	1.33	1.23
16	X9	324	TYR	CE1-CZ	-5.21	1.31	1.38
19	a9	105	TYR	CE1-CZ	-5.21	1.31	1.38
25	ka	313	TYR	CA-CB	-5.21	1.42	1.53
5	x1	90	ARG	NE-CZ	5.21	1.39	1.33
10	la	130	SER	CB-OG	-5.21	1.35	1.42
10	lo	142	ARG	CZ-NH1	5.20	1.39	1.33
12	Z9	80	PHE	CG-CD1	5.20	1.46	1.38
2	C1	185	ARG	CZ-NH2	-5.19	1.26	1.33
4	P1	94	TYR	CG-CD2	5.19	1.45	1.39
15	W9	150	TYR	CE2-CZ	-5.19	1.31	1.38
16	X5	212	PHE	CG-CD1	5.19	1.46	1.38
5	S1	116	TYR	CG-CD2	-5.18	1.32	1.39
5	r1	87	TYR	CB-CG	-5.18	1.43	1.51
21	ex	227	TRP	CZ3-CH2	5.18	1.48	1.40
4	k1	111	GLY	C-O	-5.17	1.15	1.23
10	G7	127	TYR	CG-CD2	5.17	1.45	1.39
15	R8	107	VAL	CA-CB	-5.17	1.43	1.54
10	C6	111	ALA	C-O	5.17	1.33	1.23
10	bv	89	TYR	CE2-CZ	5.17	1.45	1.38
11	n6	115	GLU	CG-CD	5.17	1.59	1.51
11	X7	95	TYR	CG-CD2	5.17	1.45	1.39
19	a8	303	TYR	CD2-CE2	5.17	1.47	1.39
1	B1	45	TYR	CG-CD1	5.16	1.45	1.39
10	W2	111	ALA	C-O	5.16	1.33	1.23
25	ka	313	TYR	CG-CD2	-5.16	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	y1	93	THR	C-O	5.16	1.33	1.23
10	g2	49	GLU	CG-CD	5.16	1.59	1.51
5	r1	18	TYR	CG-CD2	5.16	1.45	1.39
12	aY	284	TYR	CE2-CZ	5.16	1.45	1.38
10	K4	127	TYR	CE1-CZ	5.15	1.45	1.38
4	G1	88	TYR	CG-CD1	5.15	1.45	1.39
15	W9	80	VAL	CB-CG2	-5.15	1.42	1.52
10	O6	127	TYR	CE1-CZ	5.14	1.45	1.38
10	s9	95	TYR	CE1-CZ	5.14	1.45	1.38
10	as	95	TYR	CE1-CZ	5.14	1.45	1.38
17	ca	90	TYR	CG-CD1	5.14	1.45	1.39
10	cv	83	TYR	CE1-CZ	5.14	1.45	1.38
4	I1	75	GLU	CD-OE2	5.13	1.31	1.25
5	n1	78	TYR	CG-CD2	5.13	1.45	1.39
17	bi	91	TYR	CG-CD1	-5.13	1.32	1.39
14	e9	100	THR	CB-CG2	-5.13	1.35	1.52
4	K1	111	GLY	C-O	-5.12	1.15	1.23
10	m7	95	TYR	CE1-CZ	5.12	1.45	1.38
4	k1	151	PHE	CG-CD2	5.12	1.46	1.38
11	t5	92	TYR	CG-CD1	-5.12	1.32	1.39
10	f7	142	ARG	CD-NE	5.12	1.55	1.46
11	ee	92	TYR	CG-CD1	-5.11	1.32	1.39
17	cc	69	MET	CG-SD	-5.11	1.67	1.81
1	A1	84	PHE	CE2-CZ	5.11	1.47	1.37
5	U1	18	TYR	CG-CD2	5.11	1.45	1.39
5	r1	87	TYR	CE1-CZ	5.11	1.45	1.38
4	s1	69	GLY	N-CA	-5.11	1.38	1.46
8	b2	34	PHE	CB-CG	-5.11	1.42	1.51
4	o1	114	GLU	CD-OE1	5.11	1.31	1.25
4	b1	116	TYR	CE2-CZ	5.10	1.45	1.38
10	O2	18	PHE	CG-CD2	5.10	1.46	1.38
12	bY	170	TYR	CE2-CZ	5.10	1.45	1.38
10	cy	91	ARG	CZ-NH1	-5.10	1.26	1.33
11	l7	30	PHE	CG-CD1	-5.10	1.31	1.38
14	c3	158	TYR	CG-CD1	5.10	1.45	1.39
18	ab	84	ARG	CZ-NH1	5.10	1.39	1.33
10	Y7	18	PHE	CG-CD2	5.10	1.46	1.38
8	b2	592	TYR	CE1-CZ	5.09	1.45	1.38
10	dJ	131	PHE	CE1-CZ	5.09	1.47	1.37
5	p1	106	GLU	CD-OE1	5.09	1.31	1.25
4	q1	152	TYR	CG-CD1	-5.09	1.32	1.39
10	A7	95	TYR	CE1-CZ	5.08	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	ca	156	TYR	CD2-CE2	-5.08	1.31	1.39
11	X6	92	TYR	CE2-CZ	-5.08	1.31	1.38
16	bX	324	TYR	CB-CG	-5.08	1.44	1.51
12	b8	170	TYR	CE1-CZ	-5.08	1.31	1.38
11	P6	74	TYR	CE1-CZ	5.08	1.45	1.38
4	w1	152	TYR	CG-CD1	-5.07	1.32	1.39
10	C7	95	TYR	CE1-CZ	5.07	1.45	1.38
10	gm	70	GLY	N-CA	-5.07	1.38	1.46
13	b3	201	TYR	CD1-CE1	-5.07	1.31	1.39
10	s5	83	TYR	CG-CD1	5.07	1.45	1.39
10	w3	111	ALA	C-O	5.07	1.32	1.23
4	w1	128	GLU	CD-OE1	5.07	1.31	1.25
11	cR	152	GLU	CD-OE1	-5.07	1.20	1.25
4	s1	114	GLU	CG-CD	5.06	1.59	1.51
4	s1	59	PHE	CD1-CE1	5.06	1.49	1.39
15	W9	101	ASN	CB-CG	-5.06	1.39	1.51
10	m4	130	SER	CB-OG	-5.06	1.35	1.42
25	kb	351	GLU	CG-CD	5.05	1.59	1.51
7	m1	116	TYR	CE2-CZ	5.05	1.45	1.38
11	L6	95	TYR	CG-CD1	5.05	1.45	1.39
5	p1	18	TYR	CG-CD2	5.05	1.45	1.39
8	b2	316	GLU	CD-OE1	5.05	1.31	1.25
4	X1	75	GLU	CD-OE2	5.05	1.31	1.25
4	X1	151	PHE	CG-CD2	5.04	1.46	1.38
10	bM	140	VAL	C-O	5.04	1.32	1.23
11	cF	87	GLU	CG-CD	5.04	1.59	1.51
8	a2	605	ARG	NE-CZ	-5.04	1.26	1.33
11	X6	30	PHE	CG-CD1	-5.04	1.31	1.38
11	aF	87	GLU	CG-CD	5.04	1.59	1.51
17	ca	93	ARG	CZ-NH2	5.04	1.39	1.33
1	B1	46	THR	CB-CG2	-5.04	1.35	1.52
4	q1	151	PHE	CG-CD1	5.04	1.46	1.38
4	s1	82	LEU	CB-CG	5.04	1.67	1.52
10	cW	33	ARG	CZ-NH2	-5.04	1.26	1.33
10	q3	95	TYR	CE1-CZ	5.03	1.45	1.38
10	iA	1	MET	CG-SD	-5.03	1.68	1.81
5	v1	94	TYR	CB-CG	-5.03	1.44	1.51
11	J7	87	GLU	CG-CD	5.03	1.59	1.51
4	w1	27	LYS	CD-CE	5.02	1.63	1.51
8	a2	339	ARG	CZ-NH2	5.02	1.39	1.33
10	dJ	89	TYR	CE1-CZ	5.02	1.45	1.38
8	b2	647	TYR	CE1-CZ	-5.02	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	m5	130	SER	CB-OG	-5.02	1.35	1.42
4	s1	75	GLU	CD-OE2	5.02	1.31	1.25
10	y5	127	TYR	CE1-CZ	5.02	1.45	1.38
17	ag	90	TYR	CE1-CZ	5.02	1.45	1.38
25	ka	351	GLU	CG-CD	5.02	1.59	1.51
4	N1	87	TYR	CE1-CZ	5.01	1.45	1.38
10	G6	158	TYR	CG-CD2	-5.01	1.32	1.39
10	dQ	95	TYR	CE1-CZ	5.01	1.45	1.38
5	v1	106	GLU	CD-OE1	5.00	1.31	1.25
10	E3	130	SER	CB-OG	-5.00	1.35	1.42
12	aY	71	ARG	NE-CZ	5.00	1.39	1.33
10	bA	65	TYR	CE1-CZ	5.00	1.45	1.38
10	cm	117	TYR	CG-CD2	-5.00	1.32	1.39

All (3857) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	bM	140	VAL	C-N-CD	-39.22	34.32	120.60
10	bU	140	VAL	C-N-CD	-31.64	50.98	120.60
10	dc	140	VAL	C-N-CD	-27.73	59.60	120.60
10	bK	140	VAL	C-N-CD	-25.87	63.69	120.60
11	jO	108	ARG	NE-CZ-NH1	25.70	133.15	120.30
10	bG	140	VAL	C-N-CD	-24.65	66.38	120.60
11	jP	108	ARG	NE-CZ-NH1	23.96	132.28	120.30
10	bI	140	VAL	C-N-CD	-23.59	68.70	120.60
16	X9	61	ARG	NE-CZ-NH2	-23.39	108.61	120.30
10	cC	140	VAL	C-N-CD	-22.23	71.70	120.60
10	gw	140	VAL	C-N-CD	-21.49	73.33	120.60
10	bA	140	VAL	C-N-CD	-21.36	73.61	120.60
10	bQ	140	VAL	C-N-CD	-20.70	75.06	120.60
10	bC	140	VAL	C-N-CD	-20.63	75.21	120.60
22	eZ	264	GLY	C-N-CD	-20.29	75.97	120.60
10	cm	140	VAL	C-N-CD	-18.83	79.18	120.60
10	bE	140	VAL	C-N-CD	-18.68	79.52	120.60
10	cw	140	VAL	C-N-CD	-18.43	80.05	120.60
10	gq	140	VAL	C-N-CD	-18.02	80.95	120.60
5	e1	107	ARG	NE-CZ-NH1	17.98	129.29	120.30
11	dL	84	ARG	NE-CZ-NH1	-17.72	111.44	120.30
8	a2	847	ARG	NE-CZ-NH1	-17.65	111.48	120.30
11	dX	84	ARG	NE-CZ-NH1	-17.60	111.50	120.30
10	dW	91	ARG	NE-CZ-NH1	17.40	129.00	120.30
5	O1	107	ARG	NE-CZ-NH1	17.34	128.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	x5	84	ARG	NE-CZ-NH2	-17.34	111.63	120.30
17	ca	93	ARG	NE-CZ-NH2	-17.25	111.68	120.30
11	ei	84	ARG	NE-CZ-NH1	17.23	128.92	120.30
2	D1	41	LEU	C-N-CD	-17.21	82.74	120.60
10	cm	91	ARG	NE-CZ-NH2	17.05	128.83	120.30
5	e1	83	ARG	NE-CZ-NH2	-16.93	111.83	120.30
10	dJ	91	ARG	NE-CZ-NH1	16.90	128.75	120.30
10	ct	140	VAL	C-N-CD	-16.76	83.72	120.60
8	a2	605	ARG	NE-CZ-NH1	-16.37	112.11	120.30
10	bm	91	ARG	NE-CZ-NH2	16.30	128.45	120.30
10	bS	140	VAL	C-N-CD	-16.23	84.89	120.60
11	er	84	ARG	NE-CZ-NH1	16.17	128.39	120.30
3	F1	171	ARG	NE-CZ-NH2	-15.75	112.43	120.30
10	db	138	LEU	CB-CG-CD1	-15.44	84.75	111.00
10	O2	38	LEU	CB-CG-CD1	-15.35	84.91	111.00
17	ba	93	ARG	NE-CZ-NH2	-15.28	112.66	120.30
11	t5	77	ARG	NE-CZ-NH2	15.06	127.83	120.30
11	t4	77	ARG	NE-CZ-NH2	14.99	127.80	120.30
11	L6	77	ARG	NE-CZ-NH1	14.99	127.79	120.30
5	e1	76	ARG	NE-CZ-NH1	-14.87	112.86	120.30
25	kb	243	ASP	CB-CG-OD2	14.86	131.67	118.30
10	cy	91	ARG	NE-CZ-NH2	14.85	127.72	120.30
5	O1	83	ARG	NE-CZ-NH2	-14.25	113.17	120.30
5	Y1	83	ARG	NE-CZ-NH1	14.22	127.41	120.30
19	a8	303	TYR	CB-CG-CD2	-14.10	112.54	121.00
17	k5	30	ARG	NE-CZ-NH1	14.09	127.34	120.30
17	ca	30	ARG	NE-CZ-NH2	-14.08	113.26	120.30
12	A2	71	ARG	NE-CZ-NH1	14.07	127.33	120.30
18	bh	84	ARG	NE-CZ-NH1	-14.07	113.27	120.30
8	a2	847	ARG	NE-CZ-NH2	14.03	127.32	120.30
4	Z1	90	ARG	NE-CZ-NH1	13.96	127.28	120.30
11	h3	77	ARG	NE-CZ-NH2	13.95	127.28	120.30
5	O1	76	ARG	NE-CZ-NH1	-13.89	113.35	120.30
11	H2	77	ARG	NE-CZ-NH2	13.88	127.24	120.30
10	bt	84	ARG	NE-CZ-NH2	13.79	127.19	120.30
18	ch	84	ARG	NE-CZ-NH1	-13.78	113.41	120.30
19	a8	303	TYR	CB-CG-CD1	13.77	129.26	121.00
12	a3	71	ARG	NE-CZ-NH1	13.68	127.14	120.30
17	ak	17	ARG	NE-CZ-NH2	-13.67	113.46	120.30
11	er	84	ARG	NE-CZ-NH2	-13.65	113.47	120.30
10	dA	91	ARG	NE-CZ-NH1	13.64	127.12	120.30
10	cv	33	ARG	NE-CZ-NH1	13.59	127.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	X7	91	ARG	NE-CZ-NH1	13.52	127.06	120.30
10	bv	33	ARG	NE-CZ-NH1	13.51	127.05	120.30
17	ba	30	ARG	NE-CZ-NH2	-13.50	113.55	120.30
10	by	91	ARG	NE-CZ-NH2	13.49	127.04	120.30
14	c9	279	ARG	NE-CZ-NH1	13.48	127.04	120.30
10	ct	84	ARG	NE-CZ-NH2	13.38	126.99	120.30
10	dA	84	ARG	NE-CZ-NH2	13.32	126.96	120.30
4	P1	90	ARG	NE-CZ-NH2	-13.21	113.69	120.30
17	k9	17	ARG	NE-CZ-NH2	-13.10	113.75	120.30
12	bY	156	ARG	NE-CZ-NH2	-13.03	113.79	120.30
10	dA	85	ASP	CB-CG-OD2	12.98	129.99	118.30
11	D7	161	LEU	CB-CG-CD2	-12.93	89.02	111.00
11	z4	7	ARG	NE-CZ-NH1	12.91	126.76	120.30
5	U1	107	ARG	NE-CZ-NH1	12.86	126.73	120.30
14	c8	279	ARG	NE-CZ-NH2	-12.84	113.88	120.30
19	a9	303	TYR	CB-CG-CD2	-12.84	113.30	121.00
11	J7	91	ARG	NE-CZ-NH1	12.83	126.71	120.30
17	k4	30	ARG	NE-CZ-NH1	12.82	126.71	120.30
12	ey	236	LYS	CD-CE-NZ	-12.80	82.25	111.70
15	W5	96	LEU	CB-CG-CD1	-12.76	89.32	111.00
11	t5	7	ARG	NE-CZ-NH1	12.75	126.68	120.30
10	Y7	44	LEU	CB-CG-CD1	12.75	132.67	111.00
8	b2	847	ARG	NE-CZ-NH2	12.73	126.67	120.30
13	B2	90	ARG	NE-CZ-NH1	-12.71	113.95	120.30
5	H1	107	ARG	NE-CZ-NH1	12.69	126.64	120.30
14	c9	279	ARG	NE-CZ-NH2	-12.68	113.96	120.30
11	D5	7	ARG	NE-CZ-NH1	12.66	126.63	120.30
15	14	96	LEU	CB-CG-CD1	-12.64	89.52	111.00
11	t4	7	ARG	NE-CZ-NH1	12.63	126.61	120.30
13	b3	90	ARG	NE-CZ-NH1	-12.58	114.01	120.30
10	y5	91	ARG	NE-CZ-NH1	12.48	126.54	120.30
10	cA	33	ARG	NE-CZ-NH1	12.47	126.54	120.30
11	n9	108	ARG	NE-CZ-NH2	12.45	126.53	120.30
13	B2	90	ARG	NE-CZ-NH2	12.43	126.52	120.30
3	F1	198	MET	CG-SD-CE	-12.41	80.35	100.20
4	s1	151	PHE	CG-CD1-CE1	-12.40	107.16	120.80
11	an	108	ARG	NE-CZ-NH2	12.38	126.49	120.30
14	d9	77	MET	CG-SD-CE	-12.36	80.43	100.20
5	a1	107	ARG	NE-CZ-NH1	12.34	126.47	120.30
5	c1	107	ARG	NE-CZ-NH1	12.32	126.46	120.30
5	e1	107	ARG	NE-CZ-NH2	-12.32	114.14	120.30
13	b3	90	ARG	NE-CZ-NH2	12.28	126.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	c8	279	ARG	NE-CZ-NH1	12.25	126.42	120.30
4	y1	151	PHE	CG-CD1-CE1	-12.24	107.34	120.80
19	a9	303	TYR	CB-CG-CD1	12.24	128.34	121.00
16	X5	288	ARG	NE-CZ-NH2	-12.22	114.19	120.30
5	l1	107	ARG	NE-CZ-NH1	12.18	126.39	120.30
18	l9	84	ARG	NE-CZ-NH2	12.18	126.39	120.30
11	H4	7	ARG	NE-CZ-NH1	12.18	126.39	120.30
8	b2	847	ARG	NE-CZ-NH1	-12.15	114.22	120.30
11	v9	161	LEU	CB-CG-CD2	-12.12	90.40	111.00
10	go	137	ARG	NE-CZ-NH1	12.07	126.33	120.30
11	av	161	LEU	CB-CG-CD2	-12.06	90.50	111.00
10	y4	91	ARG	NE-CZ-NH1	12.05	126.33	120.30
4	d1	90	ARG	NE-CZ-NH2	-12.03	114.29	120.30
16	24	158	LEU	CB-CG-CD1	-12.03	90.56	111.00
10	G6	120	LEU	CB-CG-CD1	11.99	131.38	111.00
11	z5	7	ARG	NE-CZ-NH1	11.95	126.27	120.30
11	D3	84	ARG	NE-CZ-NH2	-11.94	114.33	120.30
17	bi	50	ARG	NE-CZ-NH2	-11.93	114.34	120.30
5	O1	107	ARG	NE-CZ-NH2	-11.86	114.37	120.30
20	dz	281	ALA	C-N-CD	-11.77	94.70	120.60
10	ct	139	CYS	CA-CB-SG	11.76	135.16	114.00
16	bX	61	ARG	NE-CZ-NH1	-11.75	114.43	120.30
11	z3	84	ARG	NE-CZ-NH2	-11.69	114.45	120.30
11	h3	84	ARG	NE-CZ-NH2	-11.69	114.45	120.30
11	J7	77	ARG	NE-CZ-NH1	11.69	126.14	120.30
5	v1	77	ARG	NE-CZ-NH1	-11.64	114.48	120.30
8	b2	423	ARG	NE-CZ-NH1	-11.63	114.49	120.30
10	dO	85	ASP	CB-CG-OD2	11.62	128.76	118.30
11	H2	84	ARG	NE-CZ-NH2	-11.60	114.50	120.30
11	X6	91	ARG	NE-CZ-NH1	11.60	126.10	120.30
17	k5	30	ARG	NE-CZ-NH2	-11.50	114.55	120.30
11	T2	91	ARG	NE-CZ-NH2	-11.49	114.55	120.30
4	b1	86	ASP	CB-CG-OD1	-11.48	107.97	118.30
15	R8	87	LEU	CA-CB-CG	11.42	141.56	115.30
16	aX	61	ARG	NE-CZ-NH1	-11.39	114.60	120.30
10	cI	33	ARG	NE-CZ-NH1	11.36	125.98	120.30
11	ei	84	ARG	NE-CZ-NH2	-11.36	114.62	120.30
11	Z2	84	ARG	NE-CZ-NH2	-11.35	114.62	120.30
18	f9	145	LEU	CB-CG-CD2	-11.35	91.71	111.00
18	af	145	LEU	CB-CG-CD2	-11.31	91.78	111.00
17	ck	30	ARG	NE-CZ-NH2	-11.27	114.67	120.30
11	N6	108	ARG	NE-CZ-NH1	11.26	125.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	lx	108	ARG	NE-CZ-NH2	11.24	125.92	120.30
12	Z9	156	ARG	NE-CZ-NH2	-11.23	114.69	120.30
12	U8	156	ARG	NE-CZ-NH2	-11.22	114.69	120.30
11	D4	84	ARG	NE-CZ-NH2	-11.21	114.69	120.30
8	a2	423	ARG	NE-CZ-NH1	-11.21	114.70	120.30
3	E1	171	ARG	NE-CZ-NH2	-11.17	114.71	120.30
4	G1	86	ASP	CB-CG-OD1	-11.14	108.27	118.30
17	a5	30	ARG	NE-CZ-NH1	11.14	125.87	120.30
18	al	84	ARG	NE-CZ-NH2	11.12	125.86	120.30
11	br	161	LEU	CB-CG-CD2	-11.09	92.14	111.00
15	W9	87	LEU	CA-CB-CG	11.07	140.75	115.30
11	N4	84	ARG	NE-CZ-NH2	-11.05	114.77	120.30
11	t6	77	ARG	NE-CZ-NH1	11.04	125.82	120.30
11	az	108	ARG	NE-CZ-NH2	10.96	125.78	120.30
17	k4	30	ARG	NE-CZ-NH2	-10.95	114.83	120.30
5	v1	83	ARG	NE-CZ-NH1	10.94	125.77	120.30
17	ci	50	ARG	NE-CZ-NH2	-10.87	114.86	120.30
13	B2	346	ARG	NE-CZ-NH2	10.85	125.73	120.30
11	J2	91	ARG	NE-CZ-NH1	10.83	125.72	120.30
15	W9	87	LEU	CB-CG-CD1	-10.83	92.58	111.00
11	v7	161	LEU	CB-CG-CD1	-10.83	92.59	111.00
11	J5	84	ARG	NE-CZ-NH2	-10.80	114.90	120.30
11	x5	129	ARG	NE-CZ-NH1	10.79	125.70	120.30
11	z9	108	ARG	NE-CZ-NH2	10.68	125.64	120.30
11	b7	91	ARG	NE-CZ-NH1	10.63	125.61	120.30
17	bk	30	ARG	NE-CZ-NH2	-10.61	115.00	120.30
11	t3	91	ARG	NE-CZ-NH2	-10.61	115.00	120.30
4	N1	90	ARG	NE-CZ-NH2	-10.60	115.00	120.30
13	b3	346	ARG	NE-CZ-NH2	10.60	125.60	120.30
11	v9	98	LEU	CB-CG-CD1	-10.60	92.99	111.00
10	as	85	ASP	CB-CG-OD2	10.59	127.83	118.30
11	L6	91	ARG	NE-CZ-NH1	10.59	125.59	120.30
11	aD	91	ARG	NE-CZ-NH1	10.57	125.58	120.30
5	e1	90	ARG	NE-CZ-NH1	10.53	125.56	120.30
11	P7	108	ARG	NE-CZ-NH1	10.53	125.56	120.30
15	R8	87	LEU	CB-CG-CD1	-10.52	93.12	111.00
11	B7	129	ARG	NE-CZ-NH1	10.52	125.56	120.30
15	W9	74	ARG	NE-CZ-NH1	-10.49	115.05	120.30
11	T6	91	ARG	NE-CZ-NH1	10.49	125.54	120.30
11	bD	91	ARG	NE-CZ-NH1	10.49	125.54	120.30
4	k1	90	ARG	NE-CZ-NH1	10.47	125.53	120.30
14	bZ	192	ARG	NE-CZ-NH2	10.46	125.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	dA	135	ARG	NE-CZ-NH1	-10.42	115.09	120.30
10	z8	85	ASP	CB-CG-OD2	10.39	127.65	118.30
11	B6	161	LEU	CB-CG-CD2	-10.38	93.35	111.00
18	cb	84	ARG	NE-CZ-NH1	10.37	125.49	120.30
16	X5	61	ARG	NE-CZ-NH1	-10.35	115.12	120.30
11	r6	161	LEU	CB-CG-CD1	-10.35	93.40	111.00
5	p1	77	ARG	NE-CZ-NH1	-10.35	115.13	120.30
10	cm	67	LYS	CD-CE-NZ	10.34	135.47	111.70
5	L1	107	ARG	NE-CZ-NH1	10.34	125.47	120.30
11	P7	161	LEU	CB-CG-CD2	-10.33	93.43	111.00
5	p1	83	ARG	NE-CZ-NH1	10.31	125.45	120.30
10	ct	84	ARG	NE-CZ-NH1	-10.29	115.15	120.30
10	W7	120	LEU	CB-CG-CD1	10.29	128.49	111.00
11	v5	91	ARG	NE-CZ-NH1	-10.28	115.16	120.30
11	N6	161	LEU	CB-CG-CD2	-10.25	93.57	111.00
17	k9	30	ARG	NE-CZ-NH1	-10.25	115.17	120.30
11	B4	91	ARG	NE-CZ-NH2	-10.23	115.19	120.30
4	y1	115	MET	CG-SD-CE	-10.21	83.87	100.20
12	a3	62	ARG	NE-CZ-NH1	-10.19	115.20	120.30
5	S1	83	ARG	NE-CZ-NH1	10.19	125.39	120.30
15	W5	197	LEU	CA-CB-CG	10.18	138.72	115.30
19	a9	401	LEU	CB-CG-CD2	-10.18	93.69	111.00
11	en	101	ASP	CB-CG-OD1	10.15	127.44	118.30
11	V7	91	ARG	NE-CZ-NH1	10.14	125.37	120.30
4	s1	115	MET	CG-SD-CE	-10.13	83.99	100.20
11	ee	101	ASP	CB-CG-OD1	10.12	127.41	118.30
5	H1	107	ARG	NE-CZ-NH2	-10.11	115.25	120.30
11	x5	50	CYS	CA-CB-SG	10.10	132.17	114.00
10	C7	156	LEU	CB-CG-CD2	-10.08	93.86	111.00
11	v3	161	LEU	CB-CG-CD2	-10.06	93.89	111.00
10	W7	137	ARG	NE-CZ-NH2	-10.06	115.27	120.30
4	d1	90	ARG	NE-CZ-NH1	10.05	125.33	120.30
11	x4	7	ARG	NE-CZ-NH1	10.05	125.33	120.30
10	iB	84	ARG	NE-CZ-NH1	-10.04	115.28	120.30
5	O1	90	ARG	NE-CZ-NH1	10.03	125.31	120.30
10	s9	85	ASP	CB-CG-OD2	10.01	127.31	118.30
4	y1	157	LEU	CB-CG-CD2	-9.99	94.02	111.00
18	l4	27	LEU	CB-CG-CD2	-9.98	94.03	111.00
11	cq	78	ARG	NE-CZ-NH2	-9.98	115.31	120.30
2	C1	133	LEU	CB-CG-CD2	-9.98	94.04	111.00
17	bk	93	ARG	NE-CZ-NH2	-9.97	115.31	120.30
5	W1	77	ARG	NE-CZ-NH2	-9.97	115.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d1	87	TYR	CB-CG-CD2	-9.96	115.02	121.00
10	la	66	LEU	CB-CG-CD2	-9.94	94.10	111.00
4	s1	84	ASP	CB-CG-OD2	9.89	127.20	118.30
11	v4	91	ARG	NE-CZ-NH1	-9.88	115.36	120.30
6	g1	108	ARG	NE-CZ-NH2	9.87	125.23	120.30
10	as	91	ARG	NE-CZ-NH2	9.87	125.23	120.30
18	l5	27	LEU	CB-CG-CD2	-9.87	94.23	111.00
4	T1	90	ARG	NE-CZ-NH1	9.85	125.22	120.30
11	x4	129	ARG	NE-CZ-NH1	9.84	125.22	120.30
11	a7	41	VAL	CG1-CB-CG2	-9.84	95.16	110.90
10	gh	137	ARG	NE-CZ-NH1	9.84	125.22	120.30
5	O1	83	ARG	NE-CZ-NH1	9.83	125.22	120.30
4	N1	38	ARG	NE-CZ-NH1	9.82	125.21	120.30
11	iC	84	ARG	NE-CZ-NH2	-9.81	115.40	120.30
11	F9	84	ARG	NE-CZ-NH1	9.80	125.20	120.30
15	W5	23	LEU	CA-CB-CG	9.80	137.83	115.30
11	e6	129	ARG	NE-CZ-NH1	9.78	125.19	120.30
10	A5	114	ARG	NE-CZ-NH2	9.77	125.19	120.30
4	N1	47	ARG	NE-CZ-NH1	9.75	125.18	120.30
17	ak	30	ARG	NE-CZ-NH1	-9.75	115.42	120.30
5	J1	107	ARG	NE-CZ-NH1	9.74	125.17	120.30
17	ak	30	ARG	NE-CZ-NH2	9.74	125.17	120.30
12	bY	270	ARG	NE-CZ-NH2	-9.72	115.44	120.30
11	at	161	LEU	CB-CG-CD2	-9.72	94.48	111.00
14	aZ	192	ARG	NE-CZ-NH2	9.71	125.16	120.30
10	cC	142	ARG	NE-CZ-NH2	-9.69	115.45	120.30
10	W7	91	ARG	NE-CZ-NH1	-9.68	115.46	120.30
4	y1	84	ASP	CB-CG-OD2	9.67	127.01	118.30
5	n1	112	LEU	CB-CG-CD1	-9.67	94.56	111.00
11	N7	88	ILE	CG1-CB-CG2	-9.67	90.14	111.40
11	cr	161	LEU	CB-CG-CD2	-9.66	94.58	111.00
11	n4	78	ARG	NE-CZ-NH2	-9.65	115.47	120.30
12	ey	62	ARG	NE-CZ-NH1	-9.64	115.48	120.30
17	k9	30	ARG	NE-CZ-NH2	9.64	125.12	120.30
5	U1	76	ARG	NE-CZ-NH2	9.63	125.12	120.30
4	y1	36	ARG	NE-CZ-NH2	9.63	125.12	120.30
22	eY	339	GLU	OE1-CD-OE2	-9.63	111.75	123.30
5	c1	107	ARG	NE-CZ-NH2	-9.62	115.49	120.30
4	d1	91	LEU	CB-CG-CD2	-9.62	94.66	111.00
10	em	91	ARG	NE-CZ-NH1	9.61	125.11	120.30
11	jO	108	ARG	NH1-CZ-NH2	-9.61	108.83	119.40
18	bf	84	ARG	NE-CZ-NH1	9.60	125.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	c9	234	ARG	NE-CZ-NH2	9.59	125.10	120.30
5	v1	85	LEU	CB-CG-CD1	-9.58	94.72	111.00
14	bZ	192	ARG	NE-CZ-NH1	-9.57	115.51	120.30
11	t4	7	ARG	NE-CZ-NH2	-9.57	115.52	120.30
11	v5	7	ARG	NE-CZ-NH1	9.56	125.08	120.30
5	e1	83	ARG	NE-CZ-NH1	9.55	125.08	120.30
10	cD	140	VAL	C-N-CD	-9.53	99.63	120.60
4	d1	47	ARG	NE-CZ-NH1	9.52	125.06	120.30
10	O2	18	PHE	CB-CG-CD1	-9.51	114.14	120.80
11	eT	77	ARG	NE-CZ-NH1	9.46	125.03	120.30
10	bt	84	ARG	NE-CZ-NH1	-9.46	115.57	120.30
10	ed	91	ARG	NE-CZ-NH1	9.46	125.03	120.30
12	A2	213	ARG	NE-CZ-NH2	9.45	125.03	120.30
11	x4	50	CYS	CA-CB-SG	9.44	131.00	114.00
11	J2	91	ARG	NE-CZ-NH2	-9.43	115.59	120.30
11	cq	78	ARG	NE-CZ-NH1	-9.41	115.59	120.30
11	A8	84	ARG	NE-CZ-NH1	9.41	125.00	120.30
11	dL	50	CYS	CA-CB-SG	9.41	130.94	114.00
18	bb	84	ARG	NE-CZ-NH1	9.40	125.00	120.30
17	ck	93	ARG	NE-CZ-NH2	-9.39	115.60	120.30
5	t1	90	ARG	NE-CZ-NH2	9.38	124.99	120.30
9	d2	41	ARG	NE-CZ-NH2	-9.37	115.61	120.30
17	ce	50	ARG	NE-CZ-NH2	-9.37	115.62	120.30
20	dz	270	ARG	NE-CZ-NH1	9.36	124.98	120.30
16	24	61	ARG	NE-CZ-NH1	-9.35	115.62	120.30
5	z1	18	TYR	CG-CD1-CE1	-9.35	113.82	121.30
17	ca	93	ARG	NH1-CZ-NH2	9.34	129.68	119.40
11	d6	108	ARG	NE-CZ-NH1	9.34	124.97	120.30
11	dL	84	ARG	NH1-CZ-NH2	9.32	129.65	119.40
11	lj	108	ARG	NE-CZ-NH2	9.31	124.95	120.30
10	s9	91	ARG	NE-CZ-NH2	9.31	124.95	120.30
8	a2	837	LEU	CB-CG-CD2	-9.30	95.18	111.00
18	g4	84	ARG	NE-CZ-NH2	-9.29	115.65	120.30
11	iC	101	ASP	CB-CG-OD2	9.27	126.65	118.30
4	u1	36	ARG	NE-CZ-NH2	9.27	124.93	120.30
11	H9	38	LEU	CB-CG-CD1	-9.26	95.26	111.00
11	t5	7	ARG	NE-CZ-NH2	-9.25	115.67	120.30
11	c6	41	VAL	CG1-CB-CG2	-9.25	96.10	110.90
18	al	77	ARG	NE-CZ-NH2	-9.24	115.68	120.30
11	y7	50	CYS	CA-CB-SG	9.24	130.64	114.00
4	o1	36	ARG	NE-CZ-NH2	9.24	124.92	120.30
10	S6	137	ARG	NE-CZ-NH2	-9.24	115.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N1	87	TYR	CB-CG-CD2	-9.24	115.46	121.00
11	T6	161	LEU	CB-CG-CD2	-9.23	95.30	111.00
14	c8	234	ARG	NE-CZ-NH2	9.23	124.92	120.30
5	L1	83	ARG	NE-CZ-NH1	-9.22	115.69	120.30
4	s1	157	LEU	CB-CG-CD2	-9.21	95.34	111.00
5	W1	112	LEU	CB-CG-CD1	-9.20	95.35	111.00
11	j3	91	ARG	NE-CZ-NH1	9.20	124.90	120.30
5	a1	107	ARG	NE-CZ-NH2	-9.19	115.70	120.30
5	Y1	107	ARG	NE-CZ-NH1	9.19	124.90	120.30
17	be	50	ARG	NE-CZ-NH2	-9.19	115.70	120.30
10	z8	37	ARG	NE-CZ-NH2	-9.18	115.71	120.30
11	jP	108	ARG	NH1-CZ-NH2	-9.17	109.31	119.40
3	F1	121	ARG	NE-CZ-NH1	-9.17	115.72	120.30
12	ez	62	ARG	NE-CZ-NH1	-9.16	115.72	120.30
11	F6	161	LEU	CB-CG-CD2	-9.15	95.44	111.00
11	av	27	LEU	CB-CG-CD2	-9.14	95.45	111.00
11	dX	84	ARG	NH1-CZ-NH2	9.14	129.45	119.40
11	D7	143	MET	CG-SD-CE	-9.13	85.59	100.20
5	h1	83	ARG	NE-CZ-NH1	-9.12	115.74	120.30
11	bq	78	ARG	NE-CZ-NH2	-9.12	115.74	120.30
10	m5	135	ARG	NE-CZ-NH1	-9.11	115.74	120.30
10	bt	85	ASP	CB-CG-OD2	9.11	126.50	118.30
5	l1	76	ARG	NE-CZ-NH2	9.10	124.85	120.30
10	fx	140	VAL	C-N-CD	-9.08	100.61	120.60
11	bH	91	ARG	NE-CZ-NH1	9.06	124.83	120.30
11	p3	77	ARG	NE-CZ-NH2	9.06	124.83	120.30
13	B2	283	LEU	CB-CG-CD2	-9.05	95.61	111.00
4	N1	91	LEU	CB-CG-CD2	-9.04	95.63	111.00
10	go	140	VAL	C-N-CD	-9.03	100.73	120.60
4	w1	77	MET	CG-SD-CE	-9.02	85.77	100.20
5	J1	77	ARG	NE-CZ-NH1	-9.01	115.80	120.30
12	bY	46	PHE	CB-CG-CD2	-9.01	114.49	120.80
11	eL	27	LEU	CB-CG-CD2	-9.01	95.68	111.00
22	eZ	111	ARG	NE-CZ-NH1	-9.00	115.80	120.30
4	q1	77	MET	CG-SD-CE	-8.99	85.82	100.20
11	L2	161	LEU	CB-CG-CD2	-8.99	95.72	111.00
11	ll	91	ARG	NE-CZ-NH1	8.98	124.79	120.30
12	A2	62	ARG	NE-CZ-NH1	-8.98	115.81	120.30
16	24	95	MET	CG-SD-CE	8.96	114.54	100.20
15	W9	113	ARG	NE-CZ-NH1	-8.96	115.82	120.30
17	bc	69	MET	CG-SD-CE	-8.96	85.86	100.20
8	b2	837	LEU	CB-CG-CD2	-8.96	95.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	aO	140	VAL	C-N-CD	-8.95	100.90	120.60
10	m4	135	ARG	NE-CZ-NH1	-8.95	115.83	120.30
5	M1	83	ARG	NE-CZ-NH1	-8.95	115.83	120.30
4	P1	90	ARG	NE-CZ-NH1	8.95	124.77	120.30
10	bO	140	VAL	C-N-CD	-8.95	100.91	120.60
18	cb	117	TYR	CB-CG-CD2	-8.94	115.63	121.00
5	t1	18	TYR	CG-CD1-CE1	-8.94	114.15	121.30
11	x4	98	LEU	CB-CG-CD1	-8.94	95.81	111.00
4	G1	90	ARG	NE-CZ-NH2	-8.93	115.84	120.30
11	r5	50	CYS	CA-CB-SG	8.93	130.07	114.00
4	s1	87	TYR	CZ-CE2-CD2	-8.92	111.77	119.80
11	B3	91	ARG	NE-CZ-NH2	-8.91	115.84	120.30
12	ez	173	ARG	NE-CZ-NH2	-8.90	115.85	120.30
11	lt	91	ARG	NE-CZ-NH1	8.90	124.75	120.30
11	v4	7	ARG	NE-CZ-NH1	8.90	124.75	120.30
12	aY	71	ARG	NE-CZ-NH1	8.89	124.75	120.30
20	dz	124	ARG	NE-CZ-NH1	-8.89	115.86	120.30
11	el	101	ASP	CB-CG-OD1	8.89	126.30	118.30
8	a2	359	PHE	CB-CG-CD1	-8.88	114.59	120.80
8	b2	707	ARG	NE-CZ-NH1	-8.88	115.86	120.30
4	Z1	17	TYR	CB-CG-CD1	-8.86	115.68	121.00
8	a2	482	LEU	CB-CG-CD1	-8.86	95.94	111.00
3	F1	174	LEU	CB-CG-CD1	-8.85	95.95	111.00
13	b3	283	LEU	CB-CG-CD2	-8.85	95.96	111.00
12	ey	173	ARG	NE-CZ-NH2	-8.85	115.88	120.30
11	lh	13	ASP	CB-CG-OD2	8.85	126.26	118.30
10	s4	135	ARG	NE-CZ-NH1	-8.84	115.88	120.30
10	I9	138	LEU	CB-CG-CD1	-8.84	95.98	111.00
11	lv	13	ASP	CB-CG-OD2	8.83	126.25	118.30
11	l3	161	LEU	CB-CG-CD2	-8.83	96.00	111.00
11	e6	161	LEU	CB-CG-CD1	-8.83	95.99	111.00
11	v9	27	LEU	CB-CG-CD2	-8.83	96.00	111.00
12	a3	213	ARG	NE-CZ-NH2	8.82	124.71	120.30
11	v7	170	ASP	CB-CG-OD2	8.82	126.24	118.30
11	dL	101	ASP	CB-CG-OD1	8.82	126.24	118.30
11	b6	91	ARG	NE-CZ-NH1	8.79	124.69	120.30
11	n9	108	ARG	NE-CZ-NH1	-8.79	115.91	120.30
11	iG	91	ARG	NE-CZ-NH2	-8.79	115.91	120.30
4	k1	87	TYR	CB-CG-CD2	-8.78	115.73	121.00
11	z5	27	LEU	CB-CG-CD2	-8.78	96.08	111.00
11	bq	78	ARG	NE-CZ-NH1	-8.78	115.91	120.30
11	H2	84	ARG	NE-CZ-NH1	8.78	124.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K1	17	TYR	CB-CG-CD1	-8.77	115.74	121.00
11	C8	38	LEU	CB-CG-CD1	-8.77	96.09	111.00
10	s5	135	ARG	NE-CZ-NH1	-8.76	115.92	120.30
11	h3	84	ARG	NE-CZ-NH1	8.76	124.68	120.30
10	dA	9	ILE	CG1-CB-CG2	-8.76	92.12	111.40
10	dS	114	ARG	NE-CZ-NH1	-8.76	115.92	120.30
10	au	37	ARG	NE-CZ-NH2	-8.76	115.92	120.30
5	n1	77	ARG	NE-CZ-NH2	-8.76	115.92	120.30
11	av	101	ASP	CB-CG-OD1	8.76	126.18	118.30
4	y1	94	TYR	CB-CG-CD1	-8.76	115.75	121.00
17	k5	24	LEU	CB-CG-CD2	-8.75	96.13	111.00
10	g7	44	LEU	CB-CG-CD1	-8.75	96.13	111.00
4	T1	87	TYR	CB-CG-CD2	-8.73	115.76	121.00
11	B6	143	MET	CG-SD-CE	-8.73	86.24	100.20
17	ba	93	ARG	NH1-CZ-NH2	8.73	129.00	119.40
10	gm	91	ARG	NE-CZ-NH1	8.71	124.66	120.30
4	N1	38	ARG	NE-CZ-NH2	-8.71	115.95	120.30
11	iH	91	ARG	NE-CZ-NH2	-8.71	115.95	120.30
10	dO	84	ARG	NE-CZ-NH2	8.70	124.65	120.30
10	gh	140	VAL	C-N-CD	-8.70	101.46	120.60
3	E1	174	LEU	CB-CG-CD1	-8.69	96.23	111.00
14	aZ	192	ARG	NE-CZ-NH1	-8.69	115.95	120.30
11	kT	91	ARG	NE-CZ-NH1	8.69	124.64	120.30
5	J1	113	LYS	CD-CE-NZ	8.69	131.68	111.70
11	L7	59	MET	CG-SD-CE	8.68	114.09	100.20
15	W9	88	ILE	CG1-CB-CG2	-8.67	92.32	111.40
10	eE	142	ARG	NE-CZ-NH1	-8.67	115.96	120.30
15	R8	113	ARG	NE-CZ-NH1	-8.67	115.97	120.30
8	a2	337	ASP	CB-CG-OD2	-8.66	110.51	118.30
4	y1	65	VAL	CG1-CB-CG2	-8.65	97.06	110.90
11	r4	50	CYS	CA-CB-SG	8.64	129.56	114.00
11	e7	91	ARG	NE-CZ-NH1	8.64	124.62	120.30
11	t9	161	LEU	CB-CG-CD2	-8.64	96.31	111.00
11	eV	27	LEU	CB-CG-CD2	-8.64	96.32	111.00
18	al	84	ARG	NE-CZ-NH1	-8.63	115.98	120.30
11	eJ	77	ARG	NE-CZ-NH1	8.62	124.61	120.30
10	u9	37	ARG	NE-CZ-NH2	-8.62	115.99	120.30
10	q5	114	ARG	NE-CZ-NH1	-8.61	115.99	120.30
5	l1	83	ARG	NE-CZ-NH1	8.61	124.61	120.30
17	a5	30	ARG	NE-CZ-NH2	-8.60	116.00	120.30
11	n5	129	ARG	NE-CZ-NH1	8.60	124.60	120.30
4	b1	90	ARG	NE-CZ-NH2	-8.59	116.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	ct	85	ASP	CB-CG-OD2	8.59	126.03	118.30
20	dy	270	ARG	NE-CZ-NH1	8.59	124.59	120.30
11	aT	91	ARG	NE-CZ-NH1	8.58	124.59	120.30
18	g5	84	ARG	NE-CZ-NH2	-8.58	116.01	120.30
10	la	91	ARG	NE-CZ-NH2	-8.57	116.01	120.30
5	z1	13	ASP	CB-CG-OD2	8.56	126.01	118.30
18	bj	57	ARG	NE-CZ-NH1	-8.56	116.02	120.30
10	E9	85	ASP	CB-CG-OD2	8.56	126.01	118.30
10	dJ	91	ARG	NH1-CZ-NH2	-8.56	109.98	119.40
4	P1	109	LEU	CB-CG-CD2	-8.56	96.45	111.00
11	T2	91	ARG	NE-CZ-NH1	8.56	124.58	120.30
10	ek	91	ARG	NE-CZ-NH1	8.55	124.58	120.30
10	dZ	91	ARG	NE-CZ-NH1	8.55	124.58	120.30
13	B2	406	ARG	NE-CZ-NH1	-8.55	116.03	120.30
16	X9	61	ARG	NH1-CZ-NH2	8.55	128.80	119.40
11	x5	7	ARG	NE-CZ-NH1	8.55	124.57	120.30
11	v5	161	LEU	CB-CG-CD2	-8.54	96.48	111.00
11	ln	77	ARG	NE-CZ-NH1	-8.54	116.03	120.30
10	iA	84	ARG	NE-CZ-NH1	-8.54	116.03	120.30
10	j7	114	ARG	NE-CZ-NH2	-8.54	116.03	120.30
11	d6	153	ILE	CG1-CB-CG2	-8.53	92.63	111.40
18	l9	84	ARG	NE-CZ-NH1	-8.53	116.03	120.30
10	dA	84	ARG	NE-CZ-NH1	-8.53	116.03	120.30
4	f1	109	LEU	CB-CG-CD2	-8.52	96.52	111.00
3	F1	200	LEU	CB-CG-CD2	-8.52	96.52	111.00
11	z4	27	LEU	CB-CG-CD2	-8.52	96.53	111.00
11	p6	91	ARG	NE-CZ-NH2	-8.51	116.05	120.30
11	aH	91	ARG	NE-CZ-NH1	8.50	124.55	120.30
14	d8	112	ARG	NE-CZ-NH2	8.49	124.55	120.30
13	b3	394	LEU	CB-CG-CD1	-8.46	96.62	111.00
11	aH	91	ARG	NE-CZ-NH2	-8.46	116.07	120.30
12	a3	151	ARG	NE-CZ-NH1	8.44	124.52	120.30
11	P2	77	ARG	NE-CZ-NH2	8.43	124.52	120.30
10	dW	91	ARG	NH1-CZ-NH2	-8.43	110.12	119.40
12	U8	71	ARG	NE-CZ-NH2	-8.43	116.08	120.30
13	b3	406	ARG	NE-CZ-NH1	-8.42	116.09	120.30
8	b2	482	LEU	CB-CG-CD1	-8.42	96.69	111.00
11	x6	84	ARG	NE-CZ-NH2	-8.41	116.09	120.30
11	v9	101	ASP	CB-CG-OD1	8.41	125.87	118.30
18	cb	84	ARG	NH1-CZ-NH2	-8.41	110.15	119.40
5	U1	107	ARG	NE-CZ-NH2	-8.40	116.10	120.30
12	34	147	ARG	NE-CZ-NH1	-8.40	116.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	s1	151	PHE	CB-CG-CD1	-8.40	114.92	120.80
9	c2	42	LEU	CB-CG-CD1	-8.40	96.72	111.00
12	a3	156	ARG	NE-CZ-NH2	-8.40	116.10	120.30
11	J3	91	ARG	NE-CZ-NH1	-8.40	116.10	120.30
12	A2	151	ARG	NE-CZ-NH1	8.39	124.50	120.30
11	j3	91	ARG	NE-CZ-NH2	-8.39	116.10	120.30
11	r7	77	ARG	NE-CZ-NH1	8.39	124.50	120.30
10	eA	33	ARG	NE-CZ-NH1	-8.39	116.10	120.30
11	V7	77	ARG	NE-CZ-NH1	8.39	124.50	120.30
10	E9	37	ARG	NE-CZ-NH1	8.39	124.49	120.30
18	ch	84	ARG	NE-CZ-NH2	8.38	124.49	120.30
9	c2	13	LEU	CA-CB-CG	8.38	134.57	115.30
14	d9	112	ARG	NE-CZ-NH1	-8.38	116.11	120.30
4	N1	90	ARG	NE-CZ-NH1	8.37	124.48	120.30
16	X5	95	MET	CG-SD-CE	8.37	113.59	100.20
11	F6	129	ARG	NE-CZ-NH1	8.36	124.48	120.30
12	bY	71	ARG	NE-CZ-NH1	8.36	124.48	120.30
13	B2	150	PHE	CB-CG-CD1	-8.36	114.95	120.80
11	an	77	ARG	NE-CZ-NH2	-8.36	116.12	120.30
10	bG	91	ARG	NE-CZ-NH2	8.35	124.47	120.30
5	L1	107	ARG	NE-CZ-NH2	-8.35	116.13	120.30
11	f2	50	CYS	CA-CB-SG	8.34	129.02	114.00
18	cf	83	LEU	CB-CG-CD2	8.34	125.18	111.00
11	r5	7	ARG	NE-CZ-NH1	8.34	124.47	120.30
11	eT	77	ARG	NE-CZ-NH2	-8.34	116.13	120.30
4	d1	38	ARG	NE-CZ-NH1	8.32	124.46	120.30
4	y1	87	TYR	CZ-CE2-CD2	-8.32	112.31	119.80
10	la	91	ARG	NE-CZ-NH1	8.31	124.46	120.30
18	cl	57	ARG	NE-CZ-NH1	8.31	124.46	120.30
11	n4	129	ARG	NE-CZ-NH1	8.31	124.45	120.30
15	R8	61	LEU	CB-CG-CD2	8.31	125.13	111.00
11	r4	7	ARG	NE-CZ-NH1	8.31	124.45	120.30
10	lu	142	ARG	NE-CZ-NH1	8.31	124.45	120.30
10	I9	163	LEU	CB-CG-CD2	-8.30	96.89	111.00
15	R8	88	ILE	CG1-CB-CG2	-8.30	93.14	111.40
4	s1	90	ARG	NE-CZ-NH1	8.30	124.45	120.30
11	r9	78	ARG	NE-CZ-NH1	-8.30	116.15	120.30
13	b3	150	PHE	CB-CG-CD1	-8.30	114.99	120.80
14	d8	112	ARG	NE-CZ-NH1	-8.30	116.15	120.30
12	Y5	147	ARG	NE-CZ-NH1	-8.29	116.15	120.30
11	dB	101	ASP	CB-CG-OD1	8.29	125.76	118.30
10	bm	84	ARG	NE-CZ-NH1	-8.28	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	r6	170	ASP	CB-CG-OD2	8.28	125.75	118.30
10	i7	91	ARG	NE-CZ-NH1	-8.28	116.16	120.30
10	bm	17	ARG	NE-CZ-NH2	-8.28	116.16	120.30
5	t1	13	ASP	CB-CG-OD2	8.27	125.75	118.30
18	bb	85	ASP	CB-CG-OD2	8.27	125.74	118.30
10	o3	18	PHE	CB-CG-CD1	-8.27	115.01	120.80
8	a2	707	ARG	NE-CZ-NH2	-8.26	116.17	120.30
5	U1	115	THR	CA-CB-CG2	-8.25	100.85	112.40
10	v8	85	ASP	CB-CG-OD2	8.25	125.73	118.30
12	Z9	71	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	D1	59	ARG	NE-CZ-NH2	-8.25	116.18	120.30
4	s1	65	VAL	CG1-CB-CG2	-8.25	97.70	110.90
10	A6	142	ARG	NE-CZ-NH2	-8.25	116.18	120.30
18	cj	57	ARG	NE-CZ-NH1	-8.24	116.18	120.30
11	F3	50	CYS	CA-CB-SG	8.23	128.82	114.00
5	j1	18	TYR	CB-CG-CD2	-8.23	116.06	121.00
10	dO	91	ARG	NE-CZ-NH1	8.23	124.42	120.30
18	bh	84	ARG	NE-CZ-NH2	8.23	124.42	120.30
11	a6	59	MET	CG-SD-CE	8.23	113.36	100.20
4	b1	94	TYR	CB-CG-CD1	-8.22	116.06	121.00
10	ay	85	ASP	CB-CG-OD2	8.22	125.70	118.30
18	j4	84	ARG	NE-CZ-NH2	8.22	124.41	120.30
4	d1	38	ARG	NE-CZ-NH2	-8.22	116.19	120.30
11	L2	98	LEU	CB-CG-CD1	-8.22	97.03	111.00
5	U1	83	ARG	NE-CZ-NH1	8.21	124.41	120.30
10	C7	138	LEU	CB-CG-CD2	-8.21	97.03	111.00
11	v4	7	ARG	NE-CZ-NH2	-8.21	116.19	120.30
15	W9	61	LEU	CB-CG-CD2	8.21	124.96	111.00
21	ex	116	ARG	NE-CZ-NH1	-8.21	116.20	120.30
11	p9	88	ILE	CG1-CB-CG2	-8.18	93.40	111.40
11	F6	66	LEU	CB-CG-CD2	-8.17	97.11	111.00
2	C1	64	ARG	NE-CZ-NH1	-8.17	116.21	120.30
10	iA	91	ARG	NE-CZ-NH1	8.17	124.38	120.30
14	e9	77	MET	CG-SD-CE	-8.17	87.13	100.20
10	j6	91	ARG	NE-CZ-NH1	-8.16	116.22	120.30
14	e8	200	MET	CA-CB-CG	8.14	127.14	113.30
11	an	108	ARG	NE-CZ-NH1	-8.14	116.23	120.30
17	bi	30	ARG	NE-CZ-NH2	-8.14	116.23	120.30
11	t3	91	ARG	NE-CZ-NH1	8.14	124.37	120.30
14	e8	200	MET	CG-SD-CE	-8.14	87.18	100.20
11	l7	91	ARG	NE-CZ-NH2	-8.12	116.24	120.30
10	gm	85	ASP	CB-CG-OD2	8.13	125.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	a4	30	ARG	NE-CZ-NH1	8.12	124.36	120.30
10	cm	17	ARG	NE-CZ-NH2	-8.12	116.24	120.30
10	aE	120	LEU	CB-CG-CD2	8.12	124.80	111.00
20	dy	124	ARG	NE-CZ-NH1	-8.11	116.24	120.30
11	x4	161	LEU	CB-CG-CD2	-8.11	97.22	111.00
11	gx	61	CYS	CA-CB-SG	8.11	128.59	114.00
18	l4	88	ILE	CG1-CB-CG2	-8.10	93.58	111.40
11	bo	101	ASP	CB-CG-OD1	8.10	125.59	118.30
4	N1	38	ARG	CD-NE-CZ	8.10	134.93	123.60
11	ar	78	ARG	NE-CZ-NH1	-8.09	116.26	120.30
10	m7	37	ARG	NE-CZ-NH2	-8.08	116.26	120.30
18	cf	84	ARG	NE-CZ-NH1	8.08	124.34	120.30
10	iB	38	LEU	CB-CG-CD2	-8.07	97.28	111.00
10	o6	66	LEU	CB-CG-CD2	-8.07	97.28	111.00
11	B7	108	ARG	NE-CZ-NH1	-8.07	116.27	120.30
18	bb	117	TYR	CB-CG-CD2	-8.06	116.16	121.00
4	G1	52	LYS	CD-CE-NZ	8.06	130.24	111.70
10	cv	33	ARG	NH1-CZ-NH2	-8.06	110.54	119.40
10	cA	33	ARG	NH1-CZ-NH2	-8.06	110.54	119.40
10	cW	33	ARG	NE-CZ-NH1	8.06	124.33	120.30
5	l1	107	ARG	NE-CZ-NH2	-8.06	116.27	120.30
5	Y1	113	LYS	CD-CE-NZ	8.05	130.22	111.70
18	cl	105	LEU	CB-CG-CD2	-8.05	97.31	111.00
18	cb	77	ARG	NE-CZ-NH2	8.05	124.32	120.30
10	cC	91	ARG	NE-CZ-NH2	8.05	124.32	120.30
5	p1	97	LEU	CB-CG-CD2	-8.04	97.33	111.00
10	k6	37	ARG	NE-CZ-NH2	-8.04	116.28	120.30
25	kb	316	MET	CG-SD-CE	8.04	113.06	100.20
5	S1	28	ARG	NE-CZ-NH2	-8.03	116.28	120.30
12	A2	156	ARG	NE-CZ-NH2	-8.03	116.28	120.30
11	Z7	59	MET	CG-SD-CE	8.03	113.05	100.20
10	x8	91	ARG	NE-CZ-NH2	8.03	124.32	120.30
11	br	91	ARG	NE-CZ-NH2	-8.03	116.29	120.30
6	Q1	11	ARG	NE-CZ-NH2	8.03	124.31	120.30
11	d6	91	ARG	NE-CZ-NH1	8.03	124.31	120.30
17	ba	28	THR	CA-CB-CG2	-8.02	101.17	112.40
11	x4	2	LEU	CB-CG-CD1	-8.02	97.37	111.00
10	A9	85	ASP	CB-CG-OD2	8.01	125.51	118.30
5	j1	28	ARG	NE-CZ-NH2	-8.01	116.30	120.30
4	b1	52	LYS	CD-CE-NZ	8.01	130.11	111.70
17	k5	28	THR	CA-CB-CG2	-8.01	101.19	112.40
11	V7	120	LEU	CB-CG-CD1	-8.00	97.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	aG	91	ARG	NE-CZ-NH2	8.00	124.30	120.30
10	bE	120	LEU	CB-CG-CD2	8.00	124.61	111.00
20	dz	270	ARG	NE-CZ-NH2	-8.00	116.30	120.30
11	dX	142	ILE	CG1-CB-CG2	-8.00	93.80	111.40
11	V2	108	ARG	NE-CZ-NH2	8.00	124.30	120.30
3	F1	171	ARG	NH1-CZ-NH2	8.00	128.19	119.40
21	ew	116	ARG	NE-CZ-NH1	-8.00	116.30	120.30
5	v1	97	LEU	CB-CG-CD2	-7.99	97.41	111.00
11	F6	37	ARG	NE-CZ-NH2	7.99	124.30	120.30
4	N1	94	TYR	CB-CG-CD1	-7.99	116.21	121.00
18	cb	84	ARG	NE-CZ-NH2	7.99	124.29	120.30
11	z4	91	ARG	NE-CZ-NH1	7.99	124.29	120.30
12	Z9	122	ARG	NE-CZ-NH2	-7.99	116.31	120.30
11	kR	37	ARG	NE-CZ-NH1	7.98	124.29	120.30
11	V6	91	ARG	NE-CZ-NH1	7.97	124.28	120.30
17	k4	24	LEU	CB-CG-CD2	-7.97	97.45	111.00
18	bb	84	ARG	NH1-CZ-NH2	-7.97	110.64	119.40
12	Y5	106	MET	CG-SD-CE	7.97	112.95	100.20
11	iG	37	ARG	NE-CZ-NH1	7.96	124.28	120.30
16	X9	288	ARG	NE-CZ-NH2	-7.96	116.32	120.30
11	jK	115	GLU	OE1-CD-OE2	-7.95	113.76	123.30
10	bt	137	ARG	NE-CZ-NH2	-7.95	116.33	120.30
4	d1	94	TYR	CB-CG-CD1	-7.94	116.23	121.00
10	eM	17	ARG	NE-CZ-NH1	-7.94	116.33	120.30
11	kQ	37	ARG	NE-CZ-NH1	7.94	124.27	120.30
11	T2	77	ARG	NE-CZ-NH2	7.94	124.27	120.30
4	k1	84	ASP	CB-CG-OD2	7.93	125.44	118.30
16	S8	288	ARG	NE-CZ-NH2	-7.93	116.34	120.30
11	n9	77	ARG	NE-CZ-NH2	-7.93	116.33	120.30
11	iH	37	ARG	NE-CZ-NH1	7.93	124.26	120.30
10	cx	85	ASP	CB-CG-OD2	7.92	125.43	118.30
18	bj	39	ASP	CB-CG-OD2	-7.92	111.17	118.30
10	bv	33	ARG	NH1-CZ-NH2	-7.92	110.69	119.40
11	x5	98	LEU	CB-CG-CD1	-7.91	97.55	111.00
10	f6	44	LEU	CB-CG-CD1	-7.91	97.56	111.00
5	U1	83	ARG	NE-CZ-NH2	-7.90	116.35	120.30
14	d9	112	ARG	NE-CZ-NH2	7.90	124.25	120.30
11	br	98	LEU	CB-CG-CD1	-7.90	97.58	111.00
25	ka	316	MET	CG-SD-CE	7.90	112.83	100.20
10	go	139	CYS	CA-CB-SG	7.89	128.21	114.00
11	j2	91	ARG	NE-CZ-NH1	-7.89	116.35	120.30
12	U8	156	ARG	NH1-CZ-NH2	7.89	128.08	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	bY	62	ARG	CG-CD-NE	-7.89	95.24	111.80
10	j6	44	LEU	CB-CG-CD1	-7.88	97.60	111.00
10	aC	85	ASP	CB-CG-OD2	7.88	125.39	118.30
11	ax	108	ARG	NE-CZ-NH2	7.88	124.24	120.30
12	Z9	156	ARG	NH1-CZ-NH2	7.88	128.06	119.40
5	c1	18	TYR	CG-CD1-CE1	-7.87	115.00	121.30
11	X6	30	PHE	CB-CG-CD2	7.87	126.31	120.80
11	x4	95	TYR	CB-CG-CD1	-7.87	116.28	121.00
4	k1	77	MET	CG-SD-CE	-7.87	87.61	100.20
11	H6	59	MET	CG-SD-CE	7.87	112.78	100.20
10	bt	140	VAL	C-N-CD	-7.87	103.30	120.60
5	M1	77	ARG	NE-CZ-NH1	-7.86	116.37	120.30
11	x5	84	ARG	NH1-CZ-NH2	7.86	128.05	119.40
11	J5	7	ARG	NE-CZ-NH1	7.86	124.23	120.30
18	bl	105	LEU	CB-CG-CD2	-7.86	97.64	111.00
12	34	106	MET	CG-SD-CE	7.85	112.77	100.20
11	v5	7	ARG	NE-CZ-NH2	-7.85	116.37	120.30
6	g1	11	ARG	NE-CZ-NH2	7.85	124.22	120.30
17	k5	50	ARG	NE-CZ-NH2	-7.85	116.38	120.30
11	l3	98	LEU	CB-CG-CD1	-7.85	97.66	111.00
14	c9	234	ARG	NE-CZ-NH1	-7.85	116.38	120.30
11	aD	91	ARG	NE-CZ-NH2	-7.85	116.38	120.30
4	R1	87	TYR	CB-CG-CD2	-7.84	116.29	121.00
11	c6	153	ILE	CG1-CB-CG2	-7.84	94.15	111.40
10	li	91	ARG	NE-CZ-NH1	7.84	124.22	120.30
5	H1	18	TYR	CG-CD1-CE1	-7.83	115.03	121.30
12	34	71	ARG	NE-CZ-NH2	-7.83	116.39	120.30
11	N4	27	LEU	CB-CG-CD2	-7.82	97.70	111.00
13	b3	346	ARG	NE-CZ-NH1	-7.82	116.39	120.30
18	bb	84	ARG	NE-CZ-NH2	7.82	124.21	120.30
11	aB	27	LEU	CB-CG-CD2	-7.82	97.71	111.00
10	K2	143	ASP	CB-CG-OD2	-7.81	111.27	118.30
10	cm	91	ARG	NH1-CZ-NH2	-7.81	110.81	119.40
4	b1	90	ARG	NE-CZ-NH1	7.81	124.20	120.30
13	B2	346	ARG	NE-CZ-NH1	-7.80	116.40	120.30
11	x9	108	ARG	NE-CZ-NH2	7.80	124.20	120.30
11	ee	84	ARG	NE-CZ-NH1	-7.80	116.40	120.30
11	lr	108	ARG	NE-CZ-NH2	7.80	124.20	120.30
11	iF	91	ARG	NE-CZ-NH2	-7.80	116.40	120.30
5	H1	83	ARG	NE-CZ-NH1	7.79	124.20	120.30
4	q1	47	ARG	NE-CZ-NH1	7.79	124.20	120.30
10	m6	17	ARG	NE-CZ-NH1	7.79	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	k7	18	PHE	CB-CG-CD1	-7.79	115.34	120.80
11	J5	27	LEU	CB-CG-CD2	-7.79	97.76	111.00
10	D8	163	LEU	CB-CG-CD2	-7.79	97.76	111.00
18	ad	85	ASP	CB-CG-OD2	7.78	125.31	118.30
11	dX	50	CYS	CA-CB-SG	7.78	128.01	114.00
14	C2	138	ARG	NE-CZ-NH2	-7.77	116.41	120.30
5	a1	67	ARG	NE-CZ-NH1	-7.77	116.42	120.30
12	A2	170	TYR	CZ-CE2-CD2	-7.77	112.81	119.80
4	G1	90	ARG	NE-CZ-NH1	7.76	124.18	120.30
10	au	85	ASP	CB-CG-OD2	7.76	125.29	118.30
11	en	84	ARG	NE-CZ-NH1	-7.76	116.42	120.30
10	q9	142	ARG	NE-CZ-NH2	7.76	124.18	120.30
10	E9	18	PHE	CB-CG-CD1	-7.76	115.37	120.80
18	cb	108	ARG	NE-CZ-NH1	-7.75	116.42	120.30
18	cb	85	ASP	CB-CG-OD2	7.75	125.27	118.30
22	eY	288	TYR	CG-CD2-CE2	-7.75	115.10	121.30
10	ao	142	ARG	NE-CZ-NH2	7.74	124.17	120.30
10	C5	135	ARG	NE-CZ-NH1	-7.74	116.43	120.30
4	b1	83	ARG	NE-CZ-NH2	-7.74	116.43	120.30
11	x5	95	TYR	CB-CG-CD1	-7.74	116.36	121.00
11	t6	77	ARG	NE-CZ-NH2	-7.74	116.43	120.30
11	Z6	37	ARG	NE-CZ-NH1	-7.74	116.43	120.30
11	t3	77	ARG	NE-CZ-NH2	7.73	124.17	120.30
11	bT	91	ARG	NE-CZ-NH1	7.73	124.17	120.30
11	v5	77	ARG	NE-CZ-NH2	7.73	124.16	120.30
18	bb	83	LEU	CB-CG-CD2	-7.72	97.87	111.00
11	h8	77	ARG	NE-CZ-NH1	7.72	124.16	120.30
11	a6	97	LEU	CB-CG-CD1	-7.72	97.88	111.00
12	U8	62	ARG	CG-CD-NE	-7.71	95.60	111.80
5	h1	77	ARG	NE-CZ-NH1	-7.71	116.44	120.30
10	u9	85	ASP	CB-CG-OD2	7.71	125.24	118.30
5	S1	18	TYR	CB-CG-CD2	-7.71	116.37	121.00
15	W9	220	LEU	CB-CG-CD1	7.71	124.11	111.00
11	bB	27	LEU	CB-CG-CD2	-7.70	97.91	111.00
11	H6	91	ARG	NE-CZ-NH1	7.70	124.15	120.30
10	y9	85	ASP	CB-CG-OD2	7.70	125.23	118.30
11	V7	30	PHE	CB-CG-CD2	7.69	126.18	120.80
17	cc	69	MET	CG-SD-CE	-7.69	87.89	100.20
12	aY	156	ARG	NE-CZ-NH2	-7.69	116.45	120.30
11	jL	115	GLU	OE1-CD-OE2	-7.69	114.07	123.30
11	L2	129	ARG	NE-CZ-NH1	7.69	124.14	120.30
4	d1	38	ARG	CD-NE-CZ	7.69	134.36	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	r4	88	ILE	CG1-CB-CG2	-7.68	94.49	111.40
11	dP	101	ASP	CB-CG-OD1	7.68	125.21	118.30
11	iD	84	ARG	NE-CZ-NH2	-7.68	116.46	120.30
12	aY	46	PHE	CB-CG-CD2	-7.68	115.43	120.80
11	ap	101	ASP	CB-CG-OD1	7.67	125.21	118.30
5	e1	67	ARG	NE-CZ-NH1	-7.67	116.46	120.30
11	v4	161	LEU	CB-CG-CD2	-7.67	97.96	111.00
4	b1	151	PHE	CG-CD1-CE1	-7.67	112.37	120.80
10	O2	18	PHE	CB-CG-CD2	7.67	126.17	120.80
5	U1	112	LEU	CB-CG-CD1	-7.67	97.97	111.00
11	v3	108	ARG	NE-CZ-NH2	7.66	124.13	120.30
12	34	156	ARG	NE-CZ-NH2	-7.66	116.47	120.30
12	Z9	62	ARG	CG-CD-NE	-7.66	95.70	111.80
10	eW	163	LEU	CB-CG-CD1	7.66	124.03	111.00
11	P6	113	LEU	CB-CG-CD1	-7.66	97.98	111.00
5	O1	67	ARG	NE-CZ-NH1	-7.66	116.47	120.30
18	c5	83	LEU	CB-CG-CD1	-7.66	97.99	111.00
10	bm	91	ARG	NH1-CZ-NH2	-7.64	110.99	119.40
5	v1	77	ARG	NH1-CZ-NH2	7.64	127.80	119.40
11	r5	91	ARG	NE-CZ-NH1	-7.64	116.48	120.30
12	a3	170	TYR	CZ-CE2-CD2	-7.63	112.93	119.80
10	j7	114	ARG	NE-CZ-NH1	7.63	124.12	120.30
10	bu	74	ASP	CB-CG-OD1	7.63	125.16	118.30
10	k3	144	MET	CG-SD-CE	-7.62	88.01	100.20
11	c6	59	MET	CG-SD-CE	7.62	112.39	100.20
10	D8	138	LEU	CB-CG-CD1	-7.62	98.05	111.00
11	Z7	97	LEU	CB-CG-CD1	-7.61	98.06	111.00
11	p9	101	ASP	CB-CG-OD1	7.61	125.15	118.30
10	f7	142	ARG	NE-CZ-NH1	7.61	124.10	120.30
5	l1	83	ARG	NE-CZ-NH2	-7.61	116.50	120.30
11	cN	84	ARG	NE-CZ-NH1	7.60	124.10	120.30
11	T6	59	MET	CG-SD-CE	7.60	112.36	100.20
16	X5	288	ARG	NE-CZ-NH1	7.59	124.10	120.30
11	X6	120	LEU	CB-CG-CD1	-7.59	98.09	111.00
10	cm	84	ARG	NE-CZ-NH1	-7.59	116.50	120.30
21	ew	124	TYR	CB-CG-CD2	-7.59	116.44	121.00
5	S1	13	ASP	CB-CG-OD2	7.59	125.13	118.30
11	Z7	91	ARG	NE-CZ-NH2	-7.59	116.51	120.30
11	F5	7	ARG	NE-CZ-NH1	7.59	124.09	120.30
12	aY	62	ARG	CG-CD-NE	-7.59	95.87	111.80
11	x5	2	LEU	CB-CG-CD1	-7.58	98.11	111.00
4	s1	131	ARG	NE-CZ-NH2	-7.58	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	b9	116	MET	CG-SD-CE	-7.58	88.07	100.20
5	W1	83	ARG	NE-CZ-NH2	7.58	124.09	120.30
13	b3	249	ARG	NE-CZ-NH1	-7.58	116.51	120.30
8	a2	605	ARG	CG-CD-NE	-7.57	95.91	111.80
12	U8	122	ARG	NE-CZ-NH2	-7.57	116.52	120.30
10	bC	85	ASP	CB-CG-OD2	7.57	125.11	118.30
5	c1	108	VAL	CG1-CB-CG2	-7.56	98.80	110.90
14	D2	251	LYS	CD-CE-NZ	7.56	129.09	111.70
11	N7	59	MET	CG-SD-CE	7.56	112.30	100.20
10	u8	138	LEU	CA-CB-CG	7.56	132.69	115.30
18	l4	78	ARG	NE-CZ-NH1	-7.56	116.52	120.30
4	G1	94	TYR	CB-CG-CD1	-7.56	116.47	121.00
5	l1	115	THR	CA-CB-CG2	-7.55	101.82	112.40
8	a2	605	ARG	NH1-CZ-NH2	7.55	127.71	119.40
14	c3	251	LYS	CD-CE-NZ	7.55	129.08	111.70
12	Y5	156	ARG	NE-CZ-NH2	-7.55	116.52	120.30
18	af	145	LEU	CA-CB-CG	7.55	132.67	115.30
10	I6	138	LEU	CA-CB-CG	7.55	132.66	115.30
14	d3	251	LYS	CD-CE-NZ	7.54	129.05	111.70
16	X9	339	ARG	NE-CZ-NH1	-7.54	116.53	120.30
17	ck	38	LEU	CB-CG-CD2	7.54	123.82	111.00
2	C1	186	LEU	CB-CG-CD1	-7.54	98.19	111.00
11	eJ	77	ARG	NE-CZ-NH2	-7.54	116.53	120.30
11	N7	153	ILE	CG1-CB-CG2	-7.53	94.83	111.40
10	bG	13	ASP	CB-CG-OD2	-7.53	111.52	118.30
10	s7	24	LEU	CB-CG-CD2	-7.53	98.20	111.00
4	y1	90	ARG	NE-CZ-NH1	7.52	124.06	120.30
10	G7	114	ARG	NE-CZ-NH2	-7.52	116.54	120.30
14	C2	251	LYS	CD-CE-NZ	7.52	128.99	111.70
10	E9	138	LEU	CB-CG-CD1	-7.52	98.22	111.00
10	Y6	138	LEU	CA-CB-CG	7.52	132.59	115.30
5	e1	77	ARG	NE-CZ-NH2	-7.51	116.54	120.30
20	dy	270	ARG	NE-CZ-NH2	-7.51	116.55	120.30
11	Z6	143	MET	CG-SD-CE	-7.50	88.19	100.20
10	iA	91	ARG	NE-CZ-NH2	7.50	124.05	120.30
10	q6	138	LEU	CA-CB-CG	7.50	132.55	115.30
17	k4	50	ARG	NE-CZ-NH2	-7.49	116.56	120.30
11	av	50	CYS	CA-CB-SG	7.49	127.48	114.00
11	c7	37	ARG	NE-CZ-NH1	-7.49	116.56	120.30
4	y1	151	PHE	CB-CG-CD1	-7.49	115.56	120.80
11	h3	77	ARG	NE-CZ-NH1	-7.48	116.56	120.30
11	dV	84	ARG	NE-CZ-NH1	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T7	91	ARG	NE-CZ-NH1	7.48	124.04	120.30
11	L4	7	ARG	NE-CZ-NH1	7.47	124.04	120.30
11	cs	2	LEU	CB-CG-CD1	-7.47	98.29	111.00
24	gz	262	ASN	C-N-CD	-7.47	104.16	120.60
11	bD	91	ARG	NE-CZ-NH2	-7.47	116.56	120.30
11	jO	134	MET	CG-SD-CE	-7.47	88.25	100.20
5	S1	83	ARG	NE-CZ-NH2	-7.47	116.56	120.30
10	Q7	138	LEU	CA-CB-CG	7.47	132.48	115.30
10	h7	17	ARG	NE-CZ-NH1	7.47	124.03	120.30
10	G7	138	LEU	CA-CB-CG	7.47	132.48	115.30
18	bb	77	ARG	NE-CZ-NH2	7.46	124.03	120.30
10	lw	91	ARG	NE-CZ-NH1	7.45	124.03	120.30
4	w1	47	ARG	NE-CZ-NH1	7.45	124.03	120.30
5	j1	18	TYR	CG-CD1-CE1	-7.45	115.34	121.30
4	b1	151	PHE	CB-CG-CD1	-7.45	115.59	120.80
4	w1	151	PHE	CG-CD1-CE1	-7.45	112.61	120.80
10	m5	85	ASP	CB-CG-OD2	7.44	125.00	118.30
10	aE	85	ASP	CB-CG-OD2	7.44	125.00	118.30
11	H2	77	ARG	NE-CZ-NH1	-7.44	116.58	120.30
16	S8	110	ARG	NE-CZ-NH1	-7.43	116.58	120.30
11	cr	91	ARG	NE-CZ-NH2	-7.43	116.58	120.30
11	l3	129	ARG	NE-CZ-NH1	7.43	124.02	120.30
14	C2	112	ARG	NE-CZ-NH1	-7.43	116.58	120.30
11	t5	77	ARG	NE-CZ-NH1	-7.43	116.58	120.30
5	h1	107	ARG	NE-CZ-NH1	7.42	124.01	120.30
11	H5	7	ARG	NE-CZ-NH1	7.42	124.01	120.30
4	G1	91	LEU	CB-CG-CD2	-7.42	98.39	111.00
18	g4	163	TYR	CG-CD1-CE1	-7.42	115.37	121.30
11	R6	77	ARG	NE-CZ-NH1	7.41	124.01	120.30
10	iA	38	LEU	CB-CG-CD2	-7.40	98.42	111.00
14	d8	234	ARG	NE-CZ-NH2	7.40	124.00	120.30
11	H4	7	ARG	NE-CZ-NH2	-7.40	116.60	120.30
11	D5	7	ARG	NE-CZ-NH2	-7.40	116.60	120.30
11	cq	108	ARG	NE-CZ-NH1	-7.39	116.60	120.30
10	cI	33	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
17	a4	30	ARG	NE-CZ-NH2	-7.39	116.60	120.30
10	lw	17	ARG	NE-CZ-NH1	7.39	124.00	120.30
11	b7	153	ILE	CG1-CB-CG2	-7.39	95.14	111.40
14	c8	234	ARG	NE-CZ-NH1	-7.39	116.61	120.30
16	X9	110	ARG	NE-CZ-NH1	-7.39	116.61	120.30
10	K7	120	LEU	CB-CG-CD2	7.39	123.56	111.00
11	R6	88	ILE	CG1-CB-CG2	-7.38	95.16	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	R7	113	LEU	CB-CG-CD1	-7.38	98.45	111.00
11	n7	88	ILE	CG1-CB-CG2	-7.38	95.16	111.40
8	b2	579	LEU	CB-CG-CD2	7.38	123.55	111.00
18	bf	83	LEU	CB-CG-CD2	7.38	123.54	111.00
10	i7	92	LEU	CB-CG-CD2	7.38	123.54	111.00
12	b9	317	ARG	NE-CZ-NH1	7.38	123.99	120.30
9	d2	42	LEU	CB-CG-CD1	-7.37	98.47	111.00
12	34	122	ARG	NE-CZ-NH2	-7.37	116.61	120.30
11	D6	161	LEU	CB-CG-CD1	-7.37	98.47	111.00
10	gb	85	ASP	CB-CG-OD2	7.37	124.94	118.30
10	q9	13	ASP	CB-CG-OD1	7.37	124.93	118.30
11	r9	19	VAL	CG1-CB-CG2	-7.37	99.11	110.90
4	b1	131	ARG	NE-CZ-NH2	-7.37	116.62	120.30
17	i5	17	ARG	NE-CZ-NH1	7.37	123.98	120.30
11	D7	59	MET	CG-SD-CE	7.36	111.97	100.20
2	C1	64	ARG	NE-CZ-NH2	-7.35	116.62	120.30
10	dA	119	THR	CA-CB-CG2	-7.35	102.11	112.40
4	T1	84	ASP	CB-CG-OD2	7.35	124.91	118.30
4	b1	91	LEU	CB-CG-CD2	-7.35	98.51	111.00
11	h3	149	ARG	NE-CZ-NH1	7.35	123.97	120.30
11	F4	161	LEU	CB-CG-CD2	-7.35	98.50	111.00
18	c4	83	LEU	CB-CG-CD1	-7.35	98.50	111.00
11	a7	59	MET	CG-SD-CE	7.35	111.96	100.20
14	d9	234	ARG	NE-CZ-NH2	7.35	123.97	120.30
10	bx	85	ASP	CB-CG-OD2	7.35	124.91	118.30
10	lg	142	ARG	NE-CZ-NH1	7.35	123.97	120.30
18	bh	85	ASP	CB-CG-OD2	7.35	124.91	118.30
12	Z9	260	ARG	NE-CZ-NH1	-7.34	116.63	120.30
11	N6	66	LEU	CB-CG-CD2	7.34	123.48	111.00
10	i7	44	LEU	CB-CG-CD1	-7.34	98.52	111.00
10	O7	138	LEU	CA-CB-CG	7.33	132.16	115.30
11	l6	91	ARG	NE-CZ-NH2	-7.33	116.64	120.30
11	dX	101	ASP	CB-CG-OD1	7.33	124.90	118.30
10	gs	114	ARG	NE-CZ-NH2	-7.33	116.63	120.30
11	t4	77	ARG	NE-CZ-NH1	-7.33	116.64	120.30
11	R6	59	MET	CG-SD-CE	7.33	111.92	100.20
11	n9	78	ARG	NE-CZ-NH2	-7.32	116.64	120.30
11	c6	50	CYS	CA-CB-SG	7.32	127.17	114.00
11	V7	88	ILE	CG1-CB-CG2	-7.32	95.30	111.40
8	b2	707	ARG	NH1-CZ-NH2	7.31	127.44	119.40
10	s5	138	LEU	CA-CB-CG	7.31	132.12	115.30
12	b9	165	ARG	NE-CZ-NH1	-7.31	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	x1	91	TYR	CZ-CE2-CD2	-7.30	113.23	119.80
10	l8	138	LEU	CA-CB-CG	7.30	132.10	115.30
18	bj	108	ARG	NE-CZ-NH1	-7.30	116.65	120.30
10	cy	54	GLU	OE1-CD-OE2	-7.30	114.54	123.30
16	S8	162	ARG	NE-CZ-NH1	7.30	123.95	120.30
11	an	78	ARG	NE-CZ-NH2	-7.30	116.65	120.30
5	a1	76	ARG	NE-CZ-NH1	-7.30	116.65	120.30
11	n6	91	ARG	NE-CZ-NH2	-7.30	116.65	120.30
5	h1	107	ARG	NE-CZ-NH2	-7.29	116.65	120.30
11	F4	13	ASP	CB-CG-OD1	7.29	124.86	118.30
10	s8	138	LEU	CA-CB-CG	7.29	132.06	115.30
10	O6	138	LEU	CA-CB-CG	7.28	132.05	115.30
10	aq	142	ARG	NE-CZ-NH2	7.28	123.94	120.30
12	34	260	ARG	NE-CZ-NH1	-7.28	116.66	120.30
10	w7	138	LEU	CA-CB-CG	7.27	132.03	115.30
4	K1	31	LEU	CB-CG-CD2	7.27	123.36	111.00
18	f9	145	LEU	CA-CB-CG	7.27	132.01	115.30
10	Q6	138	LEU	CA-CB-CG	7.26	132.01	115.30
11	cH	84	ARG	NE-CZ-NH1	7.26	123.93	120.30
11	bn	27	LEU	CB-CG-CD2	-7.26	98.66	111.00
10	gs	142	ARG	NE-CZ-NH1	-7.26	116.67	120.30
11	ap	142	ILE	CG1-CB-CG2	-7.25	95.44	111.40
10	as	92	LEU	CB-CG-CD2	7.25	123.33	111.00
11	bq	78	ARG	NH1-CZ-NH2	7.25	127.38	119.40
5	e1	77	ARG	NE-CZ-NH1	-7.25	116.67	120.30
10	q5	44	LEU	CB-CG-CD1	-7.25	98.67	111.00
11	l6	88	ILE	CG1-CB-CG2	-7.25	95.44	111.40
10	bE	85	ASP	CB-CG-OD2	7.25	124.83	118.30
17	k5	88	ILE	CG1-CB-CG2	-7.25	95.45	111.40
4	q1	26	ILE	CG1-CB-CG2	-7.25	95.45	111.40
10	dg	140	VAL	C-N-CD	-7.25	104.65	120.60
10	z8	37	ARG	NE-CZ-NH1	7.24	123.92	120.30
21	ex	124	TYR	CB-CG-CD2	-7.24	116.65	121.00
24	gz	148	ARG	NE-CZ-NH1	7.24	123.92	120.30
8	b2	707	ARG	NE-CZ-NH2	-7.24	116.68	120.30
16	X9	162	ARG	NE-CZ-NH1	7.24	123.92	120.30
15	14	177	PHE	CB-CG-CD1	-7.23	115.74	120.80
15	W5	19	SER	N-CA-C	-7.23	91.49	111.00
11	bH	13	ASP	CB-CG-OD2	7.23	124.81	118.30
11	r5	88	ILE	CG1-CB-CG2	-7.22	95.51	111.40
11	r4	91	ARG	NE-CZ-NH1	-7.22	116.69	120.30
12	Y5	260	ARG	NE-CZ-NH1	-7.22	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a7	56	ILE	CG1-CB-CG2	-7.22	95.52	111.40
12	aY	71	ARG	NE-CZ-NH2	-7.22	116.69	120.30
12	b8	165	ARG	NE-CZ-NH1	-7.22	116.69	120.30
15	W9	73	LEU	CB-CG-CD1	-7.21	98.75	111.00
4	f1	115	MET	CG-SD-CE	7.20	111.72	100.20
10	m8	138	LEU	CA-CB-CG	7.20	131.87	115.30
5	e1	19	LEU	CB-CG-CD1	-7.20	98.76	111.00
11	kX	91	ARG	NE-CZ-NH1	7.20	123.90	120.30
4	T1	47	ARG	NE-CZ-NH1	7.20	123.90	120.30
17	b4	30	ARG	NE-CZ-NH2	-7.20	116.70	120.30
17	ak	17	ARG	NE-CZ-NH1	7.20	123.90	120.30
5	c1	83	ARG	NE-CZ-NH1	7.19	123.90	120.30
10	iA	91	ARG	NH1-CZ-NH2	-7.19	111.49	119.40
5	r1	76	ARG	NE-CZ-NH2	7.19	123.89	120.30
4	w1	155	TYR	CB-CG-CD2	-7.19	116.69	121.00
17	k4	28	THR	CA-CB-CG2	-7.19	102.34	112.40
11	R7	91	ARG	NE-CZ-NH1	7.19	123.89	120.30
11	r9	50	CYS	CA-CB-SG	7.19	126.94	114.00
17	bk	38	LEU	CB-CG-CD2	7.18	123.21	111.00
11	dX	109	CYS	CA-CB-SG	7.18	126.93	114.00
7	m1	80	LEU	CB-CG-CD1	-7.18	98.80	111.00
11	J4	7	ARG	NE-CZ-NH1	7.18	123.89	120.30
5	L1	67	ARG	NE-CZ-NH1	-7.18	116.71	120.30
14	c8	240	LEU	CB-CG-CD2	7.17	123.19	111.00
17	ae	93	ARG	NE-CZ-NH2	-7.17	116.71	120.30
10	bv	85	ASP	CB-CG-OD2	7.17	124.75	118.30
5	J1	76	ARG	NE-CZ-NH2	-7.17	116.72	120.30
11	P6	91	ARG	NE-CZ-NH1	7.17	123.89	120.30
11	f3	113	LEU	CB-CG-CD1	-7.17	98.82	111.00
19	a8	76	ASP	CB-CG-OD2	-7.17	111.85	118.30
12	a3	269	TYR	CB-CG-CD2	-7.16	116.70	121.00
10	K2	144	MET	CG-SD-CE	-7.16	88.74	100.20
11	N6	88	ILE	CG1-CB-CG2	-7.16	95.64	111.40
11	d7	129	ARG	NE-CZ-NH1	7.16	123.88	120.30
10	j6	1	MET	CB-CG-SD	7.16	133.87	112.40
11	cr	98	LEU	CB-CG-CD1	-7.16	98.84	111.00
16	X5	61	ARG	NE-CZ-NH2	7.15	123.88	120.30
8	b2	359	PHE	CB-CG-CD1	-7.15	115.80	120.80
11	lh	13	ASP	CB-CG-OD1	-7.15	111.86	118.30
11	L2	109	CYS	CA-CB-SG	7.15	126.87	114.00
5	j1	13	ASP	CB-CG-OD2	7.14	124.73	118.30
11	cn	27	LEU	CB-CG-CD2	-7.14	98.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cp	108	ARG	NE-CZ-NH2	7.14	123.87	120.30
4	G1	62	ARG	NE-CZ-NH1	-7.14	116.73	120.30
5	p1	107	ARG	NE-CZ-NH1	7.14	123.87	120.30
10	f6	138	LEU	CA-CB-CG	7.14	131.72	115.30
12	U8	260	ARG	NE-CZ-NH1	-7.14	116.73	120.30
11	D9	90	LEU	CB-CG-CD1	7.14	123.13	111.00
4	G1	94	TYR	CZ-CE2-CD2	-7.13	113.38	119.80
10	w3	95	TYR	CB-CG-CD2	-7.13	116.72	121.00
11	z5	91	ARG	NE-CZ-NH1	7.13	123.86	120.30
10	G6	144	MET	CG-SD-CE	-7.13	88.79	100.20
10	h6	138	LEU	CA-CB-CG	7.13	131.70	115.30
4	T1	77	MET	CG-SD-CE	-7.12	88.80	100.20
5	O1	19	LEU	CB-CG-CD1	-7.12	98.89	111.00
4	y1	131	ARG	NE-CZ-NH2	-7.12	116.74	120.30
4	f1	94	TYR	CZ-CE2-CD2	-7.12	113.40	119.80
4	s1	90	ARG	NH1-CZ-NH2	-7.12	111.57	119.40
10	k7	33	ARG	NE-CZ-NH1	-7.12	116.74	120.30
10	gh	139	CYS	CA-CB-SG	7.12	126.81	114.00
10	i8	138	LEU	CA-CB-CG	7.11	131.66	115.30
18	l5	78	ARG	NE-CZ-NH1	-7.11	116.75	120.30
10	by	54	GLU	OE1-CD-OE2	-7.11	114.77	123.30
11	L6	77	ARG	NE-CZ-NH2	-7.10	116.75	120.30
10	q3	2	LYS	CD-CE-NZ	7.10	128.03	111.70
10	k8	138	LEU	CA-CB-CG	7.10	131.63	115.30
4	q1	151	PHE	CG-CD1-CE1	-7.10	112.99	120.80
18	g5	163	TYR	CG-CD1-CE1	-7.10	115.62	121.30
10	A6	114	ARG	NE-CZ-NH2	-7.10	116.75	120.30
11	L6	33	ASP	CB-CG-OD2	7.10	124.69	118.30
4	I1	87	TYR	CB-CG-CD2	-7.09	116.75	121.00
10	o7	17	ARG	NE-CZ-NH1	7.09	123.85	120.30
17	k9	93	ARG	NE-CZ-NH2	-7.09	116.75	120.30
5	S1	18	TYR	CG-CD1-CE1	-7.09	115.63	121.30
11	B4	91	ARG	NE-CZ-NH1	7.09	123.84	120.30
12	ez	147	ARG	NE-CZ-NH2	7.09	123.84	120.30
10	do	142	ARG	N-CA-C	7.08	130.11	111.00
5	h1	97	LEU	CB-CG-CD2	-7.07	98.98	111.00
10	lq	91	ARG	NE-CZ-NH2	-7.06	116.77	120.30
11	az	161	LEU	CB-CG-CD2	-7.06	99.00	111.00
4	q1	155	TYR	CB-CG-CD2	-7.06	116.77	121.00
15	W5	177	PHE	CB-CG-CD1	-7.05	115.86	120.80
10	q8	17	ARG	NE-CZ-NH1	7.05	123.83	120.30
11	L7	110	LEU	CB-CG-CD2	-7.05	99.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Y8	77	ARG	CG-CD-NE	-7.05	96.99	111.80
5	p1	77	ARG	NH1-CZ-NH2	7.05	127.15	119.40
17	b4	86	ARG	NE-CZ-NH1	-7.05	116.78	120.30
19	a9	401	LEU	CA-CB-CG	7.05	131.51	115.30
11	a6	88	ILE	CG1-CB-CG2	-7.05	95.90	111.40
10	I6	13	ASP	CB-CG-OD2	7.04	124.64	118.30
11	p9	91	ARG	NE-CZ-NH2	-7.04	116.78	120.30
10	G4	135	ARG	NE-CZ-NH1	-7.04	116.78	120.30
25	kb	281	LEU	CB-CG-CD2	-7.04	99.04	111.00
11	ap	98	LEU	CB-CG-CD1	-7.04	99.04	111.00
10	k6	138	LEU	CA-CB-CG	7.03	131.48	115.30
10	C9	91	ARG	NE-CZ-NH2	7.03	123.82	120.30
6	g1	120	LEU	CB-CG-CD1	-7.03	99.05	111.00
5	p1	18	TYR	CB-CG-CD2	-7.03	116.78	121.00
12	A2	269	TYR	CB-CG-CD2	-7.03	116.78	121.00
12	ey	147	ARG	NE-CZ-NH2	7.03	123.81	120.30
4	i1	87	TYR	CB-CG-CD2	-7.03	116.78	121.00
8	b2	615	VAL	CA-CB-CG1	-7.03	100.36	110.90
10	cw	91	ARG	NE-CZ-NH2	7.02	123.81	120.30
11	N6	143	MET	CG-SD-CE	-7.02	88.96	100.20
11	t6	59	MET	CG-SD-CE	7.02	111.43	100.20
11	l3	109	CYS	CA-CB-SG	7.02	126.63	114.00
11	N7	77	ARG	NE-CZ-NH1	7.02	123.81	120.30
17	Z8	93	ARG	NE-CZ-NH2	-7.02	116.79	120.30
10	as	17	ARG	NE-CZ-NH2	-7.01	116.79	120.30
11	lv	13	ASP	CB-CG-OD1	-7.01	111.99	118.30
4	w1	155	TYR	CZ-CE2-CD2	-7.01	113.49	119.80
11	B5	13	ASP	CB-CG-OD1	7.01	124.61	118.30
11	J5	142	ILE	CG1-CB-CG2	-7.00	96.00	111.40
11	ln	77	ARG	NE-CZ-NH2	7.00	123.80	120.30
11	y8	90	LEU	CB-CG-CD1	7.00	122.90	111.00
15	bW	113	ARG	NE-CZ-NH1	7.00	123.80	120.30
11	p6	66	LEU	CB-CG-CD2	-6.99	99.11	111.00
14	d9	279	ARG	NE-CZ-NH1	6.99	123.80	120.30
18	cj	39	ASP	CB-CG-OD2	-6.99	112.01	118.30
14	d8	279	ARG	NE-CZ-NH1	6.99	123.80	120.30
11	H2	149	ARG	NE-CZ-NH1	6.99	123.80	120.30
10	C7	66	LEU	CB-CG-CD2	-6.99	99.11	111.00
5	v1	107	ARG	NE-CZ-NH1	6.99	123.79	120.30
5	v1	18	TYR	CB-CG-CD2	-6.99	116.81	121.00
11	Z6	91	ARG	NE-CZ-NH2	-6.98	116.81	120.30
17	ak	93	ARG	NE-CZ-NH2	-6.98	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	s1	82	LEU	CB-CG-CD2	6.98	122.87	111.00
5	r1	91	TYR	CZ-CE2-CD2	-6.98	113.52	119.80
11	c7	143	MET	CG-SD-CE	-6.98	89.03	100.20
11	a6	91	ARG	NE-CZ-NH2	-6.98	116.81	120.30
17	ca	28	THR	CA-CB-CG2	-6.98	102.63	112.40
10	s4	138	LEU	CA-CB-CG	6.98	131.35	115.30
10	i3	91	ARG	NE-CZ-NH2	6.97	123.79	120.30
10	I5	118	ARG	NE-CZ-NH1	6.97	123.79	120.30
17	ci	30	ARG	NE-CZ-NH2	-6.97	116.81	120.30
5	H1	108	VAL	CG1-CB-CG2	-6.97	99.75	110.90
8	a2	397	ARG	NE-CZ-NH2	-6.97	116.82	120.30
11	dX	153	ILE	CG1-CB-CG2	-6.97	96.07	111.40
3	F1	179	PHE	CB-CG-CD1	-6.97	115.92	120.80
12	a3	71	ARG	NE-CZ-NH2	-6.96	116.82	120.30
10	eG	163	LEU	CB-CG-CD1	6.96	122.83	111.00
18	j5	84	ARG	NE-CZ-NH2	6.96	123.78	120.30
11	p9	176	VAL	CG1-CB-CG2	-6.96	99.77	110.90
10	go	137	ARG	NE-CZ-NH2	-6.96	116.82	120.30
5	a1	77	ARG	NE-CZ-NH2	-6.96	116.82	120.30
4	T1	9	VAL	CA-CB-CG1	-6.95	100.47	110.90
10	s9	38	LEU	CB-CG-CD2	6.95	122.82	111.00
10	u6	44	LEU	CB-CG-CD1	-6.95	99.19	111.00
11	dX	52	VAL	CG1-CB-CG2	-6.95	99.78	110.90
11	ei	38	LEU	CB-CG-CD1	-6.95	99.19	111.00
10	q4	44	LEU	CB-CG-CD1	-6.94	99.20	111.00
11	Z7	88	ILE	CG1-CB-CG2	-6.94	96.13	111.40
10	dO	9	ILE	CG1-CB-CG2	-6.94	96.13	111.40
9	d2	56	LEU	CA-CB-CG	6.94	131.26	115.30
10	gc	37	ARG	NE-CZ-NH1	-6.94	116.83	120.30
12	b8	116	MET	CG-SD-CE	-6.94	89.10	100.20
11	z9	161	LEU	CB-CG-CD2	-6.94	99.21	111.00
3	F1	200	LEU	CB-CG-CD1	6.93	122.79	111.00
11	dK	78	ARG	NE-CZ-NH2	-6.93	116.83	120.30
5	r1	77	ARG	NE-CZ-NH1	-6.93	116.83	120.30
5	x1	77	ARG	NE-CZ-NH1	-6.93	116.83	120.30
11	x4	91	ARG	NE-CZ-NH1	-6.93	116.83	120.30
11	B6	59	MET	CG-SD-CE	6.93	111.29	100.20
11	P7	88	ILE	CG1-CB-CG2	-6.93	96.15	111.40
10	t8	138	LEU	CA-CB-CG	6.93	131.24	115.30
4	P1	115	MET	CG-SD-CE	6.93	111.28	100.20
10	m4	137	ARG	NE-CZ-NH1	-6.93	116.84	120.30
22	eY	264	GLY	C-N-CD	-6.93	105.36	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	V2	90	LEU	CB-CG-CD1	6.92	122.77	111.00
11	iE	91	ARG	NE-CZ-NH2	-6.92	116.84	120.30
17	k4	88	ILE	CG1-CB-CG2	-6.92	96.17	111.40
18	cb	39	ASP	CB-CG-OD2	-6.92	112.07	118.30
11	T6	13	ASP	CB-CG-OD2	6.92	124.53	118.30
11	p7	91	ARG	NE-CZ-NH2	-6.92	116.84	120.30
11	co	7	ARG	NE-CZ-NH1	6.92	123.76	120.30
11	cs	149	ARG	NE-CZ-NH1	6.92	123.76	120.30
10	I3	24	LEU	CB-CG-CD2	-6.92	99.24	111.00
17	V8	93	ARG	NE-CZ-NH2	-6.92	116.84	120.30
10	dQ	85	ASP	CB-CG-OD2	6.92	124.52	118.30
11	E8	109	CYS	CA-CB-SG	6.91	126.44	114.00
11	p9	61	CYS	CA-CB-SG	6.91	126.44	114.00
11	bL	91	ARG	NE-CZ-NH1	6.91	123.76	120.30
11	r7	59	MET	CG-SD-CE	6.91	111.25	100.20
10	iB	38	LEU	CB-CG-CD1	-6.91	99.25	111.00
16	24	117	LYS	CD-CE-NZ	-6.91	95.81	111.70
10	bC	92	LEU	CB-CG-CD2	6.91	122.74	111.00
10	q4	85	ASP	CB-CG-OD2	6.90	124.51	118.30
10	M7	157	ASP	CB-CG-OD2	6.90	124.51	118.30
10	eW	18	PHE	CB-CG-CD1	-6.90	115.97	120.80
11	az	91	ARG	NE-CZ-NH2	-6.90	116.85	120.30
10	K7	114	ARG	NE-CZ-NH2	-6.90	116.85	120.30
16	X9	158	LEU	CB-CG-CD2	6.90	122.72	111.00
11	bq	161	LEU	CB-CG-CD2	-6.90	99.27	111.00
5	O1	77	ARG	NE-CZ-NH2	-6.90	116.85	120.30
11	ld	78	ARG	NE-CZ-NH1	-6.89	116.85	120.30
19	a9	105	TYR	CG-CD1-CE1	6.89	126.81	121.30
11	J5	7	ARG	NE-CZ-NH2	-6.89	116.86	120.30
11	ga	108	ARG	NE-CZ-NH2	-6.89	116.86	120.30
12	U8	173	ARG	NE-CZ-NH2	-6.89	116.86	120.30
10	s9	92	LEU	CB-CG-CD2	6.89	122.71	111.00
10	j7	66	LEU	CB-CG-CD2	-6.89	99.29	111.00
4	G1	151	PHE	CG-CD1-CE1	-6.88	113.23	120.80
8	a2	335	PHE	CB-CG-CD1	-6.88	115.98	120.80
10	la	85	ASP	CB-CG-OD2	6.88	124.50	118.30
10	u7	138	LEU	CA-CB-CG	6.88	131.13	115.30
11	h3	91	ARG	NE-CZ-NH1	6.88	123.74	120.30
17	b5	30	ARG	NE-CZ-NH2	-6.88	116.86	120.30
17	f5	19	LEU	CB-CG-CD1	-6.88	99.30	111.00
18	j5	85	ASP	CB-CG-OD2	6.88	124.49	118.30
11	bH	91	ARG	NE-CZ-NH2	-6.88	116.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M1	97	LEU	CB-CG-CD2	-6.88	99.31	111.00
7	V1	90	ARG	NE-CZ-NH2	6.88	123.74	120.30
16	X5	205	SER	N-CA-C	-6.88	92.43	111.00
10	s7	44	LEU	CB-CG-CD1	-6.88	99.31	111.00
5	h1	94	TYR	CZ-CE2-CD2	-6.87	113.61	119.80
11	er	38	LEU	CB-CG-CD1	-6.87	99.32	111.00
2	C1	185	ARG	NE-CZ-NH1	6.87	123.73	120.30
10	cu	91	ARG	NE-CZ-NH2	6.87	123.73	120.30
10	W7	78	LYS	CD-CE-NZ	-6.87	95.91	111.70
10	m7	138	LEU	CA-CB-CG	6.87	131.09	115.30
10	O6	91	ARG	NE-CZ-NH1	-6.87	116.87	120.30
10	eC	84	ARG	NE-CZ-NH2	-6.87	116.87	120.30
10	I2	91	ARG	NE-CZ-NH2	6.86	123.73	120.30
10	o3	18	PHE	CB-CG-CD2	6.86	125.60	120.80
10	S7	138	LEU	CA-CB-CG	6.86	131.07	115.30
8	a2	390	GLU	OE1-CD-OE2	6.85	131.52	123.30
11	H3	79	MET	CG-SD-CE	-6.85	89.24	100.20
18	al	57	ARG	NE-CZ-NH2	-6.85	116.87	120.30
11	n4	2	LEU	CB-CG-CD1	-6.85	99.36	111.00
16	X5	93	TYR	CB-CG-CD2	6.85	125.11	121.00
4	G1	131	ARG	NE-CZ-NH2	-6.85	116.88	120.30
5	n1	83	ARG	NE-CZ-NH2	6.85	123.72	120.30
10	eM	137	ARG	NE-CZ-NH1	-6.84	116.88	120.30
10	dA	137	ARG	NE-CZ-NH1	-6.84	116.88	120.30
11	eX	120	LEU	CB-CG-CD2	-6.84	99.38	111.00
12	a3	225	MET	CG-SD-CE	-6.84	89.26	100.20
10	aq	13	ASP	CB-CG-OD1	6.84	124.45	118.30
11	aL	91	ARG	NE-CZ-NH1	6.84	123.72	120.30
5	r1	62	TYR	CB-CG-CD1	-6.83	116.90	121.00
11	L6	30	PHE	CB-CG-CD2	-6.83	116.02	120.80
10	m7	44	LEU	CB-CG-CD1	-6.83	99.38	111.00
10	cv	85	ASP	CB-CG-OD2	6.83	124.45	118.30
10	eG	18	PHE	CB-CG-CD1	-6.83	116.02	120.80
10	la	137	ARG	NE-CZ-NH1	-6.83	116.89	120.30
4	G1	151	PHE	CB-CG-CD1	-6.83	116.02	120.80
10	eo	85	ASP	CB-CG-OD2	6.83	124.44	118.30
19	a9	303	TYR	CZ-CE2-CD2	-6.83	113.66	119.80
11	r9	98	LEU	CB-CG-CD1	-6.83	99.40	111.00
11	t4	38	LEU	CB-CG-CD1	-6.82	99.40	111.00
11	ar	50	CYS	CA-CB-SG	6.82	126.28	114.00
11	bq	108	ARG	NE-CZ-NH1	-6.82	116.89	120.30
11	eJ	84	ARG	NE-CZ-NH2	-6.82	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	c7	91	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	E1	171	ARG	NH1-CZ-NH2	6.82	126.90	119.40
10	lm	17	ARG	NE-CZ-NH1	6.82	123.71	120.30
11	n4	91	ARG	NE-CZ-NH1	6.82	123.71	120.30
10	C6	138	LEU	CA-CB-CG	6.82	130.98	115.30
12	bY	105	LEU	CB-CG-CD2	-6.82	99.41	111.00
10	E9	18	PHE	CB-CG-CD2	6.81	125.57	120.80
5	z1	90	ARG	NE-CZ-NH2	6.81	123.70	120.30
11	P6	161	LEU	CB-CG-CD1	-6.81	99.43	111.00
10	cu	74	ASP	CB-CG-OD1	6.81	124.43	118.30
18	cb	83	LEU	CB-CG-CD2	-6.80	99.44	111.00
10	O7	17	ARG	NE-CZ-NH1	6.80	123.70	120.30
10	dA	91	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
8	a2	605	ARG	NE-CZ-NH2	-6.80	116.90	120.30
5	l1	112	LEU	CB-CG-CD1	-6.79	99.45	111.00
18	ch	85	ASP	CB-CG-OD2	6.79	124.42	118.30
10	A4	2	LYS	CD-CE-NZ	6.79	127.33	111.70
11	F9	50	CYS	CA-CB-SG	6.79	126.23	114.00
10	aI	140	VAL	C-N-CD	-6.79	105.66	120.60
11	N2	84	ARG	NE-CZ-NH1	6.79	123.70	120.30
5	M1	107	ARG	NE-CZ-NH2	-6.79	116.91	120.30
10	k7	66	LEU	CB-CG-CD2	-6.79	99.46	111.00
10	gj	142	ARG	NE-CZ-NH2	6.79	123.69	120.30
5	W1	115	THR	CA-CB-CG2	-6.79	102.90	112.40
4	P1	94	TYR	CZ-CE2-CD2	-6.78	113.69	119.80
13	B2	153	LEU	CA-CB-CG	-6.78	99.70	115.30
14	c3	218	ARG	NE-CZ-NH1	6.78	123.69	120.30
11	kW	91	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	C1	64	ARG	NH1-CZ-NH2	6.78	126.86	119.40
16	X5	117	LYS	CD-CE-NZ	-6.78	96.10	111.70
10	as	38	LEU	CB-CG-CD2	6.78	122.53	111.00
10	iB	91	ARG	NE-CZ-NH2	6.78	123.69	120.30
12	A2	71	ARG	NE-CZ-NH2	-6.78	116.91	120.30
8	a2	707	ARG	NH1-CZ-NH2	6.78	126.86	119.40
11	eR	77	ARG	NE-CZ-NH2	-6.78	116.91	120.30
11	c6	56	ILE	CG1-CB-CG2	-6.78	96.50	111.40
14	T8	234	ARG	NE-CZ-NH2	-6.78	116.91	120.30
11	at	105	LEU	CB-CG-CD2	-6.78	99.48	111.00
11	H4	98	LEU	CB-CG-CD1	-6.77	99.48	111.00
10	M7	38	LEU	CB-CG-CD2	6.77	122.51	111.00
10	aU	140	VAL	C-N-CD	-6.77	105.70	120.60
10	g7	91	ARG	NE-CZ-NH2	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	t5	38	LEU	CB-CG-CD1	-6.77	99.49	111.00
4	y1	153	PHE	CB-CG-CD1	-6.77	116.06	120.80
10	s5	92	LEU	CB-CG-CD1	-6.77	99.50	111.00
10	aG	13	ASP	CB-CG-OD2	-6.77	112.21	118.30
11	R7	161	LEU	CB-CG-CD1	-6.76	99.50	111.00
10	ef	85	ASP	CB-CG-OD2	6.76	124.39	118.30
11	iE	78	ARG	NE-CZ-NH2	-6.76	116.92	120.30
6	g1	91	ARG	NE-CZ-NH2	6.76	123.68	120.30
18	j4	85	ASP	CB-CG-OD2	6.76	124.38	118.30
11	p7	84	ARG	NE-CZ-NH2	-6.76	116.92	120.30
11	cs	84	ARG	NE-CZ-NH2	6.75	123.68	120.30
10	o6	91	ARG	NE-CZ-NH1	-6.75	116.92	120.30
18	l9	57	ARG	NE-CZ-NH2	-6.75	116.92	120.30
5	v1	91	TYR	CZ-CE2-CD2	-6.75	113.72	119.80
13	b3	153	LEU	CA-CB-CG	-6.75	99.78	115.30
11	eD	77	ARG	NE-CZ-NH2	-6.75	116.93	120.30
5	a1	60	LEU	CB-CG-CD2	6.75	122.47	111.00
10	s9	17	ARG	NE-CZ-NH2	-6.75	116.93	120.30
18	bb	84	ARG	CD-NE-CZ	6.74	133.04	123.60
10	bv	91	ARG	NE-CZ-NH2	6.74	123.67	120.30
20	dz	124	ARG	CG-CD-NE	-6.74	97.64	111.80
11	n9	120	LEU	CB-CG-CD2	-6.74	99.54	111.00
11	jO	108	ARG	CD-NE-CZ	6.74	133.03	123.60
10	K6	138	LEU	CA-CB-CG	6.74	130.79	115.30
11	L6	105	LEU	CB-CG-CD2	-6.74	99.55	111.00
10	f6	91	ARG	NE-CZ-NH2	6.74	123.67	120.30
8	a2	837	LEU	CB-CG-CD1	-6.73	99.56	111.00
10	aS	140	VAL	C-N-CD	-6.73	105.79	120.60
11	lf	77	ARG	NE-CZ-NH2	6.73	123.67	120.30
11	z9	91	ARG	NE-CZ-NH2	-6.73	116.94	120.30
10	ct	137	ARG	NE-CZ-NH2	-6.73	116.94	120.30
12	bY	46	PHE	CB-CG-CD1	6.72	125.51	120.80
10	li	163	LEU	CB-CG-CD2	-6.72	99.57	111.00
11	L4	7	ARG	NE-CZ-NH2	-6.72	116.94	120.30
10	G7	13	ASP	CB-CG-OD2	6.72	124.35	118.30
20	dy	124	ARG	CG-CD-NE	-6.72	97.69	111.80
17	k9	17	ARG	NE-CZ-NH1	6.72	123.66	120.30
10	k7	44	LEU	CB-CG-CD1	-6.72	99.58	111.00
10	q4	135	ARG	NE-CZ-NH1	-6.71	116.94	120.30
10	A9	17	ARG	NE-CZ-NH2	-6.71	116.94	120.30
10	m5	135	ARG	NE-CZ-NH2	6.71	123.65	120.30
10	aI	38	LEU	CB-CG-CD2	6.71	122.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	la	142	ARG	CG-CD-NE	6.71	125.89	111.80
11	an	120	LEU	CB-CG-CD2	-6.70	99.61	111.00
5	L1	85	LEU	CB-CG-CD1	-6.70	99.61	111.00
11	J4	77	ARG	NE-CZ-NH2	6.70	123.65	120.30
15	R8	96	LEU	CB-CG-CD2	6.70	122.39	111.00
12	U8	66	LEU	CB-CG-CD1	-6.70	99.61	111.00
10	w5	137	ARG	NE-CZ-NH1	-6.70	116.95	120.30
11	N4	142	ILE	CG1-CB-CG2	-6.70	96.67	111.40
11	H9	27	LEU	CB-CG-CD2	-6.70	99.62	111.00
4	P1	140	LEU	CB-CG-CD2	-6.69	99.62	111.00
11	L2	44	ILE	CG1-CB-CG2	-6.69	96.68	111.40
10	bE	163	LEU	CB-CG-CD2	-6.69	99.62	111.00
4	G1	83	ARG	NE-CZ-NH2	-6.69	116.95	120.30
10	h7	44	LEU	CB-CG-CD1	-6.69	99.63	111.00
11	el	161	LEU	CB-CG-CD2	-6.69	99.63	111.00
11	J9	78	ARG	NE-CZ-NH1	-6.69	116.96	120.30
11	X6	88	ILE	CG1-CB-CG2	-6.69	96.69	111.40
10	dW	67	LYS	CA-CB-CG	6.69	128.11	113.40
12	Y5	121	LYS	CD-CE-NZ	6.68	127.07	111.70
11	b7	50	CYS	CA-CB-SG	6.68	126.03	114.00
5	S1	108	VAL	CG1-CB-CG2	-6.68	100.21	110.90
8	b2	776	LEU	CB-CG-CD2	-6.68	99.64	111.00
15	W9	96	LEU	CB-CG-CD2	6.68	122.36	111.00
18	ad	77	ARG	CG-CD-NE	-6.68	97.77	111.80
18	al	85	ASP	CB-CG-OD2	6.68	124.31	118.30
3	F1	83	ASP	CB-CG-OD1	6.68	124.31	118.30
12	Y5	195	MET	CB-CG-SD	-6.68	92.37	112.40
10	eA	33	ARG	NE-CZ-NH2	6.68	123.64	120.30
11	at	50	CYS	CA-CB-SG	6.67	126.02	114.00
10	lq	37	ARG	NE-CZ-NH1	6.67	123.64	120.30
11	jP	134	MET	CG-SD-CE	-6.67	89.52	100.20
10	bI	38	LEU	CB-CG-CD2	6.67	122.34	111.00
4	i1	131	ARG	NE-CZ-NH2	-6.67	116.97	120.30
8	a2	776	LEU	CB-CG-CD2	-6.67	99.66	111.00
11	B5	7	ARG	NE-CZ-NH1	6.67	123.63	120.30
11	H5	7	ARG	NE-CZ-NH2	-6.67	116.97	120.30
11	F4	91	ARG	NE-CZ-NH2	-6.67	116.97	120.30
14	Y9	234	ARG	NE-CZ-NH2	-6.67	116.97	120.30
8	a2	707	ARG	NE-CZ-NH1	-6.67	116.97	120.30
10	W2	95	TYR	CB-CG-CD2	-6.67	117.00	121.00
12	Y5	147	ARG	CG-CD-NE	-6.67	97.80	111.80
4	b1	94	TYR	CZ-CE2-CD2	-6.66	113.80	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J9	109	CYS	CA-CB-SG	6.66	125.99	114.00
4	G1	109	LEU	CB-CG-CD2	-6.66	99.68	111.00
5	e1	77	ARG	NH1-CZ-NH2	6.65	126.72	119.40
10	aC	92	LEU	CB-CG-CD2	6.65	122.31	111.00
11	ln	77	ARG	CG-CD-NE	6.65	125.76	111.80
11	dL	109	CYS	CA-CB-SG	6.65	125.96	114.00
10	v8	17	ARG	NE-CZ-NH2	-6.64	116.98	120.30
11	h2	79	MET	CG-SD-CE	-6.64	89.57	100.20
10	M7	44	LEU	CB-CG-CD1	-6.64	99.71	111.00
17	ci	93	ARG	NE-CZ-NH2	-6.64	116.98	120.30
10	lm	17	ARG	NE-CZ-NH2	-6.64	116.98	120.30
4	k1	47	ARG	NE-CZ-NH1	6.64	123.62	120.30
12	34	195	MET	CB-CG-SD	-6.64	92.49	112.40
10	I6	66	LEU	CB-CG-CD2	-6.64	99.72	111.00
18	cj	108	ARG	NE-CZ-NH1	-6.64	116.98	120.30
11	cR	84	ARG	NE-CZ-NH1	6.64	123.62	120.30
18	g4	120	LEU	CB-CG-CD2	-6.63	99.72	111.00
10	aM	140	VAL	C-N-CD	-6.63	106.01	120.60
25	kb	258	ARG	NE-CZ-NH2	-6.63	116.98	120.30
11	N4	7	ARG	NE-CZ-NH1	6.63	123.61	120.30
11	N4	84	ARG	CB-CG-CD	-6.63	94.37	111.60
11	eb	101	ASP	CB-CG-OD1	6.63	124.27	118.30
11	eT	84	ARG	NE-CZ-NH2	-6.63	116.99	120.30
11	d7	59	MET	CG-SD-CE	6.63	110.80	100.20
10	m7	53	LYS	CD-CE-NZ	6.63	126.94	111.70
10	q7	138	LEU	CA-CB-CG	6.63	130.54	115.30
14	c3	112	ARG	NE-CZ-NH1	-6.62	116.99	120.30
11	n3	84	ARG	NE-CZ-NH1	6.62	123.61	120.30
10	q9	142	ARG	NE-CZ-NH1	-6.62	116.99	120.30
4	k1	9	VAL	CA-CB-CG1	-6.62	100.97	110.90
16	S8	158	LEU	CB-CG-CD2	6.62	122.26	111.00
5	M1	107	ARG	NE-CZ-NH1	6.62	123.61	120.30
4	u1	90	ARG	NE-CZ-NH1	6.62	123.61	120.30
10	s6	44	LEU	CB-CG-CD1	-6.62	99.75	111.00
11	cs	38	LEU	CB-CG-CD1	-6.62	99.75	111.00
12	34	270	ARG	NE-CZ-NH2	-6.62	116.99	120.30
21	ew	49	ARG	NE-CZ-NH1	-6.62	116.99	120.30
5	j1	78	TYR	CZ-CE2-CD2	-6.62	113.84	119.80
10	dA	85	ASP	OD1-CG-OD2	-6.62	110.73	123.30
10	C6	114	ARG	NE-CZ-NH2	-6.61	116.99	120.30
12	b9	195	MET	CG-SD-CE	-6.61	89.62	100.20
17	X8	2	LYS	CD-CE-NZ	6.61	126.91	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	34	147	ARG	CG-CD-NE	-6.61	97.92	111.80
11	B6	108	ARG	NE-CZ-NH1	6.61	123.61	120.30
4	N1	45	GLU	OE1-CD-OE2	6.61	131.23	123.30
9	c2	13	LEU	CB-CG-CD1	-6.61	99.77	111.00
11	t5	61	CYS	CA-CB-SG	6.61	125.89	114.00
11	t6	113	LEU	CB-CG-CD1	-6.61	99.77	111.00
10	s6	138	LEU	CA-CB-CG	6.61	130.49	115.30
10	cy	62	LYS	CD-CE-NZ	6.61	126.89	111.70
13	b3	249	ARG	NE-CZ-NH2	-6.60	117.00	120.30
10	cv	91	ARG	NE-CZ-NH2	6.60	123.60	120.30
11	kQ	108	ARG	NE-CZ-NH1	6.60	123.60	120.30
18	cb	84	ARG	CD-NE-CZ	6.60	132.84	123.60
17	cc	30	ARG	NE-CZ-NH1	6.60	123.60	120.30
12	Y5	270	ARG	NE-CZ-NH2	-6.60	117.00	120.30
18	c5	38	LEU	CB-CG-CD2	-6.60	99.78	111.00
11	R7	59	MET	CG-SD-CE	6.59	110.75	100.20
11	ll	77	ARG	NE-CZ-NH2	6.59	123.60	120.30
4	P1	92	VAL	CG1-CB-CG2	-6.59	100.35	110.90
15	aW	222	LEU	CA-CB-CG	6.59	130.46	115.30
11	bB	109	CYS	CA-CB-SG	6.59	125.86	114.00
10	bm	81	LYS	CD-CE-NZ	-6.59	96.54	111.70
8	b2	146	ARG	NE-CZ-NH2	-6.59	117.01	120.30
10	k7	4	VAL	CG1-CB-CG2	6.59	121.44	110.90
11	P6	153	ILE	CG1-CB-CG2	-6.59	96.91	111.40
11	c7	153	ILE	CG1-CB-CG2	-6.59	96.91	111.40
11	D7	108	ARG	NE-CZ-NH1	6.58	123.59	120.30
15	bW	198	LEU	CA-CB-CG	6.58	130.43	115.30
11	F5	77	ARG	NE-CZ-NH2	6.58	123.59	120.30
10	o9	142	ARG	NE-CZ-NH2	6.58	123.59	120.30
10	A6	142	ARG	NE-CZ-NH1	6.58	123.59	120.30
16	aX	41	LEU	CB-CG-CD2	-6.58	99.82	111.00
10	li	91	ARG	NE-CZ-NH2	-6.57	117.01	120.30
5	z1	28	ARG	NE-CZ-NH2	-6.57	117.01	120.30
10	C7	159	VAL	CG1-CB-CG2	-6.57	100.38	110.90
17	ac	33	ARG	NE-CZ-NH1	-6.57	117.01	120.30
6	Q1	120	LEU	CB-CG-CD1	-6.57	99.83	111.00
11	B7	91	ARG	NE-CZ-NH1	6.57	123.58	120.30
10	u9	144	MET	CG-SD-CE	-6.57	89.69	100.20
4	Z1	31	LEU	CB-CG-CD2	6.57	122.17	111.00
5	M1	94	TYR	CZ-CE2-CD2	-6.57	113.89	119.80
10	G7	66	LEU	CB-CG-CD2	-6.57	99.84	111.00
11	p9	142	ILE	CG1-CB-CG2	-6.56	96.96	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	gb	18	PHE	CB-CG-CD1	-6.56	116.21	120.80
10	m5	137	ARG	NE-CZ-NH1	-6.56	117.02	120.30
10	I6	114	ARG	NE-CZ-NH2	-6.56	117.02	120.30
18	j9	145	LEU	CB-CG-CD2	-6.56	99.85	111.00
11	bp	108	ARG	NE-CZ-NH2	6.56	123.58	120.30
15	aW	198	LEU	CA-CB-CG	6.55	130.37	115.30
14	c3	138	ARG	NE-CZ-NH2	-6.55	117.03	120.30
11	l3	91	ARG	NE-CZ-NH2	-6.55	117.03	120.30
11	D5	98	LEU	CB-CG-CD1	-6.55	99.87	111.00
18	g5	120	LEU	CB-CG-CD2	-6.55	99.87	111.00
10	o6	138	LEU	CA-CB-CG	6.55	130.35	115.30
11	t9	108	ARG	NE-CZ-NH2	6.55	123.57	120.30
17	f4	99	LEU	CB-CG-CD2	-6.54	99.87	111.00
17	aa	93	ARG	NE-CZ-NH2	-6.54	117.03	120.30
4	R1	131	ARG	NE-CZ-NH2	-6.54	117.03	120.30
10	q8	138	LEU	CA-CB-CG	6.54	130.33	115.30
12	bY	156	ARG	NH1-CZ-NH2	6.54	126.59	119.40
10	k7	138	LEU	CA-CB-CG	6.53	130.33	115.30
10	hC	38	LEU	CB-CG-CD2	6.53	122.11	111.00
4	w1	26	ILE	CG1-CB-CG2	-6.53	97.03	111.40
10	i2	24	LEU	CB-CG-CD2	-6.53	99.90	111.00
11	cq	78	ARG	NH1-CZ-NH2	6.53	126.58	119.40
11	H4	101	ASP	CB-CG-OD1	6.53	124.17	118.30
10	w4	137	ARG	NE-CZ-NH1	-6.53	117.04	120.30
10	E9	37	ARG	NE-CZ-NH2	-6.53	117.04	120.30
10	C3	142	ARG	NE-CZ-NH2	6.53	123.56	120.30
10	dU	85	ASP	CB-CG-OD2	6.53	124.17	118.30
10	U6	138	LEU	CA-CB-CG	6.52	130.30	115.30
12	b8	195	MET	CG-SD-CE	-6.52	89.76	100.20
10	o6	18	PHE	CB-CG-CD1	-6.52	116.23	120.80
5	p1	91	TYR	CZ-CE2-CD2	-6.52	113.93	119.80
11	bo	77	ARG	NE-CZ-NH2	-6.52	117.04	120.30
6	Q1	83	LEU	CB-CG-CD2	6.52	122.08	111.00
10	aE	163	LEU	CB-CG-CD2	-6.52	99.92	111.00
15	W9	47	ILE	CA-CB-CG2	-6.52	97.87	110.90
1	A1	106	PHE	CB-CG-CD1	-6.51	116.24	120.80
4	k1	91	LEU	CB-CG-CD2	-6.51	99.92	111.00
4	y1	94	TYR	CG-CD1-CE1	-6.51	116.09	121.30
8	a2	146	ARG	NE-CZ-NH2	-6.51	117.04	120.30
11	c6	120	LEU	CB-CG-CD1	-6.51	99.92	111.00
2	C1	90	GLY	N-CA-C	6.51	129.37	113.10
6	Q1	91	ARG	NE-CZ-NH2	6.51	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	U1	76	ARG	NE-CZ-NH1	-6.51	117.05	120.30
10	q4	138	LEU	CB-CG-CD2	-6.51	99.94	111.00
4	y1	110	VAL	CG1-CB-CG2	-6.50	100.49	110.90
10	A7	23	ASP	CB-CG-OD2	-6.50	112.45	118.30
11	J5	84	ARG	CB-CG-CD	-6.50	94.70	111.60
10	k6	53	LYS	CD-CE-NZ	6.50	126.65	111.70
10	dO	85	ASP	OD1-CG-OD2	-6.50	110.95	123.30
11	kS	91	ARG	NE-CZ-NH1	6.50	123.55	120.30
11	R6	153	ILE	CG1-CB-CG2	-6.50	97.10	111.40
17	ca	33	ARG	NE-CZ-NH1	6.50	123.55	120.30
10	I5	85	ASP	CB-CG-OD2	6.50	124.15	118.30
10	j6	138	LEU	CA-CB-CG	6.50	130.24	115.30
16	X5	93	TYR	CB-CG-CD1	-6.49	117.10	121.00
18	e5	30	MET	CA-CB-CG	6.49	124.34	113.30
10	E9	91	ARG	NE-CZ-NH1	-6.49	117.05	120.30
10	C4	142	ARG	NE-CZ-NH2	6.49	123.55	120.30
5	H1	18	TYR	CB-CG-CD2	-6.49	117.11	121.00
4	N1	131	ARG	NE-CZ-NH1	6.49	123.55	120.30
5	v1	18	TYR	CG-CD1-CE1	-6.49	116.11	121.30
5	a1	76	ARG	NE-CZ-NH2	6.49	123.55	120.30
8	a2	180	LEU	CB-CG-CD2	-6.49	99.97	111.00
4	f1	140	LEU	CB-CG-CD2	-6.49	99.97	111.00
5	J1	65	ILE	CG1-CB-CG2	-6.49	97.13	111.40
10	i3	87	ASP	CB-CG-OD2	6.48	124.13	118.30
11	eb	84	ARG	NE-CZ-NH1	6.48	123.54	120.30
23	lz	293	MET	CA-CB-CG	6.48	124.32	113.30
12	a3	191	LYS	CD-CE-NZ	6.48	126.60	111.70
10	E6	38	LEU	CB-CG-CD2	6.48	122.02	111.00
17	ak	158	ILE	CG1-CB-CG2	-6.48	97.15	111.40
1	B1	97	ASP	CB-CG-OD2	-6.47	112.47	118.30
10	A3	2	LYS	CD-CE-NZ	6.47	126.58	111.70
16	X9	133	PHE	CB-CG-CD1	-6.47	116.27	120.80
10	E3	18	PHE	CB-CG-CD1	-6.47	116.27	120.80
11	c6	143	MET	CG-SD-CE	-6.47	89.85	100.20
11	z4	98	LEU	CB-CG-CD1	-6.46	100.01	111.00
11	r7	143	MET	CG-SD-CE	-6.46	89.86	100.20
10	au	144	MET	CG-SD-CE	-6.46	89.86	100.20
11	aB	98	LEU	CB-CG-CD1	-6.46	100.02	111.00
4	b1	157	LEU	CB-CG-CD2	-6.46	100.02	111.00
10	E6	23	ASP	CB-CG-OD2	-6.46	112.49	118.30
11	dX	7	ARG	NE-CZ-NH1	-6.46	117.07	120.30
10	u7	114	ARG	NE-CZ-NH1	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	s1	87	TYR	CB-CG-CD2	-6.45	117.13	121.00
11	bs	84	ARG	NE-CZ-NH1	-6.45	117.08	120.30
10	bu	84	ARG	NE-CZ-NH2	6.45	123.53	120.30
11	lx	108	ARG	NE-CZ-NH1	-6.45	117.07	120.30
18	l9	85	ASP	CB-CG-OD2	6.45	124.10	118.30
4	d1	45	GLU	OE1-CD-OE2	6.45	131.03	123.30
12	a3	44	ASP	CB-CG-OD1	6.45	124.10	118.30
10	w9	142	ARG	NE-CZ-NH2	6.45	123.52	120.30
17	bc	93	ARG	NE-CZ-NH2	-6.45	117.08	120.30
10	q5	138	LEU	CB-CG-CD2	-6.44	100.05	111.00
11	D7	91	ARG	NE-CZ-NH1	6.44	123.52	120.30
10	G3	142	ARG	NE-CZ-NH2	6.44	123.52	120.30
17	k9	158	ILE	CG1-CB-CG2	-6.44	97.23	111.40
4	X1	87	TYR	CB-CG-CD2	-6.44	117.14	121.00
17	ba	19	LEU	CB-CG-CD2	-6.44	100.06	111.00
10	lq	37	ARG	NE-CZ-NH2	-6.44	117.08	120.30
11	v4	77	ARG	NE-CZ-NH2	6.43	123.52	120.30
11	Z6	84	ARG	NE-CZ-NH2	-6.43	117.08	120.30
10	gs	37	ARG	NE-CZ-NH1	-6.43	117.08	120.30
8	b2	452	LEU	CB-CG-CD2	-6.43	100.07	111.00
10	K4	135	ARG	NE-CZ-NH1	-6.43	117.09	120.30
10	gq	17	ARG	NE-CZ-NH2	-6.43	117.09	120.30
11	c6	1	MET	CG-SD-CE	6.42	110.48	100.20
11	ln	77	ARG	CD-NE-CZ	6.42	132.59	123.60
10	gb	17	ARG	NE-CZ-NH2	-6.42	117.09	120.30
12	34	121	LYS	CD-CE-NZ	6.42	126.47	111.70
10	M7	18	PHE	CB-CG-CD2	6.42	125.30	120.80
18	bd	104	VAL	CG1-CB-CG2	6.42	121.17	110.90
16	24	143	ILE	CG1-CB-CG2	-6.42	97.28	111.40
10	k3	84	ARG	NE-CZ-NH1	6.42	123.51	120.30
5	p1	18	TYR	CG-CD1-CE1	-6.42	116.17	121.30
10	W6	138	LEU	CA-CB-CG	6.41	130.05	115.30
11	x9	108	ARG	NE-CZ-NH1	-6.41	117.09	120.30
11	J3	129	ARG	NE-CZ-NH1	6.41	123.50	120.30
11	R3	38	LEU	CB-CG-CD1	-6.41	100.11	111.00
10	q5	135	ARG	NE-CZ-NH1	-6.41	117.10	120.30
10	o6	4	VAL	CG1-CB-CG2	6.41	121.15	110.90
17	cc	30	ARG	NE-CZ-NH2	-6.41	117.10	120.30
11	eX	108	ARG	NE-CZ-NH1	-6.41	117.10	120.30
16	X5	143	ILE	CG1-CB-CG2	-6.41	97.30	111.40
10	K7	118	ARG	NE-CZ-NH1	-6.41	117.10	120.30
11	Z7	30	PHE	CB-CG-CD2	6.41	125.28	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n1	149	MET	CG-SD-CE	6.41	110.45	100.20
16	bX	143	ILE	CG1-CB-CG2	-6.41	97.31	111.40
11	H2	91	ARG	NE-CZ-NH1	6.40	123.50	120.30
11	a7	50	CYS	CA-CB-SG	6.40	125.53	114.00
18	bb	108	ARG	NE-CZ-NH1	-6.40	117.10	120.30
11	eb	161	LEU	CB-CG-CD2	-6.40	100.11	111.00
5	L1	77	ARG	NE-CZ-NH2	-6.40	117.10	120.30
4	u1	35	ARG	NE-CZ-NH2	-6.40	117.10	120.30
11	B5	161	LEU	CB-CG-CD2	-6.40	100.12	111.00
10	q9	85	ASP	CB-CG-OD2	6.40	124.06	118.30
8	a2	615	VAL	CA-CB-CG1	-6.40	101.30	110.90
10	aq	85	ASP	CB-CG-OD2	6.40	124.06	118.30
10	iA	105	LEU	CB-CG-CD1	-6.40	100.12	111.00
10	aw	142	ARG	NE-CZ-NH2	6.39	123.50	120.30
4	b1	62	ARG	NE-CZ-NH1	-6.39	117.10	120.30
10	lw	91	ARG	NE-CZ-NH2	-6.39	117.10	120.30
11	bs	149	ARG	NE-CZ-NH1	6.39	123.50	120.30
5	S1	97	LEU	CB-CG-CD2	-6.39	100.14	111.00
5	t1	28	ARG	NE-CZ-NH2	-6.39	117.11	120.30
10	m3	138	LEU	CB-CG-CD2	-6.39	100.14	111.00
11	bB	98	LEU	CB-CG-CD1	-6.39	100.14	111.00
10	g6	144	MET	CG-SD-CE	-6.38	89.99	100.20
15	W9	34	THR	CA-CB-CG2	-6.38	103.46	112.40
12	34	122	ARG	CG-CD-NE	-6.38	98.40	111.80
11	A8	50	CYS	CA-CB-SG	6.38	125.49	114.00
10	dW	84	ARG	NE-CZ-NH2	6.38	123.49	120.30
4	s1	43	LEU	CB-CG-CD2	-6.38	100.16	111.00
11	x9	109	CYS	CA-CB-SG	6.38	125.48	114.00
16	aX	143	ILE	CG1-CB-CG2	-6.38	97.37	111.40
17	i4	17	ARG	NE-CZ-NH1	6.38	123.49	120.30
10	bm	84	ARG	NE-CZ-NH2	6.37	123.49	120.30
2	C1	124	MET	CG-SD-CE	-6.37	90.01	100.20
10	w6	13	ASP	CB-CG-OD1	6.37	124.03	118.30
12	Z9	173	ARG	NE-CZ-NH2	-6.37	117.11	120.30
11	dV	79	MET	CG-SD-CE	-6.37	90.00	100.20
11	V7	30	PHE	CB-CG-CD1	-6.37	116.34	120.80
9	c2	56	LEU	CA-CB-CG	6.37	129.95	115.30
11	l7	30	PHE	CB-CG-CD2	6.37	125.26	120.80
15	aW	113	ARG	NE-CZ-NH1	6.37	123.48	120.30
10	cv	137	ARG	NE-CZ-NH2	6.37	123.48	120.30
12	dw	170	TYR	CG-CD1-CE1	-6.37	116.21	121.30
5	S1	78	TYR	CZ-CE2-CD2	-6.37	114.07	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J1	109	LEU	CB-CG-CD1	-6.36	100.18	111.00
5	a1	97	LEU	CB-CG-CD2	-6.36	100.18	111.00
11	iD	108	ARG	NE-CZ-NH1	6.36	123.48	120.30
10	G5	135	ARG	NE-CZ-NH1	-6.36	117.12	120.30
3	E1	83	ASP	CB-CG-OD1	6.36	124.02	118.30
8	a2	345	PHE	CB-CG-CD2	-6.36	116.35	120.80
8	b2	390	GLU	OE1-CD-OE2	6.36	130.93	123.30
4	y1	91	LEU	CB-CG-CD2	-6.36	100.19	111.00
11	r2	38	LEU	CB-CG-CD1	-6.36	100.19	111.00
5	r1	97	LEU	CB-CG-CD2	-6.36	100.19	111.00
8	b2	180	LEU	CB-CG-CD2	-6.35	100.20	111.00
16	24	121	ARG	NE-CZ-NH1	-6.35	117.12	120.30
11	E8	78	ARG	NE-CZ-NH1	-6.35	117.12	120.30
16	aX	319	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	B1	106	PHE	CB-CG-CD1	-6.35	116.36	120.80
4	f1	92	VAL	CG1-CB-CG2	-6.35	100.74	110.90
10	iA	38	LEU	CB-CG-CD1	-6.35	100.21	111.00
5	j1	97	LEU	CB-CG-CD2	-6.34	100.21	111.00
18	c4	38	LEU	CB-CG-CD2	-6.34	100.22	111.00
10	r8	138	LEU	CA-CB-CG	6.34	129.89	115.30
12	bY	170	TYR	CZ-CE2-CD2	-6.34	114.09	119.80
12	a3	270	ARG	NE-CZ-NH2	-6.34	117.13	120.30
11	lh	28	LYS	CB-CG-CD	6.34	128.08	111.60
4	y1	109	LEU	CB-CG-CD2	-6.34	100.23	111.00
17	b5	86	ARG	NE-CZ-NH1	-6.34	117.13	120.30
11	br	101	ASP	CB-CG-OD1	6.34	124.00	118.30
11	gx	108	ARG	NE-CZ-NH2	-6.33	117.13	120.30
5	c1	18	TYR	CB-CG-CD2	-6.33	117.20	121.00
9	d2	48	LEU	CD1-CG-CD2	-6.33	91.50	110.50
11	B9	61	CYS	CA-CB-SG	6.33	125.40	114.00
5	O1	91	TYR	CZ-CE2-CD2	-6.33	114.10	119.80
11	D6	91	ARG	NE-CZ-NH2	-6.33	117.14	120.30
11	X6	30	PHE	CB-CG-CD1	-6.33	116.37	120.80
11	aB	109	CYS	CA-CB-SG	6.33	125.39	114.00
11	dX	7	ARG	NE-CZ-NH2	6.33	123.47	120.30
4	d1	65	VAL	CG1-CB-CG2	-6.33	100.78	110.90
5	e1	91	TYR	CZ-CE2-CD2	-6.33	114.11	119.80
4	q1	155	TYR	CZ-CE2-CD2	-6.32	114.11	119.80
11	aH	108	ARG	NE-CZ-NH1	-6.32	117.14	120.30
12	A2	44	ASP	CB-CG-OD1	6.32	123.99	118.30
12	bY	147	ARG	CG-CD-NE	-6.32	98.53	111.80
5	n1	115	THR	CA-CB-CG2	-6.32	103.56	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U7	138	LEU	CA-CB-CG	6.31	129.82	115.30
11	l7	91	ARG	NE-CZ-NH1	6.31	123.46	120.30
11	jO	115	GLU	OE1-CD-OE2	-6.31	115.73	123.30
11	n5	2	LEU	CB-CG-CD1	-6.31	100.27	111.00
10	as	138	LEU	CB-CG-CD1	-6.31	100.27	111.00
5	J1	119	LEU	CB-CG-CD2	6.31	121.72	111.00
4	b1	85	LEU	CB-CG-CD2	-6.31	100.28	111.00
10	Q2	2	LYS	CD-CE-NZ	6.31	126.21	111.70
11	B4	129	ARG	NE-CZ-NH1	-6.30	117.15	120.30
11	lh	50	CYS	CA-CB-SG	6.30	125.34	114.00
5	O1	77	ARG	NE-CZ-NH1	-6.30	117.15	120.30
16	aX	249	LEU	CB-CG-CD2	-6.30	100.30	111.00
18	cl	37	ARG	NE-CZ-NH2	-6.30	117.15	120.30
11	kQ	91	ARG	NE-CZ-NH1	6.30	123.45	120.30
5	t1	94	TYR	CZ-CE2-CD2	-6.29	114.14	119.80
11	b7	108	ARG	NE-CZ-NH1	6.29	123.44	120.30
10	q7	44	LEU	CB-CG-CD1	-6.29	100.30	111.00
11	kR	91	ARG	NE-CZ-NH1	6.29	123.44	120.30
10	K7	119	THR	CA-CB-CG2	-6.29	103.59	112.40
15	R8	47	ILE	CA-CB-CG2	-6.29	98.32	110.90
10	E9	17	ARG	NE-CZ-NH2	-6.29	117.16	120.30
14	C2	112	ARG	NE-CZ-NH2	6.29	123.44	120.30
24	gz	101	LEU	CA-CB-CG	-6.29	100.84	115.30
16	S8	133	PHE	CB-CG-CD1	-6.29	116.40	120.80
10	gm	119	THR	CA-CB-CG2	-6.29	103.60	112.40
4	Z1	47	ARG	NE-CZ-NH1	6.28	123.44	120.30
11	t5	79	MET	CG-SD-CE	-6.28	90.15	100.20
11	V7	170	ASP	CB-CG-OD2	-6.28	112.64	118.30
11	lj	108	ARG	NE-CZ-NH1	-6.28	117.16	120.30
4	Z1	90	ARG	NH1-CZ-NH2	-6.28	112.49	119.40
11	cq	152	GLU	OE1-CD-OE2	-6.28	115.76	123.30
10	E6	138	LEU	CA-CB-CG	6.28	129.74	115.30
12	Z9	71	ARG	NE-CZ-NH1	6.28	123.44	120.30
4	T1	91	LEU	CB-CG-CD2	-6.28	100.33	111.00
16	24	215	MET	CG-SD-CE	-6.28	90.16	100.20
10	S6	114	ARG	NE-CZ-NH2	-6.27	117.16	120.30
11	eH	108	ARG	NE-CZ-NH1	-6.27	117.16	120.30
10	y5	74	ASP	CB-CG-OD2	-6.27	112.66	118.30
10	Y7	143	ASP	CB-CG-OD2	-6.27	112.66	118.30
16	bX	249	LEU	CB-CG-CD2	-6.27	100.34	111.00
10	M7	156	LEU	CB-CG-CD2	-6.27	100.35	111.00
18	c4	13	ASP	CB-CG-OD2	-6.26	112.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	B5	91	ARG	NE-CZ-NH2	-6.26	117.17	120.30
11	y7	153	ILE	CG1-CB-CG2	-6.26	97.63	111.40
11	w8	61	CYS	CA-CB-SG	6.26	125.27	114.00
11	t9	105	LEU	CB-CG-CD2	-6.26	100.36	111.00
11	bz	108	ARG	NE-CZ-NH1	-6.26	117.17	120.30
11	eH	120	LEU	CB-CG-CD2	-6.26	100.36	111.00
4	G1	85	LEU	CB-CG-CD2	-6.25	100.37	111.00
8	b2	730	ARG	NE-CZ-NH2	-6.25	117.17	120.30
11	at	59	MET	CG-SD-CE	6.25	110.20	100.20
8	a2	146	ARG	NE-CZ-NH1	6.25	123.42	120.30
10	j7	120	LEU	CB-CG-CD2	6.25	121.62	111.00
11	bs	38	LEU	CB-CG-CD1	-6.25	100.38	111.00
11	x3	38	LEU	CB-CG-CD1	-6.25	100.38	111.00
12	34	71	ARG	NE-CZ-NH1	6.25	123.42	120.30
11	v4	142	ILE	CG1-CB-CG2	-6.25	97.65	111.40
16	bX	93	TYR	CB-CG-CD2	-6.25	117.25	121.00
10	eA	135	ARG	NE-CZ-NH2	-6.25	117.18	120.30
12	aY	147	ARG	CG-CD-NE	-6.25	98.68	111.80
10	cm	163	LEU	CB-CG-CD2	-6.25	100.38	111.00
10	dJ	38	LEU	CB-CG-CD2	6.25	121.62	111.00
4	d1	86	ASP	CB-CG-OD1	-6.24	112.68	118.30
5	p1	76	ARG	NE-CZ-NH1	-6.24	117.18	120.30
10	db	138	LEU	CA-CB-CG	6.24	129.66	115.30
6	Q1	59	LEU	CA-CB-CG	6.24	129.66	115.30
11	H2	19	VAL	CG1-CB-CG2	-6.24	100.92	110.90
11	X7	13	ASP	CB-CG-OD2	6.24	123.92	118.30
12	b9	55	LYS	CD-CE-NZ	6.24	126.05	111.70
16	X9	339	ARG	CG-CD-NE	-6.24	98.70	111.80
17	ag	155	ASP	CB-CG-OD2	6.24	123.91	118.30
11	R3	77	ARG	NE-CZ-NH2	6.24	123.42	120.30
14	aZ	83	LYS	CD-CE-NZ	6.24	126.05	111.70
11	iC	91	ARG	NE-CZ-NH1	-6.24	117.18	120.30
19	a9	330	ARG	NE-CZ-NH2	6.23	123.42	120.30
5	J1	14	VAL	CG1-CB-CG2	6.23	120.87	110.90
4	N1	65	VAL	CG1-CB-CG2	-6.23	100.93	110.90
4	u1	151	PHE	CG-CD1-CE1	-6.23	113.95	120.80
11	r2	77	ARG	NE-CZ-NH2	6.23	123.42	120.30
10	bw	85	ASP	CB-CG-OD2	6.23	123.91	118.30
20	dy	97	TYR	CA-CB-CG	-6.23	101.57	113.40
11	x5	161	LEU	CB-CG-CD2	-6.23	100.41	111.00
10	g6	138	LEU	CA-CB-CG	6.23	129.62	115.30
10	lw	163	LEU	CB-CG-CD2	-6.23	100.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A1	97	ASP	CB-CG-OD2	-6.22	112.70	118.30
13	b3	414	ALA	N-CA-C	-6.22	94.19	111.00
10	I6	17	ARG	NE-CZ-NH1	6.22	123.41	120.30
10	bu	91	ARG	NE-CZ-NH2	6.22	123.41	120.30
11	dH	79	MET	CG-SD-CE	-6.22	90.24	100.20
11	iD	91	ARG	NE-CZ-NH1	-6.22	117.19	120.30
11	ap	176	VAL	CG1-CB-CG2	-6.22	100.94	110.90
10	eG	137	ARG	NE-CZ-NH1	-6.22	117.19	120.30
18	e5	85	ASP	CB-CG-OD2	6.22	123.90	118.30
10	I7	138	LEU	CA-CB-CG	6.22	129.61	115.30
11	p9	98	LEU	CB-CG-CD1	-6.22	100.43	111.00
10	O9	17	ARG	NE-CZ-NH2	-6.22	117.19	120.30
12	aY	105	LEU	CB-CG-CD2	-6.22	100.43	111.00
10	dJ	67	LYS	CA-CB-CG	6.22	127.08	113.40
11	L2	59	MET	CG-SD-CE	6.22	110.15	100.20
11	eN	108	ARG	NE-CZ-NH2	-6.22	117.19	120.30
5	L1	60	LEU	CB-CG-CD2	6.22	121.57	111.00
11	z5	98	LEU	CB-CG-CD1	-6.22	100.43	111.00
10	K7	1	MET	CB-CG-SD	6.22	131.05	112.40
18	bl	37	ARG	NE-CZ-NH2	-6.22	117.19	120.30
13	b3	406	ARG	CG-CD-NE	-6.21	98.75	111.80
10	C7	79	ILE	CG1-CB-CG2	-6.21	97.73	111.40
10	aA	95	TYR	CZ-CE2-CD2	-6.21	114.21	119.80
11	bs	2	LEU	CB-CG-CD1	-6.21	100.44	111.00
11	dH	84	ARG	NE-CZ-NH1	6.21	123.41	120.30
11	er	27	LEU	CB-CG-CD2	-6.21	100.44	111.00
18	c4	166	ARG	NE-CZ-NH1	-6.21	117.20	120.30
7	m1	90	ARG	NE-CZ-NH2	6.21	123.40	120.30
10	hS	38	LEU	CB-CG-CD2	6.21	121.55	111.00
13	B2	68	LEU	CA-CB-CG	-6.20	101.03	115.30
11	D5	101	ASP	CB-CG-OD1	6.20	123.88	118.30
10	h6	114	ARG	NE-CZ-NH2	-6.20	117.20	120.30
10	s4	92	LEU	CB-CG-CD1	-6.20	100.46	111.00
14	bZ	83	LYS	CD-CE-NZ	6.20	125.96	111.70
4	s1	153	PHE	CB-CG-CD1	-6.20	116.46	120.80
12	A2	191	LYS	CD-CE-NZ	6.20	125.96	111.70
18	e4	83	LEU	CB-CG-CD1	-6.20	100.46	111.00
18	l4	85	ASP	CB-CG-OD2	6.20	123.88	118.30
16	24	61	ARG	NE-CZ-NH2	6.20	123.40	120.30
10	db	137	ARG	NE-CZ-NH1	-6.20	117.20	120.30
5	O1	76	ARG	NE-CZ-NH2	6.19	123.40	120.30
10	C5	135	ARG	NE-CZ-NH2	6.19	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a8	303	TYR	CZ-CE2-CD2	-6.19	114.23	119.80
10	aK	140	VAL	C-N-CD	-6.19	106.97	120.60
5	Y1	14	VAL	CG1-CB-CG2	6.19	120.81	110.90
13	b3	287	ASP	CB-CG-OD1	6.19	123.87	118.30
18	l9	77	ARG	NE-CZ-NH2	-6.19	117.20	120.30
11	cL	149	ARG	NE-CZ-NH2	-6.19	117.20	120.30
20	dz	97	TYR	CA-CB-CG	-6.19	101.64	113.40
5	S1	19	LEU	CB-CG-CD1	-6.19	100.48	111.00
4	q1	51	VAL	CA-CB-CG1	-6.19	101.62	110.90
18	g4	83	LEU	CB-CG-CD1	-6.19	100.48	111.00
10	bw	91	ARG	NE-CZ-NH2	6.19	123.39	120.30
11	at	142	ILE	CG1-CB-CG2	-6.19	97.79	111.40
3	E1	184	ARG	NE-CZ-NH1	6.18	123.39	120.30
13	B2	406	ARG	CG-CD-NE	-6.18	98.81	111.80
11	v3	90	LEU	CB-CG-CD1	6.18	121.51	111.00
10	q4	91	ARG	NE-CZ-NH2	6.18	123.39	120.30
10	bu	84	ARG	NE-CZ-NH1	-6.18	117.21	120.30
12	A2	225	MET	CG-SD-CE	-6.18	90.32	100.20
17	X8	33	ARG	NE-CZ-NH1	-6.18	117.21	120.30
11	dN	78	ARG	NE-CZ-NH2	-6.18	117.21	120.30
11	D5	113	LEU	CB-CG-CD1	-6.17	100.50	111.00
10	z8	18	PHE	CB-CG-CD1	-6.17	116.48	120.80
4	w1	151	PHE	CB-CG-CD1	-6.17	116.48	120.80
11	X6	142	ILE	CG1-CB-CG2	-6.17	97.82	111.40
11	n6	91	ARG	NE-CZ-NH1	6.17	123.39	120.30
5	M1	39	ARG	NE-CZ-NH1	-6.17	117.22	120.30
10	dW	67	LYS	CD-CE-NZ	6.17	125.89	111.70
10	u9	92	LEU	CB-CG-CD1	-6.17	100.52	111.00
11	co	77	ARG	NE-CZ-NH2	-6.17	117.22	120.30
4	d1	44	THR	CA-CB-CG2	-6.17	103.77	112.40
18	e5	83	LEU	CB-CG-CD1	-6.17	100.52	111.00
10	h6	142	ARG	NE-CZ-NH1	-6.17	117.22	120.30
11	B6	91	ARG	NE-CZ-NH1	6.16	123.38	120.30
20	dy	350	LEU	CA-CB-CG	6.16	129.47	115.30
10	o6	33	ARG	NE-CZ-NH1	-6.16	117.22	120.30
12	U8	125	VAL	CG1-CB-CG2	6.16	120.76	110.90
4	T1	65	VAL	CG1-CB-CG2	-6.16	101.05	110.90
6	g1	149	GLN	C-N-CA	6.16	137.09	121.70
17	bc	30	ARG	NE-CZ-NH1	6.16	123.38	120.30
6	g1	59	LEU	CB-CG-CD1	-6.16	100.53	111.00
5	e1	76	ARG	NE-CZ-NH2	6.16	123.38	120.30
18	c5	166	ARG	NE-CZ-NH1	-6.16	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	O2	87	ASP	CB-CG-OD2	6.15	123.84	118.30
10	dW	38	LEU	CB-CG-CD2	6.15	121.46	111.00
11	L2	38	LEU	CB-CG-CD1	-6.15	100.55	111.00
17	ac	2	LYS	CD-CE-NZ	6.15	125.84	111.70
11	cz	108	ARG	NE-CZ-NH1	-6.15	117.22	120.30
16	X5	215	MET	CG-SD-CE	-6.15	90.36	100.20
11	J6	120	LEU	CA-CB-CG	6.15	129.44	115.30
12	U8	71	ARG	NE-CZ-NH1	6.15	123.37	120.30
20	dy	193	ARG	NE-CZ-NH2	-6.15	117.23	120.30
10	C7	44	LEU	CB-CG-CD1	-6.15	100.55	111.00
5	x1	97	LEU	CB-CG-CD2	-6.14	100.56	111.00
10	I4	135	ARG	NE-CZ-NH1	-6.14	117.23	120.30
11	z4	79	MET	CG-SD-CE	-6.14	90.37	100.20
13	b3	68	LEU	CA-CB-CG	-6.14	101.18	115.30
10	i7	1	MET	CB-CG-SD	6.14	130.82	112.40
10	cy	91	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
10	I5	91	ARG	NE-CZ-NH1	6.14	123.37	120.30
11	jP	115	GLU	OE1-CD-OE2	-6.14	115.94	123.30
12	U8	156	ARG	NE-CZ-NH1	-6.14	117.23	120.30
23	ly	202	ARG	NE-CZ-NH2	-6.14	117.23	120.30
18	bl	75	THR	N-CA-C	-6.13	94.44	111.00
11	dK	98	LEU	CB-CG-CD1	-6.13	100.57	111.00
10	A5	74	ASP	CB-CG-OD2	-6.13	112.78	118.30
18	ch	88	ILE	CG1-CB-CG2	-6.13	97.91	111.40
6	g1	83	LEU	CB-CG-CD2	6.13	121.42	111.00
6	g1	95	TYR	CZ-CE2-CD2	-6.13	114.28	119.80
11	iD	98	LEU	CB-CG-CD1	-6.13	100.58	111.00
18	bb	39	ASP	CB-CG-OD2	-6.13	112.79	118.30
4	d1	94	TYR	CZ-CE2-CD2	-6.12	114.29	119.80
10	M4	85	ASP	CB-CG-OD2	6.12	123.81	118.30
16	X5	262	LEU	CB-CG-CD1	6.12	121.41	111.00
10	cw	85	ASP	CB-CG-OD2	6.12	123.81	118.30
10	y4	138	LEU	CB-CG-CD2	-6.12	100.59	111.00
10	db	140	VAL	C-N-CD	-6.12	107.13	120.60
23	lz	212	CYS	N-CA-C	6.12	127.54	111.00
10	M7	89	TYR	CB-CG-CD2	-6.12	117.33	121.00
10	W7	114	ARG	NE-CZ-NH2	-6.12	117.24	120.30
11	dX	161	LEU	CB-CG-CD2	-6.12	100.59	111.00
4	d1	140	LEU	CB-CG-CD2	-6.12	100.60	111.00
18	W8	141	LEU	CB-CG-CD2	-6.12	100.60	111.00
5	J1	97	LEU	CB-CG-CD2	-6.12	100.60	111.00
18	bf	57	ARG	NE-CZ-NH1	-6.12	117.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B2	287	ASP	CB-CG-OD1	6.12	123.80	118.30
11	T7	59	MET	CG-SD-CE	6.12	109.99	100.20
10	dO	53	LYS	CD-CE-NZ	6.12	125.77	111.70
10	K7	66	LEU	CB-CG-CD2	-6.11	100.61	111.00
18	ab	57	ARG	NE-CZ-NH2	-6.11	117.24	120.30
10	gj	142	ARG	NE-CZ-NH1	-6.11	117.24	120.30
8	a2	626	ARG	NE-CZ-NH2	-6.11	117.24	120.30
10	aI	142	ARG	NE-CZ-NH1	-6.11	117.24	120.30
10	g2	142	ARG	NE-CZ-NH2	6.11	123.35	120.30
15	W9	107	VAL	CG1-CB-CG2	6.11	120.67	110.90
15	bW	222	LEU	CA-CB-CG	6.11	129.34	115.30
10	cm	84	ARG	NE-CZ-NH2	6.11	123.35	120.30
5	L1	97	LEU	CB-CG-CD2	-6.11	100.62	111.00
11	iE	59	MET	CG-SD-CE	6.11	109.97	100.20
10	y5	138	LEU	CB-CG-CD2	-6.10	100.62	111.00
12	Z9	156	ARG	NE-CZ-NH1	-6.10	117.25	120.30
8	a2	359	PHE	CB-CG-CD2	6.10	125.07	120.80
11	Z6	153	ILE	CG1-CB-CG2	-6.10	97.97	111.40
11	X7	59	MET	CG-SD-CE	6.10	109.96	100.20
10	h7	138	LEU	CA-CB-CG	6.10	129.33	115.30
10	A9	18	PHE	CB-CG-CD2	6.10	125.07	120.80
10	bw	140	VAL	C-N-CD	-6.10	107.18	120.60
10	eq	85	ASP	CB-CG-OD2	6.10	123.79	118.30
18	g5	83	LEU	CB-CG-CD1	-6.10	100.63	111.00
12	bY	270	ARG	NE-CZ-NH1	6.10	123.35	120.30
20	dz	193	ARG	NE-CZ-NH2	-6.10	117.25	120.30
11	j2	129	ARG	NE-CZ-NH1	6.10	123.35	120.30
10	y4	74	ASP	CB-CG-OD2	-6.10	112.81	118.30
11	v7	120	LEU	CA-CB-CG	6.10	129.33	115.30
4	w1	51	VAL	CA-CB-CG1	-6.09	101.76	110.90
17	b4	24	LEU	CB-CG-CD2	6.09	121.36	111.00
16	bX	93	TYR	CB-CG-CD1	6.09	124.66	121.00
11	L2	91	ARG	NE-CZ-NH2	-6.09	117.25	120.30
10	m5	138	LEU	CB-CG-CD2	-6.09	100.65	111.00
10	Q2	24	LEU	CB-CG-CD2	-6.09	100.65	111.00
10	M4	118	ARG	NE-CZ-NH1	6.09	123.34	120.30
12	Y5	122	ARG	NE-CZ-NH2	-6.09	117.25	120.30
12	dw	173	ARG	NE-CZ-NH2	-6.09	117.25	120.30
19	a8	401	LEU	CB-CG-CD2	-6.09	100.65	111.00
14	d9	77	MET	CB-CG-SD	-6.09	94.14	112.40
7	m1	15	LEU	CB-CG-CD1	-6.09	100.65	111.00
12	Z9	125	VAL	CG1-CB-CG2	6.09	120.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	au	92	LEU	CB-CG-CD1	-6.09	100.65	111.00
10	de	142	ARG	NE-CZ-NH1	6.09	123.34	120.30
5	Y1	109	LEU	CB-CG-CD1	-6.08	100.66	111.00
4	y1	90	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
10	E7	157	ASP	CB-CG-OD2	6.08	123.78	118.30
18	cl	83	LEU	CB-CG-CD1	-6.08	100.66	111.00
10	cu	84	ARG	NE-CZ-NH2	6.08	123.34	120.30
11	t4	79	MET	CG-SD-CE	-6.08	90.47	100.20
10	aq	142	ARG	NE-CZ-NH1	-6.08	117.26	120.30
10	C7	89	TYR	CB-CG-CD2	-6.08	117.35	121.00
10	bt	114	ARG	NE-CZ-NH2	-6.08	117.26	120.30
11	eT	129	ARG	NE-CZ-NH1	6.08	123.34	120.30
12	A2	270	ARG	NE-CZ-NH2	-6.08	117.26	120.30
14	e8	193	PHE	CB-CG-CD1	6.08	125.05	120.80
12	Y5	122	ARG	CG-CD-NE	-6.08	99.04	111.80
10	s6	91	ARG	NE-CZ-NH1	-6.07	117.26	120.30
17	X8	30	ARG	NE-CZ-NH1	-6.07	117.26	120.30
11	bz	84	ARG	NE-CZ-NH1	-6.07	117.26	120.30
10	Y7	18	PHE	CB-CG-CD2	6.07	125.05	120.80
11	bq	152	GLU	OE1-CD-OE2	-6.07	116.02	123.30
10	cx	138	LEU	CB-CG-CD2	-6.07	100.68	111.00
4	d1	43	LEU	CB-CG-CD2	-6.07	100.68	111.00
10	dA	120	LEU	CB-CG-CD2	-6.07	100.69	111.00
10	D8	85	ASP	CB-CG-OD2	6.07	123.76	118.30
11	t9	21	GLY	N-CA-C	6.07	128.26	113.10
4	k1	65	VAL	CG1-CB-CG2	-6.06	101.20	110.90
10	q5	85	ASP	CB-CG-OD2	6.06	123.76	118.30
11	t9	59	MET	CG-SD-CE	6.06	109.90	100.20
18	bh	88	ILE	CG1-CB-CG2	-6.06	98.06	111.40
19	a8	234	MET	CG-SD-CE	-6.06	90.50	100.20
18	bl	84	ARG	NE-CZ-NH2	-6.06	117.27	120.30
11	bo	153	ILE	CG1-CB-CG2	-6.06	98.07	111.40
10	lq	63	TYR	CG-CD2-CE2	-6.06	116.45	121.30
11	F4	7	ARG	NE-CZ-NH1	6.06	123.33	120.30
10	C5	85	ASP	CB-CG-OD2	6.06	123.75	118.30
10	ct	114	ARG	NE-CZ-NH2	-6.06	117.27	120.30
17	bc	30	ARG	NE-CZ-NH2	-6.05	117.27	120.30
4	G1	91	LEU	CB-CG-CD1	6.05	121.29	111.00
11	h3	149	ARG	NE-CZ-NH2	-6.05	117.27	120.30
16	S8	199	ARG	NE-CZ-NH1	-6.05	117.27	120.30
11	ar	98	LEU	CB-CG-CD1	-6.05	100.71	111.00
12	bY	293	LEU	CB-CG-CD2	-6.05	100.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D1	133	LEU	CB-CG-CD2	-6.05	100.72	111.00
11	v5	142	ILE	CG1-CB-CG2	-6.05	98.09	111.40
10	E7	33	ARG	NE-CZ-NH2	6.05	123.33	120.30
11	C8	27	LEU	CB-CG-CD2	-6.05	100.72	111.00
10	eM	18	PHE	CB-CG-CD1	-6.05	116.56	120.80
6	Q1	151	ILE	CG1-CB-CG2	-6.05	98.09	111.40
10	dO	135	ARG	NE-CZ-NH1	-6.05	117.28	120.30
9	c2	81	LEU	CB-CG-CD1	6.05	121.28	111.00
11	H6	170	ASP	CB-CG-OD2	6.05	123.74	118.30
10	s9	138	LEU	CB-CG-CD1	-6.05	100.72	111.00
10	cW	33	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
11	H6	110	LEU	CB-CG-CD2	-6.04	100.72	111.00
11	L6	59	MET	CG-SD-CE	6.04	109.87	100.20
10	K2	84	ARG	NE-CZ-NH1	6.04	123.32	120.30
18	cl	75	THR	N-CA-C	-6.04	94.68	111.00
10	gb	37	ARG	NE-CZ-NH2	6.04	123.32	120.30
11	el	84	ARG	NE-CZ-NH1	6.04	123.32	120.30
3	E1	179	PHE	CB-CG-CD1	-6.04	116.57	120.80
10	y5	156	LEU	CB-CG-CD1	-6.04	100.73	111.00
11	N7	120	LEU	CA-CB-CG	6.04	129.18	115.30
12	a3	66	LEU	CA-CB-CG	-6.04	101.42	115.30
18	c5	105	LEU	CB-CG-CD2	-6.03	100.74	111.00
10	g7	91	ARG	NE-CZ-NH1	-6.03	117.28	120.30
4	b1	91	LEU	CB-CG-CD1	6.03	121.25	111.00
4	y1	100	ASP	CB-CG-OD2	-6.03	112.88	118.30
13	b3	90	ARG	CG-CD-NE	-6.03	99.14	111.80
11	lv	50	CYS	CA-CB-SG	6.03	124.85	114.00
5	e1	78	TYR	CZ-CE2-CD2	-6.02	114.38	119.80
6	g1	59	LEU	CA-CB-CG	6.02	129.15	115.30
4	o1	151	PHE	CG-CD1-CE1	-6.02	114.18	120.80
10	E4	74	ASP	CB-CG-OD2	-6.02	112.88	118.30
8	b2	146	ARG	NE-CZ-NH1	6.02	123.31	120.30
11	l2	84	ARG	NE-CZ-NH2	-6.02	117.29	120.30
11	jP	108	ARG	CD-NE-CZ	6.02	132.03	123.60
11	J7	91	ARG	NH1-CZ-NH2	-6.02	112.78	119.40
11	X7	84	ARG	CG-CD-NE	-6.02	99.16	111.80
10	J8	17	ARG	NE-CZ-NH2	-6.02	117.29	120.30
15	bW	115	LEU	CB-CG-CD2	-6.02	100.77	111.00
5	c1	90	ARG	NE-CZ-NH1	6.01	123.31	120.30
24	gy	101	LEU	CA-CB-CG	-6.01	101.47	115.30
11	T4	50	CYS	CA-CB-SG	6.01	124.82	114.00
11	V6	59	MET	CG-SD-CE	6.01	109.82	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	a8	105	TYR	CG-CD1-CE1	6.01	126.11	121.30
11	t9	142	ILE	CG1-CB-CG2	-6.01	98.18	111.40
4	R1	94	TYR	CZ-CE2-CD2	-6.01	114.39	119.80
10	E5	135	ARG	NE-CZ-NH1	-6.01	117.30	120.30
11	ap	2	LEU	CA-CB-CG	6.01	129.12	115.30
6	g1	151	ILE	CG1-CB-CG2	-6.01	98.19	111.40
10	C6	157	ASP	CB-CG-OD2	6.01	123.71	118.30
10	i7	91	ARG	NE-CZ-NH2	6.01	123.30	120.30
11	eX	38	LEU	CB-CG-CD1	-6.01	100.79	111.00
18	e4	30	MET	CA-CB-CG	6.00	123.51	113.30
6	Q1	59	LEU	CB-CG-CD1	-6.00	100.80	111.00
11	r6	120	LEU	CA-CB-CG	6.00	129.11	115.30
25	kb	164	LYS	CD-CE-NZ	6.00	125.51	111.70
11	H4	113	LEU	CB-CG-CD1	-6.00	100.80	111.00
11	t6	33	ASP	CB-CG-OD2	-6.00	112.90	118.30
12	Z9	315	MET	CG-SD-CE	6.00	109.80	100.20
10	bQ	138	LEU	CB-CG-CD1	6.00	121.20	111.00
10	dG	163	LEU	CB-CG-CD2	-6.00	100.80	111.00
11	X6	170	ASP	CB-CG-OD2	-6.00	112.90	118.30
17	f5	99	LEU	CB-CG-CD2	-6.00	100.81	111.00
10	Q7	91	ARG	NE-CZ-NH1	-5.99	117.30	120.30
4	I1	94	TYR	CZ-CE2-CD2	-5.99	114.41	119.80
11	L6	30	PHE	CB-CG-CD1	5.99	124.99	120.80
11	a7	153	ILE	CG1-CB-CG2	-5.99	98.22	111.40
10	eM	91	ARG	NE-CZ-NH2	5.99	123.30	120.30
10	E7	114	ARG	NE-CZ-NH2	-5.99	117.31	120.30
14	d9	279	ARG	NE-CZ-NH2	-5.99	117.31	120.30
16	X9	199	ARG	NE-CZ-NH1	-5.99	117.31	120.30
16	X9	296	ARG	NE-CZ-NH2	-5.99	117.31	120.30
14	c9	169	LYS	CD-CE-NZ	5.99	125.47	111.70
10	k6	44	LEU	CB-CG-CD1	-5.99	100.83	111.00
17	ag	93	ARG	NE-CZ-NH2	-5.99	117.31	120.30
6	Q1	149	GLN	C-N-CA	5.98	136.66	121.70
5	Y1	97	LEU	CB-CG-CD2	-5.98	100.83	111.00
5	n1	38	VAL	CA-CB-CG1	-5.98	101.92	110.90
10	as	118	ARG	NE-CZ-NH2	5.98	123.29	120.30
15	aW	115	LEU	CB-CG-CD2	-5.98	100.83	111.00
11	L2	149	ARG	NE-CZ-NH1	5.98	123.29	120.30
10	C5	23	ASP	CB-CG-OD2	-5.98	112.92	118.30
11	a7	1	MET	CG-SD-CE	5.98	109.77	100.20
24	gy	148	ARG	NE-CZ-NH1	5.98	123.29	120.30
10	f6	91	ARG	NE-CZ-NH1	-5.98	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	o9	85	ASP	CB-CG-OD2	5.98	123.68	118.30
20	dz	350	LEU	CA-CB-CG	5.98	129.05	115.30
11	dN	98	LEU	CB-CG-CD1	-5.98	100.83	111.00
20	dz	128	PHE	CB-CG-CD1	-5.98	116.61	120.80
10	gh	137	ARG	NE-CZ-NH2	-5.98	117.31	120.30
4	y1	87	TYR	CG-CD1-CE1	-5.98	116.52	121.30
11	P5	50	CYS	CA-CB-SG	5.97	124.75	114.00
11	F9	108	ARG	NE-CZ-NH2	5.97	123.29	120.30
10	I2	87	ASP	CB-CG-OD2	5.97	123.68	118.30
17	ac	93	ARG	NE-CZ-NH2	-5.97	117.31	120.30
11	p9	1	MET	CG-SD-CE	5.97	109.75	100.20
20	dz	304	TYR	CB-CG-CD1	5.97	124.58	121.00
11	c7	84	ARG	NE-CZ-NH2	-5.97	117.32	120.30
11	v6	77	ARG	NE-CZ-NH1	5.97	123.28	120.30
11	bp	98	LEU	CB-CG-CD1	-5.97	100.86	111.00
10	li	23	ASP	CB-CG-OD2	-5.97	112.93	118.30
11	R6	120	LEU	CA-CB-CG	5.96	129.02	115.30
16	aX	346	VAL	CG1-CB-CG2	-5.96	101.36	110.90
4	G1	157	LEU	CB-CG-CD2	-5.96	100.87	111.00
10	K4	135	ARG	NE-CZ-NH2	5.96	123.28	120.30
17	g9	155	ASP	CB-CG-OD2	5.96	123.67	118.30
16	24	262	LEU	CB-CG-CD1	5.96	121.13	111.00
11	lh	78	ARG	NE-CZ-NH1	-5.96	117.32	120.30
11	bs	84	ARG	NE-CZ-NH2	5.96	123.28	120.30
14	Y9	178	ARG	NE-CZ-NH1	5.95	123.27	120.30
10	cD	91	ARG	NE-CZ-NH2	5.95	123.27	120.30
10	C6	1	MET	CB-CG-SD	5.95	130.24	112.40
22	eY	231	ARG	NE-CZ-NH1	5.95	123.27	120.30
11	l3	113	LEU	CB-CG-CD1	5.95	121.11	111.00
11	r5	129	ARG	NE-CZ-NH2	-5.95	117.33	120.30
11	P6	59	MET	CG-SD-CE	5.95	109.71	100.20
11	n9	108	ARG	CD-NE-CZ	5.95	131.93	123.60
18	bf	15	ARG	NE-CZ-NH1	5.95	123.27	120.30
18	c5	13	ASP	CB-CG-OD2	-5.94	112.95	118.30
10	bC	163	LEU	CB-CG-CD2	-5.94	100.89	111.00
5	O1	77	ARG	NH1-CZ-NH2	5.94	125.94	119.40
11	z5	79	MET	CG-SD-CE	-5.94	90.69	100.20
10	Y7	138	LEU	CB-CG-CD2	-5.94	100.90	111.00
16	aX	247	ILE	CG1-CB-CG2	5.94	124.47	111.40
17	ci	30	ARG	NE-CZ-NH1	5.94	123.27	120.30
11	eN	7	ARG	NE-CZ-NH1	5.94	123.27	120.30
11	N4	91	ARG	NE-CZ-NH1	-5.94	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	J7	77	ARG	NH1-CZ-NH2	-5.94	112.87	119.40
11	p6	91	ARG	NE-CZ-NH1	5.94	123.27	120.30
21	fd	223	ASP	CB-CG-OD2	5.94	123.64	118.30
13	B2	90	ARG	CG-CD-NE	-5.93	99.34	111.80
16	bX	247	ILE	CG1-CB-CG2	5.93	124.45	111.40
22	eY	111	ARG	NE-CZ-NH1	-5.93	117.33	120.30
10	q4	137	ARG	NE-CZ-NH1	-5.93	117.33	120.30
10	eC	163	LEU	CB-CG-CD2	-5.93	100.92	111.00
11	lb	108	ARG	NE-CZ-NH2	5.93	123.27	120.30
8	a2	542	TYR	CB-CG-CD1	-5.92	117.44	121.00
11	a7	161	LEU	CB-CG-CD2	-5.92	100.93	111.00
16	aX	41	LEU	CB-CG-CD1	5.92	121.07	111.00
11	gd	38	LEU	CB-CG-CD1	-5.92	100.93	111.00
8	b2	867	LEU	CB-CG-CD2	-5.92	100.93	111.00
15	R8	34	THR	CA-CB-CG2	-5.92	104.11	112.40
11	bo	28	LYS	CB-CG-CD	5.92	126.99	111.60
16	bX	116	VAL	CG1-CB-CG2	-5.92	101.42	110.90
19	a8	330	ARG	NE-CZ-NH2	5.92	123.26	120.30
10	gm	62	LYS	CD-CE-NZ	-5.92	98.09	111.70
10	iB	105	LEU	CB-CG-CD1	-5.92	100.94	111.00
25	kb	161	LEU	CB-CG-CD2	-5.92	100.94	111.00
4	i1	94	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
10	I7	8	THR	CA-CB-CG2	-5.92	104.12	112.40
11	l3	149	ARG	NE-CZ-NH1	5.91	123.26	120.30
10	K7	138	LEU	CA-CB-CG	5.91	128.90	115.30
10	W7	1	MET	CA-CB-CG	-5.91	103.25	113.30
18	W8	57	ARG	NE-CZ-NH2	-5.91	117.34	120.30
11	cp	98	LEU	CB-CG-CD1	-5.91	100.95	111.00
11	gd	108	ARG	NE-CZ-NH2	-5.91	117.34	120.30
11	a6	30	PHE	CB-CG-CD2	5.91	124.94	120.80
8	a2	535	ARG	NE-CZ-NH1	5.91	123.25	120.30
10	W2	142	ARG	NE-CZ-NH2	5.91	123.25	120.30
4	N1	86	ASP	CB-CG-OD1	-5.91	112.99	118.30
11	L2	13	ASP	CB-CG-OD2	5.91	123.62	118.30
10	y4	156	LEU	CB-CG-CD1	-5.91	100.96	111.00
17	be	30	ARG	NE-CZ-NH2	-5.91	117.35	120.30
17	ca	19	LEU	CB-CG-CD2	-5.91	100.96	111.00
4	d1	35	ARG	NE-CZ-NH2	-5.90	117.35	120.30
10	aG	57	ASP	CB-CG-OD2	5.90	123.61	118.30
12	aY	225	MET	CA-CB-CG	5.90	123.34	113.30
10	bA	95	TYR	CZ-CE2-CD2	-5.90	114.49	119.80
2	D1	124	MET	CG-SD-CE	-5.90	90.75	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P1	119	LEU	CB-CG-CD2	-5.90	100.97	111.00
17	cc	93	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	U1	65	ILE	CG1-CB-CG2	-5.90	98.43	111.40
11	dH	129	ARG	NE-CZ-NH2	-5.90	117.35	120.30
10	i6	142	ARG	CG-CD-NE	5.89	124.18	111.80
17	Z8	30	ARG	NE-CZ-NH2	5.89	123.25	120.30
12	dx	173	ARG	NE-CZ-NH2	-5.89	117.35	120.30
11	T2	109	CYS	CA-CB-SG	5.89	124.61	114.00
11	B6	50	CYS	CA-CB-SG	5.89	124.61	114.00
11	H7	91	ARG	NE-CZ-NH2	-5.89	117.35	120.30
11	ar	19	VAL	CG1-CB-CG2	-5.89	101.47	110.90
17	bc	86	ARG	NE-CZ-NH2	-5.89	117.35	120.30
4	y1	94	TYR	CZ-CE2-CD2	-5.89	114.50	119.80
8	b2	359	PHE	CB-CG-CD2	5.89	124.92	120.80
11	z2	77	ARG	NE-CZ-NH2	5.89	123.25	120.30
10	gm	37	ARG	NE-CZ-NH2	5.89	123.24	120.30
10	li	17	ARG	NE-CZ-NH1	5.89	123.24	120.30
5	W1	38	VAL	CA-CB-CG1	-5.88	102.07	110.90
17	bg	161	LEU	CB-CG-CD2	-5.88	101.00	111.00
10	bI	142	ARG	NE-CZ-NH1	-5.88	117.36	120.30
10	cu	84	ARG	NE-CZ-NH1	-5.88	117.36	120.30
10	iB	95	TYR	CZ-CE2-CD2	-5.88	114.50	119.80
4	s1	151	PHE	CD1-CG-CD2	5.88	125.95	118.30
17	f4	30	ARG	NE-CZ-NH2	-5.88	117.36	120.30
11	er	98	LEU	CB-CG-CD1	-5.88	101.00	111.00
6	g1	67	LEU	CB-CG-CD1	5.88	121.00	111.00
5	j1	62	TYR	CB-CG-CD1	-5.88	117.47	121.00
4	q1	151	PHE	CB-CG-CD1	-5.88	116.68	120.80
5	x1	62	TYR	CB-CG-CD1	-5.88	117.47	121.00
17	ca	2	LYS	CD-CE-NZ	5.88	125.23	111.70
11	dN	143	MET	CG-SD-CE	5.88	109.61	100.20
10	fp	17	ARG	NE-CZ-NH2	5.88	123.24	120.30
5	L1	83	ARG	NH1-CZ-NH2	5.88	125.87	119.40
5	Y1	74	THR	CA-CB-CG2	-5.88	104.17	112.40
5	z1	94	TYR	CZ-CE2-CD2	-5.88	114.51	119.80
8	b2	837	LEU	CB-CG-CD1	-5.88	101.01	111.00
15	aW	6	LEU	CA-CB-CG	5.88	128.82	115.30
12	A2	66	LEU	CA-CB-CG	-5.88	101.78	115.30
10	k3	163	LEU	CB-CG-CD2	-5.88	101.01	111.00
10	w9	91	ARG	NE-CZ-NH2	5.88	123.24	120.30
11	ap	91	ARG	NE-CZ-NH2	-5.88	117.36	120.30
10	la	63	TYR	CG-CD2-CE2	-5.88	116.60	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P1	62	ARG	NE-CZ-NH1	5.87	123.24	120.30
10	S7	66	LEU	CB-CG-CD2	-5.87	101.02	111.00
11	A8	108	ARG	NE-CZ-NH2	5.87	123.24	120.30
11	kT	170	ASP	CB-CG-OD1	5.87	123.59	118.30
11	L3	84	ARG	NE-CZ-NH2	-5.87	117.36	120.30
10	q5	17	ARG	NE-CZ-NH1	5.87	123.23	120.30
17	cg	161	LEU	CB-CG-CD2	-5.87	101.02	111.00
10	m4	135	ARG	NE-CZ-NH2	5.87	123.23	120.30
10	dJ	67	LYS	CD-CE-NZ	5.87	125.20	111.70
11	J7	18	TYR	CB-CG-CD1	-5.87	117.48	121.00
12	U8	315	MET	CG-SD-CE	5.87	109.59	100.20
11	aB	129	ARG	NE-CZ-NH1	-5.87	117.37	120.30
5	h1	39	ARG	NE-CZ-NH1	-5.86	117.37	120.30
11	X7	143	MET	CG-SD-CE	-5.86	90.82	100.20
16	S8	296	ARG	NE-CZ-NH2	-5.86	117.37	120.30
12	34	152	THR	CA-CB-CG2	-5.86	104.19	112.40
10	s5	17	ARG	NE-CZ-NH2	-5.86	117.37	120.30
14	d8	192	ARG	NE-CZ-NH1	5.86	123.23	120.30
10	lw	23	ASP	CB-CG-OD2	-5.86	113.03	118.30
11	H6	109	CYS	CA-CB-SG	5.86	124.55	114.00
11	e7	91	ARG	NE-CZ-NH2	-5.86	117.37	120.30
6	g1	85	ASP	CB-CG-OD2	5.86	123.57	118.30
4	q1	93	THR	CA-CB-CG2	-5.86	104.20	112.40
10	o6	44	LEU	CB-CG-CD1	-5.86	101.04	111.00
18	bl	83	LEU	CB-CG-CD1	-5.86	101.04	111.00
3	E1	106	ASP	CB-CG-OD2	5.86	123.57	118.30
12	Y5	152	THR	CA-CB-CG2	-5.86	104.20	112.40
11	F6	153	ILE	CG1-CB-CG2	-5.86	98.52	111.40
14	e9	193	PHE	CB-CG-CD1	5.86	124.90	120.80
10	dU	163	LEU	CB-CG-CD2	-5.86	101.05	111.00
10	f7	17	ARG	NE-CZ-NH2	-5.85	117.37	120.30
20	dy	128	PHE	CB-CG-CD1	-5.85	116.70	120.80
5	W1	149	MET	CG-SD-CE	5.85	109.56	100.20
16	X5	121	ARG	NE-CZ-NH1	-5.85	117.37	120.30
10	Y7	18	PHE	CB-CG-CD1	-5.85	116.70	120.80
12	bY	71	ARG	NE-CZ-NH2	-5.85	117.37	120.30
5	v1	87	TYR	CG-CD1-CE1	-5.85	116.62	121.30
16	24	316	LEU	CA-CB-CG	5.85	128.75	115.30
11	v4	21	GLY	N-CA-C	5.85	127.72	113.10
11	c6	33	ASP	CB-CG-OD2	-5.85	113.03	118.30
5	W1	13	ASP	CB-CG-OD2	5.85	123.56	118.30
5	Y1	65	ILE	CG1-CB-CG2	-5.85	98.54	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	P2	50	CYS	CA-CB-SG	5.85	124.53	114.00
11	x3	79	MET	CG-SD-CE	-5.85	90.84	100.20
18	bj	84	ARG	NE-CZ-NH2	5.85	123.22	120.30
18	cl	84	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A1	150	ARG	NE-CZ-NH2	-5.85	117.38	120.30
11	h8	84	ARG	NE-CZ-NH2	-5.85	117.38	120.30
11	F7	91	ARG	NE-CZ-NH2	-5.84	117.38	120.30
8	a2	730	ARG	NE-CZ-NH2	-5.84	117.38	120.30
14	c3	279	ARG	NE-CZ-NH2	-5.84	117.38	120.30
10	u9	37	ARG	NE-CZ-NH1	5.84	123.22	120.30
11	ln	1	MET	CG-SD-CE	5.84	109.55	100.20
10	K7	114	ARG	NE-CZ-NH1	5.84	123.22	120.30
13	B2	383	TRP	CA-CB-CG	-5.84	102.61	113.70
10	K7	137	ARG	CB-CG-CD	5.84	126.77	111.60
10	Q6	114	ARG	NE-CZ-NH2	-5.83	117.38	120.30
10	dO	84	ARG	NE-CZ-NH1	-5.83	117.38	120.30
4	f1	119	LEU	CB-CG-CD2	-5.83	101.08	111.00
11	X2	79	MET	CG-SD-CE	-5.83	90.87	100.20
11	lp	90	LEU	CB-CG-CD1	5.83	120.92	111.00
11	z3	91	ARG	NE-CZ-NH1	-5.83	117.39	120.30
11	X6	120	LEU	CA-CB-CG	5.83	128.71	115.30
19	a9	76	ASP	CB-CG-OD2	-5.83	113.05	118.30
13	B2	149	ARG	NE-CZ-NH1	5.83	123.22	120.30
12	a3	170	TYR	CE1-CZ-OH	-5.83	104.36	120.10
14	e9	46	LEU	CA-CB-CG	5.83	128.71	115.30
18	ab	141	LEU	CB-CG-CD2	-5.83	101.09	111.00
11	R6	77	ARG	NE-CZ-NH2	-5.83	117.39	120.30
18	ab	77	ARG	NE-CZ-NH2	5.83	123.21	120.30
10	db	137	ARG	NE-CZ-NH2	5.83	123.21	120.30
10	aS	137	ARG	NE-CZ-NH1	-5.83	117.39	120.30
16	bX	346	VAL	CG1-CB-CG2	-5.83	101.58	110.90
11	x4	7	ARG	NE-CZ-NH2	-5.83	117.39	120.30
10	u6	138	LEU	CB-CG-CD2	-5.83	101.10	111.00
10	i7	13	ASP	CB-CG-OD1	-5.83	113.06	118.30
10	bv	89	TYR	CB-CG-CD2	-5.83	117.50	121.00
8	b2	776	LEU	CA-CB-CG	5.82	128.68	115.30
17	d5	19	LEU	CB-CG-CD2	-5.82	101.11	111.00
14	d8	57	VAL	CG1-CB-CG2	-5.82	101.59	110.90
15	R8	107	VAL	CG1-CB-CG2	5.82	120.21	110.90
10	bC	17	ARG	NE-CZ-NH2	-5.82	117.39	120.30
3	F1	106	ASP	CB-CG-OD2	5.82	123.53	118.30
18	e5	84	ARG	NE-CZ-NH2	5.82	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q1	67	LEU	CB-CG-CD1	5.81	120.88	111.00
14	c9	279	ARG	CG-CD-NE	-5.81	99.59	111.80
15	W9	117	ARG	NE-CZ-NH1	5.81	123.21	120.30
11	eF	7	ARG	NE-CZ-NH1	5.81	123.21	120.30
11	eF	108	ARG	NE-CZ-NH2	-5.81	117.39	120.30
11	f3	27	LEU	CB-CG-CD2	-5.81	101.12	111.00
10	M4	91	ARG	NE-CZ-NH1	5.81	123.21	120.30
11	dX	44	ILE	CG1-CB-CG2	-5.81	98.61	111.40
4	q1	83	ARG	NE-CZ-NH2	-5.81	117.39	120.30
16	X5	345	LEU	CB-CG-CD2	-5.81	101.12	111.00
11	cs	90	LEU	CB-CG-CD1	-5.81	101.12	111.00
5	U1	160	LEU	CB-CG-CD2	5.81	120.87	111.00
5	x1	94	TYR	CZ-CE2-CD2	-5.81	114.58	119.80
11	H7	120	LEU	CA-CB-CG	5.80	128.65	115.30
16	aX	116	VAL	CG1-CB-CG2	-5.80	101.61	110.90
11	iH	98	LEU	CB-CG-CD1	-5.80	101.13	111.00
5	l1	65	ILE	CG1-CB-CG2	-5.80	98.64	111.40
11	V2	88	ILE	CG1-CB-CG2	-5.80	98.64	111.40
13	b3	149	ARG	NE-CZ-NH1	5.80	123.20	120.30
13	b3	249	ARG	NH1-CZ-NH2	5.80	125.78	119.40
18	c5	84	ARG	NE-CZ-NH1	5.80	123.20	120.30
11	x4	2	LEU	CA-CB-CG	5.80	128.64	115.30
14	d9	57	VAL	CG1-CB-CG2	-5.80	101.62	110.90
10	ef	91	ARG	NE-CZ-NH1	5.80	123.20	120.30
4	P1	43	LEU	CB-CG-CD2	-5.80	101.14	111.00
10	aC	163	LEU	CB-CG-CD2	-5.80	101.14	111.00
4	N1	140	LEU	CB-CG-CD2	-5.80	101.14	111.00
7	V1	15	LEU	CB-CG-CD1	-5.80	101.14	111.00
14	Y9	260	GLY	N-CA-C	-5.80	98.61	113.10
10	dk	38	LEU	CB-CG-CD2	5.80	120.86	111.00
11	H2	149	ARG	NE-CZ-NH2	-5.79	117.40	120.30
11	P7	84	ARG	CG-CD-NE	-5.79	99.63	111.80
14	T8	260	GLY	N-CA-C	-5.79	98.62	113.10
10	q4	33	ARG	NE-CZ-NH2	5.79	123.20	120.30
15	W5	154	PHE	CB-CG-CD1	-5.79	116.75	120.80
18	ah	84	ARG	NE-CZ-NH1	5.79	123.20	120.30
11	lf	78	ARG	NE-CZ-NH1	-5.79	117.40	120.30
11	br	88	ILE	CG1-CB-CG2	-5.79	98.66	111.40
23	ly	293	MET	CA-CB-CG	5.79	123.14	113.30
13	b3	393	ARG	CG-CD-NE	5.79	123.95	111.80
17	d4	19	LEU	CB-CG-CD2	-5.79	101.16	111.00
10	bm	140	VAL	C-N-CD	-5.79	107.87	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	b3	383	TRP	CA-CB-CG	-5.79	102.71	113.70
10	C7	89	TYR	CB-CG-CD1	5.79	124.47	121.00
11	an	108	ARG	CD-NE-CZ	5.79	131.70	123.60
10	au	37	ARG	NE-CZ-NH1	5.79	123.19	120.30
17	ba	2	LYS	CD-CE-NZ	5.79	125.01	111.70
18	bf	105	LEU	CB-CG-CD2	-5.79	101.17	111.00
10	cv	89	TYR	CB-CG-CD2	-5.79	117.53	121.00
10	W2	143	ASP	CB-CG-OD2	-5.78	113.10	118.30
16	X5	316	LEU	CA-CB-CG	5.78	128.60	115.30
11	L6	41	VAL	CG1-CB-CG2	-5.78	101.65	110.90
11	a7	143	MET	CG-SD-CE	-5.78	90.95	100.20
12	dx	170	TYR	CG-CD1-CE1	-5.78	116.68	121.30
10	eQ	84	ARG	NE-CZ-NH2	-5.78	117.41	120.30
18	bh	57	ARG	NE-CZ-NH1	-5.78	117.41	120.30
10	gq	18	PHE	CB-CG-CD1	-5.77	116.76	120.80
8	a2	564	ARG	NE-CZ-NH1	-5.77	117.41	120.30
8	b2	533	TYR	CB-CG-CD2	-5.77	117.54	121.00
10	K7	136	ASP	CB-CG-OD1	5.77	123.50	118.30
23	ly	109	ARG	NE-CZ-NH2	-5.77	117.41	120.30
11	p9	108	ARG	NE-CZ-NH1	-5.77	117.41	120.30
11	jO	91	ARG	NE-CZ-NH2	5.77	123.19	120.30
11	kQ	108	ARG	NE-CZ-NH2	-5.77	117.41	120.30
11	L2	133	ILE	CG1-CB-CG2	-5.77	98.71	111.40
18	c4	105	LEU	CB-CG-CD2	-5.77	101.20	111.00
10	C7	142	ARG	CG-CD-NE	5.77	123.91	111.80
17	ag	30	ARG	NE-CZ-NH1	-5.77	117.42	120.30
11	c6	91	ARG	NE-CZ-NH2	-5.77	117.42	120.30
14	C2	279	ARG	NE-CZ-NH2	-5.76	117.42	120.30
11	V2	149	ARG	NE-CZ-NH1	5.76	123.18	120.30
11	N4	7	ARG	NE-CZ-NH2	-5.76	117.42	120.30
17	ce	93	ARG	NE-CZ-NH2	-5.76	117.42	120.30
10	bU	163	LEU	CB-CG-CD2	-5.76	101.20	111.00
5	t1	107	ARG	NE-CZ-NH1	5.76	123.18	120.30
11	iH	78	ARG	NE-CZ-NH2	-5.76	117.42	120.30
4	i1	131	ARG	NE-CZ-NH1	5.76	123.18	120.30
11	aH	77	ARG	NE-CZ-NH2	-5.76	117.42	120.30
11	P7	91	ARG	NE-CZ-NH2	-5.76	117.42	120.30
11	at	98	LEU	CB-CG-CD1	-5.76	101.22	111.00
10	eI	140	VAL	C-N-CD	-5.76	107.94	120.60
10	fn	142	ARG	NE-CZ-NH2	5.76	123.18	120.30
12	34	112	CYS	CA-CB-SG	-5.75	103.64	114.00
10	j6	137	ARG	NE-CZ-NH2	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	o8	109	CYS	CA-CB-SG	5.75	124.36	114.00
10	f7	142	ARG	NE-CZ-NH2	-5.75	117.42	120.30
16	bX	282	ARG	NE-CZ-NH1	5.75	123.18	120.30
11	v3	149	ARG	NE-CZ-NH1	5.75	123.18	120.30
11	L6	1	MET	CB-CG-SD	5.75	129.66	112.40
10	Y7	4	VAL	CG1-CB-CG2	5.75	120.10	110.90
10	aC	17	ARG	NE-CZ-NH2	-5.75	117.42	120.30
11	iD	37	ARG	NE-CZ-NH1	5.75	123.17	120.30
10	q5	91	ARG	NE-CZ-NH2	5.75	123.17	120.30
17	cc	88	ILE	CG1-CB-CG2	-5.75	98.75	111.40
4	f1	82	LEU	CB-CG-CD2	-5.75	101.23	111.00
10	q8	142	ARG	CG-CD-NE	5.75	123.87	111.80
10	M7	37	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	C1	133	LEU	CB-CG-CD1	-5.75	101.23	111.00
4	k1	151	PHE	CG-CD1-CE1	-5.75	114.48	120.80
5	j1	94	TYR	CZ-CE2-CD2	-5.74	114.63	119.80
10	K2	163	LEU	CB-CG-CD2	-5.74	101.23	111.00
11	Z2	91	ARG	NE-CZ-NH1	-5.74	117.43	120.30
10	w3	142	ARG	NE-CZ-NH2	5.74	123.17	120.30
16	24	345	LEU	CB-CG-CD2	-5.74	101.24	111.00
10	C5	2	LYS	CD-CE-NZ	5.74	124.91	111.70
11	n5	91	ARG	NE-CZ-NH1	5.74	123.17	120.30
11	cL	84	ARG	NE-CZ-NH1	5.74	123.17	120.30
11	eJ	129	ARG	NE-CZ-NH1	5.74	123.17	120.30
10	E6	44	LEU	CB-CG-CD1	-5.74	101.24	111.00
11	dL	7	ARG	NE-CZ-NH2	5.74	123.17	120.30
11	H4	91	ARG	NE-CZ-NH1	-5.74	117.43	120.30
12	Y5	112	CYS	CA-CB-SG	-5.74	103.67	114.00
10	de	142	ARG	NE-CZ-NH2	-5.74	117.43	120.30
12	Z9	231	MET	CG-SD-CE	5.74	109.38	100.20
11	az	108	ARG	CD-NE-CZ	5.74	131.63	123.60
15	R8	117	ARG	NE-CZ-NH1	5.74	123.17	120.30
11	ap	44	ILE	CG1-CB-CG2	-5.74	98.78	111.40
10	eS	140	VAL	C-N-CD	-5.74	107.98	120.60
5	j1	1	MET	CG-SD-CE	5.73	109.38	100.20
5	O1	78	TYR	CZ-CE2-CD2	-5.73	114.64	119.80
17	ba	33	ARG	NE-CZ-NH1	5.73	123.17	120.30
10	ao	85	ASP	CB-CG-OD2	5.73	123.46	118.30
10	la	63	TYR	CZ-CE2-CD2	5.73	124.96	119.80
8	a2	848	PHE	CB-CG-CD1	-5.73	116.79	120.80
17	X8	93	ARG	NE-CZ-NH2	-5.73	117.44	120.30
11	aR	129	ARG	NE-CZ-NH1	5.73	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j6	92	LEU	CB-CG-CD2	5.73	120.73	111.00
11	a7	33	ASP	CB-CG-OD2	-5.73	113.15	118.30
4	y1	31	LEU	CB-CG-CD2	-5.72	101.27	111.00
10	eQ	163	LEU	CB-CG-CD2	-5.72	101.27	111.00
4	N1	94	TYR	CZ-CE2-CD2	-5.72	114.65	119.80
4	N1	43	LEU	CB-CG-CD2	-5.72	101.28	111.00
11	X2	38	LEU	CB-CG-CD1	-5.72	101.28	111.00
11	a7	51	ILE	CG1-CB-CG2	-5.72	98.82	111.40
14	d9	77	MET	CA-CB-CG	5.72	123.02	113.30
5	H1	90	ARG	NE-CZ-NH1	5.72	123.16	120.30
10	s9	118	ARG	NE-CZ-NH2	5.72	123.16	120.30
11	co	120	LEU	CB-CG-CD2	5.72	120.72	111.00
5	r1	94	TYR	CZ-CE2-CD2	-5.71	114.66	119.80
10	ft	140	VAL	C-N-CD	-5.71	108.03	120.60
11	l3	59	MET	CG-SD-CE	5.71	109.34	100.20
4	w1	119	LEU	CB-CG-CD2	-5.71	101.29	111.00
5	z1	83	ARG	NE-CZ-NH1	-5.71	117.44	120.30
4	d1	131	ARG	NE-CZ-NH1	5.71	123.15	120.30
8	b2	739	ARG	NE-CZ-NH2	5.71	123.15	120.30
11	c7	59	MET	CG-SD-CE	5.71	109.33	100.20
11	F2	129	ARG	NE-CZ-NH1	5.70	123.15	120.30
10	h7	156	LEU	CB-CG-CD2	-5.70	101.30	111.00
18	bf	120	LEU	CB-CG-CD2	-5.70	101.30	111.00
8	b2	542	TYR	CB-CG-CD1	-5.70	117.58	121.00
14	c8	169	LYS	CD-CE-NZ	5.70	124.81	111.70
14	d8	57	VAL	CA-CB-CG1	-5.70	102.35	110.90
4	X1	94	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
10	q5	137	ARG	NE-CZ-NH1	-5.70	117.45	120.30
18	cj	84	ARG	NE-CZ-NH2	5.70	123.15	120.30
4	f1	65	VAL	CG1-CB-CG2	-5.70	101.78	110.90
11	H3	18	TYR	CB-CG-CD1	-5.70	117.58	121.00
11	az	108	ARG	NE-CZ-NH1	-5.70	117.45	120.30
18	bd	131	ILE	CG1-CB-CG2	-5.70	98.87	111.40
4	y1	52	LYS	CD-CE-NZ	5.70	124.80	111.70
11	fi	27	LEU	CA-CB-CG	5.70	128.40	115.30
11	kQ	95	TYR	CG-CD2-CE2	-5.70	116.74	121.30
10	A7	138	LEU	CA-CB-CG	5.69	128.40	115.30
10	dI	91	ARG	NE-CZ-NH1	5.69	123.15	120.30
11	r7	129	ARG	NE-CZ-NH1	-5.69	117.45	120.30
11	B7	66	LEU	CB-CG-CD2	-5.69	101.33	111.00
11	cs	27	LEU	CB-CG-CD2	-5.69	101.33	111.00
11	fu	27	LEU	CA-CB-CG	5.69	128.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O1	91	TYR	CG-CD2-CE2	5.69	125.85	121.30
5	U1	97	LEU	CB-CG-CD2	-5.69	101.33	111.00
10	s6	18	PHE	CB-CG-CD2	5.69	124.78	120.80
10	A5	138	LEU	CB-CG-CD2	-5.69	101.33	111.00
11	v6	120	LEU	CA-CB-CG	5.68	128.38	115.30
10	D8	91	ARG	NE-CZ-NH1	-5.68	117.46	120.30
10	bv	13	ASP	CB-CG-OD2	-5.68	113.18	118.30
10	gl	140	VAL	C-N-CD	-5.68	108.09	120.60
5	a1	119	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	B1	150	ARG	NE-CZ-NH2	-5.68	117.46	120.30
10	I5	17	ARG	NE-CZ-NH2	-5.68	117.46	120.30
10	Q6	157	ASP	CB-CG-OD2	5.68	123.41	118.30
8	b2	535	ARG	NE-CZ-NH1	5.68	123.14	120.30
11	T6	143	MET	CG-SD-CE	-5.68	91.12	100.20
11	bB	129	ARG	NE-CZ-NH1	-5.68	117.46	120.30
11	ei	27	LEU	CB-CG-CD2	-5.68	101.35	111.00
4	d1	91	LEU	CB-CG-CD1	5.67	120.65	111.00
4	s1	109	LEU	CB-CG-CD2	-5.67	101.35	111.00
11	N6	84	ARG	CG-CD-NE	-5.67	99.89	111.80
11	b6	91	ARG	NE-CZ-NH2	-5.67	117.46	120.30
10	i7	156	LEU	CB-CG-CD2	-5.67	101.36	111.00
15	W9	75	PHE	CG-CD2-CE2	-5.67	114.56	120.80
12	aY	170	TYR	CZ-CE2-CD2	-5.67	114.70	119.80
10	cX	91	ARG	NE-CZ-NH2	5.67	123.14	120.30
4	w1	93	THR	CA-CB-CG2	-5.67	104.46	112.40
10	G4	135	ARG	NE-CZ-NH2	5.67	123.14	120.30
11	L6	88	ILE	CG1-CB-CG2	-5.67	98.93	111.40
11	F2	27	LEU	CB-CG-CD2	-5.67	101.36	111.00
10	m4	156	LEU	CB-CG-CD2	-5.67	101.36	111.00
11	v5	131	VAL	CG1-CB-CG2	-5.67	101.83	110.90
11	L7	170	ASP	CB-CG-OD2	5.67	123.40	118.30
18	j9	150	LEU	CB-CG-CD2	-5.67	101.36	111.00
10	y9	142	ARG	NE-CZ-NH2	5.67	123.13	120.30
11	J4	28	LYS	CD-CE-NZ	5.67	124.73	111.70
18	c5	88	ILE	CG1-CB-CG2	-5.67	98.94	111.40
11	J7	84	ARG	NE-CZ-NH2	-5.67	117.47	120.30
10	k7	91	ARG	NE-CZ-NH1	-5.67	117.47	120.30
10	q5	92	LEU	CB-CG-CD1	-5.66	101.37	111.00
24	gy	192	TYR	CB-CG-CD1	-5.66	117.60	121.00
4	P1	83	ARG	NE-CZ-NH2	-5.66	117.47	120.30
10	I4	163	LEU	CB-CG-CD2	-5.66	101.38	111.00
18	j5	120	LEU	CB-CG-CD2	5.66	120.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	p7	77	ARG	NE-CZ-NH2	-5.66	117.47	120.30
12	ez	78	LEU	CB-CG-CD2	5.66	120.62	111.00
10	Y7	157	ASP	CB-CG-OD2	5.66	123.39	118.30
11	t9	98	LEU	CB-CG-CD1	-5.66	101.38	111.00
10	dA	163	LEU	CB-CG-CD2	-5.66	101.38	111.00
21	ew	201	ARG	N-CA-C	-5.66	95.72	111.00
14	e8	193	PHE	CB-CG-CD2	-5.66	116.84	120.80
15	bW	74	ARG	NE-CZ-NH2	-5.66	117.47	120.30
8	b2	335	PHE	CB-CG-CD1	-5.66	116.84	120.80
11	r4	129	ARG	NE-CZ-NH2	-5.66	117.47	120.30
10	E5	163	LEU	CB-CG-CD2	-5.66	101.39	111.00
10	db	38	LEU	CB-CG-CD2	5.66	120.61	111.00
7	m1	83	ARG	NE-CZ-NH1	5.65	123.13	120.30
11	f3	129	ARG	NE-CZ-NH1	5.65	123.13	120.30
11	p7	77	ARG	NE-CZ-NH1	5.65	123.13	120.30
11	fj	27	LEU	CA-CB-CG	5.65	128.31	115.30
5	l1	76	ARG	NE-CZ-NH1	-5.65	117.47	120.30
10	u4	163	LEU	CB-CG-CD2	-5.65	101.39	111.00
11	F6	134	MET	CG-SD-CE	-5.65	91.16	100.20
11	X7	105	LEU	CB-CG-CD2	-5.65	101.39	111.00
4	N1	35	ARG	NE-CZ-NH2	-5.65	117.47	120.30
5	W1	77	ARG	NH1-CZ-NH2	5.65	125.62	119.40
10	W7	138	LEU	CA-CB-CG	5.65	128.29	115.30
3	F1	174	LEU	CA-CB-CG	5.65	128.29	115.30
5	c1	91	TYR	CG-CD2-CE2	5.65	125.82	121.30
10	I7	66	LEU	CB-CG-CD2	-5.65	101.40	111.00
12	aY	293	LEU	CB-CG-CD2	-5.65	101.40	111.00
17	b4	93	ARG	NE-CZ-NH1	-5.65	117.48	120.30
10	S6	138	LEU	CA-CB-CG	5.65	128.28	115.30
10	eQ	17	ARG	NE-CZ-NH1	-5.65	117.48	120.30
13	b3	276	LEU	CB-CG-CD2	-5.64	101.40	111.00
10	G6	19	PRO	CA-N-CD	-5.64	103.60	111.50
5	M1	76	ARG	NE-CZ-NH1	-5.64	117.48	120.30
10	cu	138	LEU	CB-CG-CD2	-5.64	101.41	111.00
11	V6	91	ARG	NE-CZ-NH2	-5.64	117.48	120.30
11	eP	27	LEU	CB-CG-CD2	-5.64	101.41	111.00
11	lh	142	ILE	CG1-CB-CG2	-5.64	98.99	111.40
11	eB	152	GLU	OE1-CD-OE2	-5.64	116.53	123.30
10	eE	142	ARG	NE-CZ-NH2	5.64	123.12	120.30
10	lc	17	ARG	NE-CZ-NH1	5.64	123.12	120.30
11	y8	13	ASP	CB-CG-OD2	5.64	123.37	118.30
11	r9	117	TYR	CG-CD2-CE2	-5.64	116.79	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	bg	63	PHE	CB-CG-CD1	-5.64	116.85	120.80
5	l1	97	LEU	CB-CG-CD2	-5.63	101.42	111.00
11	ld	84	ARG	NE-CZ-NH2	-5.63	117.48	120.30
18	e5	37	ARG	NE-CZ-NH2	-5.63	117.48	120.30
5	O1	97	LEU	CB-CG-CD2	-5.63	101.43	111.00
10	C7	18	PHE	CB-CG-CD2	5.63	124.74	120.80
18	e4	37	ARG	NE-CZ-NH2	-5.63	117.49	120.30
11	x4	84	ARG	NE-CZ-NH2	-5.63	117.49	120.30
17	k5	91	TYR	CZ-CE2-CD2	-5.63	114.74	119.80
10	dJ	2	LYS	CD-CE-NZ	5.63	124.64	111.70
5	x1	87	TYR	CG-CD2-CE2	-5.62	116.80	121.30
10	bU	142	ARG	NE-CZ-NH2	-5.62	117.49	120.30
11	N6	91	ARG	NE-CZ-NH2	-5.62	117.49	120.30
19	a8	300	ARG	NE-CZ-NH1	-5.62	117.49	120.30
11	av	84	ARG	NE-CZ-NH1	-5.62	117.49	120.30
10	eS	142	ARG	NE-CZ-NH1	-5.62	117.49	120.30
25	ka	321	VAL	N-CA-C	-5.62	95.82	111.00
10	q7	91	ARG	NE-CZ-NH1	-5.62	117.49	120.30
12	A2	147	ARG	NE-CZ-NH2	-5.62	117.49	120.30
10	q9	91	ARG	NE-CZ-NH2	5.62	123.11	120.30
11	fw	27	LEU	CA-CB-CG	5.62	128.22	115.30
11	F6	91	ARG	NE-CZ-NH1	-5.62	117.49	120.30
11	B7	84	ARG	CG-CD-NE	-5.62	100.00	111.80
11	B5	33	ASP	CB-CG-OD2	5.62	123.35	118.30
11	Z6	78	ARG	NE-CZ-NH2	5.61	123.11	120.30
11	iF	59	MET	CG-SD-CE	5.61	109.18	100.20
10	j6	91	ARG	NE-CZ-NH2	5.61	123.11	120.30
11	aB	91	ARG	NE-CZ-NH2	-5.61	117.49	120.30
11	lh	98	LEU	CB-CG-CD1	-5.61	101.46	111.00
10	y5	89	TYR	CB-CG-CD2	-5.61	117.63	121.00
10	g6	66	LEU	CB-CG-CD2	-5.61	101.46	111.00
11	eB	7	ARG	NE-CZ-NH1	5.61	123.11	120.30
4	s1	52	LYS	CD-CE-NZ	5.61	124.60	111.70
14	C2	218	ARG	NE-CZ-NH1	5.61	123.10	120.30
18	l5	15	ARG	NE-CZ-NH2	-5.61	117.50	120.30
12	Z9	270	ARG	NE-CZ-NH2	-5.61	117.50	120.30
5	j1	19	LEU	CB-CG-CD1	-5.61	101.47	111.00
5	j1	77	ARG	NE-CZ-NH1	-5.61	117.50	120.30
13	b3	149	ARG	NE-CZ-NH2	-5.60	117.50	120.30
5	n1	13	ASP	CB-CG-OD2	5.60	123.34	118.30
4	w1	29	PHE	CG-CD2-CE2	5.60	126.96	120.80
10	E6	120	LEU	CB-CG-CD2	5.60	120.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	D7	98	LEU	CB-CG-CD1	-5.60	101.47	111.00
10	E7	1	MET	CB-CG-SD	5.60	129.21	112.40
11	x9	27	LEU	CB-CG-CD2	-5.60	101.47	111.00
25	kb	195	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A1	191	ARG	NE-CZ-NH1	-5.60	117.50	120.30
10	M6	17	ARG	NE-CZ-NH1	5.60	123.10	120.30
11	J4	2	LEU	CB-CG-CD1	-5.60	101.48	111.00
10	G5	135	ARG	NE-CZ-NH2	5.60	123.10	120.30
15	bW	6	LEU	CA-CB-CG	5.60	128.18	115.30
10	eC	85	ASP	CB-CG-OD2	5.60	123.34	118.30
11	F4	33	ASP	CB-CG-OD2	5.60	123.34	118.30
10	U7	17	ARG	NE-CZ-NH1	5.60	123.10	120.30
11	ax	27	LEU	CB-CG-CD2	-5.60	101.48	111.00
11	bB	91	ARG	NE-CZ-NH2	-5.60	117.50	120.30
11	eP	7	ARG	NE-CZ-NH1	5.60	123.10	120.30
5	l1	160	LEU	CB-CG-CD2	5.59	120.51	111.00
11	v3	88	ILE	CG1-CB-CG2	-5.59	99.09	111.40
18	cf	105	LEU	CB-CG-CD2	-5.59	101.49	111.00
11	eD	129	ARG	NE-CZ-NH2	-5.59	117.50	120.30
13	B2	276	LEU	CB-CG-CD2	-5.59	101.49	111.00
10	ay	142	ARG	NE-CZ-NH2	5.59	123.10	120.30
11	B5	109	CYS	CA-CB-SG	-5.59	103.93	114.00
11	L4	91	ARG	NE-CZ-NH1	-5.59	117.50	120.30
11	z6	91	ARG	NE-CZ-NH1	5.59	123.09	120.30
11	J7	78	ARG	NE-CZ-NH1	-5.59	117.50	120.30
10	i7	92	LEU	CB-CG-CD1	-5.59	101.50	111.00
10	bm	163	LEU	CB-CG-CD2	-5.59	101.50	111.00
24	gz	192	TYR	CB-CG-CD1	-5.59	117.65	121.00
4	o1	35	ARG	NE-CZ-NH2	-5.59	117.51	120.30
12	A2	170	TYR	CE1-CZ-OH	-5.59	105.01	120.10
5	p1	75	THR	CA-CB-CG2	-5.59	104.58	112.40
18	j5	84	ARG	CB-CG-CD	-5.59	97.08	111.60
17	be	93	ARG	NE-CZ-NH2	-5.59	117.51	120.30
17	ce	30	ARG	NE-CZ-NH2	-5.59	117.51	120.30
11	P6	84	ARG	NE-CZ-NH2	-5.58	117.51	120.30
10	cu	85	ASP	CB-CG-OD1	5.58	123.32	118.30
10	cm	85	ASP	CB-CG-OD2	5.58	123.32	118.30
10	x8	142	ARG	NE-CZ-NH2	5.58	123.09	120.30
11	D5	91	ARG	NE-CZ-NH1	-5.58	117.51	120.30
15	W9	113	ARG	NE-CZ-NH2	5.58	123.09	120.30
10	K7	142	ARG	CG-CD-NE	5.58	123.51	111.80
18	bj	125	THR	CA-CB-CG2	-5.58	104.59	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	dW	2	LYS	CD-CE-NZ	5.58	124.52	111.70
10	la	65	TYR	CB-CG-CD1	5.58	124.34	121.00
11	N7	77	ARG	NE-CZ-NH2	-5.57	117.51	120.30
17	cg	63	PHE	CB-CG-CD1	-5.57	116.90	120.80
11	dL	52	VAL	CG1-CB-CG2	-5.57	101.98	110.90
5	t1	14	VAL	CG1-CB-CG2	5.57	119.82	110.90
18	bf	15	ARG	NE-CZ-NH2	-5.57	117.51	120.30
4	b1	36	ARG	NE-CZ-NH2	5.57	123.09	120.30
10	w3	143	ASP	CB-CG-OD2	-5.57	113.29	118.30
10	m5	156	LEU	CB-CG-CD2	-5.57	101.53	111.00
11	T6	113	LEU	CB-CG-CD1	-5.57	101.53	111.00
14	d8	279	ARG	NE-CZ-NH2	-5.57	117.51	120.30
10	by	91	ARG	NH1-CZ-NH2	-5.57	113.27	119.40
12	A2	152	THR	CA-CB-CG2	-5.57	104.60	112.40
18	cj	85	ASP	CB-CG-OD2	5.57	123.31	118.30
10	M7	138	LEU	CA-CB-CG	5.57	128.10	115.30
11	cz	84	ARG	NE-CZ-NH1	-5.57	117.52	120.30
10	u5	163	LEU	CB-CG-CD2	-5.57	101.54	111.00
10	Q6	38	LEU	CB-CG-CD2	5.57	120.46	111.00
11	n7	91	ARG	NE-CZ-NH2	-5.57	117.52	120.30
10	lq	63	TYR	CZ-CE2-CD2	5.57	124.81	119.80
11	B3	129	ARG	NE-CZ-NH1	-5.56	117.52	120.30
11	t6	153	ILE	CG1-CB-CG2	-5.56	99.16	111.40
11	fs	77	ARG	NE-CZ-NH1	5.56	123.08	120.30
10	q5	33	ARG	NE-CZ-NH2	5.56	123.08	120.30
17	bi	93	ARG	NE-CZ-NH2	-5.56	117.52	120.30
10	s4	135	ARG	NE-CZ-NH2	5.56	123.08	120.30
11	z4	2	LEU	CB-CG-CD1	-5.56	101.55	111.00
11	J6	37	ARG	NE-CZ-NH2	5.56	123.08	120.30
10	E7	44	LEU	CB-CG-CD1	-5.56	101.55	111.00
11	J9	2	LEU	CB-CG-CD1	5.56	120.45	111.00
21	ex	201	ARG	N-CA-C	-5.56	96.00	111.00
12	Y5	105	LEU	CB-CG-CD2	-5.56	101.56	111.00
18	e5	108	ARG	NE-CZ-NH1	5.56	123.08	120.30
4	P1	82	LEU	CB-CG-CD2	-5.55	101.56	111.00
10	cx	163	LEU	CB-CG-CD2	-5.55	101.56	111.00
11	br	50	CYS	CA-CB-SG	5.55	124.00	114.00
10	C7	67	LYS	CD-CE-NZ	5.55	124.47	111.70
10	y9	37	ARG	NE-CZ-NH1	5.55	123.08	120.30
10	W2	49	GLU	OE1-CD-OE2	5.55	129.96	123.30
10	q4	114	ARG	NE-CZ-NH1	-5.55	117.53	120.30
11	t5	113	LEU	CB-CG-CD2	-5.55	101.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	bi	57	GLN	CB-CG-CD	5.55	126.03	111.60
18	bj	38	LEU	CB-CG-CD2	5.55	120.43	111.00
18	cj	141	LEU	CB-CG-CD2	-5.55	101.56	111.00
11	ld	38	LEU	CB-CG-CD2	5.55	120.43	111.00
11	v2	91	ARG	NE-CZ-NH2	-5.55	117.53	120.30
10	j6	1	MET	CA-CB-CG	-5.55	103.87	113.30
10	C7	86	VAL	CA-CB-CG2	5.55	119.22	110.90
10	y5	91	ARG	NE-CZ-NH2	-5.54	117.53	120.30
12	ey	317	ARG	NE-CZ-NH2	5.54	123.07	120.30
10	C6	89	TYR	CB-CG-CD2	-5.54	117.67	121.00
14	d9	138	ARG	NE-CZ-NH2	-5.54	117.53	120.30
10	lu	118	ARG	NE-CZ-NH2	-5.54	117.53	120.30
5	e1	94	TYR	CB-CG-CD1	-5.54	117.67	121.00
10	o3	87	ASP	CB-CG-OD2	5.54	123.29	118.30
10	A4	143	ASP	CB-CG-OD1	5.54	123.29	118.30
11	t9	108	ARG	NE-CZ-NH1	-5.54	117.53	120.30
10	ay	120	LEU	CB-CG-CD2	5.54	120.42	111.00
4	k1	116	TYR	CB-CG-CD1	-5.54	117.68	121.00
12	a3	151	ARG	NE-CZ-NH2	-5.54	117.53	120.30
17	i5	17	ARG	NE-CZ-NH2	-5.54	117.53	120.30
10	G7	138	LEU	CB-CG-CD2	-5.54	101.58	111.00
11	az	109	CYS	CA-CB-SG	5.54	123.97	114.00
12	ey	44	ASP	CB-CG-OD1	5.54	123.29	118.30
5	r1	38	VAL	CA-CB-CG1	-5.54	102.59	110.90
4	w1	17	TYR	CB-CG-CD1	-5.54	117.68	121.00
10	G4	83	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
12	34	105	LEU	CB-CG-CD2	-5.54	101.59	111.00
18	e4	85	ASP	CB-CG-OD2	5.54	123.28	118.30
11	an	98	LEU	CB-CG-CD1	-5.54	101.58	111.00
11	v4	131	VAL	CG1-CB-CG2	-5.54	102.04	110.90
11	dN	41	VAL	CG1-CB-CG2	-5.54	102.04	110.90
13	B2	149	ARG	NE-CZ-NH2	-5.54	117.53	120.30
10	q4	92	LEU	CB-CG-CD1	-5.53	101.59	111.00
12	Z9	147	ARG	NE-CZ-NH2	5.53	123.07	120.30
10	dA	81	LYS	CG-CD-CE	5.53	128.50	111.90
4	R1	131	ARG	NE-CZ-NH1	5.53	123.06	120.30
8	a2	739	ARG	NE-CZ-NH2	5.53	123.06	120.30
10	q3	62	LYS	CD-CE-NZ	-5.53	98.98	111.70
10	q5	157	ASP	CB-CG-OD2	5.53	123.28	118.30
10	C7	52	VAL	CA-CB-CG2	-5.53	102.61	110.90
10	o7	66	LEU	CB-CG-CD2	-5.53	101.60	111.00
11	N4	84	ARG	NH1-CZ-NH2	5.53	125.48	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	cm	81	LYS	CD-CE-NZ	-5.53	98.98	111.70
4	N1	44	THR	CA-CB-CG2	-5.53	104.66	112.40
4	y1	91	LEU	CB-CG-CD1	5.53	120.40	111.00
10	I4	85	ASP	CB-CG-OD1	5.53	123.28	118.30
10	U7	39	GLU	OE1-CD-OE2	5.53	129.93	123.30
10	E9	91	ARG	NE-CZ-NH2	5.53	123.06	120.30
10	du	140	VAL	CG1-CB-CG2	-5.53	102.06	110.90
12	ez	225	MET	CG-SD-CE	-5.53	91.36	100.20
5	z1	14	VAL	CG1-CB-CG2	5.53	119.74	110.90
11	R7	153	ILE	CG1-CB-CG2	-5.53	99.24	111.40
12	34	315	MET	CG-SD-CE	5.52	109.04	100.20
15	W9	227	ASP	CB-CG-OD2	5.52	123.27	118.30
5	e1	91	TYR	CG-CD2-CE2	5.52	125.72	121.30
4	q1	29	PHE	CG-CD2-CE2	5.52	126.87	120.80
18	l5	105	LEU	CA-CB-CG	5.52	128.00	115.30
11	p6	30	PHE	CB-CG-CD2	5.52	124.67	120.80
11	N7	134	MET	CG-SD-CE	-5.52	91.36	100.20
10	s7	138	LEU	CB-CG-CD2	-5.52	101.61	111.00
12	A2	293	LEU	CB-CG-CD2	-5.52	101.61	111.00
10	k3	135	ARG	CG-CD-NE	-5.52	100.21	111.80
12	bY	225	MET	CA-CB-CG	5.52	122.69	113.30
19	a8	330	ARG	NE-CZ-NH1	-5.52	117.54	120.30
11	y7	36	LYS	CD-CE-NZ	5.52	124.39	111.70
10	o9	17	ARG	NE-CZ-NH2	-5.52	117.54	120.30
10	aU	163	LEU	CB-CG-CD2	-5.52	101.62	111.00
18	cf	15	ARG	NE-CZ-NH1	5.52	123.06	120.30
17	b4	111	LEU	CB-CG-CD1	-5.52	101.62	111.00
11	lx	108	ARG	CD-NE-CZ	5.52	131.32	123.60
5	v1	65	ILE	CG1-CB-CG2	-5.51	99.27	111.40
8	b2	239	ARG	NE-CZ-NH2	-5.51	117.54	120.30
15	14	154	PHE	CB-CG-CD1	-5.51	116.94	120.80
10	I6	138	LEU	CB-CG-CD2	-5.51	101.62	111.00
11	az	82	CYS	CA-CB-SG	-5.51	104.07	114.00
11	cs	84	ARG	NE-CZ-NH1	-5.51	117.54	120.30
12	34	191	LYS	CD-CE-NZ	5.51	124.38	111.70
10	A7	44	LEU	CB-CG-CD1	-5.51	101.63	111.00
10	M7	8	THR	CA-CB-CG2	-5.51	104.68	112.40
10	es	163	LEU	CB-CG-CD2	-5.51	101.63	111.00
11	t6	129	ARG	NE-CZ-NH1	-5.51	117.54	120.30
10	K7	89	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
14	c8	279	ARG	CG-CD-NE	-5.51	100.22	111.80
14	d9	57	VAL	CA-CB-CG1	-5.51	102.63	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	gm	84	ARG	NE-CZ-NH1	-5.51	117.54	120.30
11	z3	129	ARG	NE-CZ-NH2	-5.51	117.55	120.30
17	bk	93	ARG	NH1-CZ-NH2	5.51	125.46	119.40
17	ca	134	GLU	OE1-CD-OE2	5.51	129.91	123.30
15	bW	104	TYR	CB-CG-CD2	-5.51	117.69	121.00
12	Y5	170	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
11	X7	79	MET	CG-SD-CE	-5.51	91.39	100.20
11	n7	84	ARG	CG-CD-NE	-5.51	100.23	111.80
11	lx	84	ARG	NE-CZ-NH2	-5.51	117.55	120.30
5	x1	38	VAL	CA-CB-CG1	-5.50	102.64	110.90
2	D1	133	LEU	CB-CG-CD1	-5.50	101.64	111.00
5	O1	90	ARG	NE-CZ-NH2	-5.50	117.55	120.30
14	C2	66	ILE	CB-CG1-CD1	-5.50	98.49	113.90
11	F5	2	LEU	CB-CG-CD1	-5.50	101.65	111.00
11	dV	129	ARG	NE-CZ-NH2	-5.50	117.55	120.30
8	b2	851	LEU	N-CA-C	5.50	125.85	111.00
11	B3	79	MET	CG-SD-CE	-5.50	91.40	100.20
11	B7	50	CYS	CA-CB-SG	5.50	123.90	114.00
12	a3	152	THR	CA-CB-CG2	-5.50	104.70	112.40
10	k3	44	LEU	CB-CG-CD1	-5.50	101.66	111.00
10	o7	44	LEU	CB-CG-CD1	5.50	120.34	111.00
11	cs	170	ASP	CB-CG-OD2	-5.50	113.35	118.30
10	cv	13	ASP	CB-CG-OD2	-5.50	113.35	118.30
8	a2	533	TYR	CB-CG-CD2	-5.50	117.70	121.00
15	R8	179	LEU	CB-CG-CD2	-5.50	101.66	111.00
10	gm	37	ARG	NE-CZ-NH1	-5.50	117.55	120.30
11	R6	104	VAL	CG1-CB-CG2	5.49	119.69	110.90
11	d6	50	CYS	CA-CB-SG	5.49	123.89	114.00
17	k9	161	LEU	CB-CG-CD2	-5.49	101.66	111.00
15	bW	78	ILE	CG1-CB-CG2	-5.49	99.32	111.40
10	dW	9	ILE	CG1-CB-CG2	-5.49	99.31	111.40
11	gv	108	ARG	NE-CZ-NH1	5.49	123.05	120.30
11	an	129	ARG	NE-CZ-NH1	5.49	123.05	120.30
5	S1	78	TYR	CB-CG-CD2	-5.49	117.71	121.00
12	b8	284	TYR	CB-CG-CD1	-5.49	117.71	121.00
10	fp	17	ARG	NE-CZ-NH1	-5.49	117.56	120.30
11	J5	84	ARG	NH1-CZ-NH2	5.49	125.44	119.40
15	W5	23	LEU	CB-CG-CD2	-5.49	101.67	111.00
18	l5	67	ILE	CG1-CB-CG2	5.49	123.47	111.40
11	X7	37	ARG	NE-CZ-NH2	-5.49	117.56	120.30
10	eG	137	ARG	NE-CZ-NH2	5.49	123.04	120.30
10	A6	114	ARG	NE-CZ-NH1	5.48	123.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	lv	28	LYS	CB-CG-CD	5.48	125.86	111.60
4	G1	94	TYR	CE1-CZ-OH	-5.48	105.30	120.10
5	e1	97	LEU	CB-CG-CD2	-5.48	101.68	111.00
9	c2	52	TYR	CG-CD1-CE1	-5.48	116.92	121.30
11	F6	120	LEU	CD1-CG-CD2	-5.48	94.06	110.50
12	U8	270	ARG	NE-CZ-NH2	-5.48	117.56	120.30
11	eV	120	LEU	CB-CG-CD2	5.48	120.32	111.00
4	y1	84	ASP	OD1-CG-OD2	-5.48	112.89	123.30
4	y1	87	TYR	CB-CG-CD2	-5.48	117.71	121.00
5	W1	72	MET	CG-SD-CE	5.48	108.97	100.20
17	a4	92	LEU	CB-CG-CD1	5.48	120.31	111.00
11	r7	77	ARG	NE-CZ-NH2	-5.48	117.56	120.30
10	v8	18	PHE	CB-CG-CD2	5.48	124.64	120.80
12	34	170	TYR	CZ-CE2-CD2	-5.48	114.87	119.80
10	E5	85	ASP	CB-CG-OD1	5.48	123.23	118.30
4	b1	155	TYR	CB-CG-CD2	-5.47	117.72	121.00
11	x4	88	ILE	CG1-CB-CG2	-5.47	99.36	111.40
15	R8	227	ASP	CB-CG-OD2	5.47	123.23	118.30
10	u9	138	LEU	CB-CG-CD1	-5.47	101.69	111.00
4	G1	155	TYR	CB-CG-CD2	-5.47	117.72	121.00
5	S1	94	TYR	CZ-CE2-CD2	-5.47	114.87	119.80
4	b1	109	LEU	CB-CG-CD2	-5.47	101.70	111.00
18	cd	104	VAL	CG1-CB-CG2	5.47	119.66	110.90
11	br	13	ASP	CB-CG-OD2	5.47	123.22	118.30
10	m9	91	ARG	NE-CZ-NH2	5.47	123.03	120.30
25	ka	283	PHE	CZ-CE2-CD2	-5.47	113.53	120.10
13	b3	66	TYR	CB-CG-CD1	-5.47	117.72	121.00
11	lp	109	CYS	CA-CB-SG	5.47	123.84	114.00
6	Q1	85	ASP	CB-CG-OD2	5.47	123.22	118.30
8	a2	776	LEU	CA-CB-CG	5.47	127.87	115.30
18	l4	105	LEU	CA-CB-CG	5.47	127.87	115.30
18	l5	13	ASP	CB-CG-OD2	-5.47	113.38	118.30
10	M6	142	ARG	NE-CZ-NH1	5.47	123.03	120.30
11	e6	33	ASP	CB-CG-OD2	-5.47	113.38	118.30
11	ax	88	ILE	CG1-CB-CG2	-5.47	99.37	111.40
10	bw	163	LEU	CB-CG-CD2	-5.47	101.71	111.00
4	P1	75	GLU	OE1-CD-OE2	-5.46	116.74	123.30
10	ay	37	ARG	NE-CZ-NH1	5.46	123.03	120.30
12	dx	166	LEU	CA-CB-CG	-5.46	102.73	115.30
11	ec	77	ARG	NE-CZ-NH2	-5.46	117.57	120.30
11	ee	109	CYS	CA-CB-SG	5.46	123.84	114.00
10	eC	17	ARG	NE-CZ-NH1	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	iA	2	LYS	CD-CE-NZ	-5.46	99.13	111.70
11	kR	95	TYR	CG-CD2-CE2	-5.46	116.93	121.30
10	ef	156	LEU	CB-CG-CD2	-5.46	101.71	111.00
10	iB	95	TYR	CG-CD2-CE2	5.46	125.67	121.30
14	e8	46	LEU	CA-CB-CG	5.46	127.86	115.30
18	cj	125	THR	CA-CB-CG2	-5.46	104.76	112.40
11	F5	28	LYS	CD-CE-NZ	5.46	124.25	111.70
11	n7	107	ASP	CB-CG-OD2	-5.46	113.39	118.30
11	cR	149	ARG	NE-CZ-NH2	-5.46	117.57	120.30
5	U1	126	THR	CA-CB-CG2	-5.46	104.76	112.40
5	h1	76	ARG	NE-CZ-NH1	-5.46	117.57	120.30
11	F4	13	ASP	CB-CG-OD2	-5.46	113.39	118.30
17	k5	50	ARG	NE-CZ-NH1	5.46	123.03	120.30
10	C9	142	ARG	NE-CZ-NH2	5.46	123.03	120.30
4	T1	151	PHE	CG-CD1-CE1	-5.46	114.80	120.80
10	s4	163	LEU	CB-CG-CD2	-5.45	101.73	111.00
10	A6	156	LEU	CB-CG-CD2	-5.45	101.73	111.00
12	b9	260	ARG	NE-CZ-NH2	-5.45	117.57	120.30
4	k1	131	ARG	NE-CZ-NH2	-5.45	117.58	120.30
11	ga	37	ARG	NE-CZ-NH2	5.45	123.03	120.30
10	ao	17	ARG	NE-CZ-NH2	-5.45	117.58	120.30
10	dG	54	GLU	CA-CB-CG	5.45	125.39	113.40
16	X5	364	SER	N-CA-CB	-5.45	102.33	110.50
11	X7	91	ARG	NE-CZ-NH2	-5.45	117.58	120.30
11	H9	110	LEU	CA-CB-CG	5.45	127.83	115.30
11	ax	134	MET	CG-SD-CE	-5.45	91.48	100.20
4	s1	90	ARG	NE-CZ-NH2	5.45	123.02	120.30
10	K2	9	ILE	CG1-CB-CG2	-5.45	99.42	111.40
10	i3	90	MET	CG-SD-CE	5.45	108.91	100.20
10	G6	62	LYS	CD-CE-NZ	-5.45	99.18	111.70
10	G6	138	LEU	CA-CB-CG	5.45	127.82	115.30
16	X9	199	ARG	NE-CZ-NH2	5.45	123.02	120.30
11	bH	77	ARG	NE-CZ-NH2	-5.44	117.58	120.30
4	f1	83	ARG	NE-CZ-NH2	-5.44	117.58	120.30
10	bS	137	ARG	NE-CZ-NH1	-5.44	117.58	120.30
10	A5	2	LYS	CD-CE-NZ	5.44	124.21	111.70
12	U8	231	MET	CG-SD-CE	5.44	108.91	100.20
10	cy	17	ARG	NE-CZ-NH2	-5.44	117.58	120.30
10	m4	138	LEU	CB-CG-CD2	-5.44	101.75	111.00
11	D9	13	ASP	CB-CG-OD2	5.44	123.19	118.30
11	eH	38	LEU	CB-CG-CD1	-5.44	101.75	111.00
16	S8	199	ARG	NE-CZ-NH2	5.44	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	cd	39	ASP	CB-CG-OD2	-5.44	113.41	118.30
18	e4	84	ARG	NE-CZ-NH2	5.43	123.02	120.30
16	S8	209	MET	CG-SD-CE	5.43	108.90	100.20
23	lz	202	ARG	NE-CZ-NH2	-5.43	117.58	120.30
12	34	293	LEU	CB-CG-CD2	-5.43	101.77	111.00
18	h5	125	THR	CA-CB-CG2	-5.43	104.79	112.40
18	ch	57	ARG	NE-CZ-NH1	-5.43	117.58	120.30
4	P1	65	VAL	CG1-CB-CG2	-5.43	102.21	110.90
4	f1	62	ARG	NE-CZ-NH1	5.43	123.02	120.30
16	X9	104	LYS	CD-CE-NZ	-5.43	99.21	111.70
10	eW	137	ARG	NE-CZ-NH1	-5.43	117.58	120.30
11	Z2	129	ARG	NE-CZ-NH2	-5.43	117.58	120.30
18	j5	91	ARG	NE-CZ-NH2	5.43	123.02	120.30
11	bR	129	ARG	NE-CZ-NH1	5.43	123.02	120.30
11	dP	50	CYS	CA-CB-SG	5.43	123.78	114.00
4	s1	84	ASP	OD1-CG-OD2	-5.43	112.99	123.30
10	ej	163	LEU	CB-CG-CD2	-5.43	101.77	111.00
5	r1	91	TYR	CG-CD1-CE1	-5.43	116.96	121.30
8	b2	626	ARG	NE-CZ-NH2	-5.42	117.59	120.30
10	o2	2	LYS	CD-CE-NZ	5.42	124.18	111.70
11	F4	109	CYS	CA-CB-SG	-5.42	104.24	114.00
16	S8	104	LYS	CD-CE-NZ	-5.42	99.22	111.70
10	y9	120	LEU	CB-CG-CD2	5.42	120.22	111.00
10	bK	17	ARG	NE-CZ-NH1	5.42	123.01	120.30
11	H7	41	VAL	CG1-CB-CG2	-5.42	102.22	110.90
11	B3	91	ARG	NE-CZ-NH1	5.42	123.01	120.30
13	B2	66	TYR	CB-CG-CD1	-5.42	117.75	121.00
17	k5	154	LEU	CB-CG-CD2	-5.42	101.79	111.00
11	z9	109	CYS	CA-CB-SG	5.42	123.76	114.00
4	R1	47	ARG	NE-CZ-NH1	5.42	123.01	120.30
3	E1	59	VAL	N-CA-C	-5.42	96.38	111.00
8	b2	564	ARG	NE-CZ-NH1	-5.42	117.59	120.30
11	X6	66	LEU	CB-CG-CD2	-5.42	101.79	111.00
10	I7	1	MET	CB-CG-SD	5.42	128.65	112.40
18	h9	125	THR	CA-CB-CG2	-5.42	104.82	112.40
11	L4	84	ARG	CB-CG-CD	-5.42	97.52	111.60
10	cu	138	LEU	CA-CB-CG	5.42	127.75	115.30
8	a2	867	LEU	CB-CG-CD2	-5.41	101.80	111.00
10	j8	114	ARG	NE-CZ-NH1	5.41	123.01	120.30
11	D7	50	CYS	CA-CB-SG	5.41	123.74	114.00
11	F7	91	ARG	NE-CZ-NH1	5.41	123.01	120.30
10	i7	138	LEU	CA-CB-CG	5.41	127.75	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	bw	89	TYR	CB-CG-CD2	-5.41	117.75	121.00
20	dy	304	TYR	CB-CG-CD1	5.41	124.25	121.00
5	j1	97	LEU	CB-CG-CD1	-5.41	101.80	111.00
8	a2	579	LEU	CB-CG-CD2	5.41	120.20	111.00
10	E4	138	LEU	CB-CG-CD2	-5.41	101.80	111.00
17	k4	161	LEU	CB-CG-CD2	-5.41	101.80	111.00
23	lz	109	ARG	NE-CZ-NH2	-5.41	117.59	120.30
10	S6	17	ARG	NE-CZ-NH1	5.41	123.00	120.30
11	R7	33	ASP	CB-CG-OD2	-5.41	113.43	118.30
10	E9	157	ASP	CB-CG-OD1	-5.41	113.43	118.30
18	bj	85	ASP	CB-CG-OD2	5.41	123.17	118.30
10	gm	66	LEU	CB-CG-CD2	-5.41	101.80	111.00
5	H1	91	TYR	CG-CD2-CE2	5.41	125.63	121.30
18	l4	15	ARG	NE-CZ-NH2	-5.41	117.60	120.30
11	J7	59	MET	CG-SD-CE	5.41	108.85	100.20
10	aQ	140	VAL	C-N-CD	-5.41	108.70	120.60
18	l4	19	LEU	CB-CG-CD1	-5.41	101.81	111.00
11	r7	88	ILE	CG1-CB-CG2	-5.41	99.51	111.40
15	W9	164	ARG	NE-CZ-NH2	-5.41	117.60	120.30
10	le	142	ARG	CG-CD-NE	5.41	123.16	111.80
5	h1	126	THR	CA-CB-CG2	-5.41	104.83	112.40
4	q1	116	TYR	CG-CD2-CE2	5.41	125.62	121.30
10	W6	17	ARG	NE-CZ-NH1	5.41	123.00	120.30
11	ei	38	LEU	CA-CB-CG	5.41	127.73	115.30
12	ey	48	ARG	NE-CZ-NH2	-5.41	117.60	120.30
10	U6	66	LEU	CB-CG-CD2	-5.40	101.81	111.00
10	eq	135	ARG	NE-CZ-NH1	-5.40	117.60	120.30
11	d7	33	ASP	CB-CG-OD2	-5.40	113.44	118.30
17	cc	1	MET	CG-SD-CE	5.40	108.84	100.20
10	la	78	LYS	CD-CE-NZ	-5.40	99.27	111.70
11	t5	88	ILE	CG1-CB-CG2	-5.40	99.52	111.40
10	Q7	92	LEU	CB-CG-CD1	-5.40	101.82	111.00
15	W9	61	LEU	CB-CG-CD1	-5.40	101.82	111.00
18	al	77	ARG	CG-CD-NE	-5.40	100.46	111.80
18	bh	160	LEU	CA-CB-CG	5.40	127.72	115.30
10	eM	13	ASP	CB-CG-OD1	-5.40	113.44	118.30
10	gq	137	ARG	NE-CZ-NH2	-5.40	117.60	120.30
4	K1	112	VAL	CA-CB-CG1	5.40	119.00	110.90
11	V7	142	ILE	CG1-CB-CG2	-5.40	99.52	111.40
10	Q2	62	LYS	CD-CE-NZ	-5.40	99.29	111.70
11	N4	50	CYS	CA-CB-SG	5.40	123.72	114.00
18	h4	125	THR	CA-CB-CG2	-5.40	104.84	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	cr	88	ILE	CG1-CB-CG2	-5.40	99.53	111.40
11	X6	77	ARG	NE-CZ-NH1	5.39	123.00	120.30
17	ae	30	ARG	NE-CZ-NH2	5.39	123.00	120.30
10	E2	114	ARG	NE-CZ-NH1	-5.39	117.60	120.30
10	A4	105	LEU	CB-CG-CD1	-5.39	101.83	111.00
11	H7	77	ARG	NE-CZ-NH1	5.39	123.00	120.30
11	ap	1	MET	CG-SD-CE	5.39	108.83	100.20
12	dw	166	LEU	CA-CB-CG	-5.39	102.90	115.30
11	bH	108	ARG	NE-CZ-NH1	-5.39	117.61	120.30
10	eK	23	ASP	CB-CG-OD2	5.39	123.15	118.30
10	eO	163	LEU	CB-CG-CD2	-5.39	101.84	111.00
11	jJ	149	ARG	NE-CZ-NH2	5.39	123.00	120.30
10	q4	157	ASP	CB-CG-OD2	5.39	123.15	118.30
11	V6	30	PHE	CB-CG-CD1	-5.39	117.03	120.80
18	h9	78	ARG	NE-CZ-NH1	-5.39	117.61	120.30
18	cf	15	ARG	NE-CZ-NH2	-5.39	117.61	120.30
10	cw	163	LEU	CB-CG-CD2	-5.39	101.84	111.00
5	r1	87	TYR	CG-CD2-CE2	-5.38	116.99	121.30
10	y4	89	TYR	CB-CG-CD2	-5.38	117.77	121.00
16	S8	315	LYS	CD-CE-NZ	5.38	124.08	111.70
11	z9	82	CYS	CA-CB-SG	-5.38	104.31	114.00
17	ag	50	ARG	NE-CZ-NH1	-5.38	117.61	120.30
10	gf	114	ARG	NE-CZ-NH2	5.38	122.99	120.30
11	l3	133	ILE	CG1-CB-CG2	-5.38	99.56	111.40
10	s7	156	LEU	CA-CB-CG	5.38	127.68	115.30
17	g9	93	ARG	NE-CZ-NH2	-5.38	117.61	120.30
10	bt	84	ARG	CD-NE-CZ	-5.38	116.07	123.60
5	n1	84	ASP	CB-CG-OD1	-5.38	113.46	118.30
10	C5	83	TYR	CB-CG-CD1	-5.38	117.77	121.00
16	X9	209	MET	CG-SD-CE	5.38	108.81	100.20
18	cj	156	LEU	CB-CG-CD1	-5.38	101.86	111.00
3	E1	171	ARG	NE-CZ-NH1	-5.38	117.61	120.30
5	e1	90	ARG	NE-CZ-NH2	-5.38	117.61	120.30
10	q7	18	PHE	CB-CG-CD2	5.38	124.56	120.80
18	ch	160	LEU	CA-CB-CG	5.38	127.67	115.30
11	dY	109	CYS	CA-CB-SG	5.38	123.68	114.00
10	eK	137	ARG	NE-CZ-NH1	5.38	122.99	120.30
11	r6	41	VAL	CG1-CB-CG2	-5.38	102.30	110.90
18	cj	38	LEU	CB-CG-CD2	5.38	120.14	111.00
11	eT	88	ILE	CG1-CB-CG2	-5.38	99.58	111.40
10	I6	92	LEU	CB-CG-CD1	-5.37	101.86	111.00
10	cm	38	LEU	CB-CG-CD2	5.37	120.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	eW	13	ASP	CB-CG-OD1	-5.37	113.46	118.30
10	m5	24	LEU	CB-CG-CD2	5.37	120.13	111.00
18	ah	125	THR	CA-CB-CG2	-5.37	104.88	112.40
17	ak	161	LEU	CB-CG-CD2	-5.37	101.87	111.00
10	am	91	ARG	NE-CZ-NH2	5.37	122.99	120.30
12	Y5	293	LEU	CB-CG-CD2	-5.37	101.87	111.00
11	P6	120	LEU	CB-CG-CD2	-5.37	101.87	111.00
17	cc	86	ARG	NE-CZ-NH2	-5.37	117.61	120.30
11	cn	37	ARG	NE-CZ-NH2	5.37	122.98	120.30
11	B5	13	ASP	CB-CG-OD2	-5.37	113.47	118.30
17	a5	99	LEU	CA-CB-CG	5.37	127.65	115.30
11	cn	1	MET	CG-SD-CE	5.37	108.79	100.20
10	gu	53	LYS	CD-CE-NZ	5.37	124.05	111.70
12	34	259	LEU	CB-CG-CD2	-5.37	101.88	111.00
18	ab	19	LEU	CB-CG-CD2	-5.37	101.88	111.00
11	t9	88	ILE	CG1-CB-CG2	-5.37	99.60	111.40
10	gh	91	ARG	NE-CZ-NH1	5.37	122.98	120.30
12	a3	293	LEU	CB-CG-CD2	-5.36	101.88	111.00
11	v4	75	THR	N-CA-C	-5.36	96.52	111.00
14	e8	77	MET	CG-SD-CE	-5.36	91.62	100.20
10	bE	97	LEU	CB-CG-CD2	-5.36	101.88	111.00
11	cn	91	ARG	NE-CZ-NH1	5.36	122.98	120.30
10	dA	127	TYR	CB-CG-CD2	-5.36	117.78	121.00
10	la	163	LEU	CB-CG-CD2	-5.36	101.88	111.00
11	bo	59	MET	CG-SD-CE	5.36	108.78	100.20
5	p1	87	TYR	CG-CD1-CE1	-5.36	117.01	121.30
4	q1	27	LYS	CD-CE-NZ	5.36	124.03	111.70
10	bv	163	LEU	CB-CG-CD2	-5.36	101.89	111.00
10	bx	163	LEU	CB-CG-CD2	-5.36	101.89	111.00
12	dx	225	MET	CA-CB-CG	5.36	122.41	113.30
10	eM	131	PHE	CB-CG-CD2	-5.36	117.05	120.80
10	e2	18	PHE	CB-CG-CD1	-5.36	117.05	120.80
18	l5	125	THR	CA-CB-CG2	-5.36	104.90	112.40
10	C6	137	ARG	NE-CZ-NH2	-5.36	117.62	120.30
10	E7	89	TYR	CB-CG-CD2	-5.36	117.78	121.00
20	dy	135	ARG	NE-CZ-NH1	-5.36	117.62	120.30
4	w1	31	LEU	CB-CG-CD2	5.36	120.11	111.00
10	E6	24	LEU	CB-CG-CD2	-5.36	101.90	111.00
10	f7	120	LEU	CB-CG-CD1	5.36	120.11	111.00
12	b8	260	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	E1	243	ASP	CB-CG-OD1	5.35	123.12	118.30
11	P4	38	LEU	CB-CG-CD1	-5.35	101.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F6	170	ASP	CB-CG-OD2	5.35	123.12	118.30
11	a7	83	LEU	CB-CG-CD2	-5.35	101.90	111.00
11	at	88	ILE	CG1-CB-CG2	-5.35	99.62	111.40
16	24	111	ASP	CB-CG-OD2	5.35	123.12	118.30
18	j5	105	LEU	CA-CB-CG	5.35	127.60	115.30
10	s5	163	LEU	CB-CG-CD2	-5.35	101.91	111.00
14	d8	279	ARG	CG-CD-NE	-5.35	100.56	111.80
11	av	91	ARG	NE-CZ-NH2	-5.35	117.62	120.30
10	cm	37	ARG	NE-CZ-NH2	5.35	122.97	120.30
10	ct	38	LEU	CB-CG-CD2	5.35	120.09	111.00
10	eA	163	LEU	CB-CG-CD2	-5.35	101.91	111.00
1	B1	45	TYR	CB-CG-CD2	-5.35	117.79	121.00
4	b1	94	TYR	CE1-CZ-OH	-5.35	105.66	120.10
4	s1	87	TYR	CG-CD1-CE1	-5.35	117.02	121.30
11	B4	79	MET	CG-SD-CE	-5.35	91.64	100.20
11	L6	170	ASP	CB-CG-OD2	5.35	123.11	118.30
16	S8	296	ARG	NE-CZ-NH1	5.35	122.97	120.30
11	x9	98	LEU	CB-CG-CD1	-5.35	101.91	111.00
15	W9	61	LEU	CA-CB-CG	5.35	127.60	115.30
16	aX	282	ARG	NE-CZ-NH1	5.35	122.97	120.30
10	cK	91	ARG	NE-CZ-NH2	5.35	122.97	120.30
24	gz	188	ARG	NE-CZ-NH2	-5.35	117.63	120.30
11	iC	108	ARG	NE-CZ-NH1	5.35	122.97	120.30
16	bX	272	GLN	N-CA-C	-5.35	96.57	111.00
10	s5	135	ARG	NE-CZ-NH2	5.34	122.97	120.30
11	J7	19	VAL	CG1-CB-CG2	5.34	119.45	110.90
10	z8	18	PHE	CB-CG-CD2	5.34	124.54	120.80
17	aa	92	LEU	CB-CG-CD1	5.34	120.09	111.00
10	gq	85	ASP	CB-CG-OD2	5.34	123.11	118.30
10	h6	142	ARG	NE-CZ-NH2	5.34	122.97	120.30
12	Y5	315	MET	CG-SD-CE	5.34	108.75	100.20
10	Q7	8	THR	CA-CB-CG2	-5.34	104.92	112.40
10	aI	135	ARG	NE-CZ-NH2	-5.34	117.63	120.30
5	a1	36	LEU	CB-CG-CD1	5.34	120.08	111.00
5	h1	94	TYR	CG-CD2-CE2	5.34	125.57	121.30
17	k5	87	ASP	CB-CG-OD1	5.34	123.11	118.30
10	o5	44	LEU	CB-CG-CD1	-5.34	101.92	111.00
10	g7	33	ARG	NE-CZ-NH1	-5.34	117.63	120.30
11	r9	171	LYS	CD-CE-NZ	5.34	123.98	111.70
10	u3	91	ARG	NE-CZ-NH1	5.34	122.97	120.30
11	z9	108	ARG	CD-NE-CZ	5.34	131.07	123.60
10	Q6	89	TYR	CB-CG-CD2	-5.34	117.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	v7	41	VAL	CG1-CB-CG2	-5.34	102.36	110.90
11	bP	84	ARG	NE-CZ-NH1	-5.34	117.63	120.30
18	j5	110	LEU	CB-CG-CD2	-5.33	101.93	111.00
10	cS	91	ARG	NE-CZ-NH2	5.33	122.97	120.30
11	eL	120	LEU	CB-CG-CD2	5.33	120.07	111.00
11	Z3	77	ARG	NE-CZ-NH2	5.33	122.97	120.30
18	W8	19	LEU	CB-CG-CD1	5.33	120.06	111.00
18	bd	105	LEU	CB-CG-CD1	-5.33	101.94	111.00
12	ez	43	VAL	CG1-CB-CG2	-5.33	102.37	110.90
11	T6	91	ARG	NE-CZ-NH2	-5.33	117.64	120.30
10	A7	1	MET	CB-CG-SD	5.33	128.38	112.40
10	bE	89	TYR	CB-CG-CD2	-5.33	117.80	121.00
11	kT	120	LEU	CB-CG-CD2	5.33	120.06	111.00
2	C1	72	ARG	NE-CZ-NH2	-5.33	117.64	120.30
10	u2	17	ARG	NE-CZ-NH1	-5.33	117.64	120.30
10	M3	87	ASP	CB-CG-OD2	5.33	123.09	118.30
17	f5	30	ARG	NE-CZ-NH2	-5.33	117.64	120.30
11	t6	84	ARG	CG-CD-NE	-5.33	100.61	111.80
11	r7	84	ARG	CG-CD-NE	-5.33	100.61	111.80
18	cb	117	TYR	OH-CZ-CE2	-5.33	105.72	120.10
11	er	38	LEU	CB-CG-CD2	-5.33	101.94	111.00
11	T2	161	LEU	CB-CG-CD1	-5.33	101.95	111.00
10	G4	83	TYR	CB-CG-CD1	-5.33	117.81	121.00
16	X5	111	ASP	CB-CG-OD2	5.33	123.09	118.30
11	cL	149	ARG	NE-CZ-NH1	5.33	122.96	120.30
11	fa	27	LEU	CA-CB-CG	5.33	127.55	115.30
8	b2	345	PHE	CB-CG-CD2	-5.32	117.07	120.80
10	eW	25	GLU	OE1-CD-OE2	-5.32	116.91	123.30
10	gq	120	LEU	CB-CG-CD2	5.32	120.05	111.00
11	A8	88	ILE	CG1-CB-CG2	-5.32	99.70	111.40
11	gr	84	ARG	NE-CZ-NH2	-5.32	117.64	120.30
10	C9	85	ASP	CB-CG-OD2	5.32	123.09	118.30
15	bW	26	GLU	OE1-CD-OE2	5.32	129.68	123.30
11	H5	105	LEU	CB-CG-CD2	-5.32	101.96	111.00
10	I5	138	LEU	CB-CG-CD2	-5.32	101.96	111.00
15	R8	61	LEU	CA-CB-CG	5.32	127.53	115.30
11	eL	149	ARG	NE-CZ-NH1	5.32	122.96	120.30
23	lz	100	TYR	CG-CD2-CE2	5.32	125.55	121.30
10	k2	53	LYS	CD-CE-NZ	5.32	123.92	111.70
18	g5	125	THR	CA-CB-CG2	-5.32	104.96	112.40
10	s7	138	LEU	CA-CB-CG	5.32	127.53	115.30
10	dZ	84	ARG	NE-CZ-NH2	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	x1	91	TYR	CG-CD1-CE1	-5.31	117.05	121.30
11	N7	104	VAL	CG1-CB-CG2	5.31	119.40	110.90
11	lj	78	ARG	NE-CZ-NH1	-5.31	117.64	120.30
5	t1	107	ARG	NE-CZ-NH2	-5.31	117.64	120.30
11	v9	84	ARG	NE-CZ-NH1	-5.31	117.64	120.30
18	bj	160	LEU	CA-CB-CG	5.31	127.52	115.30
10	Y7	37	ARG	NE-CZ-NH2	-5.31	117.64	120.30
11	n4	91	ARG	NE-CZ-NH2	-5.31	117.65	120.30
10	s6	91	ARG	NE-CZ-NH2	-5.31	117.64	120.30
11	E8	2	LEU	CB-CG-CD1	5.31	120.03	111.00
10	E9	17	ARG	CG-CD-NE	-5.31	100.65	111.80
11	lv	78	ARG	NE-CZ-NH1	-5.31	117.65	120.30
11	iD	105	LEU	CB-CG-CD2	-5.31	101.97	111.00
5	r1	75	THR	CA-CB-CG2	-5.31	104.97	112.40
18	g4	166	ARG	NE-CZ-NH2	-5.31	117.65	120.30
10	k8	135	ARG	NE-CZ-NH1	5.31	122.95	120.30
10	W7	89	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
17	ag	30	ARG	NE-CZ-NH2	5.31	122.95	120.30
10	eQ	135	ARG	NE-CZ-NH2	-5.31	117.65	120.30
18	e5	160	LEU	CA-CB-CG	5.31	127.50	115.30
11	B6	28	LYS	CD-CE-NZ	5.30	123.90	111.70
10	u6	138	LEU	CA-CB-CG	5.30	127.50	115.30
10	w9	38	LEU	CB-CG-CD2	-5.30	101.98	111.00
4	f1	43	LEU	CB-CG-CD2	-5.30	101.98	111.00
10	g7	66	LEU	CB-CG-CD2	-5.30	101.98	111.00
11	h2	44	ILE	CG1-CB-CG2	-5.30	99.73	111.40
11	T2	120	LEU	CB-CG-CD2	-5.30	101.99	111.00
12	a3	269	TYR	CA-CB-CG	5.30	123.47	113.40
11	n9	98	LEU	CB-CG-CD1	-5.30	101.99	111.00
12	ez	48	ARG	NE-CZ-NH2	-5.30	117.65	120.30
5	S1	1	MET	CG-SD-CE	5.30	108.68	100.20
5	j1	78	TYR	CB-CG-CD2	-5.30	117.82	121.00
5	x1	83	ARG	NE-CZ-NH2	5.30	122.95	120.30
18	e4	160	LEU	CA-CB-CG	5.30	127.49	115.30
18	l4	125	THR	CA-CB-CG2	-5.30	104.98	112.40
11	L6	84	ARG	CG-CD-NE	-5.30	100.67	111.80
18	cj	160	LEU	CA-CB-CG	5.30	127.49	115.30
22	eY	141	ARG	NE-CZ-NH1	-5.30	117.65	120.30
11	n6	43	CYS	CA-CB-SG	-5.30	104.46	114.00
10	A9	163	LEU	CB-CG-CD2	-5.30	101.99	111.00
20	dy	264	LYS	CB-CG-CD	5.30	125.37	111.60
11	X7	120	LEU	CB-CG-CD2	-5.30	102.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	e8	64	GLY	N-CA-C	5.30	126.34	113.10
11	dX	45	VAL	CG1-CB-CG2	-5.30	102.42	110.90
11	lv	142	ILE	CG1-CB-CG2	-5.30	99.75	111.40
10	w3	78	LYS	CD-CE-NZ	-5.29	99.52	111.70
10	i3	83	TYR	CB-CG-CD1	-5.29	117.82	121.00
10	eU	23	ASP	CB-CG-OD2	5.29	123.06	118.30
4	K1	86	ASP	CB-CG-OD1	5.29	123.06	118.30
8	b2	161	LEU	CA-CB-CG	-5.29	103.13	115.30
11	v5	79	MET	CG-SD-CE	-5.29	91.73	100.20
10	bw	92	LEU	CB-CG-CD2	5.29	120.00	111.00
10	le	37	ARG	NE-CZ-NH2	5.29	122.95	120.30
14	d8	251	LYS	CD-CE-NZ	5.29	123.87	111.70
17	be	30	ARG	NE-CZ-NH1	5.29	122.94	120.30
11	cq	161	LEU	CB-CG-CD2	-5.29	102.01	111.00
11	H4	110	LEU	CA-CB-CG	5.29	127.47	115.30
5	h1	75	THR	CA-CB-CG2	-5.29	105.00	112.40
10	m7	157	ASP	CB-CG-OD2	5.29	123.06	118.30
10	I9	17	ARG	NE-CZ-NH2	-5.29	117.66	120.30
10	g2	18	PHE	CB-CG-CD1	-5.29	117.10	120.80
16	X5	158	LEU	CB-CG-CD1	-5.29	102.02	111.00
12	Y5	259	LEU	CB-CG-CD2	-5.29	102.02	111.00
18	g5	117	TYR	CB-CG-CD1	-5.29	117.83	121.00
10	k6	1	MET	CB-CG-SD	5.29	128.25	112.40
15	W9	73	LEU	CA-CB-CG	5.29	127.45	115.30
11	eB	108	ARG	NE-CZ-NH2	-5.29	117.66	120.30
5	M1	75	THR	CA-CB-CG2	-5.28	105.00	112.40
5	z1	18	TYR	CB-CG-CD2	-5.28	117.83	121.00
8	b2	201	ARG	NE-CZ-NH2	-5.28	117.66	120.30
11	L4	105	LEU	CB-CG-CD2	-5.28	102.02	111.00
11	v7	28	LYS	CD-CE-NZ	5.28	123.85	111.70
12	b9	317	ARG	NE-CZ-NH2	-5.28	117.66	120.30
20	dz	350	LEU	CB-CG-CD1	-5.28	102.02	111.00
24	gy	188	ARG	NE-CZ-NH2	-5.28	117.66	120.30
5	x1	83	ARG	NE-CZ-NH1	-5.28	117.66	120.30
5	c1	90	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
17	k5	99	LEU	CA-CB-CG	5.28	127.44	115.30
11	T6	84	ARG	CG-CD-NE	-5.28	100.71	111.80
17	g9	30	ARG	NE-CZ-NH1	-5.28	117.66	120.30
10	bC	92	LEU	CB-CG-CD1	-5.28	102.03	111.00
10	lq	122	LEU	CB-CG-CD1	-5.28	102.03	111.00
2	C1	45	GLY	N-CA-C	-5.28	99.91	113.10
4	o1	151	PHE	CB-CG-CD1	-5.28	117.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	bt	163	LEU	CB-CG-CD2	-5.28	102.03	111.00
10	lo	142	ARG	CG-CD-NE	5.28	122.88	111.80
8	a2	161	LEU	CA-CB-CG	-5.28	103.17	115.30
11	F3	7	ARG	NE-CZ-NH2	-5.28	117.66	120.30
11	T3	91	ARG	NE-CZ-NH2	-5.28	117.66	120.30
18	bb	83	LEU	CB-CG-CD1	-5.28	102.03	111.00
12	A2	151	ARG	NE-CZ-NH2	-5.27	117.66	120.30
11	b6	120	LEU	CB-CG-CD2	-5.27	102.03	111.00
12	b9	284	TYR	CB-CG-CD1	-5.27	117.84	121.00
11	ar	171	LYS	CD-CE-NZ	5.27	123.83	111.70
11	X7	129	ARG	NE-CZ-NH1	5.27	122.94	120.30
5	n1	72	MET	CG-SD-CE	5.27	108.63	100.20
11	eR	129	ARG	NE-CZ-NH2	-5.27	117.66	120.30
11	l6	107	ASP	CB-CG-OD2	-5.27	113.56	118.30
10	A7	120	LEU	CB-CG-CD2	5.27	119.96	111.00
11	T7	30	PHE	CB-CG-CD1	-5.27	117.11	120.80
11	F9	88	ILE	CG1-CB-CG2	-5.27	99.81	111.40
25	kb	283	PHE	CZ-CE2-CD2	-5.27	113.78	120.10
4	w1	27	LYS	CD-CE-NZ	5.27	123.81	111.70
10	I2	83	TYR	CB-CG-CD1	-5.27	117.84	121.00
10	S6	95	TYR	CZ-CE2-CD2	-5.27	115.06	119.80
10	G7	17	ARG	NE-CZ-NH1	5.27	122.93	120.30
10	k7	18	PHE	CB-CG-CD2	5.27	124.49	120.80
12	a3	106	MET	CG-SD-CE	5.27	108.62	100.20
5	n1	77	ARG	NH1-CZ-NH2	5.26	125.19	119.40
10	s4	83	TYR	CD1-CE1-CZ	-5.26	115.06	119.80
25	ka	307	ASP	CB-CG-OD2	-5.26	113.56	118.30
4	s1	44	THR	CA-CB-CG2	-5.26	105.03	112.40
17	aa	139	ASP	CB-CG-OD2	5.26	123.04	118.30
20	dz	210	MET	CG-SD-CE	5.26	108.62	100.20
10	Q2	91	ARG	NE-CZ-NH1	5.26	122.93	120.30
19	a8	303	TYR	CG-CD1-CE1	-5.26	117.09	121.30
11	aJ	108	ARG	NE-CZ-NH1	-5.26	117.67	120.30
18	bb	117	TYR	OH-CZ-CE2	-5.26	105.90	120.10
10	gj	53	LYS	CD-CE-NZ	5.26	123.80	111.70
3	E1	196	TYR	CB-CG-CD2	-5.26	117.84	121.00
4	q1	43	LEU	CB-CG-CD1	-5.26	102.06	111.00
10	ef	84	ARG	NE-CZ-NH2	5.26	122.93	120.30
5	O1	94	TYR	CB-CG-CD1	-5.26	117.85	121.00
10	m4	85	ASP	CB-CG-OD2	5.26	123.03	118.30
11	z6	50	CYS	CA-CB-SG	5.26	123.46	114.00
15	R8	81	LYS	CD-CE-NZ	-5.26	99.61	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	aW	104	TYR	CB-CG-CD2	-5.26	117.85	121.00
5	Y1	77	ARG	NE-CZ-NH1	-5.25	117.67	120.30
11	n3	116	THR	CA-CB-CG2	-5.25	105.04	112.40
17	d5	139	ASP	CB-CG-OD2	5.25	123.03	118.30
12	bY	260	ARG	NE-CZ-NH1	-5.25	117.67	120.30
8	a2	698	ARG	NE-CZ-NH2	5.25	122.93	120.30
13	b3	206	LEU	CB-CG-CD1	-5.25	102.07	111.00
10	s4	138	LEU	CB-CG-CD2	-5.25	102.07	111.00
10	I5	17	ARG	NE-CZ-NH1	5.25	122.93	120.30
10	j7	44	LEU	CB-CG-CD1	-5.25	102.07	111.00
17	ce	86	ARG	NE-CZ-NH2	-5.25	117.67	120.30
17	ci	108	ASP	CB-CG-OD1	-5.25	113.57	118.30
5	S1	62	TYR	CB-CG-CD1	-5.25	117.85	121.00
10	k3	159	VAL	CG1-CB-CG2	-5.25	102.50	110.90
10	s4	85	ASP	CB-CG-OD2	5.25	123.03	118.30
11	L6	89	ILE	CG1-CB-CG2	-5.25	99.84	111.40
18	f9	120	LEU	CB-CG-CD2	5.25	119.93	111.00
10	by	17	ARG	NE-CZ-NH2	-5.25	117.67	120.30
11	lr	50	CYS	CA-CB-SG	5.25	123.45	114.00
17	f4	139	ASP	CB-CG-OD2	5.25	123.03	118.30
4	q1	29	PHE	CZ-CE2-CD2	-5.25	113.80	120.10
8	a2	361	LYS	CD-CE-NZ	5.25	123.77	111.70
10	j7	37	ARG	NE-CZ-NH2	-5.25	117.68	120.30
11	ec	91	ARG	NE-CZ-NH2	-5.25	117.68	120.30
11	ei	38	LEU	CB-CG-CD2	-5.25	102.08	111.00
12	ey	43	VAL	CG1-CB-CG2	-5.25	102.50	110.90
5	W1	107	ARG	NE-CZ-NH2	-5.25	117.68	120.30
10	I2	95	TYR	CZ-CE2-CD2	-5.25	115.08	119.80
11	r4	7	ARG	NE-CZ-NH2	-5.25	117.68	120.30
11	v5	75	THR	N-CA-C	-5.25	96.83	111.00
17	ac	139	ASP	CB-CG-OD2	5.25	123.02	118.30
11	L6	120	LEU	CB-CG-CD2	5.25	119.92	111.00
10	D8	163	LEU	CB-CG-CD1	5.25	119.92	111.00
4	b1	61	LYS	CD-CE-NZ	5.24	123.76	111.70
17	b4	139	ASP	CB-CG-OD2	5.24	123.02	118.30
10	E6	91	ARG	NE-CZ-NH2	-5.24	117.68	120.30
11	ar	117	TYR	CG-CD2-CE2	-5.24	117.11	121.30
10	bx	135	ARG	NE-CZ-NH1	-5.24	117.68	120.30
14	T8	178	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	D1	64	ARG	NE-CZ-NH1	-5.24	117.68	120.30
4	i1	119	LEU	CB-CG-CD2	-5.24	102.09	111.00
11	x4	129	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a6	30	PHE	CB-CG-CD1	-5.24	117.13	120.80
17	ag	139	ASP	CB-CG-OD2	5.24	123.01	118.30
10	bt	85	ASP	OD1-CG-OD2	-5.24	113.35	123.30
10	bt	138	LEU	CB-CG-CD1	-5.24	102.09	111.00
11	N2	116	THR	CA-CB-CG2	-5.24	105.07	112.40
11	t4	88	ILE	CG1-CB-CG2	-5.24	99.88	111.40
3	F1	268	ARG	NE-CZ-NH1	-5.24	117.68	120.30
5	j1	50	THR	CA-CB-CG2	-5.24	105.07	112.40
10	q5	157	ASP	CB-CG-OD1	-5.24	113.59	118.30
10	U7	66	LEU	CB-CG-CD2	-5.24	102.10	111.00
16	S8	41	LEU	CB-CG-CD1	5.24	119.90	111.00
18	l5	19	LEU	CB-CG-CD1	-5.23	102.10	111.00
25	kb	307	ASP	CB-CG-OD1	-5.23	113.59	118.30
14	d8	208	TYR	CB-CG-CD2	-5.23	117.86	121.00
17	g9	50	ARG	NE-CZ-NH1	-5.23	117.68	120.30
17	i9	139	ASP	CB-CG-OD2	5.23	123.01	118.30
11	aP	129	ARG	NE-CZ-NH1	-5.23	117.68	120.30
18	cb	2	LEU	CB-CG-CD2	5.23	119.89	111.00
4	G1	119	LEU	CB-CG-CD2	-5.23	102.11	111.00
5	W1	119	LEU	CB-CG-CD2	-5.23	102.11	111.00
17	i4	139	ASP	CB-CG-OD2	5.23	123.01	118.30
11	ev	101	ASP	CB-CG-OD1	5.23	123.01	118.30
11	et	45	VAL	CG1-CB-CG2	-5.23	102.53	110.90
11	eF	1	MET	CG-SD-CE	5.23	108.57	100.20
10	w4	18	PHE	CB-CG-CD1	-5.23	117.14	120.80
17	V8	139	ASP	CB-CG-OD2	5.23	123.01	118.30
16	X9	296	ARG	NE-CZ-NH1	5.23	122.91	120.30
11	az	84	ARG	NE-CZ-NH2	-5.23	117.69	120.30
10	bt	38	LEU	CB-CG-CD2	5.23	119.89	111.00
10	dM	91	ARG	NE-CZ-NH1	5.23	122.91	120.30
11	L3	120	LEU	CB-CG-CD2	5.23	119.89	111.00
14	bZ	77	MET	CA-CB-CG	5.23	122.18	113.30
5	e1	85	LEU	CB-CG-CD1	-5.22	102.12	111.00
10	m3	137	ARG	NE-CZ-NH2	-5.22	117.69	120.30
10	M4	17	ARG	NE-CZ-NH1	5.22	122.91	120.30
17	i5	139	ASP	CB-CG-OD2	5.22	123.00	118.30
16	S8	215	MET	CG-SD-CE	-5.22	91.84	100.20
11	v9	110	LEU	CA-CB-CG	5.22	127.31	115.30
11	eX	61	CYS	CA-CB-SG	-5.22	104.60	114.00
10	lw	2	LYS	CD-CE-NZ	5.22	123.72	111.70
18	g4	117	TYR	CB-CG-CD1	-5.22	117.87	121.00
17	b5	111	LEU	CB-CG-CD1	-5.22	102.12	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Y7	138	LEU	CA-CB-CG	5.22	127.31	115.30
10	A9	18	PHE	CB-CG-CD1	-5.22	117.14	120.80
17	ak	139	ASP	CB-CG-OD2	5.22	123.00	118.30
10	as	85	ASP	OD1-CG-OD2	-5.22	113.38	123.30
10	aA	85	ASP	CB-CG-OD2	5.22	123.00	118.30
13	B2	206	LEU	CB-CG-CD1	-5.22	102.12	111.00
11	H9	88	ILE	CG1-CB-CG2	-5.22	99.92	111.40
11	et	91	ARG	NE-CZ-NH2	5.22	122.91	120.30
24	gz	204	ARG	NE-CZ-NH1	-5.22	117.69	120.30
5	S1	97	LEU	CB-CG-CD1	-5.22	102.13	111.00
10	m9	17	ARG	NE-CZ-NH2	-5.22	117.69	120.30
10	aQ	138	LEU	CB-CG-CD1	5.22	119.87	111.00
17	bc	88	ILE	CG1-CB-CG2	-5.22	99.92	111.40
10	lw	17	ARG	NE-CZ-NH2	-5.22	117.69	120.30
12	U8	147	ARG	NE-CZ-NH2	5.22	122.91	120.30
15	W9	6	LEU	CB-CG-CD2	-5.22	102.13	111.00
17	bc	139	ASP	CB-CG-OD2	5.22	123.00	118.30
11	bn	91	ARG	NE-CZ-NH1	5.22	122.91	120.30
17	cc	139	ASP	CB-CG-OD2	5.22	122.99	118.30
4	u1	151	PHE	CB-CG-CD1	-5.21	117.15	120.80
8	a2	201	ARG	NE-CZ-NH2	-5.21	117.69	120.30
9	c2	13	LEU	CD1-CG-CD2	-5.21	94.86	110.50
11	f2	7	ARG	NE-CZ-NH2	-5.21	117.69	120.30
10	U3	17	ARG	NE-CZ-NH1	-5.21	117.69	120.30
12	a3	179	LEU	CB-CG-CD2	5.21	119.86	111.00
10	aq	91	ARG	NE-CZ-NH2	5.21	122.91	120.30
11	dK	143	MET	CG-SD-CE	5.21	108.54	100.20
22	eY	263	ARG	NE-CZ-NH2	-5.21	117.69	120.30
11	r7	75	THR	N-CA-CB	5.21	120.20	110.30
18	cf	120	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	B1	238	LEU	CA-CB-CG	5.21	127.29	115.30
5	t1	18	TYR	CB-CG-CD2	-5.21	117.87	121.00
5	v1	91	TYR	CG-CD2-CE2	5.21	125.47	121.30
17	i4	99	LEU	CB-CG-CD2	-5.21	102.14	111.00
17	i5	99	LEU	CB-CG-CD2	-5.21	102.14	111.00
18	W8	19	LEU	CB-CG-CD2	-5.21	102.14	111.00
16	X9	215	MET	CG-SD-CE	-5.21	91.86	100.20
10	aw	38	LEU	CB-CG-CD2	-5.21	102.14	111.00
18	cd	160	LEU	CA-CB-CG	5.21	127.29	115.30
17	cg	139	ASP	CB-CG-OD2	5.21	122.99	118.30
18	bb	84	ARG	CA-CB-CG	5.21	124.86	113.40
11	cs	129	ARG	NE-CZ-NH1	-5.21	117.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	ek	84	ARG	NE-CZ-NH2	5.21	122.91	120.30
5	h1	76	ARG	NE-CZ-NH2	-5.21	117.69	120.30
11	N3	77	ARG	NE-CZ-NH2	5.21	122.91	120.30
11	J6	2	LEU	CB-CG-CD2	-5.21	102.15	111.00
10	bm	118	ARG	NE-CZ-NH2	-5.21	117.69	120.30
11	bn	1	MET	CG-SD-CE	5.21	108.53	100.20
13	b3	212	TYR	N-CA-C	5.21	125.06	111.00
11	B7	143	MET	CG-SD-CE	-5.21	91.87	100.20
10	U7	8	THR	CA-CB-CG2	-5.21	105.11	112.40
11	d7	2	LEU	CB-CG-CD1	-5.21	102.15	111.00
11	co	170	ASP	CB-CG-OD2	5.21	122.99	118.30
11	eJ	13	ASP	CB-CG-OD2	5.21	122.99	118.30
11	gx	37	ARG	NE-CZ-NH2	5.21	122.90	120.30
4	G1	36	ARG	NE-CZ-NH2	5.20	122.90	120.30
4	q1	76	GLU	OE1-CD-OE2	5.20	129.54	123.30
17	d4	139	ASP	CB-CG-OD2	5.20	122.98	118.30
10	z8	92	LEU	CB-CG-CD2	5.20	119.85	111.00
16	X9	116	VAL	CG1-CB-CG2	-5.20	102.57	110.90
17	bi	139	ASP	CB-CG-OD2	5.20	122.98	118.30
14	c3	66	ILE	CB-CG1-CD1	-5.20	99.34	113.90
17	d4	19	LEU	CB-CG-CD1	5.20	119.84	111.00
14	d9	251	LYS	CD-CE-NZ	5.20	123.66	111.70
4	b1	116	TYR	CZ-CE2-CD2	-5.20	115.12	119.80
11	v7	37	ARG	CG-CD-NE	-5.20	100.88	111.80
12	b9	279	VAL	CG1-CB-CG2	5.20	119.22	110.90
11	H9	105	LEU	CB-CG-CD1	-5.20	102.16	111.00
10	aw	91	ARG	NE-CZ-NH2	5.20	122.90	120.30
5	j1	76	ARG	NE-CZ-NH2	-5.20	117.70	120.30
10	U2	91	ARG	NE-CZ-NH1	5.20	122.90	120.30
11	B3	50	CYS	CA-CB-SG	5.20	123.36	114.00
10	K3	53	LYS	CD-CE-NZ	5.20	123.66	111.70
10	i3	95	TYR	CZ-CE2-CD2	-5.20	115.12	119.80
11	x4	95	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
17	a5	139	ASP	CB-CG-OD2	5.20	122.98	118.30
15	W9	16	ARG	N-CA-C	5.20	125.03	111.00
17	ae	139	ASP	CB-CG-OD2	5.20	122.98	118.30
11	ax	77	ARG	NE-CZ-NH1	-5.20	117.70	120.30
4	q1	31	LEU	CB-CG-CD2	5.20	119.84	111.00
17	bk	139	ASP	CB-CG-OD2	5.20	122.98	118.30
10	eh	163	LEU	CB-CG-CD2	-5.20	102.16	111.00
17	k4	139	ASP	CB-CG-OD2	5.20	122.98	118.30
10	E5	138	LEU	CB-CG-CD2	-5.20	102.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L5	38	LEU	CB-CG-CD1	-5.20	102.17	111.00
17	f5	18	PHE	N-CA-CB	-5.20	101.25	110.60
10	z8	142	ARG	NE-CZ-NH2	5.20	122.90	120.30
11	at	45	VAL	CG1-CB-CG2	-5.20	102.59	110.90
17	ca	139	ASP	CB-CG-OD2	5.20	122.98	118.30
5	p1	77	ARG	NE-CZ-NH2	-5.19	117.70	120.30
16	X5	95	MET	CB-CG-SD	5.19	127.98	112.40
16	X9	315	LYS	CD-CE-NZ	5.19	123.65	111.70
17	ca	30	ARG	NE-CZ-NH1	5.19	122.90	120.30
11	co	28	LYS	CB-CG-CD	5.19	125.10	111.60
10	G6	1	MET	CA-CB-CG	-5.19	104.47	113.30
11	R7	84	ARG	NE-CZ-NH2	-5.19	117.70	120.30
17	ci	139	ASP	CB-CG-OD2	5.19	122.97	118.30
10	iB	1	MET	CG-SD-CE	-5.19	91.89	100.20
10	G4	23	ASP	CB-CG-OD2	-5.19	113.63	118.30
11	T7	91	ARG	NE-CZ-NH2	-5.19	117.70	120.30
14	e9	62	GLY	N-CA-C	5.19	126.07	113.10
15	R8	43	MET	CG-SD-CE	-5.19	91.90	100.20
17	k9	139	ASP	CB-CG-OD2	5.19	122.97	118.30
18	g4	108	ARG	NE-CZ-NH1	5.19	122.89	120.30
16	X5	123	LEU	CB-CG-CD1	-5.19	102.18	111.00
11	co	153	ILE	CG1-CB-CG2	-5.19	99.99	111.40
11	J5	90	LEU	CB-CG-CD2	-5.19	102.18	111.00
17	k5	139	ASP	CB-CG-OD2	5.19	122.97	118.30
10	h6	114	ARG	NE-CZ-NH1	5.19	122.89	120.30
17	ai	139	ASP	CB-CG-OD2	5.19	122.97	118.30
17	ba	139	ASP	CB-CG-OD2	5.19	122.97	118.30
18	bd	160	LEU	CA-CB-CG	5.19	127.23	115.30
21	fz	203	ALA	N-CA-C	5.19	125.00	111.00
11	r3	91	ARG	NE-CZ-NH1	-5.18	117.71	120.30
10	t8	24	LEU	CB-CG-CD2	5.18	119.81	111.00
17	Z8	139	ASP	CB-CG-OD2	5.18	122.97	118.30
18	bb	93	VAL	CG1-CB-CG2	-5.18	102.61	110.90
17	be	139	ASP	CB-CG-OD2	5.18	122.97	118.30
4	N1	29	PHE	CB-CG-CD2	-5.18	117.17	120.80
5	t1	11	THR	CA-CB-CG2	-5.18	105.15	112.40
14	Z5	194	MET	CG-SD-CE	-5.18	91.91	100.20
10	A6	1	MET	CB-CG-SD	5.18	127.94	112.40
10	C7	138	LEU	CD1-CG-CD2	5.18	126.04	110.50
17	bk	19	LEU	CB-CG-CD2	-5.18	102.19	111.00
17	ce	139	ASP	CB-CG-OD2	5.18	122.96	118.30
17	ck	139	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	eT	13	ASP	CB-CG-OD2	5.18	122.96	118.30
10	hA	38	LEU	CB-CG-CD2	5.18	119.81	111.00
11	D5	110	LEU	CA-CB-CG	5.18	127.21	115.30
17	f5	139	ASP	CB-CG-OD2	5.18	122.96	118.30
17	g9	139	ASP	CB-CG-OD2	5.18	122.96	118.30
11	x9	91	ARG	NE-CZ-NH2	-5.18	117.71	120.30
10	I4	138	LEU	CB-CG-CD2	-5.18	102.20	111.00
11	bo	115	GLU	CA-CB-CG	-5.18	102.01	113.40
10	bM	17	ARG	NE-CZ-NH2	-5.18	117.71	120.30
7	m1	83	ARG	NE-CZ-NH2	-5.18	117.71	120.30
17	b5	24	LEU	CB-CG-CD2	5.18	119.80	111.00
17	ac	30	ARG	NE-CZ-NH1	-5.18	117.71	120.30
14	aZ	77	MET	CA-CB-CG	5.18	122.10	113.30
10	ct	138	LEU	CB-CG-CD1	-5.18	102.20	111.00
10	cy	85	ASP	CB-CG-OD2	5.18	122.96	118.30
4	y1	8	ILE	CG1-CB-CG2	-5.17	100.02	111.40
25	ka	161	LEU	CB-CG-CD2	-5.17	102.20	111.00
12	a3	147	ARG	NE-CZ-NH2	-5.17	117.71	120.30
17	k9	19	LEU	CB-CG-CD2	5.17	119.79	111.00
17	bg	1	MET	CG-SD-CE	5.17	108.48	100.20
4	s1	30	VAL	CG1-CB-CG2	5.17	119.17	110.90
10	E4	2	LYS	CD-CE-NZ	5.17	123.59	111.70
17	a4	139	ASP	CB-CG-OD2	5.17	122.95	118.30
11	J6	98	LEU	CB-CG-CD2	5.17	119.79	111.00
10	u6	156	LEU	CA-CB-CG	5.17	127.19	115.30
11	p7	59	MET	CG-SD-CE	5.17	108.47	100.20
12	U8	129	VAL	CG1-CB-CG2	-5.17	102.62	110.90
4	w1	29	PHE	CZ-CE2-CD2	-5.17	113.90	120.10
17	b5	139	ASP	CB-CG-OD2	5.17	122.95	118.30
5	U1	91	TYR	CG-CD1-CE1	-5.17	117.17	121.30
16	X5	133	PHE	CB-CG-CD1	-5.17	117.18	120.80
10	s6	91	ARG	NH1-CZ-NH2	5.17	125.08	119.40
18	bh	27	LEU	CB-CG-CD2	5.17	119.79	111.00
11	jJ	50	CYS	CA-CB-SG	5.17	123.30	114.00
5	v1	77	ARG	NE-CZ-NH2	-5.17	117.72	120.30
11	D3	50	CYS	CA-CB-SG	5.17	123.30	114.00
17	i4	17	ARG	NE-CZ-NH2	-5.17	117.72	120.30
10	s5	138	LEU	CB-CG-CD2	-5.17	102.22	111.00
10	M6	142	ARG	CG-CD-NE	5.17	122.65	111.80
11	b6	84	ARG	CG-CD-NE	-5.17	100.95	111.80
10	i7	1	MET	CA-CB-CG	-5.17	104.52	113.30
17	X8	139	ASP	CB-CG-OD2	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	ln	84	ARG	NE-CZ-NH2	-5.17	117.72	120.30
15	R8	8	TYR	CG-CD1-CE1	5.17	125.43	121.30
11	x9	134	MET	CG-SD-CE	-5.17	91.94	100.20
10	S6	89	TYR	CZ-CE2-CD2	-5.16	115.15	119.80
11	n6	19	VAL	CG1-CB-CG2	-5.16	102.64	110.90
11	o8	78	ARG	NE-CZ-NH2	-5.16	117.72	120.30
11	b7	37	ARG	NE-CZ-NH1	-5.16	117.72	120.30
10	cm	74	ASP	CB-CG-OD2	5.16	122.95	118.30
16	S8	116	VAL	CG1-CB-CG2	-5.16	102.64	110.90
12	bY	263	ILE	CG1-CB-CG2	-5.16	100.04	111.40
5	O1	85	LEU	CB-CG-CD1	-5.16	102.23	111.00
17	k4	50	ARG	NE-CZ-NH1	5.16	122.88	120.30
10	C5	83	TYR	CD1-CE1-CZ	-5.16	115.16	119.80
17	d5	19	LEU	CB-CG-CD1	5.16	119.77	111.00
10	j8	142	ARG	NE-CZ-NH1	-5.16	117.72	120.30
10	i7	159	VAL	CG1-CB-CG2	-5.16	102.64	110.90
5	t1	28	ARG	NE-CZ-NH1	5.16	122.88	120.30
18	ch	27	LEU	CB-CG-CD2	5.16	119.77	111.00
4	f1	36	ARG	NE-CZ-NH1	5.16	122.88	120.30
10	S7	86	VAL	CG1-CB-CG2	-5.16	102.65	110.90
11	ld	77	ARG	NE-CZ-NH2	5.16	122.88	120.30
10	w3	49	GLU	OE1-CD-OE2	5.16	129.49	123.30
17	k5	101	VAL	CG1-CB-CG2	-5.16	102.65	110.90
11	D6	75	THR	N-CA-CB	5.16	120.09	110.30
17	V8	92	LEU	CB-CG-CD1	5.16	119.76	111.00
11	p9	2	LEU	CA-CB-CG	5.16	127.16	115.30
10	m3	17	ARG	NE-CZ-NH1	-5.15	117.72	120.30
11	eJ	88	ILE	CG1-CB-CG2	-5.15	100.06	111.40
4	f1	100	ASP	CB-CG-OD1	5.15	122.94	118.30
10	M4	137	ARG	NE-CZ-NH1	-5.15	117.72	120.30
17	ci	155	ASP	CB-CG-OD2	5.15	122.94	118.30
11	F3	91	ARG	NE-CZ-NH2	-5.15	117.72	120.30
18	j4	120	LEU	CB-CG-CD2	5.15	119.76	111.00
11	v5	27	LEU	CB-CG-CD2	-5.15	102.25	111.00
10	K6	142	ARG	NE-CZ-NH1	5.15	122.88	120.30
11	c6	161	LEU	CB-CG-CD2	-5.15	102.24	111.00
11	H7	2	LEU	CB-CG-CD2	-5.15	102.24	111.00
10	aK	138	LEU	CB-CG-CD2	-5.15	102.24	111.00
10	bm	38	LEU	CB-CG-CD2	5.15	119.76	111.00
10	bI	135	ARG	NE-CZ-NH2	-5.15	117.72	120.30
10	eS	142	ARG	NE-CZ-NH2	5.15	122.88	120.30
11	l2	84	ARG	CB-CG-CD	-5.15	98.21	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K7	33	ARG	NE-CZ-NH1	-5.15	117.72	120.30
11	J9	84	ARG	NE-CZ-NH2	-5.15	117.72	120.30
17	bg	139	ASP	CB-CG-OD2	5.15	122.94	118.30
11	H4	75	THR	N-CA-C	-5.15	97.10	111.00
11	D5	75	THR	N-CA-C	-5.15	97.10	111.00
11	x5	129	ARG	NE-CZ-NH2	-5.15	117.73	120.30
11	z5	2	LEU	CB-CG-CD1	-5.15	102.25	111.00
11	J6	91	ARG	NE-CZ-NH1	5.15	122.87	120.30
11	bP	129	ARG	NE-CZ-NH1	-5.15	117.73	120.30
20	dy	350	LEU	CB-CG-CD1	-5.15	102.25	111.00
11	R7	120	LEU	CB-CG-CD2	-5.15	102.25	111.00
11	D4	84	ARG	NE-CZ-NH1	5.14	122.87	120.30
10	j6	159	VAL	CG1-CB-CG2	-5.14	102.67	110.90
4	i1	47	ARG	NE-CZ-NH1	5.14	122.87	120.30
5	j1	91	TYR	CZ-CE2-CD2	-5.14	115.17	119.80
11	r3	78	ARG	NE-CZ-NH2	-5.14	117.73	120.30
5	t1	36	LEU	CA-CB-CG	5.14	127.12	115.30
11	P6	33	ASP	CB-CG-OD2	-5.14	113.67	118.30
23	hZ	203	ARG	NE-CZ-NH2	5.14	122.87	120.30
4	q1	119	LEU	CB-CG-CD2	-5.14	102.26	111.00
4	s1	119	LEU	CB-CG-CD1	-5.14	102.26	111.00
10	o6	18	PHE	CB-CG-CD2	5.14	124.40	120.80
11	T7	142	ILE	CG1-CB-CG2	-5.14	100.09	111.40
14	44	194	MET	CG-SD-CE	-5.14	91.98	100.20
18	cd	131	ILE	CG1-CB-CG2	-5.14	100.10	111.40
10	dJ	120	LEU	CB-CG-CD2	5.14	119.73	111.00
11	f2	91	ARG	NE-CZ-NH2	-5.14	117.73	120.30
11	at	27	LEU	CB-CG-CD2	-5.14	102.27	111.00
10	bM	142	ARG	NE-CZ-NH1	-5.14	117.73	120.30
5	z1	11	THR	CA-CB-CG2	-5.13	105.21	112.40
5	z1	36	LEU	CA-CB-CG	5.13	127.11	115.30
14	d9	279	ARG	CG-CD-NE	-5.13	101.02	111.80
18	bd	75	THR	N-CA-C	-5.13	97.14	111.00
11	dB	50	CYS	CA-CB-SG	5.13	123.24	114.00
9	c2	63	TYR	CA-CB-CG	-5.13	103.65	113.40
10	K2	159	VAL	CG1-CB-CG2	-5.13	102.69	110.90
24	gy	39	PHE	CB-CG-CD1	-5.13	117.21	120.80
11	l7	13	ASP	CB-CG-OD2	5.13	122.92	118.30
11	p7	37	ARG	NE-CZ-NH1	5.13	122.87	120.30
11	z9	108	ARG	NE-CZ-NH1	-5.13	117.73	120.30
11	bq	113	LEU	CB-CG-CD1	5.13	119.72	111.00
10	lu	118	ARG	NE-CZ-NH1	5.13	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	n6	77	ARG	NE-CZ-NH1	5.13	122.86	120.30
5	j1	61	LEU	CB-CG-CD2	-5.13	102.28	111.00
16	24	364	SER	N-CA-CB	-5.13	102.81	110.50
10	f6	144	MET	CG-SD-CE	-5.13	92.00	100.20
10	bm	85	ASP	CB-CG-OD2	5.13	122.92	118.30
5	e1	119	LEU	CB-CG-CD2	-5.13	102.28	111.00
5	v1	14	VAL	CG1-CB-CG2	5.13	119.10	110.90
5	v1	76	ARG	NE-CZ-NH2	-5.12	117.74	120.30
10	Q6	18	PHE	CB-CG-CD2	5.12	124.39	120.80
10	S6	138	LEU	CB-CG-CD2	-5.12	102.29	111.00
4	G1	38	ARG	NE-CZ-NH2	-5.12	117.74	120.30
5	M1	28	ARG	NE-CZ-NH2	-5.12	117.74	120.30
11	F6	51	ILE	CG1-CB-CG2	-5.12	100.13	111.40
11	dN	118	ILE	CG1-CB-CG2	-5.12	100.13	111.40
11	fy	27	LEU	CA-CB-CG	5.12	127.08	115.30
10	y5	144	MET	CG-SD-CE	-5.12	92.00	100.20
10	I9	85	ASP	CB-CG-OD2	5.12	122.91	118.30
11	er	105	LEU	CB-CG-CD1	-5.12	102.30	111.00
10	gb	18	PHE	CB-CG-CD2	5.12	124.38	120.80
4	b1	107	ILE	CG1-CB-CG2	-5.12	100.14	111.40
4	s1	155	TYR	CB-CG-CD2	-5.12	117.93	121.00
17	k4	87	ASP	CB-CG-OD1	5.12	122.91	118.30
18	ad	84	ARG	NE-CZ-NH1	5.12	122.86	120.30
11	co	77	ARG	CA-CB-CG	5.12	124.66	113.40
11	dL	153	ILE	CG1-CB-CG2	-5.12	100.14	111.40
11	x5	2	LEU	CA-CB-CG	5.12	127.07	115.30
15	W9	8	TYR	CG-CD1-CE1	5.12	125.39	121.30
18	bl	74	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
25	kb	243	ASP	CB-CG-OD1	-5.12	113.69	118.30
10	q3	91	ARG	NE-CZ-NH1	5.12	122.86	120.30
18	g5	163	TYR	CB-CG-CD1	-5.12	117.93	121.00
11	el	129	ARG	NE-CZ-NH1	-5.11	117.74	120.30
10	gh	17	ARG	NE-CZ-NH2	-5.11	117.74	120.30
5	M1	94	TYR	CG-CD2-CE2	5.11	125.39	121.30
4	P1	100	ASP	CB-CG-OD1	5.11	122.90	118.30
10	C4	17	ARG	NE-CZ-NH2	5.11	122.86	120.30
12	Y5	49	LYS	CA-CB-CG	5.11	124.64	113.40
12	Z9	129	VAL	CG1-CB-CG2	-5.11	102.72	110.90
12	bY	315	MET	CG-SD-CE	5.11	108.38	100.20
17	cg	1	MET	CG-SD-CE	5.11	108.38	100.20
11	co	33	ASP	CB-CG-OD2	5.11	122.90	118.30
10	m2	87	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G3	91	ARG	NE-CZ-NH1	5.11	122.85	120.30
11	D4	50	CYS	CA-CB-SG	5.11	123.19	114.00
16	24	130	ARG	CG-CD-NE	-5.11	101.08	111.80
10	q4	157	ASP	CB-CG-OD1	-5.11	113.70	118.30
10	C7	2	LYS	CB-CG-CD	-5.11	98.32	111.60
18	ah	39	ASP	CB-CG-OD2	-5.11	113.70	118.30
10	by	17	ARG	NE-CZ-NH1	5.11	122.85	120.30
11	jO	115	GLU	CA-CB-CG	5.11	124.64	113.40
10	e2	9	ILE	CG1-CB-CG2	-5.11	100.17	111.40
11	F6	149	ARG	NE-CZ-NH1	-5.11	117.75	120.30
11	ev	27	LEU	CB-CG-CD2	-5.11	102.32	111.00
25	ka	357	ASP	CB-CG-OD2	-5.11	113.70	118.30
5	c1	90	ARG	NE-CZ-NH2	5.10	122.85	120.30
4	q1	91	LEU	CB-CG-CD2	-5.10	102.33	111.00
11	N2	77	ARG	NE-CZ-NH2	5.10	122.85	120.30
11	P5	84	ARG	NE-CZ-NH1	5.10	122.85	120.30
10	G6	137	ARG	CB-CG-CD	5.10	124.87	111.60
17	ci	57	GLN	CB-CG-CD	5.10	124.86	111.60
11	ev	105	LEU	CA-CB-CG	5.10	127.04	115.30
17	f4	129	TYR	CB-CG-CD2	-5.10	117.94	121.00
10	ek	85	ASP	CB-CG-OD2	5.10	122.89	118.30
25	kb	175	LEU	CB-CG-CD1	-5.10	102.33	111.00
18	l5	108	ARG	NE-CZ-NH1	5.10	122.85	120.30
11	bs	90	LEU	CB-CG-CD1	-5.10	102.33	111.00
10	bv	142	ARG	NE-CZ-NH2	5.10	122.85	120.30
5	r1	87	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
13	B2	308	ARG	NE-CZ-NH2	-5.10	117.75	120.30
17	g9	161	LEU	CB-CG-CD2	-5.10	102.33	111.00
17	bg	30	ARG	NE-CZ-NH2	-5.10	117.75	120.30
25	kb	195	ARG	NE-CZ-NH2	-5.10	117.75	120.30
10	eu	85	ASP	CB-CG-OD2	5.10	122.89	118.30
11	lj	38	LEU	CB-CG-CD1	-5.10	102.34	111.00
5	O1	38	VAL	CA-CB-CG1	-5.09	103.26	110.90
5	h1	36	LEU	CA-CB-CG	5.09	127.02	115.30
4	k1	119	LEU	CB-CG-CD2	-5.09	102.34	111.00
4	y1	29	PHE	CB-CG-CD2	-5.09	117.23	120.80
11	R2	91	ARG	NE-CZ-NH1	-5.09	117.75	120.30
11	p9	44	ILE	CG1-CB-CG2	-5.09	100.19	111.40
16	X9	41	LEU	CB-CG-CD1	5.09	119.66	111.00
10	am	17	ARG	NE-CZ-NH2	-5.09	117.75	120.30
11	av	110	LEU	CA-CB-CG	5.09	127.02	115.30
11	bV	91	ARG	NE-CZ-NH1	5.09	122.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	cv	163	LEU	CB-CG-CD2	-5.09	102.34	111.00
4	y1	94	TYR	CE1-CZ-OH	-5.09	106.35	120.10
11	p5	122	VAL	CG1-CB-CG2	-5.09	102.75	110.90
10	dA	138	LEU	CA-CB-CG	-5.09	103.58	115.30
11	P7	143	MET	CG-SD-CE	-5.09	92.05	100.20
14	c9	81	VAL	CA-CB-CG2	-5.09	103.26	110.90
12	aY	62	ARG	NE-CZ-NH1	5.09	122.84	120.30
10	M3	62	LYS	CD-CE-NZ	-5.09	100.00	111.70
17	b4	87	ASP	CB-CG-OD2	5.09	122.88	118.30
10	u4	137	ARG	NE-CZ-NH2	5.09	122.84	120.30
10	y5	17	ARG	NE-CZ-NH1	5.09	122.84	120.30
11	t6	75	THR	N-CA-CB	5.09	119.97	110.30
11	cn	91	ARG	NE-CZ-NH2	-5.09	117.76	120.30
11	cr	50	CYS	CA-CB-SG	5.09	123.16	114.00
3	E1	174	LEU	CA-CB-CG	5.09	127.00	115.30
11	r3	108	ARG	NE-CZ-NH2	5.09	122.84	120.30
11	z4	7	ARG	NE-CZ-NH2	-5.09	117.76	120.30
18	g4	125	THR	CA-CB-CG2	-5.09	105.28	112.40
11	B5	82	CYS	CA-CB-SG	-5.09	104.84	114.00
10	K6	114	ARG	NE-CZ-NH2	-5.09	117.76	120.30
16	S8	64	VAL	CG1-CB-CG2	-5.09	102.76	110.90
10	do	38	LEU	CB-CG-CD2	5.09	119.65	111.00
11	en	98	LEU	CB-CG-CD1	-5.09	102.35	111.00
21	ew	116	ARG	NE-CZ-NH2	5.08	122.84	120.30
13	b3	236	GLY	N-CA-C	-5.08	100.39	113.10
10	E5	66	LEU	CB-CG-CD1	5.08	119.64	111.00
23	hY	203	ARG	NE-CZ-NH2	5.08	122.84	120.30
12	A2	269	TYR	CA-CB-CG	5.08	123.05	113.40
11	L3	84	ARG	CB-CG-CD	-5.08	98.39	111.60
11	D4	91	ARG	NE-CZ-NH1	-5.08	117.76	120.30
12	34	117	LEU	CB-CG-CD1	-5.08	102.36	111.00
15	R8	61	LEU	CB-CG-CD1	-5.08	102.36	111.00
18	W8	110	LEU	CB-CG-CD1	-5.08	102.36	111.00
18	bf	75	THR	N-CA-C	-5.08	97.28	111.00
10	ct	84	ARG	CD-NE-CZ	-5.08	116.49	123.60
4	w1	83	ARG	NE-CZ-NH2	-5.08	117.76	120.30
10	k7	138	LEU	CB-CG-CD1	5.08	119.64	111.00
14	c8	81	VAL	CA-CB-CG2	-5.08	103.28	110.90
10	de	140	VAL	C-N-CD	-5.08	109.42	120.60
5	l1	126	THR	CA-CB-CG2	-5.08	105.29	112.40
4	s1	29	PHE	CB-CG-CD2	-5.08	117.25	120.80
4	y1	44	THR	CA-CB-CG2	-5.08	105.29	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	F4	82	CYS	CA-CB-SG	-5.08	104.86	114.00
18	j4	91	ARG	NE-CZ-NH2	5.08	122.84	120.30
11	B7	88	ILE	CG1-CB-CG2	-5.08	100.23	111.40
17	ak	19	LEU	CB-CG-CD2	5.08	119.63	111.00
11	bn	91	ARG	NE-CZ-NH2	-5.08	117.76	120.30
18	cd	75	THR	N-CA-C	-5.08	97.29	111.00
12	dw	112	CYS	CA-CB-SG	-5.08	104.86	114.00
10	I5	137	ARG	NE-CZ-NH1	-5.08	117.76	120.30
11	el	1	MET	CB-CG-SD	5.08	127.63	112.40
11	h2	149	ARG	NE-CZ-NH1	5.08	122.84	120.30
16	24	162	ARG	NE-CZ-NH1	5.08	122.84	120.30
17	k5	111	LEU	CB-CG-CD1	-5.08	102.37	111.00
10	f6	158	TYR	CB-CG-CD2	-5.08	117.95	121.00
11	bD	120	LEU	CB-CG-CD2	-5.08	102.37	111.00
10	k8	66	LEU	CB-CG-CD2	-5.07	102.38	111.00
11	y7	7	ARG	NE-CZ-NH2	5.07	122.84	120.30
16	S8	329	MET	CG-SD-CE	5.07	108.32	100.20
10	aE	97	LEU	CB-CG-CD2	-5.07	102.38	111.00
11	bB	28	LYS	CB-CG-CD	5.07	124.79	111.60
18	ch	38	LEU	CB-CG-CD2	5.07	119.62	111.00
18	cl	1	MET	CG-SD-CE	5.07	108.32	100.20
18	cl	74	TYR	CZ-CE2-CD2	-5.07	115.23	119.80
4	y1	90	ARG	NE-CZ-NH2	5.07	122.84	120.30
11	R2	108	ARG	NE-CZ-NH2	5.07	122.84	120.30
10	G6	1	MET	CB-CG-SD	5.07	127.62	112.40
11	X7	110	LEU	CA-CB-CG	5.07	126.97	115.30
11	t7	120	LEU	CA-CB-CG	5.07	126.97	115.30
11	co	115	GLU	CA-CB-CG	-5.07	102.24	113.40
11	jP	91	ARG	NE-CZ-NH2	5.07	122.84	120.30
13	B2	382	PHE	CG-CD2-CE2	5.07	126.38	120.80
10	I2	90	MET	CG-SD-CE	5.07	108.31	100.20
13	b3	155	PHE	CB-CG-CD2	-5.07	117.25	120.80
11	a7	44	ILE	CG1-CB-CG2	-5.07	100.25	111.40
10	aq	38	LEU	CB-CG-CD2	5.07	119.62	111.00
10	by	62	LYS	CD-CE-NZ	5.07	123.36	111.70
11	fm	27	LEU	CA-CB-CG	5.07	126.96	115.30
11	V6	30	PHE	CB-CG-CD2	5.07	124.35	120.80
5	M1	36	LEU	CA-CB-CG	5.07	126.95	115.30
10	E4	135	ARG	NE-CZ-NH1	-5.07	117.77	120.30
10	M4	138	LEU	CB-CG-CD2	-5.07	102.39	111.00
10	K7	91	ARG	NE-CZ-NH2	-5.07	117.77	120.30
10	u5	137	ARG	NE-CZ-NH2	5.07	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	x5	95	TYR	CD1-CE1-CZ	-5.07	115.24	119.80
10	A6	89	TYR	CB-CG-CD2	-5.07	117.96	121.00
10	o6	144	MET	CG-SD-CE	-5.07	92.09	100.20
17	X8	19	LEU	CB-CG-CD1	-5.07	102.39	111.00
11	fc	27	LEU	CA-CB-CG	5.07	126.95	115.30
10	go	141	PRO	N-CA-C	5.07	125.27	112.10
11	jP	115	GLU	CA-CB-CG	5.07	124.54	113.40
11	at	77	ARG	NE-CZ-NH1	-5.06	117.77	120.30
18	bj	156	LEU	CB-CG-CD1	-5.06	102.39	111.00
10	la	33	ARG	NE-CZ-NH1	-5.06	117.77	120.30
7	V1	91	LEU	CB-CG-CD2	-5.06	102.39	111.00
5	c1	91	TYR	CZ-CE2-CD2	-5.06	115.24	119.80
11	bo	77	ARG	CA-CB-CG	5.06	124.54	113.40
10	ct	163	LEU	CB-CG-CD2	-5.06	102.39	111.00
21	ex	116	ARG	NE-CZ-NH2	5.06	122.83	120.30
12	ey	225	MET	CG-SD-CE	-5.06	92.10	100.20
11	jI	149	ARG	NE-CZ-NH2	5.06	122.83	120.30
11	J4	153	ILE	CG1-CB-CG2	-5.06	100.27	111.40
10	s5	83	TYR	CD1-CE1-CZ	-5.06	115.25	119.80
11	N7	66	LEU	CB-CG-CD2	-5.06	102.40	111.00
18	bh	38	LEU	CB-CG-CD2	5.06	119.60	111.00
8	a2	331	PHE	CB-CG-CD1	-5.06	117.26	120.80
17	k4	99	LEU	CA-CB-CG	5.06	126.94	115.30
18	j5	108	ARG	NE-CZ-NH1	5.06	122.83	120.30
11	H7	98	LEU	CB-CG-CD2	5.06	119.60	111.00
14	c8	208	TYR	CB-CG-CD2	-5.06	117.96	121.00
11	aD	120	LEU	CB-CG-CD2	-5.06	102.40	111.00
10	aK	17	ARG	NE-CZ-NH1	5.06	122.83	120.30
11	el	38	LEU	CB-CG-CD1	-5.06	102.40	111.00
10	gc	163	LEU	CB-CG-CD2	-5.06	102.40	111.00
10	iA	106	ASP	CB-CG-OD1	5.06	122.85	118.30
11	T6	110	LEU	CA-CB-CG	5.06	126.93	115.30
11	kT	170	ASP	CB-CG-OD2	-5.06	113.75	118.30
11	er	38	LEU	CA-CB-CG	5.06	126.93	115.30
11	V5	84	ARG	NE-CZ-NH2	-5.05	117.77	120.30
11	V7	77	ARG	NE-CZ-NH2	-5.05	117.77	120.30
10	bu	85	ASP	CB-CG-OD1	5.05	122.85	118.30
11	bJ	161	LEU	CB-CG-CD2	-5.05	102.41	111.00
10	dA	145	SER	N-CA-CB	5.05	118.08	110.50
5	p1	14	VAL	CG1-CB-CG2	5.05	118.98	110.90
16	24	123	LEU	CB-CG-CD1	-5.05	102.41	111.00
10	G6	90	MET	CB-CG-SD	-5.05	97.24	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	al	77	ARG	NE-CZ-NH1	5.05	122.83	120.30
4	K1	47	ARG	NE-CZ-NH1	5.05	122.83	120.30
4	y1	103	PRO	N-CD-CG	5.05	110.78	103.20
9	d2	81	LEU	CB-CG-CD1	5.05	119.59	111.00
11	L2	77	ARG	NE-CZ-NH2	5.05	122.83	120.30
11	n6	84	ARG	NE-CZ-NH2	-5.05	117.77	120.30
17	k9	38	LEU	CA-CB-CG	-5.05	103.68	115.30
17	ac	19	LEU	CB-CG-CD1	-5.05	102.41	111.00
11	dV	50	CYS	CA-CB-SG	5.05	123.09	114.00
10	lg	137	ARG	NE-CZ-NH2	5.05	122.83	120.30
11	lx	61	CYS	CA-CB-SG	5.05	123.09	114.00
11	H4	79	MET	CG-SD-CE	-5.05	92.12	100.20
10	du	140	VAL	C-N-CD	-5.05	109.49	120.60
25	ka	186	GLY	C-N-CD	5.05	139.00	128.40
4	w1	52	LYS	CA-CB-CG	5.05	124.51	113.40
11	H5	84	ARG	CB-CG-CD	-5.05	98.48	111.60
10	G6	18	PHE	CB-CG-CD1	5.05	124.33	120.80
11	F7	120	LEU	CB-CG-CD2	-5.05	102.42	111.00
10	z8	119	THR	CA-CB-CG2	-5.05	105.33	112.40
5	a1	38	VAL	CA-CB-CG1	-5.04	103.33	110.90
4	y1	43	LEU	CB-CG-CD2	-5.04	102.42	111.00
10	C3	17	ARG	NE-CZ-NH2	5.04	122.82	120.30
4	N1	91	LEU	CB-CG-CD1	5.04	119.57	111.00
4	y1	61	LYS	CD-CE-NZ	5.04	123.30	111.70
11	l3	41	VAL	CG1-CB-CG2	-5.04	102.83	110.90
3	E1	184	ARG	CG-CD-NE	-5.04	101.21	111.80
11	R6	129	ARG	NE-CZ-NH1	5.04	122.82	120.30
11	br	13	ASP	CB-CG-OD1	-5.04	113.76	118.30
10	ct	97	LEU	CB-CG-CD2	-5.04	102.43	111.00
11	z4	91	ARG	NE-CZ-NH2	-5.04	117.78	120.30
18	e5	105	LEU	CB-CG-CD2	-5.04	102.43	111.00
11	l7	120	LEU	CA-CB-CG	5.04	126.89	115.30
10	s9	18	PHE	CB-CG-CD2	5.04	124.33	120.80
10	E9	135	ARG	NE-CZ-NH1	5.04	122.82	120.30
18	bb	120	LEU	CB-CG-CD2	-5.04	102.43	111.00
11	l2	91	ARG	NE-CZ-NH1	-5.04	117.78	120.30
12	A2	46	PHE	CB-CG-CD1	-5.04	117.27	120.80
11	V2	134	MET	CG-SD-CE	-5.04	92.14	100.20
10	C6	44	LEU	CB-CG-CD1	-5.04	102.44	111.00
10	G6	142	ARG	CG-CD-NE	5.04	122.38	111.80
11	gv	108	ARG	NE-CZ-NH2	-5.04	117.78	120.30
13	B2	155	PHE	CB-CG-CD2	-5.04	117.28	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	V7	66	LEU	CB-CG-CD2	-5.04	102.44	111.00
17	ak	38	LEU	CA-CB-CG	-5.04	103.72	115.30
20	dy	244	VAL	N-CA-C	-5.04	97.40	111.00
10	gh	141	PRO	N-CA-C	5.04	125.19	112.10
5	e1	94	TYR	CD1-CE1-CZ	-5.03	115.27	119.80
18	g5	166	ARG	NE-CZ-NH2	-5.03	117.78	120.30
11	x6	79	MET	CG-SD-CE	-5.03	92.15	100.20
10	aA	91	ARG	NE-CZ-NH2	5.03	122.82	120.30
11	eb	38	LEU	CB-CG-CD1	-5.03	102.44	111.00
11	ee	77	ARG	NE-CZ-NH2	-5.03	117.78	120.30
25	kb	186	GLY	C-N-CD	5.03	138.97	128.40
8	b2	616	TYR	CB-CG-CD1	-5.03	117.98	121.00
11	n7	59	MET	CG-SD-CE	5.03	108.25	100.20
10	bK	138	LEU	CB-CG-CD2	-5.03	102.45	111.00
4	y1	151	PHE	CD1-CG-CD2	5.03	124.84	118.30
12	34	190	PHE	CB-CG-CD2	-5.03	117.28	120.80
10	y4	144	MET	CG-SD-CE	-5.03	92.15	100.20
11	P6	170	ASP	CB-CG-OD2	5.03	122.83	118.30
15	R8	113	ARG	NE-CZ-NH2	5.03	122.82	120.30
18	cd	117	TYR	CB-CG-CD1	-5.03	117.98	121.00
10	ef	105	LEU	CB-CG-CD1	-5.03	102.45	111.00
11	H5	91	ARG	NE-CZ-NH1	-5.03	117.78	120.30
10	dA	67	LYS	CD-CE-NZ	5.03	123.27	111.70
11	ev	153	ILE	CG1-CB-CG2	-5.03	100.34	111.40
5	W1	97	LEU	CB-CG-CD2	-5.03	102.45	111.00
11	t6	10	VAL	CG1-CB-CG2	-5.03	102.86	110.90
10	i7	137	ARG	NE-CZ-NH2	-5.03	117.79	120.30
11	ev	105	LEU	CB-CG-CD1	-5.03	102.45	111.00
10	iB	91	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
4	b1	140	LEU	CB-CG-CD1	-5.03	102.46	111.00
10	u3	95	TYR	CB-CG-CD2	-5.03	117.98	121.00
11	Z4	84	ARG	NE-CZ-NH2	-5.03	117.79	120.30
10	q9	38	LEU	CB-CG-CD2	5.03	119.54	111.00
10	cZ	24	LEU	CB-CG-CD2	5.03	119.54	111.00
10	eG	25	GLU	OE1-CD-OE2	-5.03	117.27	123.30
11	x2	13	ASP	CB-CG-OD1	5.02	122.82	118.30
10	y9	119	THR	CA-CB-CG2	-5.02	105.37	112.40
17	ak	111	LEU	CB-CG-CD1	-5.02	102.46	111.00
10	as	18	PHE	CB-CG-CD2	5.02	124.32	120.80
10	eE	62	LYS	CD-CE-NZ	-5.02	100.15	111.70
5	t1	78	TYR	CB-CG-CD1	5.02	124.01	121.00
14	e9	193	PHE	CB-CG-CD2	-5.02	117.28	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	fz	223	ASP	CB-CG-OD2	5.02	122.82	118.30
18	l4	13	ASP	CB-CG-OD2	-5.02	113.78	118.30
18	ah	78	ARG	NE-CZ-NH1	-5.02	117.79	120.30
4	k1	16	ARG	NE-CZ-NH1	-5.02	117.79	120.30
5	z1	107	ARG	NE-CZ-NH2	-5.02	117.79	120.30
10	e3	114	ARG	NE-CZ-NH1	-5.02	117.79	120.30
12	bY	121	LYS	CD-CE-NZ	5.02	123.25	111.70
4	G1	107	ILE	CG1-CB-CG2	-5.02	100.36	111.40
10	w4	18	PHE	CB-CG-CD2	5.02	124.31	120.80
11	F6	78	ARG	NE-CZ-NH1	-5.02	117.79	120.30
10	Q6	44	LEU	CB-CG-CD1	-5.02	102.47	111.00
11	lf	90	LEU	CB-CG-CD1	5.02	119.53	111.00
10	s9	85	ASP	OD1-CG-OD2	-5.02	113.77	123.30
1	A1	87	LEU	CB-CG-CD1	-5.01	102.47	111.00
4	K1	115	MET	CG-SD-CE	-5.01	92.18	100.20
5	S1	61	LEU	CB-CG-CD2	-5.01	102.47	111.00
5	S1	85	LEU	CB-CG-CD1	-5.01	102.48	111.00
4	Z1	112	VAL	CA-CB-CG1	5.01	118.42	110.90
11	v7	66	LEU	CB-CG-CD2	-5.01	102.47	111.00
10	dJ	84	ARG	NE-CZ-NH2	5.01	122.81	120.30
4	G1	116	TYR	CZ-CE2-CD2	-5.01	115.29	119.80
5	L1	36	LEU	CB-CG-CD1	5.01	119.52	111.00
5	t1	78	TYR	CB-CG-CD2	-5.01	117.99	121.00
10	G4	85	ASP	CB-CG-OD2	5.01	122.81	118.30
11	p4	122	VAL	CG1-CB-CG2	-5.01	102.88	110.90
11	H6	161	LEU	CB-CG-CD2	-5.01	102.48	111.00
11	z6	110	LEU	CA-CB-CG	5.01	126.83	115.30
10	ls	38	LEU	CB-CG-CD2	5.01	119.52	111.00
5	Y1	83	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
11	cr	13	ASP	CB-CG-OD2	5.01	122.81	118.30
11	dL	142	ILE	CG1-CB-CG2	-5.01	100.38	111.40
10	M6	33	ARG	NE-CZ-NH1	-5.01	117.80	120.30
11	J2	7	ARG	NE-CZ-NH2	-5.01	117.80	120.30
10	G6	114	ARG	NE-CZ-NH2	-5.01	117.80	120.30
11	H7	10	VAL	CG1-CB-CG2	-5.01	102.89	110.90
17	bc	24	LEU	CB-CG-CD2	5.01	119.51	111.00
17	ce	30	ARG	NE-CZ-NH1	5.01	122.80	120.30
10	gh	142	ARG	NE-CZ-NH1	-5.01	117.80	120.30
11	Z7	30	PHE	CB-CG-CD1	-5.00	117.30	120.80
18	aj	145	LEU	CB-CG-CD1	5.00	119.51	111.00
10	i3	91	ARG	NH1-CZ-NH2	-5.00	113.90	119.40
10	I4	66	LEU	CB-CG-CD1	5.00	119.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	y7	18	TYR	CB-CG-CD1	-5.00	118.00	121.00
11	az	157	ASP	CB-CG-OD1	5.00	122.80	118.30
10	dA	92	LEU	CB-CG-CD2	5.00	119.51	111.00
21	ex	200	MET	CA-CB-CG	5.00	121.81	113.30
10	M4	156	LEU	CB-CG-CD2	-5.00	102.50	111.00
17	k5	161	LEU	CB-CG-CD2	-5.00	102.50	111.00
11	n7	27	LEU	CB-CG-CD1	5.00	119.50	111.00
19	a8	99	GLU	OE1-CD-OE2	-5.00	117.30	123.30
10	la	87	ASP	CB-CG-OD1	-5.00	113.80	118.30
11	gr	61	CYS	CA-CB-SG	5.00	123.00	114.00

There are no chirality outliers.

All (493) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	44	183	GLU	Peptide
10	A5	69	SER	Peptide
10	A7	69	SER	Peptide
11	A8	33	ASP	Peptide
11	A8	47	ASN	Peptide
11	A8	74	TYR	Peptide
11	B3	46	SER	Peptide
11	B9	33	ASP	Peptide
11	B9	47	ASN	Peptide
11	B9	74	TYR	Peptide
10	C3	144	MET	Peptide
10	C4	144	MET	Peptide
10	C5	68	ASN	Peptide
10	C5	69	SER	Peptide
10	C6	69	SER	Peptide
10	C7	69	SER	Peptide
11	D3	46	SER	Peptide
11	D4	46	SER	Peptide
11	D9	33	ASP	Peptide
11	D9	47	ASN	Peptide
10	E3	144	MET	Peptide
10	E4	69	SER	Peptide
10	E5	69	SER	Peptide
10	E6	69	SER	Peptide
10	E7	69	SER	Peptide
11	E8	33	ASP	Peptide
11	F2	46	SER	Peptide

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Mol	Chain	Res	Type	Group
11	F9	33	ASP	Peptide
11	F9	47	ASN	Peptide
11	F9	74	TYR	Peptide
10	G2	144	MET	Peptide
10	G3	144	MET	Peptide
10	G4	68	ASN	Peptide
10	G4	69	SER	Peptide
10	G5	69	SER	Peptide
10	G7	69	SER	Peptide
11	G8	33	ASP	Peptide
11	G8	47	ASN	Peptide
11	G8	74	TYR	Peptide
11	H9	33	ASP	Peptide
10	I3	144	MET	Peptide
10	I4	69	SER	Peptide
10	I5	69	SER	Peptide
10	I6	69	SER	Peptide
10	I7	69	SER	Peptide
11	I8	33	ASP	Peptide
11	I8	47	ASN	Peptide
11	I8	74	TYR	Peptide
11	J9	33	ASP	Peptide
10	K3	144	MET	Peptide
10	K4	69	SER	Peptide
10	K5	69	SER	Peptide
10	K6	69	SER	Peptide
10	K7	127	TYR	Sidechain
10	K7	69	SER	Peptide
11	K8	33	ASP	Peptide
11	K8	74	TYR	Peptide
11	L2	46	SER	Peptide
11	L3	46	SER	Peptide
11	L9	33	ASP	Peptide
11	L9	47	ASN	Peptide
11	L9	74	TYR	Peptide
5	M1	73	TYR	Peptide
10	M3	144	MET	Peptide
10	M4	69	SER	Peptide
10	M5	69	SER	Peptide
10	M7	69	SER	Peptide
11	M8	33	ASP	Peptide
11	M8	47	ASN	Peptide

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Mol	Chain	Res	Type	Group
11	M8	74	TYR	Peptide
11	N2	46	SER	Peptide
11	N9	33	ASP	Peptide
11	N9	47	ASN	Peptide
11	N9	74	TYR	Peptide
5	O1	73	TYR	Peptide
10	O3	144	MET	Peptide
10	O4	69	SER	Peptide
10	O5	69	SER	Peptide
10	O6	69	SER	Peptide
10	O7	69	SER	Peptide
11	O8	33	ASP	Peptide
11	O8	47	ASN	Peptide
11	P2	46	SER	Peptide
11	P3	46	SER	Peptide
11	P9	33	ASP	Peptide
6	Q1	150	ASN	Peptide
10	Q2	144	MET	Peptide
10	Q3	144	MET	Peptide
10	Q4	69	SER	Peptide
10	Q5	69	SER	Peptide
10	Q6	69	SER	Peptide
10	Q7	69	SER	Peptide
11	Q8	33	ASP	Peptide
11	R3	46	SER	Peptide
11	R9	33	ASP	Peptide
11	R9	47	ASN	Peptide
11	R9	74	TYR	Peptide
10	S3	144	MET	Peptide
10	S4	69	SER	Peptide
10	S5	69	SER	Peptide
10	S6	69	SER	Peptide
10	S7	69	SER	Peptide
16	S8	206	ASN	Peptide
11	T3	46	SER	Peptide
14	T8	183	GLU	Peptide
14	T8	212	CYS	Peptide
11	T9	33	ASP	Peptide
11	T9	47	ASN	Peptide
5	U1	73	TYR	Peptide
10	U2	144	MET	Peptide
10	U3	144	MET	Peptide

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Mol	Chain	Res	Type	Group
10	U4	69	SER	Peptide
10	U5	69	SER	Peptide
10	U6	69	SER	Peptide
10	U7	69	SER	Peptide
11	V3	46	SER	Peptide
11	V9	33	ASP	Peptide
11	V9	47	ASN	Peptide
5	W1	73	TYR	Peptide
10	W2	144	MET	Peptide
10	W3	144	MET	Peptide
10	W4	69	SER	Peptide
10	W7	69	SER	Peptide
15	W9	101	ASN	Peptide
11	X2	46	SER	Peptide
11	X3	46	SER	Peptide
16	X5	285	HIS	Peptide
16	X5	286	GLY	Peptide
16	X9	206	ASN	Peptide
16	X9	285	HIS	Peptide
10	Y3	144	MET	Peptide
10	Y4	69	SER	Peptide
10	Y6	69	SER	Peptide
10	Y7	69	SER	Peptide
14	Y9	183	GLU	Peptide
14	Y9	212	CYS	Peptide
11	Z2	46	SER	Peptide
14	Z5	183	GLU	Peptide
8	a2	140	VAL	Peptide
8	a2	605	ARG	Sidechain
8	a2	765	GLN	Sidechain
19	a8	303	TYR	Sidechain
10	aA	69	SER	Peptide
10	aC	69	SER	Peptide
10	aE	69	SER	Peptide
10	aG	69	SER	Peptide
10	aI	69	SER	Peptide
10	aK	69	SER	Peptide
10	aO	69	SER	Peptide
10	aQ	69	SER	Peptide
10	aS	69	SER	Peptide
10	aU	69	SER	Peptide
16	aX	277	GLY	Peptide

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Mol	Chain	Res	Type	Group
14	aZ	212	CYS	Peptide
11	an	33	ASP	Peptide
11	an	47	ASN	Peptide
11	an	74	TYR	Peptide
11	ar	47	ASN	Peptide
11	ar	74	TYR	Peptide
11	ax	33	ASP	Peptide
11	az	47	ASN	Peptide
8	b2	14	PRO	Peptide
8	b2	140	VAL	Peptide
8	b2	34	PHE	Peptide
8	b2	765	GLN	Sidechain
11	b7	74	TYR	Peptide
10	bA	69	SER	Peptide
10	bC	69	SER	Peptide
10	bE	69	SER	Peptide
10	bG	69	SER	Peptide
10	bI	69	SER	Peptide
10	bK	69	SER	Peptide
11	bL	74	TYR	Peptide
10	bM	69	SER	Peptide
11	bN	74	TYR	Peptide
10	bO	69	SER	Peptide
11	bP	74	TYR	Peptide
10	bQ	69	SER	Peptide
11	bR	74	TYR	Peptide
10	bS	69	SER	Peptide
11	bT	74	TYR	Peptide
10	bU	69	SER	Peptide
16	bX	206	ASN	Peptide
16	bX	277	GLY	Peptide
16	bX	69	ARG	Peptide
14	bZ	212	CYS	Peptide
14	bZ	43	ARG	Peptide
10	bt	69	SER	Peptide
5	c1	73	TYR	Peptide
18	c5	68	GLN	Peptide
14	c9	176	CYS	Peptide
10	cA	69	SER	Peptide
11	cB	74	TYR	Peptide
10	cC	69	SER	Peptide
10	cD	69	SER	Peptide

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Mol	Chain	Res	Type	Group
11	cE	74	TYR	Peptide
11	cF	74	TYR	Peptide
10	cG	69	SER	Peptide
11	cH	74	TYR	Peptide
10	cI	141	PRO	Peptide
10	cI	69	SER	Peptide
11	cJ	74	TYR	Peptide
10	cK	141	PRO	Peptide
10	cK	69	SER	Peptide
11	cL	74	TYR	Peptide
11	cM	74	TYR	Peptide
11	cN	74	TYR	Peptide
11	cO	74	TYR	Peptide
11	cP	74	TYR	Peptide
11	cQ	74	TYR	Peptide
11	cR	74	TYR	Peptide
10	cS	69	SER	Peptide
10	cT	141	PRO	Peptide
10	cT	69	SER	Peptide
10	cV	69	SER	Peptide
10	cW	69	SER	Peptide
10	cX	69	SER	Peptide
11	cY	74	TYR	Peptide
10	cZ	69	SER	Peptide
10	cm	67	LYS	Mainchain
11	cp	74	TYR	Peptide
11	cq	74	TYR	Peptide
10	ct	69	SER	Peptide
11	cz	74	TYR	Peptide
14	d3	176	CYS	Peptide
10	dA	69	SER	Peptide
10	dC	69	SER	Peptide
11	dD	33	ASP	Peptide
10	dE	69	SER	Peptide
11	dF	33	ASP	Peptide
10	dG	69	SER	Peptide
11	dH	33	ASP	Peptide
10	dI	69	SER	Peptide
10	dJ	69	SER	Peptide
11	dK	33	ASP	Peptide
11	dL	33	ASP	Peptide
10	dM	69	SER	Peptide

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Mol	Chain	Res	Type	Group
10	dO	69	SER	Peptide
10	dQ	69	SER	Peptide
11	dR	33	ASP	Peptide
10	dS	69	SER	Peptide
11	dT	33	ASP	Peptide
10	dU	69	SER	Peptide
10	dW	69	SER	Peptide
11	dY	33	ASP	Peptide
10	dZ	69	SER	Peptide
10	da	69	SER	Peptide
10	db	69	SER	Peptide
10	dc	69	SER	Peptide
11	dd	74	TYR	Peptide
10	de	69	SER	Peptide
11	df	74	TYR	Peptide
11	dh	74	TYR	Peptide
11	di	74	TYR	Peptide
11	dj	74	TYR	Peptide
10	dk	69	SER	Peptide
11	dl	74	TYR	Peptide
10	dm	69	SER	Peptide
11	dn	74	TYR	Peptide
11	dp	74	TYR	Peptide
10	dq	69	SER	Peptide
11	dt	74	TYR	Peptide
11	dv	74	TYR	Peptide
20	dy	297	VAL	Peptide
20	dz	297	VAL	Peptide
5	e1	73	TYR	Peptide
10	e2	144	MET	Peptide
10	eA	69	SER	Peptide
10	eC	69	SER	Peptide
10	eE	69	SER	Peptide
10	eG	69	SER	Peptide
10	eI	69	SER	Peptide
10	eK	69	SER	Peptide
10	eM	69	SER	Peptide
10	eO	69	SER	Peptide
10	eQ	69	SER	Peptide
10	eS	69	SER	Peptide
10	ea	69	SER	Peptide
11	eb	33	ASP	Peptide

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Mol	Chain	Res	Type	Group
11	ec	33	ASP	Peptide
10	ed	141	PRO	Peptide
10	ed	69	SER	Peptide
11	ee	33	ASP	Peptide
10	ef	69	SER	Peptide
11	eg	33	ASP	Peptide
10	eh	69	SER	Peptide
11	ei	33	ASP	Peptide
10	ej	141	PRO	Peptide
10	ej	69	SER	Peptide
10	ek	69	SER	Peptide
10	em	141	PRO	Peptide
10	em	69	SER	Peptide
10	eo	69	SER	Peptide
11	ep	33	ASP	Peptide
10	eq	69	SER	Peptide
10	es	141	PRO	Peptide
10	es	69	SER	Peptide
12	ey	214	THR	Peptide
12	ez	214	THR	Peptide
10	f6	69	SER	Peptide
10	f7	69	SER	Peptide
11	fa	74	TYR	Peptide
10	fb	140	VAL	Peptide
10	fb	69	SER	Peptide
10	fb	70	GLY	Peptide
11	fc	74	TYR	Peptide
21	fd	201	ARG	Peptide
10	fe	140	VAL	Peptide
10	fe	69	SER	Peptide
10	fe	70	GLY	Peptide
11	ff	74	TYR	Peptide
10	fg	137	ARG	Peptide
10	fg	140	VAL	Peptide
10	fg	141	PRO	Peptide
10	fg	69	SER	Peptide
10	fg	70	GLY	Peptide
10	fh	140	VAL	Peptide
10	fh	69	SER	Peptide
10	fh	70	GLY	Peptide
11	fi	74	TYR	Peptide
11	fj	74	TYR	Peptide

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Mol	Chain	Res	Type	Group
10	fk	140	VAL	Peptide
10	fk	69	SER	Peptide
10	fk	70	GLY	Peptide
10	fl	137	ARG	Peptide
10	fl	140	VAL	Peptide
10	fl	141	PRO	Peptide
10	fl	69	SER	Peptide
10	fl	70	GLY	Peptide
11	fm	74	TYR	Peptide
10	fn	69	SER	Peptide
10	fn	70	GLY	Peptide
11	fo	74	TYR	Peptide
10	fp	140	VAL	Peptide
10	fp	69	SER	Peptide
10	fp	70	GLY	Peptide
11	fq	74	TYR	Peptide
10	fr	140	VAL	Peptide
10	fr	69	SER	Peptide
10	fr	70	GLY	Peptide
11	fs	74	TYR	Peptide
10	ft	69	SER	Peptide
10	ft	70	GLY	Peptide
11	fu	74	TYR	Peptide
10	fv	69	SER	Peptide
10	fv	70	GLY	Peptide
11	fw	74	TYR	Peptide
10	fx	69	SER	Peptide
10	fx	70	GLY	Peptide
11	fy	74	TYR	Peptide
6	g1	150	ASN	Peptide
10	g2	144	MET	Peptide
10	g3	144	MET	Peptide
10	g6	69	SER	Peptide
10	g7	69	SER	Peptide
10	gb	69	SER	Peptide
10	gc	69	SER	Peptide
10	gh	69	SER	Peptide
10	gj	69	SER	Peptide
10	gl	69	SER	Peptide
10	gm	67	LYS	Mainchain
10	gm	69	SER	Peptide
10	go	69	SER	Peptide

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Mol	Chain	Res	Type	Group
10	gq	69	SER	Peptide
11	gr	74	TYR	Peptide
10	gs	69	SER	Peptide
10	gu	69	SER	Peptide
10	gw	69	SER	Peptide
24	gy	117	GLY	Peptide
24	gz	117	GLY	Peptide
24	gz	63	GLY	Peptide
5	h1	73	TYR	Peptide
11	h2	46	SER	Peptide
10	h7	69	SER	Peptide
10	hA	69	SER	Peptide
10	hC	69	SER	Peptide
10	hE	69	SER	Peptide
10	hF	69	SER	Peptide
10	hI	69	SER	Peptide
10	hK	69	SER	Peptide
10	hM	69	SER	Peptide
10	hO	69	SER	Peptide
10	hQ	69	SER	Peptide
10	hS	69	SER	Peptide
10	hU	69	SER	Peptide
10	hW	69	SER	Peptide
10	i2	144	MET	Peptide
10	i6	69	SER	Peptide
10	i7	69	SER	Peptide
10	i8	69	SER	Peptide
11	iC	75	THR	Peptide
11	iD	75	THR	Peptide
11	j2	46	SER	Peptide
10	j6	69	SER	Peptide
10	j7	69	SER	Peptide
10	j8	69	SER	Peptide
10	k2	144	MET	Peptide
17	k4	91	TYR	Sidechain
17	k5	91	TYR	Sidechain
10	k6	69	SER	Peptide
10	k7	69	SER	Peptide
10	k8	69	SER	Peptide
11	kS	33	ASP	Peptide
11	kT	149	ARG	Peptide
25	kb	118	GLU	Peptide

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Mol	Chain	Res	Type	Group
5	l1	73	TYR	Peptide
10	l8	69	SER	Peptide
10	la	69	SER	Peptide
10	la	71	GLU	Peptide
10	lc	62	LYS	Peptide
10	lc	69	SER	Peptide
10	lc	71	GLU	Peptide
10	le	69	SER	Peptide
10	le	71	GLU	Peptide
10	lg	69	SER	Peptide
10	lg	71	GLU	Peptide
10	li	69	SER	Peptide
10	lk	69	SER	Peptide
10	lk	71	GLU	Peptide
10	lm	69	SER	Peptide
10	lm	71	GLU	Peptide
10	lo	69	SER	Peptide
10	lo	71	GLU	Peptide
10	lq	69	SER	Peptide
10	lq	71	GLU	Peptide
10	ls	69	SER	Peptide
10	ls	71	GLU	Peptide
10	lu	69	SER	Peptide
10	lu	71	GLU	Peptide
10	m2	144	MET	Peptide
10	m3	144	MET	Peptide
10	m4	69	SER	Peptide
10	m5	69	SER	Peptide
10	m6	69	SER	Peptide
10	m7	69	SER	Peptide
10	m8	69	SER	Peptide
5	n1	73	TYR	Peptide
11	n2	46	SER	Peptide
11	n3	46	SER	Peptide
11	n9	33	ASP	Peptide
11	n9	47	ASN	Peptide
11	n9	74	TYR	Peptide
10	o4	69	SER	Peptide
10	o5	69	SER	Peptide
10	o6	69	SER	Peptide
10	o7	69	SER	Peptide
11	p2	46	SER	Peptide

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Mol	Chain	Res	Type	Group
10	q2	144	MET	Peptide
10	q3	144	MET	Peptide
10	q4	69	SER	Peptide
10	q5	69	SER	Peptide
10	q6	69	SER	Peptide
10	q7	69	SER	Peptide
10	q8	69	SER	Peptide
5	r1	73	TYR	Peptide
11	r2	46	SER	Peptide
10	r8	69	SER	Peptide
11	r9	74	TYR	Peptide
10	s2	144	MET	Peptide
10	s3	144	MET	Peptide
10	s4	69	SER	Peptide
10	s5	68	ASN	Peptide
10	s5	69	SER	Peptide
10	s6	69	SER	Peptide
10	s7	69	SER	Peptide
10	s8	69	SER	Peptide
11	t2	46	SER	Peptide
10	t8	69	SER	Peptide
10	u2	144	MET	Peptide
10	u3	144	MET	Peptide
10	u4	69	SER	Peptide
10	u5	69	SER	Peptide
10	u6	69	SER	Peptide
10	u7	69	SER	Peptide
10	u8	69	SER	Peptide
11	v2	46	SER	Peptide
10	w2	144	MET	Peptide
10	w3	144	MET	Peptide
10	w4	69	SER	Peptide
10	w5	69	SER	Peptide
10	w6	69	SER	Peptide
10	w7	69	SER	Peptide
11	w8	33	ASP	Peptide
11	w8	47	ASN	Peptide
11	w8	74	TYR	Peptide
11	x2	46	SER	Peptide
11	x9	33	ASP	Peptide
10	y2	144	MET	Peptide
10	y5	100	GLY	Peptide

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Mol	Chain	Res	Type	Group
10	y5	69	SER	Peptide
11	z2	46	SER	Peptide
11	z3	46	SER	Peptide
11	z9	47	ASN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A1	217/260 (84%)	204 (94%)	13 (6%)	0	100 100
1	B1	218/260 (84%)	202 (93%)	16 (7%)	0	100 100
2	C1	152/192 (79%)	139 (91%)	12 (8%)	1 (1%)	22 61
2	D1	151/192 (79%)	135 (89%)	13 (9%)	3 (2%)	7 39
3	E1	257/307 (84%)	244 (95%)	10 (4%)	3 (1%)	13 50
3	F1	257/307 (84%)	243 (95%)	11 (4%)	3 (1%)	13 50
4	G1	158/161 (98%)	155 (98%)	3 (2%)	0	100 100
4	I1	158/161 (98%)	155 (98%)	3 (2%)	0	100 100
4	K1	158/161 (98%)	154 (98%)	4 (2%)	0	100 100
4	N1	158/161 (98%)	154 (98%)	4 (2%)	0	100 100
4	P1	158/161 (98%)	153 (97%)	5 (3%)	0	100 100
4	R1	158/161 (98%)	153 (97%)	3 (2%)	2 (1%)	12 48
4	T1	158/161 (98%)	155 (98%)	3 (2%)	0	100 100
4	X1	158/161 (98%)	155 (98%)	3 (2%)	0	100 100
4	Z1	158/161 (98%)	155 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	b1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	d1	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
4	f1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	i1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	k1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	o1	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
4	q1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	s1	158/161 (98%)	151 (96%)	6 (4%)	1 (1%)	25	64
4	u1	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
4	w1	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
4	y1	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
5	H1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	J1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	L1	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	M1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	O1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	S1	159/161 (99%)	154 (97%)	4 (2%)	1 (1%)	25	64
5	U1	159/161 (99%)	156 (98%)	2 (1%)	1 (1%)	25	64
5	W1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	Y1	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	a1	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	c1	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
5	e1	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
5	h1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	j1	159/161 (99%)	154 (97%)	4 (2%)	1 (1%)	25	64
5	l1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	n1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	p1	159/161 (99%)	156 (98%)	3 (2%)	0	100	100
5	r1	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
5	t1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	v1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	x1	159/161 (99%)	155 (98%)	4 (2%)	0	100	100
5	z1	159/161 (99%)	154 (97%)	5 (3%)	0	100	100
6	Q1	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	9	42
6	g1	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	9	42
7	V1	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
7	m1	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
8	a2	795/885 (90%)	746 (94%)	43 (5%)	6 (1%)	19	58
8	b2	795/885 (90%)	730 (92%)	56 (7%)	9 (1%)	14	52
9	c2	89/93 (96%)	79 (89%)	8 (9%)	2 (2%)	6	37
9	d2	89/93 (96%)	82 (92%)	6 (7%)	1 (1%)	14	52
10	A3	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	A4	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	A5	162/164 (99%)	146 (90%)	14 (9%)	2 (1%)	13	50
10	A6	162/164 (99%)	156 (96%)	2 (1%)	4 (2%)	5	34
10	A7	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	A9	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
10	B8	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
10	C3	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	C4	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	C5	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	C6	162/164 (99%)	148 (91%)	10 (6%)	4 (2%)	5	34
10	C7	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	C9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	D8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	E2	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
10	E3	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	E4	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
10	E5	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
10	E6	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	E7	162/164 (99%)	150 (93%)	8 (5%)	4 (2%)	5	34
10	E9	162/164 (99%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	F8	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	G2	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	G3	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	G4	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	G5	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	G6	162/164 (99%)	154 (95%)	4 (2%)	4 (2%)	5	34
10	G7	161/164 (98%)	152 (94%)	5 (3%)	4 (2%)	5	34
10	G9	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	H8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	I2	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	I3	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	I4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
10	I5	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	I6	161/164 (98%)	153 (95%)	4 (2%)	4 (2%)	5	34
10	I7	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	I9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	J8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	K2	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	K3	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	K4	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	K5	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	K6	162/164 (99%)	153 (94%)	6 (4%)	3 (2%)	8	40
10	K7	162/164 (99%)	149 (92%)	9 (6%)	4 (2%)	5	34
10	K9	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	L8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	M2	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	M3	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	M4	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	M5	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	M6	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
10	M7	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	M9	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	N8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	O2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	O3	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	O4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	O5	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	O6	162/164 (99%)	150 (93%)	8 (5%)	4 (2%)	5	34
10	O7	162/164 (99%)	151 (93%)	8 (5%)	3 (2%)	8	40
10	O9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	P8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	Q2	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	Q3	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	Q4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	Q5	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	Q6	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	Q7	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	Q9	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	S2	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	S3	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	S4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	S5	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	S6	162/164 (99%)	152 (94%)	7 (4%)	3 (2%)	8	40
10	S7	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	S9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	U2	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	U3	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	U4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	U5	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	U6	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	U7	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	U9	162/164 (99%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	W2	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	W3	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	W4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	W6	162/164 (99%)	156 (96%)	2 (1%)	4 (2%)	5	34
10	W7	162/164 (99%)	154 (95%)	4 (2%)	4 (2%)	5	34
10	Y2	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	Y3	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	Y4	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	Y6	162/164 (99%)	152 (94%)	7 (4%)	3 (2%)	8	40
10	Y7	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	aA	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	50
10	aC	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	aE	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	50
10	aG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	aI	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	aK	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	aM	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	aO	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	aQ	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	aS	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	aU	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	am	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
10	ao	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
10	aq	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
10	as	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	au	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
10	aw	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	ay	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	bA	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	bC	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	50
10	bE	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	bG	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	bI	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	bK	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	50
10	bM	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	bO	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	bQ	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	bS	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	bU	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	bm	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	bt	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	bu	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	bv	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
10	bw	162/164 (99%)	154 (95%)	6 (4%)	2 (1%)	13	50
10	bx	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	by	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
10	cA	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	cC	162/164 (99%)	155 (96%)	5 (3%)	2 (1%)	13	50
10	cD	162/164 (99%)	152 (94%)	7 (4%)	3 (2%)	8	40
10	cG	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
10	cI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	cK	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	cS	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	cT	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	cU	162/164 (99%)	157 (97%)	2 (1%)	3 (2%)	8	40
10	cV	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
10	cW	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	cX	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
10	cZ	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	cm	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	ct	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	cu	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	cv	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
10	cw	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	50
10	cx	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	cy	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
10	dA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	dC	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
10	dE	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	dG	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	dI	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	dJ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	dM	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	dO	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	dQ	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
10	dS	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	dU	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	dW	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	dZ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	da	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	50
10	db	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
10	dc	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	de	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	50
10	dg	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
10	dk	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
10	dm	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
10	do	162/164 (99%)	154 (95%)	6 (4%)	2 (1%)	13	50
10	dq	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	ds	162/164 (99%)	156 (96%)	4 (2%)	2 (1%)	13	50
10	du	162/164 (99%)	159 (98%)	2 (1%)	1 (1%)	25	64
10	e2	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	e3	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	eA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	eC	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	eE	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	eG	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	eI	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	eK	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	eM	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	eO	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	eQ	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	eS	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25	64
10	eU	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13	50
10	eW	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	ea	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	ed	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
10	ef	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	eh	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
10	ej	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	ek	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
10	em	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	eo	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	eq	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
10	es	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	eu	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
10	f6	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	f7	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	50
10	fb	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40
10	fe	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40
10	fg	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40
10	fh	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40
10	fk	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40
10	fl	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40
10	fn	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	fp	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8 40
10	fr	162/164 (99%)	150 (93%)	9 (6%)	3 (2%)	8 40
10	ft	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25 64
10	fv	162/164 (99%)	157 (97%)	5 (3%)	0	100 100
10	fx	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25 64
10	g2	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25 64
10	g3	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25 64
10	g6	162/164 (99%)	152 (94%)	5 (3%)	5 (3%)	4 30
10	g7	162/164 (99%)	153 (94%)	8 (5%)	1 (1%)	25 64
10	gb	162/164 (99%)	158 (98%)	4 (2%)	0	100 100
10	gc	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25 64
10	gf	162/164 (99%)	156 (96%)	3 (2%)	3 (2%)	8 40
10	gh	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25 64
10	gj	162/164 (99%)	156 (96%)	4 (2%)	2 (1%)	13 50
10	gl	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25 64
10	gm	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	25 64
10	go	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25 64
10	gq	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25 64
10	gs	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25 64
10	gu	162/164 (99%)	156 (96%)	6 (4%)	0	100 100
10	gw	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	13 50
10	h6	162/164 (99%)	154 (95%)	3 (2%)	5 (3%)	4 30
10	h7	162/164 (99%)	149 (92%)	9 (6%)	4 (2%)	5 34
10	hA	162/164 (99%)	152 (94%)	10 (6%)	0	100 100
10	hC	162/164 (99%)	151 (93%)	11 (7%)	0	100 100
10	hE	162/164 (99%)	152 (94%)	10 (6%)	0	100 100
10	hF	162/164 (99%)	151 (93%)	11 (7%)	0	100 100
10	hI	162/164 (99%)	151 (93%)	11 (7%)	0	100 100
10	hK	162/164 (99%)	152 (94%)	10 (6%)	0	100 100
10	hM	162/164 (99%)	151 (93%)	11 (7%)	0	100 100
10	hO	162/164 (99%)	152 (94%)	10 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	hQ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	hS	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	hU	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	hW	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
10	i2	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	i3	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25	64
10	i6	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	25	64
10	i7	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	i8	162/164 (99%)	154 (95%)	4 (2%)	4 (2%)	5	34
10	iA	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	iB	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	j6	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	j7	162/164 (99%)	149 (92%)	9 (6%)	4 (2%)	5	34
10	j8	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
10	k2	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	k3	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	k6	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	k7	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	k8	162/164 (99%)	153 (94%)	6 (4%)	3 (2%)	8	40
10	l8	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	la	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	lc	162/164 (99%)	147 (91%)	15 (9%)	0	100	100
10	le	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	lg	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
10	li	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25	64
10	lk	162/164 (99%)	145 (90%)	16 (10%)	1 (1%)	25	64
10	lm	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	lo	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
10	lq	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
10	ls	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
10	lu	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	lw	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	50
10	m2	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	m3	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	m4	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	m5	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	m6	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	m7	162/164 (99%)	150 (93%)	8 (5%)	4 (2%)	5	34
10	m8	162/164 (99%)	154 (95%)	4 (2%)	4 (2%)	5	34
10	m9	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	25	64
10	o2	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
10	o3	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
10	o4	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	o5	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	o6	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	o7	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	o9	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
10	q2	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
10	q3	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	q4	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	q5	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
10	q6	162/164 (99%)	154 (95%)	5 (3%)	3 (2%)	8	40
10	q7	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	q8	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5	34
10	q9	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
10	r8	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5	34
10	s2	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
10	s3	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
10	s4	162/164 (99%)	148 (91%)	12 (7%)	2 (1%)	13	50
10	s5	162/164 (99%)	148 (91%)	12 (7%)	2 (1%)	13	50
10	s6	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	34
10	s7	162/164 (99%)	154 (95%)	4 (2%)	4 (2%)	5	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	s8	162/164 (99%)	153 (94%)	6 (4%)	3 (2%)	8 40
10	s9	162/164 (99%)	156 (96%)	6 (4%)	0	100 100
10	t8	162/164 (99%)	153 (94%)	5 (3%)	4 (2%)	5 34
10	u2	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25 64
10	u3	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25 64
10	u4	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25 64
10	u5	162/164 (99%)	150 (93%)	10 (6%)	2 (1%)	13 50
10	u6	162/164 (99%)	152 (94%)	6 (4%)	4 (2%)	5 34
10	u7	162/164 (99%)	153 (94%)	6 (4%)	3 (2%)	8 40
10	u8	162/164 (99%)	154 (95%)	5 (3%)	3 (2%)	8 40
10	u9	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25 64
10	v8	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25 64
10	w2	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25 64
10	w3	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	25 64
10	w4	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25 64
10	w5	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25 64
10	w6	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25 64
10	w7	162/164 (99%)	153 (94%)	6 (4%)	3 (2%)	8 40
10	w9	162/164 (99%)	155 (96%)	7 (4%)	0	100 100
10	x8	162/164 (99%)	156 (96%)	6 (4%)	0	100 100
10	y2	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25 64
10	y3	162/164 (99%)	151 (93%)	11 (7%)	0	100 100
10	y4	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13 50
10	y5	162/164 (99%)	149 (92%)	12 (7%)	1 (1%)	25 64
10	y9	162/164 (99%)	155 (96%)	7 (4%)	0	100 100
10	z8	162/164 (99%)	154 (95%)	8 (5%)	0	100 100
11	A8	175/177 (99%)	166 (95%)	9 (5%)	0	100 100
11	B3	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25 64
11	B4	175/177 (99%)	172 (98%)	3 (2%)	0	100 100
11	B5	175/177 (99%)	173 (99%)	2 (1%)	0	100 100
11	B6	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	B7	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	B9	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25	64
11	C8	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	D3	175/177 (99%)	172 (98%)	2 (1%)	1 (1%)	25	64
11	D4	175/177 (99%)	172 (98%)	2 (1%)	1 (1%)	25	64
11	D5	175/177 (99%)	172 (98%)	2 (1%)	1 (1%)	25	64
11	D6	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	D7	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25	64
11	D9	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	E8	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	F2	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	F3	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	F4	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
11	F5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	F6	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	F7	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	F9	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
11	G8	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	H2	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	H3	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	H4	175/177 (99%)	172 (98%)	2 (1%)	1 (1%)	25	64
11	H5	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	H6	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	H7	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	H9	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25	64
11	I8	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	J2	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	J3	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	J4	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	J5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	J6	175/177 (99%)	167 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J7	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	J9	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	K8	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	L2	175/177 (99%)	171 (98%)	2 (1%)	2 (1%)	14	52
11	L3	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	L4	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	L5	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	L6	175/177 (99%)	167 (95%)	6 (3%)	2 (1%)	14	52
11	L7	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	L9	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	M8	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
11	N2	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	N3	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	N4	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	N5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	N6	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	N7	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	N9	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	O8	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	P2	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	P3	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	P4	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	P5	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	P6	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	P7	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	P9	175/177 (99%)	165 (94%)	9 (5%)	1 (1%)	25	64
11	Q8	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	R2	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	R3	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	R4	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	R5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	R6	175/177 (99%)	169 (97%)	4 (2%)	2 (1%)	14 52
11	R7	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25 64
11	R9	175/177 (99%)	166 (95%)	9 (5%)	0	100 100
11	T2	175/177 (99%)	171 (98%)	2 (1%)	2 (1%)	14 52
11	T3	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25 64
11	T4	175/177 (99%)	171 (98%)	4 (2%)	0	100 100
11	T5	175/177 (99%)	173 (99%)	2 (1%)	0	100 100
11	T6	175/177 (99%)	168 (96%)	7 (4%)	0	100 100
11	T7	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25 64
11	T9	175/177 (99%)	167 (95%)	8 (5%)	0	100 100
11	V2	175/177 (99%)	173 (99%)	2 (1%)	0	100 100
11	V3	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25 64
11	V4	175/177 (99%)	172 (98%)	3 (2%)	0	100 100
11	V5	175/177 (99%)	172 (98%)	3 (2%)	0	100 100
11	V6	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25 64
11	V7	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25 64
11	V9	175/177 (99%)	167 (95%)	8 (5%)	0	100 100
11	X2	175/177 (99%)	171 (98%)	2 (1%)	2 (1%)	14 52
11	X3	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25 64
11	X4	175/177 (99%)	173 (99%)	2 (1%)	0	100 100
11	X6	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25 64
11	X7	175/177 (99%)	167 (95%)	8 (5%)	0	100 100
11	Z2	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25 64
11	Z3	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25 64
11	Z4	175/177 (99%)	172 (98%)	3 (2%)	0	100 100
11	Z6	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25 64
11	Z7	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25 64
11	a6	175/177 (99%)	166 (95%)	9 (5%)	0	100 100
11	a7	175/177 (99%)	169 (97%)	6 (3%)	0	100 100
11	aB	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25 64
11	aD	175/177 (99%)	170 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	aF	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	aH	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	aJ	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	aL	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	aN	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	aP	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	aR	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	aT	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	aV	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	an	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
11	ap	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	ar	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	at	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	av	175/177 (99%)	169 (97%)	3 (2%)	3 (2%)	9	42
11	ax	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	az	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	b6	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	b7	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	bB	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	bD	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	bF	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	bH	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	bJ	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	bL	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	bN	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	bP	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	bR	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	bT	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	bV	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	bn	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	bo	175/177 (99%)	167 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	bp	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	bq	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	br	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	bs	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	bz	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	c6	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	c7	175/177 (99%)	165 (94%)	8 (5%)	2 (1%)	14	52
11	cB	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	cE	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	cF	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	cH	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	cJ	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	cL	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	cM	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	cN	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	cO	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	cP	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	cQ	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	cR	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	cY	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	cn	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	co	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	cp	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	cq	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	cr	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	cs	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	cz	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	d6	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
11	d7	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	dB	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	dD	175/177 (99%)	169 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	dF	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	dH	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	dK	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	dL	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	dN	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	dP	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	dR	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	dT	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	dV	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	dX	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	dY	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	dd	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	df	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	dh	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	di	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	dj	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	dl	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	dn	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	dp	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	dr	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	dt	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	dv	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	e6	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	e7	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	eB	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	eD	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	eF	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	eH	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	eJ	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	eL	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	eN	175/177 (99%)	168 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	eP	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	eR	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	eT	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	eV	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	eX	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	eb	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	ec	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	ee	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	eg	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	ei	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	el	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	en	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	ep	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	er	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	et	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	ev	175/177 (99%)	169 (97%)	4 (2%)	2 (1%)	14	52
11	f2	175/177 (99%)	173 (99%)	1 (1%)	1 (1%)	25	64
11	f3	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	f8	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	fa	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	fc	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	ff	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	fi	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	fj	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	fm	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	fo	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	fq	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	fs	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	fu	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	fw	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	fy	175/177 (99%)	171 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	g8	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	ga	175/177 (99%)	172 (98%)	2 (1%)	1 (1%)	25	64
11	gd	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	ge	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	gg	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	gi	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	gk	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	gn	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	gp	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	gr	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	gt	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
11	gv	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	gx	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	h2	175/177 (99%)	170 (97%)	3 (2%)	2 (1%)	14	52
11	h3	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	h8	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	hB	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	hD	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	hG	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hH	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hJ	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	hL	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hN	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hP	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hR	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	hT	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hV	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	hX	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	iC	175/177 (99%)	155 (89%)	18 (10%)	2 (1%)	14	52
11	iD	175/177 (99%)	156 (89%)	18 (10%)	1 (1%)	25	64
11	iE	144/177 (81%)	137 (95%)	5 (4%)	2 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	iF	144/177 (81%)	127 (88%)	15 (10%)	2 (1%)	11 46
11	iG	146/177 (82%)	136 (93%)	9 (6%)	1 (1%)	22 61
11	iH	146/177 (82%)	136 (93%)	9 (6%)	1 (1%)	22 61
11	j2	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25 64
11	j3	175/177 (99%)	173 (99%)	2 (1%)	0	100 100
11	jI	142/177 (80%)	134 (94%)	7 (5%)	1 (1%)	22 61
11	jJ	142/177 (80%)	134 (94%)	7 (5%)	1 (1%)	22 61
11	jK	143/177 (81%)	132 (92%)	10 (7%)	1 (1%)	22 61
11	jL	143/177 (81%)	133 (93%)	10 (7%)	0	100 100
11	jM	143/177 (81%)	132 (92%)	11 (8%)	0	100 100
11	jN	143/177 (81%)	132 (92%)	11 (8%)	0	100 100
11	jO	143/177 (81%)	132 (92%)	10 (7%)	1 (1%)	22 61
11	jP	143/177 (81%)	133 (93%)	10 (7%)	0	100 100
11	kQ	142/177 (80%)	133 (94%)	9 (6%)	0	100 100
11	kR	142/177 (80%)	133 (94%)	9 (6%)	0	100 100
11	kS	145/177 (82%)	134 (92%)	8 (6%)	3 (2%)	7 38
11	kT	144/177 (81%)	134 (93%)	9 (6%)	1 (1%)	22 61
11	kU	142/177 (80%)	132 (93%)	10 (7%)	0	100 100
11	kV	142/177 (80%)	132 (93%)	10 (7%)	0	100 100
11	kW	145/177 (82%)	134 (92%)	10 (7%)	1 (1%)	22 61
11	kX	145/177 (82%)	134 (92%)	10 (7%)	1 (1%)	22 61
11	l2	175/177 (99%)	172 (98%)	3 (2%)	0	100 100
11	l3	175/177 (99%)	173 (99%)	2 (1%)	0	100 100
11	l6	175/177 (99%)	168 (96%)	7 (4%)	0	100 100
11	l7	175/177 (99%)	167 (95%)	8 (5%)	0	100 100
11	lb	175/177 (99%)	167 (95%)	8 (5%)	0	100 100
11	ld	175/177 (99%)	169 (97%)	6 (3%)	0	100 100
11	lf	175/177 (99%)	167 (95%)	8 (5%)	0	100 100
11	lh	175/177 (99%)	170 (97%)	5 (3%)	0	100 100
11	lj	175/177 (99%)	168 (96%)	7 (4%)	0	100 100
11	ll	175/177 (99%)	168 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	ln	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
11	lp	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	lr	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	lt	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	lv	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	lx	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	n2	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	n3	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	n4	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	n5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	n6	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	n7	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	n8	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	n9	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
11	o8	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	p2	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	p3	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	p4	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	p5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	p6	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	p7	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	p8	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	p9	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	r2	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	r3	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	r4	175/177 (99%)	172 (98%)	2 (1%)	1 (1%)	25	64
11	r5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	r6	175/177 (99%)	168 (96%)	4 (2%)	3 (2%)	9	42
11	r7	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	r9	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	t2	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	t3	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	t4	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
11	t5	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	t6	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	t7	175/177 (99%)	166 (95%)	9 (5%)	0	100	100
11	t9	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	v2	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	v3	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	v4	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
11	v5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	v6	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	v7	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	v9	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	w8	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	x2	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	x3	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	x4	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	x5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	x6	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
11	x7	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
11	x9	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	y6	175/177 (99%)	168 (96%)	6 (3%)	1 (1%)	25	64
11	y7	175/177 (99%)	166 (95%)	8 (5%)	1 (1%)	25	64
11	y8	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64
11	z2	175/177 (99%)	169 (97%)	5 (3%)	1 (1%)	25	64
11	z3	175/177 (99%)	171 (98%)	3 (2%)	1 (1%)	25	64
11	z4	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	z5	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
11	z6	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
11	z7	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	z9	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	34	275/318 (86%)	257 (94%)	14 (5%)	4 (2%)	10	45
12	A2	275/318 (86%)	262 (95%)	10 (4%)	3 (1%)	14	52
12	U8	275/318 (86%)	257 (94%)	15 (6%)	3 (1%)	14	52
12	Y5	275/318 (86%)	259 (94%)	11 (4%)	5 (2%)	8	41
12	Z9	275/318 (86%)	257 (94%)	14 (5%)	4 (2%)	10	45
12	a3	275/318 (86%)	260 (94%)	12 (4%)	3 (1%)	14	52
12	aY	275/318 (86%)	254 (92%)	19 (7%)	2 (1%)	22	61
12	b8	275/318 (86%)	255 (93%)	15 (6%)	5 (2%)	8	41
12	b9	275/318 (86%)	250 (91%)	19 (7%)	6 (2%)	6	37
12	bY	275/318 (86%)	253 (92%)	17 (6%)	5 (2%)	8	41
12	dw	275/318 (86%)	252 (92%)	20 (7%)	3 (1%)	14	52
12	dx	275/318 (86%)	259 (94%)	14 (5%)	2 (1%)	22	61
12	ey	275/318 (86%)	262 (95%)	11 (4%)	2 (1%)	22	61
12	ez	274/318 (86%)	258 (94%)	15 (6%)	1 (0%)	34	72
13	B2	372/477 (78%)	351 (94%)	18 (5%)	3 (1%)	19	58
13	b3	372/477 (78%)	351 (94%)	17 (5%)	4 (1%)	14	52
14	44	243/285 (85%)	230 (95%)	10 (4%)	3 (1%)	13	50
14	C2	243/285 (85%)	236 (97%)	7 (3%)	0	100	100
14	D2	237/285 (83%)	226 (95%)	11 (5%)	0	100	100
14	T8	243/285 (85%)	227 (93%)	16 (7%)	0	100	100
14	Y9	243/285 (85%)	227 (93%)	16 (7%)	0	100	100
14	Z5	243/285 (85%)	228 (94%)	12 (5%)	3 (1%)	13	50
14	aZ	243/285 (85%)	231 (95%)	12 (5%)	0	100	100
14	bZ	243/285 (85%)	230 (95%)	13 (5%)	0	100	100
14	c3	243/285 (85%)	235 (97%)	8 (3%)	0	100	100
14	c8	243/285 (85%)	232 (96%)	10 (4%)	1 (0%)	34	72
14	c9	243/285 (85%)	232 (96%)	7 (3%)	4 (2%)	9	43
14	d3	237/285 (83%)	225 (95%)	12 (5%)	0	100	100
14	d8	237/285 (83%)	224 (94%)	10 (4%)	3 (1%)	12	48
14	d9	237/285 (83%)	226 (95%)	9 (4%)	2 (1%)	19	58
14	e8	237/285 (83%)	222 (94%)	13 (6%)	2 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
14	e9	237/285 (83%)	219 (92%)	17 (7%)	1 (0%)	34 72
15	14	225/232 (97%)	202 (90%)	18 (8%)	5 (2%)	6 37
15	R8	224/232 (97%)	204 (91%)	17 (8%)	3 (1%)	12 48
15	W5	225/232 (97%)	199 (88%)	22 (10%)	4 (2%)	8 41
15	W9	224/232 (97%)	203 (91%)	17 (8%)	4 (2%)	8 41
15	aW	226/232 (97%)	203 (90%)	16 (7%)	7 (3%)	4 30
15	bW	226/232 (97%)	202 (89%)	17 (8%)	7 (3%)	4 30
16	24	329/371 (89%)	307 (93%)	17 (5%)	5 (2%)	10 45
16	S8	329/371 (89%)	296 (90%)	29 (9%)	4 (1%)	13 50
16	X5	329/371 (89%)	304 (92%)	18 (6%)	7 (2%)	7 38
16	X9	329/371 (89%)	296 (90%)	29 (9%)	4 (1%)	13 50
16	aX	329/371 (89%)	296 (90%)	25 (8%)	8 (2%)	6 35
16	bX	329/371 (89%)	301 (92%)	22 (7%)	6 (2%)	8 41
17	V8	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	X8	160/162 (99%)	159 (99%)	1 (1%)	0	100 100
17	Z8	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	a4	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	a5	160/162 (99%)	155 (97%)	5 (3%)	0	100 100
17	aa	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	ac	160/162 (99%)	159 (99%)	1 (1%)	0	100 100
17	ae	161/162 (99%)	158 (98%)	3 (2%)	0	100 100
17	ag	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	ai	160/162 (99%)	159 (99%)	1 (1%)	0	100 100
17	ak	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	b4	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
17	b5	160/162 (99%)	157 (98%)	3 (2%)	0	100 100
17	ba	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	bc	160/162 (99%)	156 (98%)	4 (2%)	0	100 100
17	be	161/162 (99%)	158 (98%)	3 (2%)	0	100 100
17	bg	160/162 (99%)	154 (96%)	6 (4%)	0	100 100
17	bi	160/162 (99%)	157 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	bk	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
17	ca	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
17	cc	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
17	ce	161/162 (99%)	156 (97%)	5 (3%)	0	100	100
17	cg	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
17	ci	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
17	ck	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
17	d4	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
17	d5	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
17	f4	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
17	f5	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
17	g9	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
17	i4	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
17	i5	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
17	i9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
17	k4	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	25	64
17	k5	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
17	k9	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
18	W8	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
18	Y8	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25	64
18	ab	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
18	ad	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	25	64
18	af	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
18	ah	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
18	aj	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
18	al	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25	64
18	bb	170/172 (99%)	164 (96%)	4 (2%)	2 (1%)	13	50
18	bd	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
18	bf	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
18	bh	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
18	bj	171/172 (99%)	165 (96%)	5 (3%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	bl	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	25	64
18	c4	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
18	c5	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
18	cb	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
18	cd	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	25	64
18	cf	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
18	ch	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
18	cj	171/172 (99%)	165 (96%)	5 (3%)	1 (1%)	25	64
18	cl	170/172 (99%)	165 (97%)	5 (3%)	0	100	100
18	e4	170/172 (99%)	166 (98%)	3 (2%)	1 (1%)	25	64
18	e5	170/172 (99%)	168 (99%)	1 (1%)	1 (1%)	25	64
18	f9	170/172 (99%)	166 (98%)	4 (2%)	0	100	100
18	g4	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
18	g5	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
18	h4	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25	64
18	h5	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
18	h9	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
18	j4	171/172 (99%)	166 (97%)	5 (3%)	0	100	100
18	j5	171/172 (99%)	166 (97%)	5 (3%)	0	100	100
18	j9	170/172 (99%)	168 (99%)	2 (1%)	0	100	100
18	l4	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
18	l5	170/172 (99%)	163 (96%)	7 (4%)	0	100	100
18	l9	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25	64
19	a8	360/514 (70%)	326 (91%)	29 (8%)	5 (1%)	11	46
19	a9	360/514 (70%)	329 (91%)	26 (7%)	5 (1%)	11	46
20	dy	301/352 (86%)	279 (93%)	21 (7%)	1 (0%)	41	75
20	dz	301/352 (86%)	278 (92%)	22 (7%)	1 (0%)	41	75
21	ew	231/276 (84%)	210 (91%)	20 (9%)	1 (0%)	34	72
21	ex	231/276 (84%)	212 (92%)	19 (8%)	0	100	100
21	fd	194/276 (70%)	177 (91%)	15 (8%)	2 (1%)	15	54
21	fz	194/276 (70%)	177 (91%)	15 (8%)	2 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	eY	307/352 (87%)	279 (91%)	26 (8%)	2 (1%)	22 61
22	eZ	307/352 (87%)	276 (90%)	27 (9%)	4 (1%)	12 48
23	hY	227/350 (65%)	218 (96%)	8 (4%)	1 (0%)	34 72
23	hZ	227/350 (65%)	217 (96%)	9 (4%)	1 (0%)	34 72
23	ly	249/350 (71%)	237 (95%)	12 (5%)	0	100 100
23	lz	249/350 (71%)	236 (95%)	11 (4%)	2 (1%)	19 58
24	gy	258/297 (87%)	244 (95%)	14 (5%)	0	100 100
24	gz	258/297 (87%)	238 (92%)	18 (7%)	2 (1%)	19 58
25	ka	271/362 (75%)	240 (89%)	21 (8%)	10 (4%)	3 26
25	kb	271/362 (75%)	240 (89%)	26 (10%)	5 (2%)	8 41
All	All	151518/157478 (96%)	144159 (95%)	6533 (4%)	826 (0%)	32 68

All (826) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D1	41	LEU
2	D1	42	PRO
2	D1	44	PRO
6	Q1	151	ILE
4	R1	9	VAL
6	g1	151	ILE
4	s1	14	GLU
8	a2	476	ARG
8	a2	505	CYS
8	a2	542	TYR
8	a2	692	ILE
8	b2	542	TYR
8	b2	686	ASP
8	b2	687	ASN
11	f2	18	TYR
11	h2	18	TYR
11	h2	47	ASN
11	j2	47	ASN
11	n2	47	ASN
11	p2	47	ASN
11	r2	47	ASN
11	t2	47	ASN
11	v2	47	ASN

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Mol	Chain	Res	Type
11	x2	47	ASN
11	z2	47	ASN
13	B2	212	TYR
13	B2	416	THR
11	F2	47	ASN
11	L2	47	ASN
11	N2	47	ASN
11	P2	47	ASN
11	T2	47	ASN
11	X2	47	ASN
11	Z2	47	ASN
11	B3	47	ASN
11	D3	47	ASN
11	L3	47	ASN
11	P3	47	ASN
11	R3	47	ASN
11	T3	47	ASN
11	V3	47	ASN
11	X3	47	ASN
13	b3	53	LEU
13	b3	213	THR
13	b3	376	SER
13	b3	416	THR
11	n3	47	ASN
11	z3	47	ASN
11	D4	47	ASN
11	L4	75	THR
11	N4	75	THR
15	14	31	CYS
15	14	183	ARG
16	24	289	GLN
16	24	341	ASN
12	34	52	SER
14	44	260	GLY
10	s4	146	SER
10	y4	72	ALA
11	H5	75	THR
15	W5	183	ARG
16	X5	44	VAL
16	X5	48	SER
16	X5	340	ALA
12	Y5	51	GLN

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Mol	Chain	Res	Type
12	Y5	73	GLY
12	Y5	214	THR
12	Y5	215	VAL
14	Z5	260	GLY
10	s5	146	SER
10	u5	18	PHE
10	k8	138	LEU
10	k8	139	CYS
10	l8	139	CYS
10	m8	139	CYS
10	A6	139	CYS
10	C6	139	CYS
10	E6	139	CYS
10	G6	138	LEU
10	G6	139	CYS
10	I6	139	CYS
10	K6	138	LEU
10	K6	139	CYS
10	M6	69	SER
10	O6	139	CYS
10	Q6	139	CYS
10	S6	139	CYS
10	U6	138	LEU
10	U6	139	CYS
10	W6	139	CYS
10	f6	138	LEU
10	f6	139	CYS
10	g6	138	LEU
10	g6	139	CYS
10	h6	139	CYS
10	j6	139	CYS
10	k6	139	CYS
10	m6	138	LEU
10	m6	139	CYS
10	o6	139	CYS
11	r6	74	TYR
10	s6	139	CYS
10	u6	138	LEU
10	u6	139	CYS
10	q8	139	CYS
10	r8	139	CYS
10	s8	139	CYS

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Mol	Chain	Res	Type
10	t8	138	LEU
10	t8	139	CYS
10	u8	139	CYS
10	A7	139	CYS
10	C7	139	CYS
10	E7	138	LEU
10	E7	139	CYS
10	G7	139	CYS
10	I7	138	LEU
10	I7	139	CYS
10	K7	138	LEU
10	K7	139	CYS
10	M7	138	LEU
10	M7	139	CYS
10	O7	139	CYS
10	Q7	139	CYS
10	S7	139	CYS
10	U7	139	CYS
10	W7	139	CYS
10	Y7	138	LEU
10	Y7	139	CYS
11	c7	75	THR
10	h7	139	CYS
10	i7	139	CYS
10	j7	139	CYS
10	k7	139	CYS
10	m7	139	CYS
11	n7	75	THR
10	o7	138	LEU
10	o7	139	CYS
10	q7	139	CYS
10	s7	138	LEU
10	s7	139	CYS
10	w7	139	CYS
19	a8	53	ASP
19	a8	327	PHE
12	b8	136	GLU
19	a9	327	PHE
14	c9	47	ARG
16	S8	207	LEU
18	l9	76	SER
11	x9	75	THR

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Mol	Chain	Res	Type
11	z9	75	THR
15	W9	57	GLU
16	X9	207	LEU
18	al	76	SER
11	av	34	GLY
11	av	110	LEU
10	aI	141	PRO
10	aK	141	PRO
10	aM	141	PRO
10	aO	141	PRO
10	aQ	141	PRO
10	aS	141	PRO
10	aU	141	PRO
15	aW	35	ASP
15	aW	182	PRO
15	aW	183	ARG
18	bd	75	THR
18	bj	75	THR
18	bl	4	ALA
10	bm	141	PRO
10	bt	141	PRO
10	bu	70	GLY
10	bw	70	GLY
10	bw	141	PRO
10	by	70	GLY
10	bA	141	PRO
10	bC	141	PRO
10	bE	141	PRO
10	bG	141	PRO
10	bI	141	PRO
10	bK	141	PRO
10	bM	141	PRO
10	bO	141	PRO
10	bQ	141	PRO
10	bS	141	PRO
10	bU	141	PRO
15	bW	35	ASP
16	bX	207	LEU
12	bY	51	GLN
18	cd	75	THR
10	cm	141	PRO
10	ct	141	PRO

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Mol	Chain	Res	Type
10	cu	70	GLY
10	cw	70	GLY
10	cw	141	PRO
10	cy	70	GLY
10	cA	141	PRO
10	cC	141	PRO
10	cD	140	VAL
10	cS	140	VAL
10	cU	69	SER
10	cU	140	VAL
10	cW	141	PRO
10	db	141	PRO
10	dc	141	PRO
10	de	141	PRO
10	de	142	ARG
10	dg	141	PRO
10	dk	141	PRO
10	do	141	PRO
10	do	142	ARG
10	dq	141	PRO
11	dX	75	THR
11	er	34	GLY
10	eI	141	PRO
10	eQ	121	ASN
10	eU	73	GLY
22	eY	155	LYS
22	eZ	265	PRO
10	lw	72	ALA
23	lz	212	CYS
10	fb	138	LEU
21	fd	202	LEU
10	fe	138	LEU
10	fh	138	LEU
10	fk	138	LEU
10	fn	138	LEU
10	fn	139	CYS
10	fp	138	LEU
10	fx	141	PRO
21	fz	203	ALA
10	gf	71	GLU
10	gf	72	ALA
10	gj	141	PRO

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Mol	Chain	Res	Type
10	gq	141	PRO
10	gw	141	PRO
11	iF	75	THR
11	kS	71	GLY
11	kS	75	THR
11	kT	75	THR
25	ka	188	VAL
25	ka	274	ALA
25	ka	276	GLY
3	E1	74	THR
3	F1	73	TRP
6	Q1	150	ASN
8	b2	464	LEU
9	c2	39	GLU
12	A2	128	GLY
13	B2	214	PRO
10	K2	145	SER
11	Z3	46	SER
12	a3	128	GLY
10	k3	145	SER
11	r3	74	TYR
15	14	186	LYS
16	24	250	ALA
18	h4	118	GLN
16	X5	284	SER
10	i8	138	LEU
10	i8	139	CYS
10	l8	138	LEU
10	m8	138	LEU
10	A6	138	LEU
11	B6	75	THR
10	C6	138	LEU
10	E6	138	LEU
10	I6	138	LEU
11	L6	34	GLY
10	O6	138	LEU
10	Q6	138	LEU
11	R6	35	ASN
11	R6	75	THR
10	S6	138	LEU
11	V6	75	THR
10	W6	138	LEU

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Mol	Chain	Res	Type
11	X6	75	THR
10	Y6	138	LEU
10	Y6	139	CYS
10	h6	138	LEU
10	j6	138	LEU
10	k6	138	LEU
10	o6	138	LEU
10	q6	138	LEU
10	q6	139	CYS
11	r6	75	THR
10	s6	138	LEU
11	t6	75	THR
10	w6	141	PRO
10	q8	138	LEU
10	r8	138	LEU
10	s8	138	LEU
10	u8	138	LEU
10	A7	138	LEU
10	C7	138	LEU
10	G7	138	LEU
11	N7	75	THR
10	O7	138	LEU
10	Q7	138	LEU
10	S7	138	LEU
11	T7	75	THR
10	U7	138	LEU
10	W7	138	LEU
11	Z7	75	THR
11	c7	74	TYR
10	g7	140	VAL
10	h7	138	LEU
10	i7	138	LEU
10	j7	138	LEU
10	k7	138	LEU
10	m7	138	LEU
10	q7	138	LEU
11	r7	75	THR
10	u7	138	LEU
10	u7	139	CYS
11	v7	75	THR
10	w7	138	LEU
11	y7	75	THR

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Mol	Chain	Res	Type
12	b8	51	GLN
19	a9	53	ASP
12	b9	51	GLN
12	b9	137	ALA
14	c9	259	HIS
11	E8	75	THR
12	U8	73	GLY
10	o9	76	GLN
11	v9	75	THR
15	W9	30	LYS
12	Z9	73	GLY
10	ao	76	GLN
11	at	75	THR
11	av	75	THR
10	aA	141	PRO
16	aX	291	LYS
12	aY	51	GLN
10	bx	70	GLY
15	bW	182	PRO
16	bX	231	ARG
10	cx	70	GLY
10	cV	141	PRO
10	cW	142	ARG
10	cZ	141	PRO
10	cZ	142	ARG
10	da	141	PRO
10	da	142	ARG
10	dm	141	PRO
10	ds	81	LYS
10	du	141	PRO
12	dw	51	GLN
11	dP	35	ASN
11	en	35	ASN
21	ew	244	LEU
10	eE	141	PRO
10	eS	141	PRO
22	eZ	156	PRO
10	fg	138	LEU
10	fl	138	LEU
10	ft	141	PRO
10	gc	141	PRO
10	gh	141	PRO

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Mol	Chain	Res	Type
10	go	141	PRO
10	gs	141	PRO
11	iE	34	GLY
25	ka	186	GLY
25	ka	256	VAL
25	ka	304	ALA
25	kb	276	GLY
3	E1	72	ASP
6	g1	75	THR
6	g1	150	ASN
8	a2	297	ASN
8	a2	301	SER
8	b2	14	PRO
8	b2	301	SER
18	e4	3	ASP
18	e5	3	ASP
11	D6	75	THR
11	b6	75	THR
10	i6	141	PRO
11	n6	75	THR
11	n8	75	THR
11	o8	75	THR
11	D7	75	THR
11	V7	75	THR
11	p7	75	THR
19	a8	323	PRO
14	d8	259	HIS
19	a9	323	PRO
14	c9	213	ASN
14	d9	259	HIS
14	e9	259	HIS
10	v8	72	ALA
11	y8	75	THR
15	R8	25	ASN
15	R8	40	ALA
15	R8	61	LEU
18	Y8	76	SER
10	m9	74	ASP
11	r9	75	THR
11	t9	75	THR
10	A9	72	ALA
11	D9	75	THR

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Mol	Chain	Res	Type
11	J9	75	THR
15	W9	40	ALA
11	ap	75	THR
11	ar	75	THR
10	aE	141	PRO
15	aW	76	ASN
15	aW	219	ALA
16	aX	111	ASP
16	aX	231	ARG
16	aX	284	SER
11	br	75	THR
15	bW	76	ASN
15	bW	168	ALA
15	bW	219	ALA
16	bX	111	ASP
16	bX	284	SER
12	bY	137	ALA
18	cj	75	THR
10	cm	69	SER
11	cn	75	THR
11	cr	75	THR
10	cC	143	ASP
10	cD	141	PRO
10	cD	142	ARG
11	dL	75	THR
11	eb	75	THR
11	el	75	THR
11	ev	75	THR
12	ey	51	GLN
12	ez	51	GLN
10	eM	141	PRO
10	la	63	TYR
10	li	63	TYR
10	lq	63	TYR
10	lw	63	TYR
23	lz	346	SER
11	ga	75	THR
10	gl	141	PRO
10	gm	141	PRO
10	gw	146	SER
11	gx	75	THR
11	iC	75	THR

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Mol	Chain	Res	Type
11	iD	75	THR
11	iF	71	GLY
25	ka	187	PRO
25	kb	278	ILE
2	C1	51	ASP
3	F1	217	PRO
3	F1	219	VAL
6	Q1	75	THR
4	R1	8	ILE
8	b2	498	VAL
8	b2	852	PRO
9	c2	9	GLY
11	L2	46	SER
10	M3	145	SER
10	u3	145	SER
10	A4	145	SER
11	H4	75	THR
15	14	56	SER
16	24	284	SER
12	34	194	PRO
10	s4	62	LYS
11	t4	75	THR
11	D5	75	THR
15	W5	22	TYR
15	W5	25	ASN
16	X5	111	ASP
16	X5	273	THR
12	Y5	217	PRO
14	Z5	44	THR
11	t5	75	THR
11	h8	75	THR
11	Z6	72	ASN
10	g6	71	GLU
10	h6	70	GLY
11	p6	75	THR
11	F7	75	THR
11	H7	75	THR
11	R7	75	THR
11	e7	75	THR
10	f7	140	VAL
14	c8	67	SER
14	d8	105	LYS

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Mol	Chain	Res	Type
14	e8	259	HIS
14	c9	67	SER
16	S8	111	ASP
16	S8	208	SER
16	S8	250	ALA
12	U8	83	ALA
11	p9	75	THR
11	H9	75	THR
16	X9	111	ASP
16	X9	208	SER
16	X9	250	ALA
12	Z9	83	ALA
18	ad	76	SER
10	am	74	ASP
10	aA	140	VAL
11	aB	75	THR
11	aH	75	THR
15	aW	30	LYS
16	aX	250	ALA
18	bb	6	ALA
18	bf	75	THR
11	bB	75	THR
10	bK	145	SER
15	bW	9	SER
16	bX	250	ALA
12	bY	194	PRO
18	ch	75	THR
10	cU	142	ARG
10	dq	142	ARG
10	ds	141	PRO
20	dz	282	PRO
11	dN	75	THR
11	ec	75	THR
10	eC	141	PRO
22	eY	345	TRP
22	eZ	345	TRP
10	le	63	TYR
10	lg	63	TYR
10	lo	63	TYR
10	lu	63	TYR
21	fd	201	ARG
10	fh	139	CYS

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Mol	Chain	Res	Type
10	fk	139	CYS
10	fp	139	CYS
10	fr	139	CYS
21	fz	204	PRO
10	gf	141	PRO
11	gr	75	THR
11	gv	75	THR
11	iC	16	ALA
11	jO	34	GLY
25	kb	187	PRO
5	S1	74	THR
5	j1	74	THR
10	e2	145	SER
10	k2	145	SER
10	m2	145	SER
10	s2	145	SER
10	u2	145	SER
10	w2	145	SER
10	y2	145	SER
12	A2	194	PRO
10	E2	146	SER
10	G2	145	SER
10	Q2	145	SER
10	U2	145	SER
11	X2	46	SER
10	A3	145	SER
10	C3	145	SER
10	E3	145	SER
10	K3	145	SER
10	O3	145	SER
10	S3	145	SER
10	U3	145	SER
10	W3	145	SER
10	Y3	145	SER
12	a3	194	PRO
10	g3	145	SER
10	m3	145	SER
10	q3	145	SER
10	s3	145	SER
10	C4	145	SER
10	E4	62	LYS
10	G4	62	LYS

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Mol	Chain	Res	Type
10	I4	62	LYS
10	K4	62	LYS
10	M4	62	LYS
16	24	111	ASP
12	34	43	VAL
14	44	44	THR
14	44	184	THR
17	k4	75	ALA
10	o4	62	LYS
10	q4	62	LYS
11	r4	75	THR
10	u4	62	LYS
10	y4	62	LYS
10	A5	62	LYS
10	C5	62	LYS
10	E5	62	LYS
10	G5	62	LYS
10	I5	62	LYS
16	X5	74	SER
14	Z5	184	THR
10	m5	62	LYS
10	o5	62	LYS
10	q5	62	LYS
10	s5	62	LYS
10	u5	62	LYS
10	y5	62	LYS
10	E6	140	VAL
11	H6	4	ALA
11	L6	75	THR
10	Q6	140	VAL
11	r6	20	GLY
10	M7	140	VAL
11	P7	75	THR
10	S7	140	VAL
10	Y7	140	VAL
11	d7	75	THR
10	h7	140	VAL
14	d8	63	ARG
12	b9	52	SER
11	w8	75	THR
11	C8	75	THR
12	U8	217	PRO

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Mol	Chain	Res	Type
10	u9	72	ALA
11	B9	75	THR
15	W9	209	GLN
12	Z9	217	PRO
10	au	72	ALA
11	ax	75	THR
15	aW	9	SER
12	aY	194	PRO
11	bn	75	THR
11	bH	75	THR
11	bJ	75	THR
15	bW	30	LYS
12	bY	83	ALA
18	cf	75	THR
11	cs	75	THR
12	dw	217	PRO
12	dx	217	PRO
20	dy	298	CYS
11	dK	75	THR
10	eU	141	PRO
10	lk	63	TYR
10	ls	63	TYR
10	fb	139	CYS
10	fb	140	VAL
10	fe	139	CYS
10	fe	140	VAL
10	fg	139	CYS
10	fh	140	VAL
10	fk	140	VAL
10	fl	139	CYS
10	fp	140	VAL
10	fr	138	LEU
10	fr	140	VAL
11	gg	75	THR
11	gn	75	THR
11	gp	75	THR
24	gz	255	TYR
11	iE	107	ASP
11	kS	34	GLY
3	E1	217	PRO
5	U1	74	THR
8	b2	508	PRO

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Mol	Chain	Res	Type
9	d2	10	SER
10	g2	145	SER
12	A2	217	PRO
11	T2	46	SER
10	W2	145	SER
10	G3	145	SER
10	Q3	145	SER
12	a3	217	PRO
10	i3	146	SER
10	w3	145	SER
10	Y4	62	LYS
15	14	9	SER
10	m4	62	LYS
10	w4	62	LYS
10	A5	63	TYR
10	U5	62	LYS
15	W5	9	SER
10	w5	62	LYS
10	A6	141	PRO
10	C6	140	VAL
11	F6	75	THR
10	I6	141	PRO
10	S6	141	PRO
10	W6	140	VAL
10	f6	141	PRO
10	g6	140	VAL
10	j6	141	PRO
10	o6	140	VAL
10	o6	141	PRO
10	u6	140	VAL
10	A7	140	VAL
10	C7	140	VAL
10	E7	140	VAL
10	G7	141	PRO
10	i7	141	PRO
10	k7	140	VAL
10	k7	141	PRO
10	s7	140	VAL
14	d9	63	ARG
11	P9	75	THR
10	aq	72	ALA
11	aJ	75	THR

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Mol	Chain	Res	Type
16	aX	47	ASN
16	aX	70	PRO
16	aX	341	ASN
18	bb	75	THR
16	bX	341	ASN
10	dG	73	GLY
10	fn	141	PRO
11	iG	34	GLY
11	iH	34	GLY
11	jI	75	THR
11	jJ	75	THR
25	ka	255	ASP
10	k8	141	PRO
10	m8	141	PRO
10	C6	141	PRO
10	G6	140	VAL
10	K6	141	PRO
10	O6	140	VAL
10	O6	141	PRO
10	Q6	141	PRO
10	U6	140	VAL
10	U6	141	PRO
10	f6	140	VAL
10	h6	141	PRO
10	j6	140	VAL
10	k6	140	VAL
10	m6	141	PRO
10	q8	140	VAL
10	r8	140	VAL
10	r8	141	PRO
10	C7	141	PRO
10	E7	141	PRO
10	I7	141	PRO
10	Q7	140	VAL
10	Q7	141	PRO
10	U7	140	VAL
10	W7	141	PRO
10	Y7	141	PRO
10	f7	141	PRO
10	i7	140	VAL
10	j7	140	VAL
10	m7	140	VAL

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Mol	Chain	Res	Type
10	m7	141	PRO
10	s7	141	PRO
10	w7	141	PRO
19	a8	69	PRO
12	b8	245	VAL
14	e8	53	GLY
19	a9	69	PRO
12	b9	245	VAL
12	Z9	194	PRO
10	aC	73	GLY
10	bC	73	GLY
10	fg	140	VAL
10	fl	140	VAL
25	ka	176	PRO
25	kb	176	PRO
10	i8	141	PRO
10	E6	141	PRO
10	G6	141	PRO
10	I6	140	VAL
10	W6	141	PRO
10	k6	141	PRO
10	s6	140	VAL
10	u6	141	PRO
10	q8	141	PRO
10	s8	141	PRO
10	t8	140	VAL
10	t8	141	PRO
10	u8	141	PRO
10	A7	141	PRO
10	G7	140	VAL
10	M7	141	PRO
10	O7	141	PRO
10	U7	141	PRO
10	h7	141	PRO
10	j7	141	PRO
10	q7	140	VAL
12	b8	194	PRO
12	b9	194	PRO
12	b9	244	PRO
10	aE	73	GLY
12	bY	73	GLY
12	dw	194	PRO

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Mol	Chain	Res	Type
12	dx	194	PRO
10	dO	73	GLY
12	ey	194	PRO
24	gz	263	PRO
10	iB	73	GLY
11	jK	34	GLY
11	kX	34	GLY
25	kb	186	GLY
10	l8	141	PRO
10	Y6	141	PRO
10	q6	141	PRO
10	s6	141	PRO
10	I7	140	VAL
10	K7	141	PRO
10	S7	141	PRO
10	o7	140	VAL
10	u7	141	PRO
19	a8	339	GLY
19	a9	339	GLY
10	B8	141	PRO
10	ct	73	GLY
10	dU	73	GLY
11	ev	34	GLY
10	gj	150	VAL
23	hY	223	PRO
23	hZ	223	PRO
10	iA	73	GLY
25	ka	325	PRO
12	34	73	GLY
10	i8	140	VAL
10	l8	140	VAL
10	g6	141	PRO
10	m6	140	VAL
10	K7	140	VAL
10	W7	140	VAL
10	o7	141	PRO
10	q7	141	PRO
10	bE	73	GLY
10	dc	123	PRO
10	eG	141	PRO
11	kW	34	GLY
10	m8	140	VAL

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Mol	Chain	Res	Type
10	A6	140	VAL
10	h6	140	VAL
11	y6	34	GLY
12	b8	244	PRO
22	eZ	155	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A1	184/218 (84%)	184 (100%)	0	100 100
1	B1	184/218 (84%)	184 (100%)	0	100 100
2	C1	124/154 (80%)	123 (99%)	1 (1%)	81 91
2	D1	123/154 (80%)	122 (99%)	1 (1%)	81 91
3	E1	214/249 (86%)	212 (99%)	2 (1%)	78 90
3	F1	214/249 (86%)	211 (99%)	3 (1%)	67 85
4	G1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	I1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	K1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	N1	132/133 (99%)	131 (99%)	1 (1%)	81 91
4	P1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	R1	132/133 (99%)	131 (99%)	1 (1%)	81 91
4	T1	132/133 (99%)	131 (99%)	1 (1%)	81 91
4	X1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	Z1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	b1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	d1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	f1	132/133 (99%)	131 (99%)	1 (1%)	81 91
4	i1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	k1	132/133 (99%)	130 (98%)	2 (2%)	65 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	o1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	q1	132/133 (99%)	131 (99%)	1 (1%)	81 91
4	s1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	u1	132/133 (99%)	130 (98%)	2 (2%)	65 84
4	w1	132/133 (99%)	131 (99%)	1 (1%)	81 91
4	y1	132/133 (99%)	131 (99%)	1 (1%)	81 91
5	H1	126/126 (100%)	124 (98%)	2 (2%)	62 83
5	J1	126/126 (100%)	126 (100%)	0	100 100
5	L1	126/126 (100%)	125 (99%)	1 (1%)	81 91
5	M1	126/126 (100%)	126 (100%)	0	100 100
5	O1	126/126 (100%)	126 (100%)	0	100 100
5	S1	126/126 (100%)	126 (100%)	0	100 100
5	U1	126/126 (100%)	126 (100%)	0	100 100
5	W1	126/126 (100%)	126 (100%)	0	100 100
5	Y1	126/126 (100%)	126 (100%)	0	100 100
5	a1	126/126 (100%)	125 (99%)	1 (1%)	81 91
5	c1	126/126 (100%)	126 (100%)	0	100 100
5	e1	125/126 (99%)	125 (100%)	0	100 100
5	h1	126/126 (100%)	126 (100%)	0	100 100
5	j1	126/126 (100%)	124 (98%)	2 (2%)	62 83
5	l1	126/126 (100%)	126 (100%)	0	100 100
5	n1	126/126 (100%)	126 (100%)	0	100 100
5	p1	126/126 (100%)	126 (100%)	0	100 100
5	r1	126/126 (100%)	126 (100%)	0	100 100
5	t1	126/126 (100%)	126 (100%)	0	100 100
5	v1	126/126 (100%)	126 (100%)	0	100 100
5	x1	126/126 (100%)	126 (100%)	0	100 100
5	z1	126/126 (100%)	126 (100%)	0	100 100
6	Q1	158/158 (100%)	156 (99%)	2 (1%)	69 86
6	g1	158/158 (100%)	156 (99%)	2 (1%)	69 86
7	V1	139/140 (99%)	138 (99%)	1 (1%)	84 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	m1	139/140 (99%)	139 (100%)	0	100	100
8	a2	712/785 (91%)	702 (99%)	10 (1%)	67	85
8	b2	712/785 (91%)	703 (99%)	9 (1%)	69	86
9	c2	77/79 (98%)	77 (100%)	0	100	100
9	d2	77/79 (98%)	77 (100%)	0	100	100
10	A3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	A4	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	A5	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	A6	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	A7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	A9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	B8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	C3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	C4	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	C5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	C6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	C7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	C9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	D8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	E2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	E3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	E4	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	E5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	E6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	E7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	E9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	F8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	G2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	G3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	G4	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	G5	132/132 (100%)	129 (98%)	3 (2%)	50	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	G6	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	G7	131/132 (99%)	126 (96%)	5 (4%)	33	65
10	G9	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	H8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	I2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	I3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	I4	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	I5	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	I6	131/132 (99%)	126 (96%)	5 (4%)	33	65
10	I7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	I9	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	J8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	K2	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	K3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	K4	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	K5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	K6	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	K7	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	K9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	L8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	M2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	M3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	M4	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	M5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	M6	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	M7	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	M9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	N8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	O2	132/132 (100%)	131 (99%)	1 (1%)	81	91
10	O3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	O4	132/132 (100%)	128 (97%)	4 (3%)	41	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	O5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	O6	132/132 (100%)	125 (95%)	7 (5%)	22	55
10	O7	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	O9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	P8	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	Q2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	Q3	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	Q4	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	Q5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	Q6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	Q7	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	Q9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	S2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	S3	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	S4	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	S5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	S6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	S7	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	S9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	U2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	U3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	U4	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	U5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	U6	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	U7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	U9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	W2	132/132 (100%)	131 (99%)	1 (1%)	81	91
10	W3	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	W4	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	W6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	W7	132/132 (100%)	126 (96%)	6 (4%)	27	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	Y2	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	Y3	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	Y4	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	Y6	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	Y7	132/132 (100%)	124 (94%)	8 (6%)	18 51
10	aA	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	aC	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	aE	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	aG	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	aI	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	aK	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	aM	132/132 (100%)	131 (99%)	1 (1%)	81 91
10	aO	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	aQ	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	aS	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	aU	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	am	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	ao	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	aq	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	as	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	au	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	aw	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	ay	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	bA	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	bC	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	bE	132/132 (100%)	124 (94%)	8 (6%)	18 51
10	bG	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	bI	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	bK	132/132 (100%)	125 (95%)	7 (5%)	22 55
10	bM	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	bO	132/132 (100%)	129 (98%)	3 (2%)	50 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	bQ	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	bS	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	bU	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	bm	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	bt	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	bu	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	bv	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	bw	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	bx	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	by	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	cA	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	cC	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	cD	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	cG	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	cI	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	cK	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	cS	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	cT	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	cU	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	cV	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	cW	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	cX	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	cZ	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	cm	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	ct	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	cu	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	cv	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	cw	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	cx	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	cy	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	dA	132/132 (100%)	130 (98%)	2 (2%)	65 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	dC	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dE	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dG	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	dI	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dJ	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dM	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dO	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dQ	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dS	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dU	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dW	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dZ	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	da	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	db	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	dc	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	de	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	dg	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	dk	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	dm	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	do	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	dq	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	ds	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	du	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	e2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	e3	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	eA	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	eC	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	eE	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	eG	132/132 (100%)	125 (95%)	7 (5%)	22	55
10	eI	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	eK	132/132 (100%)	127 (96%)	5 (4%)	33	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	eM	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	eO	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	eQ	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	eS	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	eU	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	eW	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	ea	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	ed	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	ef	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	eh	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	ej	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	ek	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	em	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	eo	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	eq	132/132 (100%)	131 (99%)	1 (1%)	81	91
10	es	132/132 (100%)	131 (99%)	1 (1%)	81	91
10	eu	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	f6	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	f7	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	fb	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	fe	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	fg	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	fh	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	fk	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	fl	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	fn	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	fp	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	fr	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	ft	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	fv	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	fx	132/132 (100%)	128 (97%)	4 (3%)	41	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	g2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	g3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	g6	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	g7	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gb	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gc	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	gf	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gh	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gj	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	gl	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gm	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	go	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	gq	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	gs	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gu	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	gw	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	h6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	h7	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	hA	132/132 (100%)	127 (96%)	5 (4%)	33	65
10	hC	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hE	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hF	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hI	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hK	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hM	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hO	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hQ	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hS	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hU	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	hW	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	i2	132/132 (100%)	130 (98%)	2 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	i3	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	i6	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	i7	132/132 (100%)	125 (95%)	7 (5%)	22 55
10	i8	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	iA	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	iB	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	j6	132/132 (100%)	124 (94%)	8 (6%)	18 51
10	j7	132/132 (100%)	125 (95%)	7 (5%)	22 55
10	j8	132/132 (100%)	131 (99%)	1 (1%)	81 91
10	k2	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	k3	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	k6	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	k7	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	k8	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	l8	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	la	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	lc	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	le	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	lg	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	li	132/132 (100%)	125 (95%)	7 (5%)	22 55
10	lk	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	lm	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	lo	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	lq	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	ls	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	lu	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	lw	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	m2	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	m3	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	m4	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	m5	132/132 (100%)	127 (96%)	5 (4%)	33 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	m6	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	m7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	m8	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	m9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	o2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	o3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	o4	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	o5	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	o6	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	o7	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	o9	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	q2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	q3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	q4	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	q5	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	q6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	q7	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	q8	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	q9	132/132 (100%)	129 (98%)	3 (2%)	50	77
10	r8	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	s2	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	s3	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	s4	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	s5	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	s6	132/132 (100%)	128 (97%)	4 (3%)	41	71
10	s7	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	s8	132/132 (100%)	126 (96%)	6 (4%)	27	61
10	s9	132/132 (100%)	130 (98%)	2 (2%)	65	84
10	t8	132/132 (100%)	125 (95%)	7 (5%)	22	55
10	u2	132/132 (100%)	131 (99%)	1 (1%)	81	91
10	u3	132/132 (100%)	130 (98%)	2 (2%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	u4	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	u5	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	u6	132/132 (100%)	129 (98%)	3 (2%)	50 77
10	u7	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	u8	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	u9	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	v8	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	w2	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	w3	132/132 (100%)	131 (99%)	1 (1%)	81 91
10	w4	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	w5	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	w6	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	w7	132/132 (100%)	126 (96%)	6 (4%)	27 61
10	w9	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	x8	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	y2	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	y3	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	y4	132/132 (100%)	127 (96%)	5 (4%)	33 65
10	y5	132/132 (100%)	128 (97%)	4 (3%)	41 71
10	y9	132/132 (100%)	130 (98%)	2 (2%)	65 84
10	z8	132/132 (100%)	130 (98%)	2 (2%)	65 84
11	A8	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	B3	138/138 (100%)	138 (100%)	0	100 100
11	B4	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	B5	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	B6	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	B7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	B9	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	C8	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	D3	138/138 (100%)	138 (100%)	0	100 100
11	D4	138/138 (100%)	138 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	D5	138/138 (100%)	138 (100%)	0	100	100
11	D6	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	D7	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	D9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	E8	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	F2	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	F3	138/138 (100%)	138 (100%)	0	100	100
11	F4	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	F5	138/138 (100%)	138 (100%)	0	100	100
11	F6	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	F7	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	F9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	G8	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	H2	138/138 (100%)	138 (100%)	0	100	100
11	H3	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	H4	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	H5	138/138 (100%)	138 (100%)	0	100	100
11	H6	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	H7	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	H9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	I8	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	J2	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	J3	138/138 (100%)	138 (100%)	0	100	100
11	J4	138/138 (100%)	138 (100%)	0	100	100
11	J5	138/138 (100%)	138 (100%)	0	100	100
11	J6	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	J7	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	J9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	K8	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	L2	138/138 (100%)	138 (100%)	0	100	100
11	L3	138/138 (100%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L4	138/138 (100%)	138 (100%)	0	100	100
11	L5	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	L6	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	L7	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	L9	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	M8	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	N2	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	N3	138/138 (100%)	138 (100%)	0	100	100
11	N4	138/138 (100%)	138 (100%)	0	100	100
11	N5	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	N6	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	N7	138/138 (100%)	134 (97%)	4 (3%)	42	71
11	N9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	O8	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	P2	138/138 (100%)	138 (100%)	0	100	100
11	P3	138/138 (100%)	138 (100%)	0	100	100
11	P4	138/138 (100%)	138 (100%)	0	100	100
11	P5	138/138 (100%)	138 (100%)	0	100	100
11	P6	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	P7	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	P9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	Q8	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	R2	138/138 (100%)	138 (100%)	0	100	100
11	R3	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	R4	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	R5	138/138 (100%)	138 (100%)	0	100	100
11	R6	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	R7	138/138 (100%)	134 (97%)	4 (3%)	42	71
11	R9	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	T2	138/138 (100%)	138 (100%)	0	100	100
11	T3	138/138 (100%)	138 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	T4	138/138 (100%)	138 (100%)	0	100	100
11	T5	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	T6	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	T7	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	T9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	V2	138/138 (100%)	138 (100%)	0	100	100
11	V3	138/138 (100%)	138 (100%)	0	100	100
11	V4	138/138 (100%)	138 (100%)	0	100	100
11	V5	138/138 (100%)	138 (100%)	0	100	100
11	V6	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	V7	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	V9	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	X2	138/138 (100%)	138 (100%)	0	100	100
11	X3	138/138 (100%)	138 (100%)	0	100	100
11	X4	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	X6	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	X7	138/138 (100%)	133 (96%)	5 (4%)	35	66
11	Z2	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	Z3	138/138 (100%)	138 (100%)	0	100	100
11	Z4	138/138 (100%)	138 (100%)	0	100	100
11	Z6	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	Z7	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	a6	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	a7	138/138 (100%)	134 (97%)	4 (3%)	42	71
11	aB	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	aD	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	aF	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	aH	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	aJ	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	aL	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	aN	138/138 (100%)	137 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	aP	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	aR	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	aT	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	aV	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	an	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	ap	138/138 (100%)	134 (97%)	4 (3%)	42	71
11	ar	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	at	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	av	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	ax	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	az	138/138 (100%)	134 (97%)	4 (3%)	42	71
11	b6	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	b7	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	bB	138/138 (100%)	133 (96%)	5 (4%)	35	66
11	bD	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	bF	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bH	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bJ	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bL	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bN	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	bP	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	bR	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bT	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bV	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	bn	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	bo	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bp	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	bq	138/138 (100%)	138 (100%)	0	100	100
11	br	138/138 (100%)	138 (100%)	0	100	100
11	bs	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	bz	138/138 (100%)	136 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	c6	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	c7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	cB	138/138 (100%)	138 (100%)	0	100 100
11	cE	138/138 (100%)	138 (100%)	0	100 100
11	cF	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	cH	138/138 (100%)	138 (100%)	0	100 100
11	cJ	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	cL	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	cM	138/138 (100%)	138 (100%)	0	100 100
11	cN	138/138 (100%)	138 (100%)	0	100 100
11	cO	138/138 (100%)	138 (100%)	0	100 100
11	cP	138/138 (100%)	138 (100%)	0	100 100
11	cQ	138/138 (100%)	138 (100%)	0	100 100
11	cR	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	cY	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	cn	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	co	138/138 (100%)	134 (97%)	4 (3%)	42 71
11	cp	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	cq	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	cr	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	cs	138/138 (100%)	133 (96%)	5 (4%)	35 66
11	cz	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	d6	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	d7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	dB	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	dD	138/138 (100%)	138 (100%)	0	100 100
11	dF	138/138 (100%)	138 (100%)	0	100 100
11	dH	138/138 (100%)	138 (100%)	0	100 100
11	dK	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	dL	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	dN	138/138 (100%)	137 (99%)	1 (1%)	84 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	dP	138/138 (100%)	138 (100%)	0	100	100
11	dR	138/138 (100%)	138 (100%)	0	100	100
11	dT	138/138 (100%)	138 (100%)	0	100	100
11	dV	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dX	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dY	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dd	138/138 (100%)	138 (100%)	0	100	100
11	df	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	dh	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	di	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dj	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dl	138/138 (100%)	138 (100%)	0	100	100
11	dn	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dp	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dr	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	dt	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	dv	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	e6	138/138 (100%)	138 (100%)	0	100	100
11	e7	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	eB	138/138 (100%)	138 (100%)	0	100	100
11	eD	138/138 (100%)	138 (100%)	0	100	100
11	eF	138/138 (100%)	138 (100%)	0	100	100
11	eH	138/138 (100%)	138 (100%)	0	100	100
11	eJ	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	eL	138/138 (100%)	138 (100%)	0	100	100
11	eN	138/138 (100%)	138 (100%)	0	100	100
11	eP	138/138 (100%)	138 (100%)	0	100	100
11	eR	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	eT	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	eV	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	eX	138/138 (100%)	137 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	eb	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	ec	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	ee	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	eg	138/138 (100%)	138 (100%)	0	100	100
11	ei	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	el	138/138 (100%)	138 (100%)	0	100	100
11	en	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	ep	138/138 (100%)	138 (100%)	0	100	100
11	er	138/138 (100%)	138 (100%)	0	100	100
11	et	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	ev	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	f2	138/138 (100%)	138 (100%)	0	100	100
11	f3	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	f8	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	fa	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fc	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	ff	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fi	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fj	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fm	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fo	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fq	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fs	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fu	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fw	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	fy	138/138 (100%)	137 (99%)	1 (1%)	84	93
11	g8	138/138 (100%)	135 (98%)	3 (2%)	52	78
11	ga	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	gd	138/138 (100%)	133 (96%)	5 (4%)	35	66
11	ge	138/138 (100%)	136 (99%)	2 (1%)	67	85
11	gg	138/138 (100%)	136 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	gi	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	gk	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	gn	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	gp	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	gr	138/138 (100%)	134 (97%)	4 (3%)	42 71
11	gt	138/138 (100%)	134 (97%)	4 (3%)	42 71
11	gv	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	gx	138/138 (100%)	134 (97%)	4 (3%)	42 71
11	h2	138/138 (100%)	138 (100%)	0	100 100
11	h3	138/138 (100%)	138 (100%)	0	100 100
11	h8	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	hB	138/138 (100%)	138 (100%)	0	100 100
11	hD	138/138 (100%)	138 (100%)	0	100 100
11	hG	138/138 (100%)	138 (100%)	0	100 100
11	hH	138/138 (100%)	138 (100%)	0	100 100
11	hJ	138/138 (100%)	138 (100%)	0	100 100
11	hL	138/138 (100%)	138 (100%)	0	100 100
11	hN	138/138 (100%)	138 (100%)	0	100 100
11	hP	138/138 (100%)	138 (100%)	0	100 100
11	hR	138/138 (100%)	138 (100%)	0	100 100
11	hT	138/138 (100%)	138 (100%)	0	100 100
11	hV	138/138 (100%)	138 (100%)	0	100 100
11	hX	138/138 (100%)	138 (100%)	0	100 100
11	iC	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	iD	138/138 (100%)	133 (96%)	5 (4%)	35 66
11	iE	112/138 (81%)	109 (97%)	3 (3%)	44 73
11	iF	112/138 (81%)	112 (100%)	0	100 100
11	iG	114/138 (83%)	111 (97%)	3 (3%)	46 74
11	iH	114/138 (83%)	114 (100%)	0	100 100
11	j2	138/138 (100%)	138 (100%)	0	100 100
11	j3	138/138 (100%)	137 (99%)	1 (1%)	84 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	jI	110/138 (80%)	108 (98%)	2 (2%)	59 81
11	jJ	110/138 (80%)	108 (98%)	2 (2%)	59 81
11	jK	111/138 (80%)	109 (98%)	2 (2%)	59 81
11	jL	111/138 (80%)	110 (99%)	1 (1%)	78 90
11	jM	111/138 (80%)	109 (98%)	2 (2%)	59 81
11	jN	111/138 (80%)	109 (98%)	2 (2%)	59 81
11	jO	111/138 (80%)	108 (97%)	3 (3%)	44 73
11	jP	111/138 (80%)	109 (98%)	2 (2%)	59 81
11	kQ	110/138 (80%)	109 (99%)	1 (1%)	78 90
11	kR	110/138 (80%)	109 (99%)	1 (1%)	78 90
11	kS	113/138 (82%)	111 (98%)	2 (2%)	59 81
11	kT	112/138 (81%)	110 (98%)	2 (2%)	59 81
11	kU	110/138 (80%)	108 (98%)	2 (2%)	59 81
11	kV	110/138 (80%)	108 (98%)	2 (2%)	59 81
11	kW	113/138 (82%)	111 (98%)	2 (2%)	59 81
11	kX	113/138 (82%)	111 (98%)	2 (2%)	59 81
11	l2	138/138 (100%)	138 (100%)	0	100 100
11	l3	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	l6	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	l7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	lb	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	ld	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	lf	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	lh	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	lj	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	ll	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	ln	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	lp	138/138 (100%)	138 (100%)	0	100 100
11	lr	138/138 (100%)	138 (100%)	0	100 100
11	lt	138/138 (100%)	138 (100%)	0	100 100
11	lv	138/138 (100%)	136 (99%)	2 (1%)	67 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	lx	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	n2	138/138 (100%)	138 (100%)	0	100 100
11	n3	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	n4	138/138 (100%)	138 (100%)	0	100 100
11	n5	138/138 (100%)	138 (100%)	0	100 100
11	n6	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	n7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	n8	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	n9	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	o8	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	p2	138/138 (100%)	138 (100%)	0	100 100
11	p3	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	p4	138/138 (100%)	138 (100%)	0	100 100
11	p5	138/138 (100%)	138 (100%)	0	100 100
11	p6	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	p7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	p8	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	p9	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	r2	138/138 (100%)	138 (100%)	0	100 100
11	r3	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	r4	138/138 (100%)	138 (100%)	0	100 100
11	r5	138/138 (100%)	138 (100%)	0	100 100
11	r6	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	r7	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	r9	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	t2	138/138 (100%)	138 (100%)	0	100 100
11	t3	138/138 (100%)	138 (100%)	0	100 100
11	t4	138/138 (100%)	138 (100%)	0	100 100
11	t5	138/138 (100%)	138 (100%)	0	100 100
11	t6	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	t7	138/138 (100%)	136 (99%)	2 (1%)	67 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	t9	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	v2	138/138 (100%)	138 (100%)	0	100 100
11	v3	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	v4	138/138 (100%)	138 (100%)	0	100 100
11	v5	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	v6	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	v7	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	v9	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	w8	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	x2	138/138 (100%)	138 (100%)	0	100 100
11	x3	138/138 (100%)	138 (100%)	0	100 100
11	x4	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	x5	138/138 (100%)	138 (100%)	0	100 100
11	x6	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	x7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	x9	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	y6	138/138 (100%)	135 (98%)	3 (2%)	52 78
11	y7	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	y8	138/138 (100%)	138 (100%)	0	100 100
11	z2	138/138 (100%)	138 (100%)	0	100 100
11	z3	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	z4	138/138 (100%)	137 (99%)	1 (1%)	84 93
11	z5	138/138 (100%)	138 (100%)	0	100 100
11	z6	138/138 (100%)	136 (99%)	2 (1%)	67 85
11	z7	138/138 (100%)	134 (97%)	4 (3%)	42 71
11	z9	138/138 (100%)	134 (97%)	4 (3%)	42 71
12	34	213/246 (87%)	211 (99%)	2 (1%)	78 90
12	A2	213/246 (87%)	207 (97%)	6 (3%)	43 72
12	U8	213/246 (87%)	209 (98%)	4 (2%)	57 80
12	Y5	213/246 (87%)	210 (99%)	3 (1%)	67 85
12	Z9	213/246 (87%)	208 (98%)	5 (2%)	50 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	a3	213/246 (87%)	209 (98%)	4 (2%)	57 80
12	aY	213/246 (87%)	208 (98%)	5 (2%)	50 77
12	b8	213/246 (87%)	209 (98%)	4 (2%)	57 80
12	b9	213/246 (87%)	209 (98%)	4 (2%)	57 80
12	bY	213/246 (87%)	207 (97%)	6 (3%)	43 72
12	dw	213/246 (87%)	207 (97%)	6 (3%)	43 72
12	dx	213/246 (87%)	208 (98%)	5 (2%)	50 77
12	ey	213/246 (87%)	208 (98%)	5 (2%)	50 77
12	ez	212/246 (86%)	209 (99%)	3 (1%)	67 85
13	B2	309/393 (79%)	304 (98%)	5 (2%)	62 83
13	b3	309/393 (79%)	302 (98%)	7 (2%)	50 77
14	44	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	C2	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	D2	188/225 (84%)	187 (100%)	1 (0%)	88 94
14	T8	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	Y9	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	Z5	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	aZ	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	bZ	193/225 (86%)	190 (98%)	3 (2%)	62 83
14	c3	193/225 (86%)	191 (99%)	2 (1%)	76 88
14	c8	193/225 (86%)	190 (98%)	3 (2%)	62 83
14	c9	193/225 (86%)	189 (98%)	4 (2%)	53 79
14	d3	188/225 (84%)	186 (99%)	2 (1%)	73 88
14	d8	188/225 (84%)	187 (100%)	1 (0%)	88 94
14	d9	188/225 (84%)	187 (100%)	1 (0%)	88 94
14	e8	188/225 (84%)	187 (100%)	1 (0%)	88 94
14	e9	188/225 (84%)	188 (100%)	0	100 100
15	14	205/209 (98%)	203 (99%)	2 (1%)	76 88
15	R8	203/209 (97%)	199 (98%)	4 (2%)	55 79
15	W5	205/209 (98%)	204 (100%)	1 (0%)	88 94
15	W9	203/209 (97%)	195 (96%)	8 (4%)	32 64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	aW	206/209 (99%)	204 (99%)	2 (1%)	76 88
15	bW	206/209 (99%)	203 (98%)	3 (2%)	65 84
16	24	265/298 (89%)	262 (99%)	3 (1%)	73 88
16	S8	266/298 (89%)	263 (99%)	3 (1%)	73 88
16	X5	266/298 (89%)	256 (96%)	10 (4%)	33 65
16	X9	266/298 (89%)	259 (97%)	7 (3%)	46 74
16	aX	266/298 (89%)	260 (98%)	6 (2%)	50 77
16	bX	266/298 (89%)	257 (97%)	9 (3%)	37 68
17	V8	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	X8	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	Z8	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	a4	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	a5	126/126 (100%)	125 (99%)	1 (1%)	81 91
17	aa	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	ac	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	ae	127/126 (101%)	125 (98%)	2 (2%)	62 83
17	ag	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	ai	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	ak	126/126 (100%)	122 (97%)	4 (3%)	39 69
17	b4	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	b5	126/126 (100%)	123 (98%)	3 (2%)	49 76
17	ba	126/126 (100%)	125 (99%)	1 (1%)	81 91
17	bc	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	be	127/126 (101%)	125 (98%)	2 (2%)	62 83
17	bg	126/126 (100%)	125 (99%)	1 (1%)	81 91
17	bi	126/126 (100%)	125 (99%)	1 (1%)	81 91
17	bk	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	ca	126/126 (100%)	124 (98%)	2 (2%)	62 83
17	cc	126/126 (100%)	122 (97%)	4 (3%)	39 69
17	ce	127/126 (101%)	125 (98%)	2 (2%)	62 83
17	cg	126/126 (100%)	124 (98%)	2 (2%)	62 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	ci	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	ck	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	d4	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	d5	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	f4	126/126 (100%)	125 (99%)	1 (1%)	81	91
17	f5	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	g9	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	i4	126/126 (100%)	125 (99%)	1 (1%)	81	91
17	i5	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	i9	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	k4	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	k5	126/126 (100%)	124 (98%)	2 (2%)	62	83
17	k9	126/126 (100%)	125 (99%)	1 (1%)	81	91
18	W8	136/136 (100%)	133 (98%)	3 (2%)	52	78
18	Y8	136/136 (100%)	132 (97%)	4 (3%)	42	71
18	ab	136/136 (100%)	133 (98%)	3 (2%)	52	78
18	ad	136/136 (100%)	133 (98%)	3 (2%)	52	78
18	af	136/136 (100%)	132 (97%)	4 (3%)	42	71
18	ah	136/136 (100%)	132 (97%)	4 (3%)	42	71
18	aj	136/136 (100%)	133 (98%)	3 (2%)	52	78
18	al	136/136 (100%)	134 (98%)	2 (2%)	65	84
18	bb	136/136 (100%)	136 (100%)	0	100	100
18	bd	136/136 (100%)	133 (98%)	3 (2%)	52	78
18	bf	136/136 (100%)	136 (100%)	0	100	100
18	bh	136/136 (100%)	136 (100%)	0	100	100
18	bj	137/136 (101%)	136 (99%)	1 (1%)	84	93
18	bl	136/136 (100%)	136 (100%)	0	100	100
18	c4	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	c5	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	cb	136/136 (100%)	134 (98%)	2 (2%)	65	84
18	cd	136/136 (100%)	135 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	cf	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	ch	136/136 (100%)	134 (98%)	2 (2%)	65	84
18	cj	137/136 (101%)	136 (99%)	1 (1%)	84	93
18	cl	136/136 (100%)	134 (98%)	2 (2%)	65	84
18	e4	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	e5	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	f9	136/136 (100%)	134 (98%)	2 (2%)	65	84
18	g4	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	g5	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	h4	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	h5	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	h9	136/136 (100%)	133 (98%)	3 (2%)	52	78
18	j4	137/136 (101%)	136 (99%)	1 (1%)	84	93
18	j5	137/136 (101%)	137 (100%)	0	100	100
18	j9	136/136 (100%)	135 (99%)	1 (1%)	84	93
18	l4	136/136 (100%)	136 (100%)	0	100	100
18	l5	136/136 (100%)	134 (98%)	2 (2%)	65	84
18	l9	136/136 (100%)	134 (98%)	2 (2%)	65	84
19	a8	301/428 (70%)	298 (99%)	3 (1%)	76	88
19	a9	301/428 (70%)	297 (99%)	4 (1%)	69	86
20	dy	257/295 (87%)	251 (98%)	6 (2%)	50	77
20	dz	257/295 (87%)	249 (97%)	8 (3%)	40	70
21	ew	195/233 (84%)	191 (98%)	4 (2%)	53	79
21	ex	195/233 (84%)	190 (97%)	5 (3%)	46	74
21	fd	166/233 (71%)	162 (98%)	4 (2%)	49	76
21	fz	166/233 (71%)	162 (98%)	4 (2%)	49	76
22	eY	228/261 (87%)	222 (97%)	6 (3%)	46	74
22	eZ	228/261 (87%)	223 (98%)	5 (2%)	52	78
23	hY	180/277 (65%)	178 (99%)	2 (1%)	73	88
23	hZ	180/277 (65%)	178 (99%)	2 (1%)	73	88
23	ly	197/277 (71%)	195 (99%)	2 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	lz	197/277 (71%)	194 (98%)	3 (2%)	65 84
24	gy	213/246 (87%)	210 (99%)	3 (1%)	67 85
24	gz	213/246 (87%)	210 (99%)	3 (1%)	67 85
25	ka	225/307 (73%)	221 (98%)	4 (2%)	59 81
25	kb	225/307 (73%)	221 (98%)	4 (2%)	59 81
All	All	121716/125196 (97%)	119749 (98%)	1967 (2%)	64 83

All (1967) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C1	126	LYS
2	D1	126	LYS
3	E1	62	TYR
3	E1	213	LYS
3	F1	67	PHE
3	F1	132	TRP
3	F1	213	LYS
4	G1	47	ARG
4	G1	71	ASN
5	H1	74	THR
5	H1	75	THR
4	I1	47	ARG
4	I1	71	ASN
4	K1	47	ARG
4	K1	71	ASN
5	L1	20	ASP
4	N1	47	ARG
4	P1	47	ARG
4	P1	71	ASN
6	Q1	101	ASN
6	Q1	163	ASN
4	R1	47	ARG
4	T1	47	ARG
7	V1	81	CYS
4	X1	47	ARG
4	X1	71	ASN
4	Z1	47	ARG
4	Z1	71	ASN
5	a1	87	TYR
4	b1	47	ARG

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Mol	Chain	Res	Type
4	b1	71	ASN
4	d1	47	ARG
4	d1	71	ASN
4	f1	71	ASN
6	g1	101	ASN
6	g1	163	ASN
4	i1	47	ARG
4	i1	71	ASN
5	j1	109	LEU
5	j1	112	LEU
4	k1	47	ARG
4	k1	71	ASN
4	o1	47	ARG
4	o1	71	ASN
4	q1	47	ARG
4	s1	47	ARG
4	s1	71	ASN
4	u1	47	ARG
4	u1	81	CYS
4	w1	47	ARG
4	y1	47	ARG
8	a2	34	PHE
8	a2	245	ASP
8	a2	296	TYR
8	a2	297	ASN
8	a2	328	ARG
8	a2	423	ARG
8	a2	449	ASN
8	a2	495	ASN
8	a2	503	LEU
8	a2	851	LEU
8	b2	245	ASP
8	b2	328	ARG
8	b2	423	ARG
8	b2	449	ASN
8	b2	503	LEU
8	b2	505	CYS
8	b2	612	PHE
8	b2	750	PHE
8	b2	851	LEU
10	e2	30	ASN
10	e2	121	ASN

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Mol	Chain	Res	Type
10	g2	30	ASN
10	g2	121	ASN
10	i2	30	ASN
10	i2	121	ASN
10	k2	30	ASN
10	k2	121	ASN
10	m2	30	ASN
10	m2	121	ASN
10	o2	30	ASN
10	o2	121	ASN
10	q2	30	ASN
10	q2	121	ASN
10	s2	30	ASN
10	s2	121	ASN
10	u2	121	ASN
10	w2	30	ASN
10	w2	121	ASN
10	y2	30	ASN
10	y2	121	ASN
12	A2	147	ARG
12	A2	150	ASN
12	A2	193	MET
12	A2	216	ARG
12	A2	299	ASN
12	A2	317	ARG
13	B2	99	ASN
13	B2	121	ASN
13	B2	161	ARG
13	B2	209	ARG
13	B2	254	ARG
14	C2	43	ARG
14	C2	129	LYS
14	D2	129	LYS
10	E2	30	ASN
10	E2	121	ASN
11	F2	109	CYS
11	F2	113	LEU
10	G2	30	ASN
10	G2	121	ASN
10	I2	30	ASN
10	I2	121	ASN
11	J2	25	GLN

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Mol	Chain	Res	Type
10	K2	30	ASN
10	K2	121	ASN
10	K2	135	ARG
10	M2	30	ASN
10	M2	121	ASN
11	N2	25	GLN
10	O2	30	ASN
10	Q2	30	ASN
10	Q2	121	ASN
10	S2	30	ASN
10	S2	121	ASN
10	U2	30	ASN
10	U2	121	ASN
10	W2	30	ASN
10	Y2	30	ASN
10	Y2	121	ASN
11	Z2	50	CYS
10	A3	30	ASN
10	A3	121	ASN
10	C3	30	ASN
10	C3	121	ASN
10	E3	30	ASN
10	E3	121	ASN
10	G3	30	ASN
10	G3	121	ASN
11	H3	47	ASN
11	H3	150	LYS
10	I3	30	ASN
10	I3	121	ASN
10	K3	30	ASN
10	K3	121	ASN
10	M3	30	ASN
10	M3	121	ASN
10	O3	30	ASN
10	O3	121	ASN
10	Q3	30	ASN
10	Q3	37	ARG
10	Q3	121	ASN
11	R3	50	CYS
10	S3	30	ASN
10	S3	37	ARG
10	S3	121	ASN

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Mol	Chain	Res	Type
10	U3	37	ARG
10	U3	121	ASN
10	W3	30	ASN
10	W3	37	ARG
10	W3	121	ASN
10	Y3	30	ASN
10	Y3	37	ARG
10	Y3	121	ASN
12	a3	147	ARG
12	a3	150	ASN
12	a3	193	MET
12	a3	216	ARG
13	b3	51	ASP
13	b3	99	ASN
13	b3	121	ASN
13	b3	161	ARG
13	b3	209	ARG
13	b3	254	ARG
13	b3	357	HIS
14	c3	43	ARG
14	c3	129	LYS
14	d3	129	LYS
14	d3	176	CYS
10	e3	30	ASN
10	e3	121	ASN
10	e3	147	GLN
11	f3	44	ILE
11	f3	108	ARG
10	g3	30	ASN
10	g3	121	ASN
10	i3	30	ASN
10	i3	121	ASN
10	i3	138	LEU
11	j3	13	ASP
10	k3	28	GLN
10	k3	31	ILE
10	k3	121	ASN
11	l3	44	ILE
11	l3	50	CYS
10	m3	30	ASN
10	m3	121	ASN
11	n3	25	GLN

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Mol	Chain	Res	Type
10	o3	30	ASN
10	o3	121	ASN
11	p3	50	CYS
10	q3	30	ASN
10	q3	121	ASN
11	r3	44	ILE
11	r3	50	CYS
10	s3	30	ASN
10	s3	121	ASN
10	u3	30	ASN
10	u3	121	ASN
11	v3	47	ASN
10	w3	30	ASN
10	y3	30	ASN
10	y3	121	ASN
11	z3	50	CYS
10	A4	30	ASN
10	A4	121	ASN
11	B4	44	ILE
10	C4	30	ASN
10	C4	121	ASN
10	E4	30	ASN
10	E4	108	TRP
10	E4	121	ASN
10	E4	135	ARG
10	E4	142	ARG
11	F4	109	CYS
10	G4	30	ASN
10	G4	121	ASN
10	G4	135	ARG
11	H4	50	CYS
10	I4	30	ASN
10	I4	108	TRP
10	I4	135	ARG
10	I4	142	ARG
10	K4	30	ASN
10	K4	108	TRP
10	K4	135	ARG
10	M4	30	ASN
10	M4	108	TRP
10	M4	121	ASN
10	M4	135	ARG

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Mol	Chain	Res	Type
10	M4	142	ARG
10	O4	30	ASN
10	O4	108	TRP
10	O4	121	ASN
10	O4	135	ARG
10	Q4	30	ASN
10	Q4	108	TRP
10	Q4	121	ASN
10	Q4	135	ARG
11	R4	50	CYS
10	S4	30	ASN
10	S4	108	TRP
10	S4	121	ASN
10	S4	135	ARG
10	U4	30	ASN
10	U4	108	TRP
10	U4	121	ASN
10	U4	135	ARG
10	W4	30	ASN
10	W4	108	TRP
10	W4	121	ASN
10	W4	135	ARG
11	X4	50	CYS
10	Y4	30	ASN
10	Y4	108	TRP
10	Y4	121	ASN
10	Y4	135	ARG
15	14	198	LEU
15	14	199	TRP
16	24	158	LEU
16	24	193	TYR
16	24	262	LEU
12	34	147	ARG
12	34	150	ASN
14	44	43	ARG
14	44	159	LYS
17	a4	21	ASN
17	a4	30	ARG
17	b4	21	ASN
17	b4	30	ARG
18	c4	21	ASN
17	d4	21	ASN

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Mol	Chain	Res	Type
17	d4	30	ARG
18	e4	21	ASN
17	f4	30	ARG
18	g4	21	ASN
18	h4	21	ASN
17	i4	30	ARG
18	j4	21	ASN
17	k4	21	ASN
17	k4	30	ARG
10	m4	30	ASN
10	m4	108	TRP
10	m4	121	ASN
10	m4	135	ARG
10	m4	142	ARG
10	o4	30	ASN
10	o4	108	TRP
10	o4	135	ARG
10	q4	30	ASN
10	q4	108	TRP
10	q4	135	ARG
10	s4	30	ASN
10	s4	43	LYS
10	s4	67	LYS
10	s4	108	TRP
10	s4	121	ASN
10	s4	135	ARG
10	u4	17	ARG
10	u4	30	ASN
10	u4	108	TRP
10	u4	121	ASN
10	u4	135	ARG
10	u4	142	ARG
10	w4	30	ASN
10	w4	108	TRP
10	w4	121	ASN
10	w4	135	ARG
11	x4	25	GLN
10	y4	30	ASN
10	y4	108	TRP
10	y4	121	ASN
10	y4	135	ARG
10	y4	142	ARG

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Mol	Chain	Res	Type
11	z4	25	GLN
10	A5	30	ASN
10	A5	108	TRP
10	A5	121	ASN
10	A5	135	ARG
10	A5	142	ARG
11	B5	50	CYS
11	B5	109	CYS
10	C5	17	ARG
10	C5	30	ASN
10	C5	121	ASN
10	C5	135	ARG
10	E5	30	ASN
10	E5	108	TRP
10	E5	135	ARG
10	E5	142	ARG
10	G5	30	ASN
10	G5	108	TRP
10	G5	135	ARG
10	I5	30	ASN
10	I5	108	TRP
10	I5	121	ASN
10	I5	135	ARG
10	I5	142	ARG
10	K5	30	ASN
10	K5	108	TRP
10	K5	121	ASN
10	K5	135	ARG
11	L5	50	CYS
10	M5	30	ASN
10	M5	108	TRP
10	M5	121	ASN
10	M5	135	ARG
11	N5	50	CYS
10	O5	30	ASN
10	O5	108	TRP
10	O5	121	ASN
10	O5	135	ARG
10	Q5	30	ASN
10	Q5	108	TRP
10	Q5	121	ASN
10	Q5	135	ARG

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Mol	Chain	Res	Type
10	S5	30	ASN
10	S5	108	TRP
10	S5	121	ASN
10	S5	135	ARG
11	T5	50	CYS
10	U5	30	ASN
10	U5	108	TRP
10	U5	121	ASN
10	U5	135	ARG
15	W5	20	PHE
16	X5	45	LEU
16	X5	262	LEU
16	X5	270	SER
16	X5	271	TRP
16	X5	272	GLN
16	X5	273	THR
16	X5	326	MET
16	X5	327	ARG
16	X5	338	ARG
16	X5	339	ARG
12	Y5	147	ARG
12	Y5	150	ASN
12	Y5	192	ASN
14	Z5	43	ARG
14	Z5	159	LYS
17	a5	30	ARG
17	b5	21	ASN
17	b5	30	ARG
17	b5	124	LEU
18	c5	75	THR
17	d5	21	ASN
17	d5	30	ARG
18	e5	21	ASN
17	f5	21	ASN
17	f5	30	ARG
18	g5	21	ASN
18	h5	21	ASN
17	i5	23	GLU
17	i5	30	ARG
17	k5	21	ASN
17	k5	30	ARG
18	l5	21	ASN

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Mol	Chain	Res	Type
18	l5	88	ILE
10	m5	30	ASN
10	m5	108	TRP
10	m5	121	ASN
10	m5	135	ARG
10	m5	142	ARG
10	o5	30	ASN
10	o5	108	TRP
10	o5	135	ARG
10	q5	30	ASN
10	q5	135	ARG
10	s5	30	ASN
10	s5	43	LYS
10	s5	121	ASN
10	s5	135	ARG
10	u5	30	ASN
10	u5	108	TRP
10	u5	121	ASN
10	u5	135	ARG
10	u5	142	ARG
11	v5	50	CYS
10	w5	30	ASN
10	w5	108	TRP
10	w5	121	ASN
10	w5	135	ARG
10	y5	30	ASN
10	y5	108	TRP
10	y5	121	ASN
10	y5	135	ARG
11	f8	111	ASN
11	f8	149	ARG
11	g8	50	CYS
11	g8	111	ASN
11	g8	149	ARG
11	h8	149	ARG
10	i8	30	ASN
10	i8	84	ARG
10	i8	121	ASN
10	i8	138	LEU
10	j8	121	ASN
10	k8	30	ASN
10	k8	121	ASN

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Mol	Chain	Res	Type
10	l8	30	ASN
10	l8	121	ASN
10	l8	138	LEU
10	m8	30	ASN
10	m8	37	ARG
10	m8	121	ASN
10	m8	138	LEU
10	A6	30	ASN
10	A6	37	ARG
10	A6	121	ASN
10	A6	138	LEU
10	A6	142	ARG
11	B6	25	GLN
11	B6	111	ASN
11	B6	149	ARG
10	C6	19	PRO
10	C6	30	ASN
10	C6	121	ASN
10	C6	138	LEU
11	D6	111	ASN
11	D6	149	ARG
10	E6	30	ASN
10	E6	121	ASN
10	E6	138	LEU
10	E6	142	ARG
11	F6	110	LEU
11	F6	111	ASN
11	F6	149	ARG
10	G6	30	ASN
10	G6	37	ARG
10	G6	89	TYR
10	G6	121	ASN
10	G6	138	LEU
11	H6	25	GLN
11	H6	111	ASN
11	H6	149	ARG
10	I6	30	ASN
10	I6	114	ARG
10	I6	121	ASN
10	I6	138	LEU
10	I6	142	ARG
11	J6	50	CYS

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Mol	Chain	Res	Type
11	J6	149	ARG
10	K6	30	ASN
10	K6	32	GLN
10	K6	37	ARG
10	K6	121	ASN
10	K6	138	LEU
10	K6	142	ARG
11	L6	25	GLN
11	L6	149	ARG
10	M6	30	ASN
10	M6	37	ARG
10	M6	85	ASP
10	M6	121	ASN
10	M6	142	ARG
11	N6	149	ARG
10	O6	30	ASN
10	O6	37	ARG
10	O6	82	CYS
10	O6	84	ARG
10	O6	121	ASN
10	O6	138	LEU
10	O6	142	ARG
11	P6	111	ASN
11	P6	149	ARG
10	Q6	30	ASN
10	Q6	121	ASN
10	Q6	138	LEU
10	Q6	142	ARG
11	R6	149	ARG
10	S6	30	ASN
10	S6	121	ASN
10	S6	138	LEU
10	S6	142	ARG
11	T6	25	GLN
11	T6	111	ASN
11	T6	149	ARG
10	U6	30	ASN
10	U6	37	ARG
10	U6	84	ARG
10	U6	121	ASN
10	U6	138	LEU
10	U6	142	ARG

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Mol	Chain	Res	Type
11	V6	149	ARG
10	W6	30	ASN
10	W6	32	GLN
10	W6	121	ASN
10	W6	138	LEU
11	X6	50	CYS
11	X6	111	ASN
11	X6	149	ARG
10	Y6	30	ASN
10	Y6	37	ARG
10	Y6	121	ASN
10	Y6	138	LEU
11	Z6	111	ASN
11	Z6	149	ARG
11	a6	27	LEU
11	a6	111	ASN
11	a6	149	ARG
11	b6	50	CYS
11	b6	111	ASN
11	b6	149	ARG
11	c6	27	LEU
11	c6	111	ASN
11	c6	149	ARG
11	d6	149	ARG
10	f6	30	ASN
10	f6	84	ARG
10	f6	121	ASN
10	f6	138	LEU
10	f6	142	ARG
10	g6	30	ASN
10	g6	37	ARG
10	g6	121	ASN
10	g6	138	LEU
10	g6	142	ARG
10	h6	30	ASN
10	h6	37	ARG
10	h6	121	ASN
10	h6	138	LEU
10	i6	30	ASN
10	i6	121	ASN
10	i6	142	ARG
10	j6	30	ASN

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Mol	Chain	Res	Type
10	j6	37	ARG
10	j6	84	ARG
10	j6	89	TYR
10	j6	114	ARG
10	j6	121	ASN
10	j6	138	LEU
10	j6	142	ARG
10	k6	30	ASN
10	k6	37	ARG
10	k6	121	ASN
10	k6	138	LEU
11	l6	15	LYS
11	l6	111	ASN
10	m6	138	LEU
10	m6	142	ARG
11	n6	87	GLU
11	n6	149	ARG
10	o6	30	ASN
10	o6	82	CYS
10	o6	138	LEU
11	p6	149	ARG
10	q6	30	ASN
10	q6	121	ASN
10	q6	138	LEU
10	q6	142	ARG
11	r6	27	LEU
11	r6	111	ASN
11	r6	149	ARG
10	s6	30	ASN
10	s6	121	ASN
10	s6	138	LEU
10	s6	142	ARG
11	t6	25	GLN
11	t6	149	ARG
10	u6	30	ASN
10	u6	121	ASN
10	u6	142	ARG
11	v6	111	ASN
11	v6	149	ARG
10	w6	30	ASN
10	w6	121	ASN
11	x6	111	ASN

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Mol	Chain	Res	Type
11	x6	149	ARG
11	y6	50	CYS
11	y6	111	ASN
11	y6	149	ARG
11	z6	111	ASN
11	z6	149	ARG
11	n8	27	LEU
11	n8	149	ARG
11	o8	149	ARG
11	p8	111	ASN
11	p8	149	ARG
10	q8	30	ASN
10	q8	37	ARG
10	q8	121	ASN
10	q8	138	LEU
10	q8	142	ARG
10	q8	144	MET
10	r8	30	ASN
10	r8	37	ARG
10	r8	84	ARG
10	r8	121	ASN
10	r8	138	LEU
10	r8	142	ARG
10	s8	30	ASN
10	s8	37	ARG
10	s8	84	ARG
10	s8	121	ASN
10	s8	138	LEU
10	s8	142	ARG
10	t8	30	ASN
10	t8	37	ARG
10	t8	84	ARG
10	t8	114	ARG
10	t8	121	ASN
10	t8	138	LEU
10	t8	142	ARG
10	u8	30	ASN
10	u8	37	ARG
10	u8	84	ARG
10	u8	121	ASN
10	u8	138	LEU
10	u8	142	ARG

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Mol	Chain	Res	Type
10	A7	30	ASN
10	A7	114	ARG
10	A7	121	ASN
10	A7	138	LEU
11	B7	73	CYS
11	B7	109	CYS
10	C7	30	ASN
10	C7	37	ARG
10	C7	121	ASN
10	C7	142	ARG
11	D7	25	GLN
11	D7	111	ASN
11	D7	149	ARG
10	E7	30	ASN
10	E7	121	ASN
10	E7	138	LEU
10	E7	142	ARG
11	F7	111	ASN
11	F7	149	ARG
10	G7	30	ASN
10	G7	37	ARG
10	G7	82	CYS
10	G7	121	ASN
10	G7	138	LEU
11	H7	149	ARG
10	I7	30	ASN
10	I7	82	CYS
10	I7	121	ASN
10	I7	138	LEU
11	J7	149	ARG
10	K7	30	ASN
10	K7	37	ARG
10	K7	82	CYS
10	K7	121	ASN
10	K7	138	LEU
10	K7	142	ARG
11	L7	25	GLN
11	L7	111	ASN
11	L7	149	ARG
10	M7	30	ASN
10	M7	37	ARG
10	M7	121	ASN

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Mol	Chain	Res	Type
10	M7	138	LEU
10	M7	142	ARG
11	N7	25	GLN
11	N7	111	ASN
11	N7	149	ARG
11	N7	159	GLN
10	O7	30	ASN
10	O7	37	ARG
10	O7	82	CYS
10	O7	121	ASN
10	O7	138	LEU
10	O7	142	ARG
11	P7	149	ARG
10	Q7	30	ASN
10	Q7	37	ARG
10	Q7	84	ARG
10	Q7	121	ASN
10	Q7	138	LEU
10	Q7	142	ARG
11	R7	27	LEU
11	R7	47	ASN
11	R7	111	ASN
11	R7	149	ARG
10	S7	30	ASN
10	S7	82	CYS
10	S7	84	ARG
10	S7	121	ASN
10	S7	138	LEU
11	T7	27	LEU
11	T7	149	ARG
10	U7	30	ASN
10	U7	84	ARG
10	U7	121	ASN
10	U7	138	LEU
11	V7	111	ASN
11	V7	149	ARG
10	W7	30	ASN
10	W7	82	CYS
10	W7	85	ASP
10	W7	121	ASN
10	W7	138	LEU
10	W7	142	ARG

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Mol	Chain	Res	Type
11	X7	1	MET
11	X7	25	GLN
11	X7	72	ASN
11	X7	111	ASN
11	X7	149	ARG
10	Y7	30	ASN
10	Y7	37	ARG
10	Y7	53	LYS
10	Y7	84	ARG
10	Y7	114	ARG
10	Y7	121	ASN
10	Y7	138	LEU
10	Y7	142	ARG
11	Z7	27	LEU
11	Z7	111	ASN
11	Z7	149	ARG
11	a7	25	GLN
11	a7	27	LEU
11	a7	111	ASN
11	a7	149	ARG
11	b7	149	ARG
11	c7	111	ASN
11	c7	149	ARG
11	d7	27	LEU
11	d7	149	ARG
11	e7	111	ASN
11	e7	149	ARG
10	f7	30	ASN
10	f7	84	ARG
10	f7	121	ASN
10	f7	138	LEU
10	f7	142	ARG
10	g7	30	ASN
10	g7	114	ARG
10	g7	121	ASN
10	h7	30	ASN
10	h7	82	CYS
10	h7	84	ARG
10	h7	114	ARG
10	h7	138	LEU
10	i7	30	ASN
10	i7	37	ARG

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Mol	Chain	Res	Type
10	i7	84	ARG
10	i7	89	TYR
10	i7	114	ARG
10	i7	121	ASN
10	i7	142	ARG
10	j7	30	ASN
10	j7	37	ARG
10	j7	82	CYS
10	j7	84	ARG
10	j7	121	ASN
10	j7	138	LEU
10	j7	142	ARG
10	k7	30	ASN
10	k7	32	GLN
10	k7	82	CYS
10	k7	138	LEU
11	l7	50	CYS
11	l7	149	ARG
10	m7	30	ASN
10	m7	37	ARG
10	m7	84	ARG
10	m7	121	ASN
11	n7	111	ASN
11	n7	149	ARG
10	o7	30	ASN
10	o7	138	LEU
10	o7	142	ARG
11	p7	111	ASN
11	p7	149	ARG
10	q7	30	ASN
10	q7	121	ASN
10	q7	138	LEU
10	q7	142	ARG
11	r7	25	GLN
11	r7	111	ASN
11	r7	149	ARG
10	s7	30	ASN
10	s7	32	GLN
10	s7	84	ARG
10	s7	121	ASN
10	s7	138	LEU
10	s7	142	ARG

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Mol	Chain	Res	Type
11	t7	82	CYS
11	t7	149	ARG
10	u7	30	ASN
10	u7	82	CYS
10	u7	84	ARG
10	u7	121	ASN
10	u7	138	LEU
11	v7	27	LEU
11	v7	111	ASN
11	v7	149	ARG
10	w7	30	ASN
10	w7	37	ARG
10	w7	84	ARG
10	w7	121	ASN
10	w7	138	LEU
10	w7	142	ARG
11	x7	111	ASN
11	x7	149	ARG
11	y7	111	ASN
11	y7	149	ARG
11	z7	25	GLN
11	z7	27	LEU
11	z7	111	ASN
11	z7	149	ARG
19	a8	203	ARG
19	a8	340	LYS
19	a8	358	ARG
12	b8	95	CYS
12	b8	147	ARG
12	b8	150	ASN
12	b8	216	ARG
14	c8	43	ARG
14	c8	46	LEU
14	c8	129	LYS
14	d8	60	TYR
14	e8	60	TYR
19	a9	47	THR
19	a9	203	ARG
19	a9	340	LYS
19	a9	358	ARG
12	b9	147	ARG
12	b9	150	ASN

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Mol	Chain	Res	Type
12	b9	213	ARG
12	b9	216	ARG
14	c9	43	ARG
14	c9	63	ARG
14	c9	72	LYS
14	c9	129	LYS
14	d9	60	TYR
10	v8	30	ASN
10	v8	121	ASN
11	w8	111	ASN
10	x8	30	ASN
10	x8	121	ASN
10	z8	30	ASN
10	z8	121	ASN
11	A8	82	CYS
11	A8	111	ASN
10	B8	30	ASN
10	B8	121	ASN
11	C8	111	ASN
10	D8	30	ASN
10	D8	121	ASN
11	E8	1	MET
11	E8	109	CYS
11	E8	111	ASN
10	F8	30	ASN
10	F8	121	ASN
11	G8	111	ASN
10	H8	30	ASN
10	H8	121	ASN
11	I8	111	ASN
10	J8	30	ASN
10	J8	121	ASN
11	K8	111	ASN
10	L8	30	ASN
10	L8	121	ASN
11	M8	111	ASN
10	N8	30	ASN
10	N8	121	ASN
11	O8	111	ASN
10	P8	30	ASN
10	P8	121	ASN
11	Q8	111	ASN

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Mol	Chain	Res	Type
15	R8	20	PHE
15	R8	105	ARG
15	R8	204	HIS
15	R8	205	ARG
16	S8	231	ARG
16	S8	241	GLN
16	S8	327	ARG
14	T8	159	LYS
14	T8	218	ARG
12	U8	147	ARG
12	U8	150	ASN
12	U8	212	TYR
12	U8	216	ARG
17	V8	21	ASN
17	V8	30	ARG
18	W8	68	GLN
18	W8	108	ARG
18	W8	111	ASN
17	X8	21	ASN
17	X8	30	ARG
18	Y8	7	LYS
18	Y8	72	ASN
18	Y8	84	ARG
18	Y8	111	ASN
17	Z8	21	ASN
17	Z8	30	ARG
18	f9	108	ARG
18	f9	111	ASN
17	g9	21	ASN
17	g9	30	ARG
18	h9	7	LYS
18	h9	65	GLN
18	h9	111	ASN
17	i9	21	ASN
17	i9	30	ARG
18	j9	111	ASN
17	k9	30	ARG
18	l9	7	LYS
18	l9	111	ASN
10	m9	30	ASN
10	m9	121	ASN
11	n9	111	ASN

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Mol	Chain	Res	Type
10	o9	30	ASN
10	o9	47	ASN
10	o9	121	ASN
11	p9	25	GLN
11	p9	77	ARG
11	p9	111	ASN
10	q9	30	ASN
10	q9	65	TYR
10	q9	121	ASN
11	r9	35	ASN
11	r9	111	ASN
10	s9	30	ASN
10	s9	121	ASN
11	t9	25	GLN
10	u9	30	ASN
10	u9	121	ASN
11	v9	25	GLN
11	v9	111	ASN
10	w9	30	ASN
10	w9	121	ASN
11	x9	109	CYS
10	y9	30	ASN
10	y9	121	ASN
11	z9	1	MET
11	z9	35	ASN
11	z9	50	CYS
11	z9	111	ASN
10	A9	30	ASN
10	A9	121	ASN
11	B9	61	CYS
11	B9	111	ASN
10	C9	30	ASN
10	C9	121	ASN
11	D9	61	CYS
10	E9	30	ASN
10	E9	121	ASN
11	F9	111	ASN
10	G9	30	ASN
10	G9	74	ASP
10	G9	121	ASN
11	H9	111	ASN
10	I9	30	ASN

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Mol	Chain	Res	Type
10	I9	82	CYS
10	I9	121	ASN
11	J9	111	ASN
10	K9	30	ASN
10	K9	121	ASN
11	L9	61	CYS
11	L9	111	ASN
10	M9	30	ASN
10	M9	121	ASN
11	N9	111	ASN
10	O9	30	ASN
10	O9	121	ASN
11	P9	111	ASN
10	Q9	30	ASN
10	Q9	121	ASN
11	R9	111	ASN
11	R9	115	GLU
10	S9	30	ASN
10	S9	121	ASN
11	T9	111	ASN
10	U9	30	ASN
10	U9	121	ASN
11	V9	111	ASN
15	W9	20	PHE
15	W9	52	ARG
15	W9	105	ARG
15	W9	204	HIS
15	W9	206	PHE
15	W9	210	GLU
15	W9	220	LEU
15	W9	225	VAL
16	X9	190	TYR
16	X9	235	ASN
16	X9	239	LEU
16	X9	241	GLN
16	X9	327	ARG
16	X9	341	ASN
16	X9	345	LEU
14	Y9	159	LYS
14	Y9	218	ARG
12	Z9	44	ASP
12	Z9	66	LEU

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Mol	Chain	Res	Type
12	Z9	147	ARG
12	Z9	150	ASN
12	Z9	216	ARG
17	aa	21	ASN
17	aa	30	ARG
18	ab	68	GLN
18	ab	108	ARG
18	ab	111	ASN
17	ac	21	ASN
17	ac	30	ARG
18	ad	7	LYS
18	ad	72	ASN
18	ad	111	ASN
17	ae	21	ASN
17	ae	30	ARG
18	af	7	LYS
18	af	72	ASN
18	af	108	ARG
18	af	111	ASN
17	ag	21	ASN
17	ag	30	ARG
18	ah	7	LYS
18	ah	65	GLN
18	ah	66	LEU
18	ah	111	ASN
17	ai	21	ASN
17	ai	30	ARG
18	aj	7	LYS
18	aj	111	ASN
18	aj	145	LEU
17	ak	19	LEU
17	ak	21	ASN
17	ak	30	ARG
17	ak	127	SER
18	al	7	LYS
18	al	111	ASN
10	am	30	ASN
10	am	121	ASN
11	an	61	CYS
11	an	111	ASN
10	ao	30	ASN
10	ao	71	GLU

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Mol	Chain	Res	Type
10	ao	121	ASN
11	ap	38	LEU
11	ap	77	ARG
11	ap	109	CYS
11	ap	159	GLN
10	aq	30	ASN
10	aq	121	ASN
11	ar	35	ASN
11	ar	111	ASN
10	as	30	ASN
10	as	121	ASN
11	at	25	GLN
10	au	30	ASN
10	au	121	ASN
11	av	62	GLU
11	av	98	LEU
11	av	111	ASN
10	aw	30	ASN
10	aw	121	ASN
11	ax	111	ASN
10	ay	30	ASN
10	ay	121	ASN
11	az	35	ASN
11	az	50	CYS
11	az	66	LEU
11	az	111	ASN
10	aA	30	ASN
10	aA	121	ASN
10	aA	137	ARG
11	aB	105	LEU
11	aB	111	ASN
10	aC	30	ASN
10	aC	121	ASN
10	aC	142	ARG
11	aD	111	ASN
10	aE	30	ASN
10	aE	82	CYS
10	aE	121	ASN
10	aE	143	ASP
10	aE	145	SER
11	aF	25	GLN
11	aF	107	ASP

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Mol	Chain	Res	Type
11	aF	111	ASN
10	aG	30	ASN
10	aG	82	CYS
10	aG	138	LEU
11	aH	50	CYS
11	aH	111	ASN
10	aI	30	ASN
10	aI	121	ASN
11	aJ	111	ASN
10	aK	30	ASN
10	aK	121	ASN
10	aK	142	ARG
11	aL	111	ASN
10	aM	30	ASN
11	aN	111	ASN
10	aO	30	ASN
10	aO	121	ASN
11	aP	76	ASN
11	aP	111	ASN
10	aQ	30	ASN
10	aQ	121	ASN
11	aR	50	CYS
11	aR	111	ASN
10	aS	30	ASN
10	aS	121	ASN
10	aS	143	ASP
11	aT	111	ASN
10	aU	30	ASN
10	aU	121	ASN
10	aU	136	ASP
11	aV	111	ASN
15	aW	25	ASN
15	aW	207	ARG
16	aX	95	MET
16	aX	104	LYS
16	aX	164	LYS
16	aX	239	LEU
16	aX	241	GLN
16	aX	327	ARG
12	aY	46	PHE
12	aY	147	ARG
12	aY	150	ASN

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Mol	Chain	Res	Type
12	aY	193	MET
12	aY	216	ARG
14	aZ	159	LYS
14	aZ	256	SER
17	ba	30	ARG
17	bc	21	ASN
17	bc	30	ARG
18	bd	82	CYS
18	bd	84	ARG
18	bd	85	ASP
17	be	21	ASN
17	be	30	ARG
17	bg	30	ARG
17	bi	30	ARG
18	bj	104	VAL
17	bk	21	ASN
17	bk	30	ARG
10	bm	30	ASN
10	bm	68	ASN
10	bm	82	CYS
11	bn	111	ASN
11	bo	77	ARG
11	bo	111	ASN
11	bp	73	CYS
11	bp	111	ASN
11	bs	50	CYS
11	bs	111	ASN
11	bs	116	THR
10	bt	30	ASN
10	bt	121	ASN
10	bt	143	ASP
10	bt	147	GLN
10	bu	30	ASN
10	bu	121	ASN
10	bu	138	LEU
10	bv	30	ASN
10	bv	121	ASN
10	bv	138	LEU
10	bw	30	ASN
10	bw	82	CYS
10	bw	121	ASN
10	bw	136	ASP

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Mol	Chain	Res	Type
10	bx	30	ASN
10	bx	82	CYS
10	bx	121	ASN
10	by	30	ASN
10	by	77	GLU
10	by	121	ASN
11	bz	50	CYS
11	bz	111	ASN
10	bA	30	ASN
10	bA	121	ASN
10	bA	137	ARG
11	bB	1	MET
11	bB	105	LEU
11	bB	109	CYS
11	bB	111	ASN
11	bB	161	LEU
10	bC	30	ASN
10	bC	121	ASN
10	bC	138	LEU
10	bC	140	VAL
10	bC	142	ARG
10	bC	143	ASP
11	bD	75	THR
11	bD	111	ASN
11	bD	161	LEU
10	bE	30	ASN
10	bE	82	CYS
10	bE	121	ASN
10	bE	137	ARG
10	bE	138	LEU
10	bE	140	VAL
10	bE	142	ARG
10	bE	143	ASP
11	bF	25	GLN
11	bF	111	ASN
10	bG	30	ASN
10	bG	121	ASN
10	bG	143	ASP
11	bH	50	CYS
11	bH	111	ASN
10	bI	30	ASN
10	bI	121	ASN

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Mol	Chain	Res	Type
11	bJ	1	MET
11	bJ	111	ASN
10	bK	30	ASN
10	bK	82	CYS
10	bK	137	ARG
10	bK	140	VAL
10	bK	141	PRO
10	bK	142	ARG
10	bK	144	MET
11	bL	50	CYS
11	bL	111	ASN
10	bM	30	ASN
10	bM	121	ASN
10	bM	136	ASP
11	bN	111	ASN
10	bO	30	ASN
10	bO	121	ASN
10	bO	138	LEU
11	bP	111	ASN
10	bQ	30	ASN
10	bQ	121	ASN
11	bR	50	CYS
11	bR	111	ASN
10	bS	30	ASN
10	bS	121	ASN
10	bS	140	VAL
10	bS	143	ASP
11	bT	50	CYS
11	bT	111	ASN
10	bU	30	ASN
10	bU	121	ASN
10	bU	136	ASP
10	bU	138	LEU
11	bV	111	ASN
15	bW	61	LEU
15	bW	169	GLN
15	bW	207	ARG
16	bX	95	MET
16	bX	98	GLU
16	bX	104	LYS
16	bX	158	LEU
16	bX	164	LYS

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Mol	Chain	Res	Type
16	bX	239	LEU
16	bX	241	GLN
16	bX	273	THR
16	bX	327	ARG
12	bY	46	PHE
12	bY	92	LEU
12	bY	147	ARG
12	bY	193	MET
12	bY	213	ARG
12	bY	216	ARG
14	bZ	43	ARG
14	bZ	66	ILE
14	bZ	159	LYS
17	ca	21	ASN
17	ca	30	ARG
18	cb	72	ASN
18	cb	149	PRO
17	cc	21	ASN
17	cc	30	ARG
17	cc	77	ASN
17	cc	79	ILE
18	cd	83	LEU
17	ce	21	ASN
17	ce	30	ARG
18	cf	72	ASN
17	cg	21	ASN
17	cg	30	ARG
18	ch	72	ASN
18	ch	77	ARG
17	ci	21	ASN
17	ci	30	ARG
18	cj	72	ASN
17	ck	21	ASN
17	ck	30	ARG
18	cl	72	ASN
18	cl	150	LEU
10	cm	30	ASN
10	cm	82	CYS
10	cm	121	ASN
10	cm	140	VAL
10	cm	143	ASP
11	cn	50	CYS

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Mol	Chain	Res	Type
11	cn	111	ASN
11	cn	161	LEU
11	co	75	THR
11	co	77	ARG
11	co	111	ASN
11	co	161	LEU
11	cp	50	CYS
11	cp	111	ASN
11	cp	161	LEU
11	cq	50	CYS
11	cq	75	THR
11	cq	111	ASN
11	cr	110	LEU
11	cr	161	LEU
11	cs	23	ASP
11	cs	50	CYS
11	cs	111	ASN
11	cs	115	GLU
11	cs	161	LEU
10	ct	30	ASN
10	ct	121	ASN
10	ct	140	VAL
10	ct	143	ASP
10	cu	30	ASN
10	cu	121	ASN
10	cu	136	ASP
10	cu	138	LEU
10	cu	139	CYS
10	cu	143	ASP
10	cv	30	ASN
10	cv	59	CYS
10	cv	68	ASN
10	cv	121	ASN
10	cv	137	ARG
10	cv	138	LEU
10	cw	30	ASN
10	cw	74	ASP
10	cw	82	CYS
10	cw	121	ASN
10	cw	136	ASP
10	cx	30	ASN
10	cx	82	CYS

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Mol	Chain	Res	Type
10	cx	121	ASN
10	cx	143	ASP
10	cy	30	ASN
10	cy	43	LYS
10	cy	121	ASN
11	cz	50	CYS
11	cz	111	ASN
10	cA	30	ASN
10	cA	121	ASN
10	cA	138	LEU
10	cA	143	ASP
10	cC	30	ASN
10	cC	121	ASN
10	cC	140	VAL
10	cD	30	ASN
10	cD	121	ASN
11	cF	50	CYS
10	cG	30	ASN
10	cG	121	ASN
10	cG	143	ASP
10	cI	30	ASN
10	cI	121	ASN
11	cJ	23	ASP
10	cK	30	ASN
10	cK	121	ASN
10	cK	142	ARG
10	cK	144	MET
11	cL	50	CYS
11	cL	127	THR
11	cR	50	CYS
10	cS	30	ASN
10	cS	121	ASN
10	cS	138	LEU
10	cS	142	ARG
10	cS	143	ASP
10	cS	144	MET
10	cT	30	ASN
10	cT	121	ASN
10	cT	142	ARG
10	cU	30	ASN
10	cU	142	ARG
10	cV	30	ASN

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Mol	Chain	Res	Type
10	cV	121	ASN
10	cV	138	LEU
10	cW	30	ASN
10	cW	121	ASN
10	cW	138	LEU
10	cW	139	CYS
10	cX	30	ASN
10	cX	121	ASN
11	cY	50	CYS
10	cZ	30	ASN
10	cZ	121	ASN
10	da	30	ASN
10	da	121	ASN
10	db	30	ASN
10	db	121	ASN
10	db	144	MET
10	dc	30	ASN
10	dc	121	ASN
10	dc	140	VAL
10	dc	142	ARG
10	de	30	ASN
10	de	121	ASN
10	de	143	ASP
11	df	50	CYS
11	df	115	GLU
10	dg	30	ASN
10	dg	121	ASN
10	dg	143	ASP
11	dh	50	CYS
11	di	50	CYS
11	dj	50	CYS
10	dk	30	ASN
10	dk	121	ASN
10	dk	142	ARG
10	dm	30	ASN
10	dm	121	ASN
11	dn	50	CYS
10	do	30	ASN
10	do	121	ASN
11	dp	50	CYS
10	dq	30	ASN
10	dq	121	ASN

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Mol	Chain	Res	Type
11	dr	50	CYS
11	dr	72	ASN
10	ds	30	ASN
10	ds	121	ASN
10	ds	143	ASP
11	dt	50	CYS
10	du	30	ASN
10	du	121	ASN
11	dv	50	CYS
12	dw	95	CYS
12	dw	135	THR
12	dw	147	ARG
12	dw	150	ASN
12	dw	193	MET
12	dw	213	ARG
12	dx	95	CYS
12	dx	147	ARG
12	dx	150	ASN
12	dx	193	MET
12	dx	213	ARG
20	dy	85	ASN
20	dy	124	ARG
20	dy	142	ARG
20	dy	198	TYR
20	dy	260	PHE
20	dy	286	ASN
20	dz	85	ASN
20	dz	124	ARG
20	dz	142	ARG
20	dz	201	CYS
20	dz	224	ARG
20	dz	227	THR
20	dz	260	PHE
20	dz	286	ASN
10	dA	30	ASN
10	dA	121	ASN
11	dB	7	ARG
11	dB	109	CYS
10	dC	30	ASN
10	dC	121	ASN
10	dE	30	ASN
10	dE	121	ASN

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Mol	Chain	Res	Type
10	dG	30	ASN
10	dG	121	ASN
10	dG	147	GLN
10	dI	30	ASN
10	dI	121	ASN
10	dJ	30	ASN
10	dJ	121	ASN
11	dK	15	LYS
11	dL	7	ARG
11	dL	61	CYS
11	dL	161	LEU
10	dM	30	ASN
10	dM	121	ASN
11	dN	50	CYS
10	dO	30	ASN
10	dO	121	ASN
10	dQ	30	ASN
10	dQ	121	ASN
10	dS	30	ASN
10	dS	121	ASN
10	dU	30	ASN
10	dU	121	ASN
11	dV	35	ASN
10	dW	30	ASN
10	dW	121	ASN
11	dX	33	ASP
11	dY	161	LEU
10	dZ	30	ASN
10	dZ	121	ASN
10	ea	30	ASN
10	ea	121	ASN
11	eb	61	CYS
11	eb	161	LEU
11	ec	23	ASP
11	ec	50	CYS
11	ec	161	LEU
10	ed	30	ASN
10	ed	121	ASN
11	ee	7	ARG
11	ee	108	ARG
11	ee	161	LEU
10	ef	30	ASN

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Mol	Chain	Res	Type
10	ef	53	LYS
10	ef	121	ASN
10	eh	30	ASN
10	eh	121	ASN
11	ei	23	ASP
11	ei	38	LEU
10	ej	30	ASN
10	ej	121	ASN
10	ej	147	GLN
10	ek	30	ASN
10	ek	121	ASN
10	em	30	ASN
10	em	121	ASN
11	en	7	ARG
10	eo	30	ASN
10	eo	53	LYS
10	eo	121	ASN
10	eq	30	ASN
10	es	30	ASN
11	et	61	CYS
11	et	109	CYS
10	eu	30	ASN
10	eu	121	ASN
11	ev	7	ARG
21	ew	67	ARG
21	ew	191	ASN
21	ew	226	ASN
21	ew	257	LYS
21	ex	67	ARG
21	ex	191	ASN
21	ex	226	ASN
21	ex	245	CYS
21	ex	257	LYS
12	ey	55	LYS
12	ey	147	ARG
12	ey	150	ASN
12	ey	193	MET
12	ey	318	TYR
12	ez	147	ARG
12	ez	150	ASN
12	ez	193	MET
10	eA	30	ASN

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Mol	Chain	Res	Type
10	eA	84	ARG
10	eA	121	ASN
10	eC	30	ASN
10	eC	84	ARG
10	eC	121	ASN
10	eE	30	ASN
10	eE	84	ARG
10	eE	121	ASN
10	eG	30	ASN
10	eG	84	ARG
10	eG	121	ASN
10	eG	138	LEU
10	eG	139	CYS
10	eG	142	ARG
10	eG	143	ASP
10	eI	30	ASN
10	eI	84	ARG
10	eI	121	ASN
10	eI	137	ARG
11	eJ	1	MET
11	eJ	109	CYS
10	eK	30	ASN
10	eK	84	ARG
10	eK	117	TYR
10	eK	121	ASN
10	eK	142	ARG
10	eM	30	ASN
10	eM	84	ARG
10	eM	121	ASN
10	eM	138	LEU
10	eM	142	ARG
10	eO	30	ASN
10	eO	84	ARG
10	eO	121	ASN
10	eO	143	ASP
10	eQ	30	ASN
10	eQ	84	ARG
10	eQ	121	ASN
10	eQ	142	ARG
10	eQ	146	SER
11	eR	23	ASP
10	eS	30	ASN

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Mol	Chain	Res	Type
10	eS	84	ARG
10	eS	121	ASN
10	eS	138	LEU
10	eS	143	ASP
11	eT	1	MET
11	eT	23	ASP
10	eU	30	ASN
10	eU	84	ARG
10	eU	121	ASN
10	eU	143	ASP
11	eV	115	GLU
10	eW	30	ASN
10	eW	84	ARG
10	eW	121	ASN
10	eW	139	CYS
11	eX	23	ASP
22	eY	111	ARG
22	eY	141	ARG
22	eY	150	ARG
22	eY	220	TYR
22	eY	300	ARG
22	eY	317	MET
22	eZ	111	ARG
22	eZ	141	ARG
22	eZ	148	CYS
22	eZ	150	ARG
22	eZ	300	ARG
10	la	30	ASN
10	la	62	LYS
10	la	67	LYS
10	la	121	ASN
11	lb	77	ARG
10	lc	30	ASN
10	lc	121	ASN
11	ld	50	CYS
10	le	30	ASN
10	le	62	LYS
10	le	121	ASN
11	lf	77	ARG
10	lg	30	ASN
10	lg	62	LYS
10	lg	67	LYS

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Mol	Chain	Res	Type
10	lg	121	ASN
10	lg	142	ARG
11	lh	7	ARG
11	lh	77	ARG
10	li	30	ASN
10	li	62	LYS
10	li	67	LYS
10	li	121	ASN
10	li	142	ARG
10	li	145	SER
10	li	156	LEU
11	lj	38	LEU
11	lj	50	CYS
11	lj	77	ARG
10	lk	30	ASN
10	lk	62	LYS
10	lk	121	ASN
10	lk	142	ARG
11	ll	50	CYS
10	lm	30	ASN
10	lm	121	ASN
11	ln	77	ARG
10	lo	30	ASN
10	lo	62	LYS
10	lo	121	ASN
10	lq	30	ASN
10	lq	121	ASN
10	lq	142	ARG
10	ls	30	ASN
10	ls	142	ARG
10	lu	30	ASN
10	lu	142	ARG
11	lv	7	ARG
11	lv	77	ARG
10	lw	30	ASN
10	lw	62	LYS
10	lw	142	ARG
11	lx	61	CYS
23	ly	203	ARG
23	ly	344	ARG
23	lz	161	THR
23	lz	203	ARG

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Mol	Chain	Res	Type
23	lz	344	ARG
11	fa	27	LEU
10	fb	30	ASN
10	fb	121	ASN
10	fb	135	ARG
10	fb	140	VAL
11	fc	27	LEU
21	fd	67	ARG
21	fd	160	LEU
21	fd	191	ASN
21	fd	226	ASN
10	fe	30	ASN
10	fe	121	ASN
10	fe	135	ARG
10	fe	140	VAL
11	ff	27	LEU
10	fg	30	ASN
10	fg	121	ASN
10	fg	135	ARG
10	fh	30	ASN
10	fh	121	ASN
10	fh	135	ARG
10	fh	140	VAL
11	fi	27	LEU
11	fj	27	LEU
10	fk	30	ASN
10	fk	121	ASN
10	fk	135	ARG
10	fk	140	VAL
10	fl	30	ASN
10	fl	121	ASN
10	fl	135	ARG
11	fm	27	LEU
10	fn	17	ARG
10	fn	30	ASN
10	fn	121	ASN
10	fn	135	ARG
10	fn	140	VAL
11	fo	27	LEU
10	fp	30	ASN
10	fp	121	ASN
10	fp	135	ARG

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Mol	Chain	Res	Type
10	fp	140	VAL
11	fq	27	LEU
10	fr	2	LYS
10	fr	30	ASN
10	fr	121	ASN
10	fr	135	ARG
10	fr	140	VAL
11	fs	27	LEU
10	ft	30	ASN
10	ft	121	ASN
10	ft	135	ARG
11	fu	27	LEU
10	fv	30	ASN
10	fv	121	ASN
10	fv	135	ARG
10	fv	142	ARG
11	fw	27	LEU
10	fx	30	ASN
10	fx	121	ASN
10	fx	135	ARG
10	fx	140	VAL
11	fy	27	LEU
21	fz	67	ARG
21	fz	160	LEU
21	fz	191	ASN
21	fz	226	ASN
11	ga	61	CYS
11	ga	78	ARG
10	gb	30	ASN
10	gb	121	ASN
10	gb	138	LEU
10	gc	30	ASN
10	gc	121	ASN
11	gd	61	CYS
11	gd	62	GLU
11	gd	73	CYS
11	gd	77	ARG
11	gd	78	ARG
11	ge	50	CYS
11	ge	78	ARG
10	gf	30	ASN
10	gf	71	GLU

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Mol	Chain	Res	Type
10	gf	121	ASN
11	gg	50	CYS
11	gg	72	ASN
10	gh	30	ASN
10	gh	121	ASN
10	gh	138	LEU
11	gi	72	ASN
11	gi	78	ARG
10	gj	30	ASN
10	gj	121	ASN
10	gj	138	LEU
10	gj	142	ARG
11	gk	77	ARG
11	gk	78	ARG
10	gl	30	ASN
10	gl	121	ASN
10	gl	143	ASP
10	gm	30	ASN
10	gm	121	ASN
10	gm	142	ARG
11	gn	50	CYS
11	gn	61	CYS
10	go	30	ASN
10	go	121	ASN
10	go	136	ASP
10	go	143	ASP
11	gp	75	THR
10	gq	30	ASN
10	gq	121	ASN
10	gq	138	LEU
10	gq	139	CYS
10	gq	143	ASP
11	gr	50	CYS
11	gr	61	CYS
11	gr	75	THR
11	gr	78	ARG
10	gs	30	ASN
10	gs	121	ASN
10	gs	143	ASP
11	gt	23	ASP
11	gt	50	CYS
11	gt	75	THR

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Mol	Chain	Res	Type
11	gt	78	ARG
10	gu	30	ASN
10	gu	121	ASN
10	gu	138	LEU
11	gv	75	THR
11	gv	78	ARG
10	gw	30	ASN
10	gw	121	ASN
10	gw	137	ARG
10	gw	140	VAL
11	gx	50	CYS
11	gx	61	CYS
11	gx	75	THR
11	gx	78	ARG
24	gy	131	MET
24	gy	169	MET
24	gy	253	PHE
24	gz	131	MET
24	gz	157	GLU
24	gz	169	MET
10	hA	30	ASN
10	hA	121	ASN
10	hA	140	VAL
10	hA	142	ARG
10	hA	144	MET
10	hC	30	ASN
10	hC	121	ASN
10	hC	140	VAL
10	hC	144	MET
10	hE	30	ASN
10	hE	121	ASN
10	hE	140	VAL
10	hE	144	MET
10	hF	30	ASN
10	hF	121	ASN
10	hF	140	VAL
10	hF	144	MET
10	hI	30	ASN
10	hI	121	ASN
10	hI	140	VAL
10	hI	144	MET
10	hK	30	ASN

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Mol	Chain	Res	Type
10	hK	121	ASN
10	hK	140	VAL
10	hK	144	MET
10	hM	30	ASN
10	hM	121	ASN
10	hM	140	VAL
10	hM	144	MET
10	hO	30	ASN
10	hO	121	ASN
10	hO	140	VAL
10	hO	144	MET
10	hQ	30	ASN
10	hQ	121	ASN
10	hQ	140	VAL
10	hQ	144	MET
10	hS	30	ASN
10	hS	121	ASN
10	hS	140	VAL
10	hS	144	MET
10	hU	30	ASN
10	hU	121	ASN
10	hU	140	VAL
10	hU	144	MET
10	hW	30	ASN
10	hW	121	ASN
10	hW	140	VAL
10	hW	144	MET
23	hY	203	ARG
23	hY	344	ARG
23	hZ	203	ARG
23	hZ	344	ARG
10	iA	2	LYS
10	iA	30	ASN
10	iA	135	ARG
10	iA	138	LEU
10	iA	161	ASN
10	iB	30	ASN
10	iB	135	ARG
10	iB	161	ASN
11	iC	76	ASN
11	iD	3	ASP
11	iD	19	VAL

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Mol	Chain	Res	Type
11	iD	23	ASP
11	iD	24	LEU
11	iD	76	ASN
11	iE	47	ASN
11	iE	66	LEU
11	iE	76	ASN
11	iG	76	ASN
11	iG	95	TYR
11	iG	107	ASP
11	jI	35	ASN
11	jI	76	ASN
11	jJ	35	ASN
11	jJ	76	ASN
11	jK	35	ASN
11	jK	76	ASN
11	jL	35	ASN
11	jM	35	ASN
11	jM	76	ASN
11	jN	35	ASN
11	jN	76	ASN
11	jO	35	ASN
11	jO	76	ASN
11	jO	161	LEU
11	jP	35	ASN
11	jP	76	ASN
11	kQ	35	ASN
11	kR	35	ASN
11	kS	35	ASN
11	kS	75	THR
11	kT	35	ASN
11	kT	75	THR
11	kU	35	ASN
11	kU	76	ASN
11	kV	35	ASN
11	kV	76	ASN
11	kW	35	ASN
11	kW	76	ASN
11	kX	35	ASN
11	kX	76	ASN
25	ka	117	LEU
25	ka	242	ASP
25	ka	316	MET

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Mol	Chain	Res	Type
25	ka	348	ARG
25	kb	238	LEU
25	kb	249	TYR
25	kb	316	MET
25	kb	348	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2627) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	147	HIS
1	A1	231	GLN
1	B1	64	GLN
1	B1	113	ASN
1	B1	147	HIS
1	B1	231	GLN
2	C1	136	GLN
2	C1	140	ASN
2	C1	161	ASN
2	D1	50	GLN
2	D1	60	HIS
2	D1	136	GLN
2	D1	140	ASN
2	D1	161	ASN
3	E1	61	GLN
3	E1	280	ASN
3	F1	60	ASN
3	F1	61	GLN
3	F1	280	ASN
4	G1	161	GLN
4	I1	161	GLN
5	J1	71	ASN
4	K1	161	GLN
5	L1	117	ASN
4	N1	46	ASN
4	N1	71	ASN
4	N1	161	GLN
5	O1	110	ASN
5	O1	131	GLN
4	P1	41	GLN
4	P1	46	ASN
4	P1	161	GLN
6	Q1	2	GLN

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Mol	Chain	Res	Type
6	Q1	72	ASN
4	R1	71	ASN
4	R1	161	GLN
5	S1	10	ASN
4	T1	71	ASN
4	T1	161	GLN
5	U1	10	ASN
7	V1	25	ASN
7	V1	145	GLN
4	X1	60	GLN
4	X1	161	GLN
5	Y1	71	ASN
4	Z1	161	GLN
5	a1	10	ASN
5	a1	15	GLN
5	a1	117	ASN
4	b1	161	GLN
4	d1	161	GLN
5	e1	110	ASN
5	e1	131	GLN
4	f1	41	GLN
4	f1	161	GLN
6	g1	72	ASN
4	i1	161	GLN
5	j1	10	ASN
4	k1	161	GLN
5	l1	10	ASN
7	m1	25	ASN
7	m1	145	GLN
5	n1	71	ASN
4	o1	161	GLN
5	p1	10	ASN
4	q1	71	ASN
4	q1	117	ASN
4	q1	161	GLN
5	r1	71	ASN
4	s1	161	GLN
5	t1	15	GLN
4	u1	56	GLN
4	u1	71	ASN
4	u1	161	GLN
5	v1	10	ASN

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Mol	Chain	Res	Type
4	w1	71	ASN
4	w1	117	ASN
4	w1	161	GLN
4	y1	71	ASN
4	y1	161	GLN
5	z1	15	GLN
5	z1	128	GLN
8	a2	58	ASN
8	a2	171	ASN
8	a2	297	ASN
8	a2	330	GLN
8	a2	347	HIS
8	a2	401	GLN
8	a2	404	GLN
8	a2	442	GLN
8	a2	491	ASN
8	a2	495	ASN
8	a2	524	ASN
8	a2	527	GLN
8	a2	661	ASN
8	a2	665	ASN
8	a2	694	ASN
8	a2	760	ASN
8	a2	797	HIS
8	a2	806	GLN
8	a2	813	ASN
8	a2	821	GLN
8	b2	58	ASN
8	b2	171	ASN
8	b2	347	HIS
8	b2	380	ASN
8	b2	401	GLN
8	b2	466	ASN
8	b2	491	ASN
8	b2	492	GLN
8	b2	501	GLN
8	b2	665	ASN
8	b2	752	ASN
8	b2	797	HIS
8	b2	806	GLN
8	b2	813	ASN
8	b2	864	ASN

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Mol	Chain	Res	Type
9	c2	49	GLN
9	c2	50	ASN
9	c2	67	GLN
9	c2	70	GLN
9	c2	86	GLN
9	d2	50	ASN
9	d2	67	GLN
9	d2	70	GLN
9	d2	86	GLN
10	e2	30	ASN
10	e2	121	ASN
10	e2	161	ASN
11	f2	35	ASN
10	g2	30	ASN
10	g2	121	ASN
10	i2	121	ASN
10	k2	30	ASN
10	k2	121	ASN
10	k2	161	ASN
11	l2	35	ASN
10	m2	30	ASN
10	m2	121	ASN
11	n2	35	ASN
11	n2	42	ASN
10	o2	30	ASN
10	o2	94	ASN
10	o2	121	ASN
10	q2	30	ASN
10	q2	121	ASN
10	s2	30	ASN
10	s2	32	GLN
10	s2	121	ASN
11	t2	35	ASN
10	u2	121	ASN
11	v2	35	ASN
10	w2	30	ASN
10	w2	94	ASN
10	w2	121	ASN
10	w2	161	ASN
11	x2	35	ASN
10	y2	30	ASN
10	y2	80	ASN

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Mol	Chain	Res	Type
10	y2	94	ASN
10	y2	121	ASN
11	z2	35	ASN
12	A2	150	ASN
12	A2	299	ASN
12	A2	300	HIS
13	B2	58	GLN
13	B2	79	ASN
13	B2	99	ASN
13	B2	121	ASN
13	B2	147	GLN
13	B2	154	ASN
13	B2	177	HIS
13	B2	202	ASN
13	B2	389	ASN
14	C2	90	ASN
14	C2	98	GLN
14	C2	150	HIS
14	C2	213	ASN
14	D2	90	ASN
14	D2	98	GLN
14	D2	146	HIS
14	D2	213	ASN
14	D2	262	ASN
10	E2	30	ASN
10	E2	94	ASN
10	E2	121	ASN
11	F2	35	ASN
10	G2	30	ASN
10	G2	94	ASN
10	G2	121	ASN
10	I2	30	ASN
10	I2	121	ASN
10	I2	161	ASN
11	J2	35	ASN
11	J2	47	ASN
11	J2	111	ASN
10	K2	28	GLN
10	K2	30	ASN
10	K2	32	GLN
10	K2	121	ASN
10	K2	161	ASN

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Mol	Chain	Res	Type
11	L2	35	ASN
10	M2	30	ASN
10	M2	121	ASN
11	N2	35	ASN
10	O2	30	ASN
10	O2	161	ASN
11	P2	35	ASN
10	Q2	30	ASN
10	Q2	121	ASN
11	R2	35	ASN
10	S2	30	ASN
10	S2	121	ASN
11	T2	35	ASN
10	U2	30	ASN
10	U2	121	ASN
11	V2	35	ASN
11	V2	42	ASN
11	V2	159	GLN
10	W2	30	ASN
10	W2	161	ASN
11	X2	35	ASN
10	Y2	30	ASN
10	Y2	32	GLN
10	Y2	121	ASN
11	Z2	35	ASN
10	A3	30	ASN
10	A3	94	ASN
10	A3	121	ASN
10	A3	161	ASN
11	B3	35	ASN
11	B3	76	ASN
10	C3	30	ASN
10	C3	76	GLN
10	C3	121	ASN
11	D3	35	ASN
10	E3	30	ASN
10	E3	94	ASN
10	E3	121	ASN
11	F3	35	ASN
11	F3	47	ASN
10	G3	30	ASN
10	G3	121	ASN

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Mol	Chain	Res	Type
10	G3	161	ASN
11	H3	47	ASN
10	I3	121	ASN
10	I3	161	ASN
11	J3	47	ASN
10	K3	30	ASN
10	K3	121	ASN
10	K3	161	ASN
11	L3	35	ASN
10	M3	30	ASN
10	M3	121	ASN
11	N3	35	ASN
11	N3	42	ASN
11	N3	47	ASN
10	O3	30	ASN
10	O3	94	ASN
10	O3	121	ASN
10	O3	161	ASN
10	Q3	28	GLN
10	Q3	30	ASN
10	Q3	80	ASN
10	Q3	121	ASN
11	R3	35	ASN
10	S3	30	ASN
10	S3	32	GLN
10	S3	121	ASN
11	T3	35	ASN
10	U3	121	ASN
11	V3	35	ASN
10	W3	30	ASN
10	W3	94	ASN
10	W3	121	ASN
10	W3	161	ASN
11	X3	35	ASN
10	Y3	30	ASN
10	Y3	80	ASN
10	Y3	94	ASN
10	Y3	121	ASN
11	Z3	35	ASN
11	Z3	47	ASN
12	a3	150	ASN
12	a3	238	ASN

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Mol	Chain	Res	Type
12	a3	252	HIS
12	a3	300	HIS
12	a3	304	GLN
13	b3	58	GLN
13	b3	79	ASN
13	b3	99	ASN
13	b3	121	ASN
13	b3	154	ASN
13	b3	177	HIS
13	b3	202	ASN
13	b3	389	ASN
14	c3	90	ASN
14	c3	98	GLN
14	c3	150	HIS
14	c3	213	ASN
14	d3	90	ASN
14	d3	98	GLN
14	d3	146	HIS
14	d3	213	ASN
14	d3	262	ASN
10	e3	30	ASN
10	e3	121	ASN
10	e3	161	ASN
11	f3	35	ASN
10	g3	30	ASN
10	g3	121	ASN
11	h3	35	ASN
10	i3	30	ASN
10	i3	76	GLN
10	i3	121	ASN
10	i3	147	GLN
10	i3	161	ASN
11	j3	47	ASN
11	j3	111	ASN
10	k3	30	ASN
10	k3	32	GLN
10	k3	121	ASN
10	k3	161	ASN
11	l3	35	ASN
11	l3	47	ASN
10	m3	30	ASN
10	m3	48	HIS

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Mol	Chain	Res	Type
10	m3	94	ASN
10	m3	121	ASN
10	m3	161	ASN
11	n3	35	ASN
10	o3	30	ASN
10	o3	121	ASN
10	o3	161	ASN
11	p3	35	ASN
11	p3	42	ASN
11	p3	47	ASN
10	q3	30	ASN
10	q3	121	ASN
10	q3	161	ASN
11	r3	35	ASN
11	r3	47	ASN
11	r3	72	ASN
10	s3	30	ASN
10	s3	121	ASN
11	t3	35	ASN
11	t3	47	ASN
10	u3	30	ASN
10	u3	121	ASN
10	u3	161	ASN
11	v3	35	ASN
11	v3	47	ASN
11	v3	159	GLN
10	w3	30	ASN
10	w3	121	ASN
10	w3	161	ASN
11	x3	35	ASN
11	x3	47	ASN
10	y3	30	ASN
10	y3	32	GLN
10	y3	121	ASN
10	y3	161	ASN
11	z3	35	ASN
10	A4	30	ASN
10	A4	94	ASN
10	A4	121	ASN
10	A4	161	ASN
11	B4	35	ASN
11	B4	47	ASN

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Mol	Chain	Res	Type
10	C4	30	ASN
10	C4	76	GLN
10	C4	121	ASN
10	C4	161	ASN
11	D4	35	ASN
10	E4	28	GLN
10	E4	30	ASN
10	E4	121	ASN
11	F4	35	ASN
11	F4	72	ASN
10	G4	30	ASN
10	G4	48	HIS
10	G4	94	ASN
10	G4	121	ASN
11	H4	35	ASN
11	H4	72	ASN
10	I4	28	GLN
10	I4	30	ASN
10	I4	161	ASN
11	J4	35	ASN
11	J4	72	ASN
10	K4	30	ASN
10	K4	147	GLN
11	L4	72	ASN
10	M4	28	GLN
10	M4	30	ASN
10	M4	121	ASN
10	M4	147	GLN
11	N4	35	ASN
11	N4	72	ASN
10	O4	28	GLN
10	O4	30	ASN
10	O4	121	ASN
11	P4	35	ASN
11	P4	42	ASN
11	P4	72	ASN
10	Q4	30	ASN
10	Q4	121	ASN
11	R4	35	ASN
11	R4	72	ASN
10	S4	28	GLN
10	S4	30	ASN

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Mol	Chain	Res	Type
10	S4	121	ASN
10	S4	161	ASN
11	T4	35	ASN
11	T4	72	ASN
10	U4	28	GLN
10	U4	30	ASN
10	U4	121	ASN
11	V4	35	ASN
11	V4	72	ASN
10	W4	28	GLN
10	W4	30	ASN
10	W4	121	ASN
11	X4	35	ASN
11	X4	72	ASN
10	Y4	30	ASN
10	Y4	121	ASN
11	Z4	72	ASN
15	14	7	ASN
15	14	28	GLN
15	14	58	HIS
15	14	59	GLN
15	14	66	GLN
15	14	178	ASN
15	14	204	HIS
16	24	160	HIS
16	24	206	ASN
16	24	236	GLN
16	24	241	GLN
16	24	285	HIS
16	24	289	GLN
16	24	341	ASN
12	34	51	GLN
12	34	139	GLN
12	34	150	ASN
12	34	238	ASN
12	34	296	HIS
12	34	300	HIS
14	44	65	ASN
14	44	98	GLN
14	44	117	ASN
14	44	137	ASN
14	44	149	HIS

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Mol	Chain	Res	Type
14	44	230	ASN
14	44	259	HIS
14	44	262	ASN
17	a4	135	ASN
17	b4	135	ASN
18	c4	21	ASN
17	d4	32	GLN
17	d4	135	ASN
18	e4	21	ASN
18	e4	45	ASN
17	f4	135	ASN
18	g4	25	ASN
18	g4	63	GLN
18	g4	68	GLN
18	h4	21	ASN
18	h4	65	GLN
18	h4	72	ASN
17	i4	32	GLN
17	i4	135	ASN
18	j4	21	ASN
18	j4	65	GLN
17	k4	135	ASN
18	l4	35	ASN
18	l4	72	ASN
18	l4	118	GLN
10	m4	30	ASN
10	m4	121	ASN
11	n4	35	ASN
11	n4	72	ASN
10	o4	30	ASN
10	o4	147	GLN
11	p4	72	ASN
11	p4	162	GLN
10	q4	28	GLN
10	q4	30	ASN
10	q4	48	HIS
11	r4	35	ASN
11	r4	72	ASN
10	s4	30	ASN
10	s4	94	ASN
10	s4	121	ASN
11	t4	35	ASN

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Mol	Chain	Res	Type
11	t4	72	ASN
11	t4	76	ASN
10	u4	28	GLN
10	u4	30	ASN
10	u4	94	ASN
10	u4	121	ASN
11	v4	35	ASN
11	v4	72	ASN
10	w4	30	ASN
10	w4	48	HIS
10	w4	121	ASN
10	w4	161	ASN
11	x4	35	ASN
11	x4	72	ASN
10	y4	30	ASN
10	y4	32	GLN
10	y4	121	ASN
11	z4	25	GLN
11	z4	72	ASN
11	z4	162	GLN
10	A5	28	GLN
10	A5	30	ASN
10	A5	48	HIS
10	A5	121	ASN
10	A5	147	GLN
11	B5	35	ASN
11	B5	72	ASN
10	C5	30	ASN
10	C5	48	HIS
10	C5	94	ASN
10	C5	121	ASN
11	D5	35	ASN
11	D5	72	ASN
10	E5	28	GLN
10	E5	30	ASN
10	E5	48	HIS
10	E5	161	ASN
11	F5	35	ASN
11	F5	72	ASN
10	G5	30	ASN
10	G5	147	GLN
11	H5	35	ASN

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Mol	Chain	Res	Type
11	H5	72	ASN
10	I5	28	GLN
10	I5	30	ASN
10	I5	48	HIS
10	I5	121	ASN
10	I5	147	GLN
11	J5	35	ASN
11	J5	72	ASN
10	K5	28	GLN
10	K5	30	ASN
10	K5	121	ASN
11	L5	35	ASN
11	L5	42	ASN
11	L5	72	ASN
10	M5	30	ASN
10	M5	121	ASN
11	N5	35	ASN
11	N5	72	ASN
10	O5	28	GLN
10	O5	30	ASN
10	O5	121	ASN
10	O5	161	ASN
11	P5	35	ASN
11	P5	72	ASN
10	Q5	28	GLN
10	Q5	30	ASN
10	Q5	121	ASN
11	R5	35	ASN
11	R5	72	ASN
10	S5	28	GLN
10	S5	30	ASN
10	S5	121	ASN
11	T5	35	ASN
11	T5	72	ASN
10	U5	28	GLN
10	U5	30	ASN
10	U5	121	ASN
11	V5	35	ASN
11	V5	72	ASN
15	W5	25	ASN
15	W5	58	HIS
15	W5	59	GLN

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Mol	Chain	Res	Type
15	W5	77	GLN
15	W5	178	ASN
16	X5	47	ASN
16	X5	65	ASN
16	X5	160	HIS
16	X5	206	ASN
16	X5	229	ASN
16	X5	241	GLN
16	X5	285	HIS
16	X5	289	GLN
16	X5	328	ASN
16	X5	341	ASN
16	X5	359	HIS
12	Y5	51	GLN
12	Y5	139	GLN
12	Y5	150	ASN
12	Y5	192	ASN
12	Y5	238	ASN
12	Y5	299	ASN
14	Z5	65	ASN
14	Z5	90	ASN
14	Z5	98	GLN
14	Z5	117	ASN
14	Z5	137	ASN
14	Z5	146	HIS
14	Z5	149	HIS
14	Z5	230	ASN
14	Z5	259	HIS
14	Z5	262	ASN
17	a5	25	GLN
17	a5	135	ASN
17	b5	15	GLN
17	b5	135	ASN
17	d5	32	GLN
17	d5	135	ASN
18	e5	21	ASN
18	e5	45	ASN
17	f5	32	GLN
17	f5	135	ASN
18	g5	21	ASN
18	g5	25	ASN
18	g5	63	GLN

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Mol	Chain	Res	Type
18	h5	21	ASN
18	h5	65	GLN
18	h5	111	ASN
17	i5	32	GLN
17	i5	135	ASN
18	j5	65	GLN
17	k5	135	ASN
18	l5	21	ASN
18	l5	25	ASN
18	l5	118	GLN
10	m5	30	ASN
10	m5	121	ASN
11	n5	72	ASN
10	o5	30	ASN
10	o5	147	GLN
11	p5	72	ASN
11	p5	162	GLN
10	q5	28	GLN
10	q5	30	ASN
10	q5	48	HIS
11	r5	35	ASN
11	r5	72	ASN
11	r5	162	GLN
10	s5	30	ASN
10	s5	94	ASN
10	s5	121	ASN
11	t5	35	ASN
11	t5	72	ASN
11	t5	76	ASN
10	u5	28	GLN
10	u5	30	ASN
10	u5	48	HIS
10	u5	94	ASN
10	u5	121	ASN
11	v5	35	ASN
11	v5	72	ASN
10	w5	28	GLN
10	w5	30	ASN
10	w5	48	HIS
10	w5	121	ASN
10	w5	147	GLN
10	w5	161	ASN

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Mol	Chain	Res	Type
11	x5	35	ASN
11	x5	72	ASN
10	y5	28	GLN
10	y5	30	ASN
10	y5	32	GLN
10	y5	48	HIS
10	y5	121	ASN
11	z5	35	ASN
11	z5	72	ASN
11	z5	162	GLN
11	f8	35	ASN
11	f8	47	ASN
11	f8	162	GLN
11	g8	35	ASN
11	g8	47	ASN
11	h8	42	ASN
11	h8	47	ASN
11	h8	162	GLN
10	i8	28	GLN
10	i8	30	ASN
10	i8	121	ASN
10	j8	121	ASN
10	j8	147	GLN
10	j8	161	ASN
10	k8	30	ASN
10	k8	121	ASN
10	k8	147	GLN
10	l8	30	ASN
10	l8	121	ASN
10	l8	161	ASN
10	m8	30	ASN
10	m8	121	ASN
10	m8	147	GLN
10	A6	28	GLN
10	A6	30	ASN
10	A6	121	ASN
11	B6	35	ASN
11	B6	47	ASN
11	B6	162	GLN
10	C6	28	GLN
10	C6	30	ASN
10	C6	121	ASN

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Mol	Chain	Res	Type
10	C6	161	ASN
11	D6	35	ASN
11	D6	47	ASN
11	D6	111	ASN
10	E6	30	ASN
10	E6	121	ASN
10	E6	147	GLN
11	F6	47	ASN
11	F6	72	ASN
11	F6	111	ASN
10	G6	30	ASN
10	G6	76	GLN
10	G6	88	HIS
10	G6	121	ASN
11	H6	35	ASN
11	H6	47	ASN
11	H6	111	ASN
10	I6	30	ASN
10	I6	121	ASN
10	I6	161	ASN
11	J6	35	ASN
11	J6	47	ASN
11	J6	162	GLN
10	K6	28	GLN
10	K6	30	ASN
10	K6	121	ASN
10	K6	147	GLN
11	L6	35	ASN
11	L6	47	ASN
11	L6	76	ASN
11	L6	111	ASN
10	M6	28	GLN
10	M6	30	ASN
10	M6	94	ASN
10	M6	121	ASN
10	M6	161	ASN
11	N6	35	ASN
11	N6	47	ASN
11	N6	162	GLN
10	O6	28	GLN
10	O6	30	ASN
10	O6	121	ASN

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Mol	Chain	Res	Type
11	P6	35	ASN
11	P6	47	ASN
11	P6	111	ASN
10	Q6	30	ASN
10	Q6	121	ASN
10	Q6	147	GLN
11	R6	47	ASN
10	S6	30	ASN
10	S6	32	GLN
10	S6	48	HIS
10	S6	121	ASN
10	S6	147	GLN
10	S6	161	ASN
11	T6	25	GLN
11	T6	47	ASN
11	T6	162	GLN
10	U6	30	ASN
10	U6	121	ASN
10	U6	147	GLN
10	U6	161	ASN
11	V6	35	ASN
11	V6	47	ASN
11	V6	111	ASN
10	W6	30	ASN
10	W6	121	ASN
10	W6	147	GLN
10	W6	161	ASN
11	X6	42	ASN
11	X6	47	ASN
11	X6	111	ASN
11	X6	162	GLN
10	Y6	28	GLN
10	Y6	30	ASN
10	Y6	121	ASN
10	Y6	161	ASN
11	Z6	35	ASN
11	Z6	47	ASN
11	Z6	63	ASN
11	Z6	111	ASN
11	a6	35	ASN
11	a6	47	ASN
11	a6	111	ASN

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Mol	Chain	Res	Type
11	a6	162	GLN
11	b6	47	ASN
11	b6	111	ASN
11	c6	35	ASN
11	c6	47	ASN
11	d6	35	ASN
11	d6	42	ASN
11	d6	47	ASN
11	d6	111	ASN
11	d6	162	GLN
11	e6	35	ASN
11	e6	47	ASN
10	f6	30	ASN
10	f6	48	HIS
10	f6	121	ASN
10	g6	28	GLN
10	g6	30	ASN
10	g6	121	ASN
10	g6	147	GLN
10	h6	28	GLN
10	h6	30	ASN
10	h6	121	ASN
10	h6	161	ASN
10	i6	30	ASN
10	i6	48	HIS
10	i6	88	HIS
10	i6	121	ASN
10	i6	147	GLN
10	i6	161	ASN
10	j6	30	ASN
10	j6	121	ASN
10	j6	161	ASN
10	k6	30	ASN
10	k6	48	HIS
10	k6	121	ASN
10	k6	161	ASN
11	l6	35	ASN
11	l6	76	ASN
11	l6	111	ASN
10	m6	28	GLN
10	m6	147	GLN
10	m6	161	ASN

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Mol	Chain	Res	Type
11	n6	35	ASN
11	n6	42	ASN
11	n6	47	ASN
10	o6	30	ASN
10	o6	32	GLN
10	o6	161	ASN
11	p6	35	ASN
11	p6	47	ASN
11	p6	111	ASN
10	q6	30	ASN
10	q6	88	HIS
10	q6	121	ASN
10	q6	147	GLN
10	q6	161	ASN
11	r6	35	ASN
11	r6	47	ASN
11	r6	72	ASN
11	r6	111	ASN
10	s6	30	ASN
10	s6	48	HIS
10	s6	121	ASN
10	s6	161	ASN
11	t6	35	ASN
11	t6	47	ASN
10	u6	30	ASN
10	u6	88	HIS
10	u6	121	ASN
10	u6	147	GLN
10	u6	161	ASN
11	v6	47	ASN
11	v6	111	ASN
10	w6	28	GLN
10	w6	30	ASN
10	w6	94	ASN
10	w6	121	ASN
10	w6	147	GLN
10	w6	161	ASN
11	x6	35	ASN
11	x6	47	ASN
11	x6	111	ASN
11	x6	162	GLN
11	y6	35	ASN

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Mol	Chain	Res	Type
11	y6	47	ASN
11	y6	111	ASN
11	y6	162	GLN
11	z6	47	ASN
11	z6	111	ASN
11	z6	162	GLN
11	n8	35	ASN
11	n8	47	ASN
11	o8	35	ASN
11	o8	42	ASN
11	o8	47	ASN
11	o8	162	GLN
11	p8	35	ASN
11	p8	47	ASN
11	p8	111	ASN
11	p8	162	GLN
10	q8	28	GLN
10	q8	30	ASN
10	q8	121	ASN
10	r8	30	ASN
10	r8	121	ASN
10	r8	147	GLN
10	r8	161	ASN
10	s8	28	GLN
10	s8	30	ASN
10	s8	121	ASN
10	t8	30	ASN
10	t8	88	HIS
10	t8	94	ASN
10	t8	121	ASN
10	t8	161	ASN
10	u8	30	ASN
10	u8	121	ASN
10	u8	161	ASN
10	A7	28	GLN
10	A7	30	ASN
10	A7	121	ASN
11	B7	35	ASN
11	B7	76	ASN
11	B7	159	GLN
10	C7	28	GLN
10	C7	30	ASN

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Mol	Chain	Res	Type
10	C7	121	ASN
10	C7	147	GLN
11	D7	35	ASN
11	D7	47	ASN
11	D7	111	ASN
11	D7	162	GLN
10	E7	28	GLN
10	E7	30	ASN
10	E7	121	ASN
10	E7	161	ASN
11	F7	35	ASN
11	F7	47	ASN
11	F7	111	ASN
10	G7	28	GLN
10	G7	30	ASN
10	G7	121	ASN
10	G7	161	ASN
11	H7	35	ASN
11	H7	47	ASN
11	H7	162	GLN
10	I7	30	ASN
10	I7	121	ASN
10	I7	147	GLN
11	J7	47	ASN
11	J7	76	ASN
11	J7	111	ASN
10	K7	28	GLN
10	K7	30	ASN
10	K7	121	ASN
10	K7	147	GLN
11	L7	35	ASN
11	L7	47	ASN
11	L7	111	ASN
10	M7	30	ASN
10	M7	121	ASN
10	M7	147	GLN
11	N7	35	ASN
11	N7	47	ASN
11	N7	111	ASN
10	O7	30	ASN
10	O7	121	ASN
10	O7	147	GLN

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Mol	Chain	Res	Type
10	O7	161	ASN
11	P7	35	ASN
11	P7	47	ASN
11	P7	162	GLN
10	Q7	30	ASN
10	Q7	121	ASN
11	R7	47	ASN
11	R7	111	ASN
10	S7	30	ASN
10	S7	121	ASN
10	S7	147	GLN
10	S7	161	ASN
11	T7	35	ASN
11	T7	47	ASN
11	T7	111	ASN
10	U7	30	ASN
10	U7	121	ASN
10	U7	161	ASN
11	V7	42	ASN
11	V7	47	ASN
11	V7	111	ASN
11	V7	162	GLN
10	W7	30	ASN
10	W7	48	HIS
10	W7	121	ASN
10	W7	147	GLN
11	X7	25	GLN
11	X7	47	ASN
11	X7	76	ASN
11	X7	162	GLN
10	Y7	30	ASN
10	Y7	48	HIS
10	Y7	121	ASN
11	Z7	35	ASN
11	Z7	47	ASN
11	Z7	111	ASN
11	a7	35	ASN
11	a7	47	ASN
11	a7	162	GLN
11	b7	42	ASN
11	b7	47	ASN
11	b7	111	ASN

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Mol	Chain	Res	Type
11	b7	162	GLN
11	c7	35	ASN
11	c7	47	ASN
11	c7	111	ASN
11	c7	162	GLN
11	d7	35	ASN
11	d7	47	ASN
11	e7	35	ASN
11	e7	47	ASN
11	e7	111	ASN
11	e7	162	GLN
10	f7	28	GLN
10	f7	30	ASN
10	f7	121	ASN
10	f7	161	ASN
10	g7	30	ASN
10	g7	121	ASN
10	g7	161	ASN
10	h7	28	GLN
10	h7	30	ASN
10	h7	48	HIS
10	h7	147	GLN
10	h7	161	ASN
10	i7	28	GLN
10	i7	30	ASN
10	i7	121	ASN
10	i7	161	ASN
10	j7	30	ASN
10	j7	32	GLN
10	j7	121	ASN
10	j7	147	GLN
10	j7	161	ASN
10	k7	30	ASN
10	k7	32	GLN
10	k7	94	ASN
10	k7	161	ASN
11	l7	35	ASN
11	l7	47	ASN
11	l7	76	ASN
10	m7	48	HIS
10	m7	121	ASN
10	m7	161	ASN

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Mol	Chain	Res	Type
11	n7	35	ASN
11	n7	47	ASN
11	n7	111	ASN
10	o7	28	GLN
10	o7	30	ASN
10	o7	48	HIS
10	o7	147	GLN
11	p7	35	ASN
11	p7	47	ASN
11	p7	111	ASN
10	q7	30	ASN
10	q7	48	HIS
10	q7	121	ASN
10	q7	147	GLN
10	q7	161	ASN
11	r7	35	ASN
11	r7	47	ASN
11	r7	111	ASN
11	r7	162	GLN
10	s7	28	GLN
10	s7	30	ASN
10	s7	121	ASN
11	t7	35	ASN
11	t7	47	ASN
11	t7	76	ASN
10	u7	28	GLN
10	u7	30	ASN
10	u7	121	ASN
10	u7	147	GLN
10	u7	161	ASN
11	v7	35	ASN
11	v7	47	ASN
11	v7	111	ASN
10	w7	30	ASN
10	w7	121	ASN
10	w7	161	ASN
11	x7	35	ASN
11	x7	47	ASN
11	x7	111	ASN
11	x7	162	GLN
11	y7	47	ASN
11	y7	111	ASN

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Mol	Chain	Res	Type
11	z7	47	ASN
11	z7	111	ASN
19	a8	84	ASN
19	a8	141	GLN
19	a8	148	ASN
19	a8	160	GLN
19	a8	210	ASN
19	a8	213	ASN
12	b8	150	ASN
12	b8	157	GLN
12	b8	238	ASN
12	b8	292	GLN
12	b8	299	ASN
12	b8	300	HIS
14	c8	98	GLN
14	c8	146	HIS
14	c8	149	HIS
14	c8	197	GLN
14	d8	149	HIS
14	d8	197	GLN
14	e8	117	ASN
14	e8	237	GLN
14	e8	262	ASN
19	a9	84	ASN
19	a9	141	GLN
19	a9	148	ASN
19	a9	159	ASN
19	a9	160	GLN
19	a9	210	ASN
19	a9	213	ASN
19	a9	333	ASN
12	b9	150	ASN
12	b9	157	GLN
12	b9	238	ASN
12	b9	292	GLN
12	b9	299	ASN
12	b9	300	HIS
14	c9	146	HIS
14	c9	149	HIS
14	c9	262	ASN
14	d9	98	GLN
14	d9	149	HIS

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Mol	Chain	Res	Type
14	d9	197	GLN
14	d9	262	ASN
14	e9	117	ASN
14	e9	237	GLN
14	e9	262	ASN
10	v8	30	ASN
10	v8	121	ASN
10	v8	147	GLN
11	w8	47	ASN
11	w8	111	ASN
10	x8	30	ASN
10	x8	121	ASN
11	y8	47	ASN
11	y8	63	ASN
11	y8	111	ASN
11	y8	159	GLN
10	z8	30	ASN
10	z8	94	ASN
10	z8	121	ASN
10	z8	161	ASN
11	A8	35	ASN
11	A8	47	ASN
11	A8	111	ASN
10	B8	30	ASN
10	B8	121	ASN
11	C8	47	ASN
11	C8	111	ASN
10	D8	30	ASN
10	D8	121	ASN
10	D8	161	ASN
11	E8	35	ASN
11	E8	47	ASN
11	E8	111	ASN
10	F8	28	GLN
10	F8	30	ASN
10	F8	32	GLN
10	F8	121	ASN
11	G8	35	ASN
11	G8	111	ASN
10	H8	30	ASN
10	H8	32	GLN
10	H8	121	ASN

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Mol	Chain	Res	Type
10	H8	161	ASN
11	I8	47	ASN
11	I8	111	ASN
10	J8	30	ASN
10	J8	121	ASN
11	K8	35	ASN
11	K8	111	ASN
10	L8	30	ASN
10	L8	94	ASN
10	L8	121	ASN
11	M8	35	ASN
11	M8	111	ASN
10	N8	30	ASN
10	N8	32	GLN
10	N8	94	ASN
10	N8	121	ASN
11	O8	47	ASN
11	O8	111	ASN
10	P8	30	ASN
10	P8	32	GLN
10	P8	121	ASN
10	P8	161	ASN
11	Q8	111	ASN
15	R8	28	GLN
15	R8	59	GLN
15	R8	76	ASN
15	R8	101	ASN
15	R8	135	GLN
15	R8	153	ASN
15	R8	209	GLN
16	S8	236	GLN
16	S8	241	GLN
16	S8	289	GLN
16	S8	317	GLN
16	S8	359	HIS
14	T8	98	GLN
14	T8	146	HIS
14	T8	149	HIS
14	T8	150	HIS
14	T8	230	ASN
14	T8	262	ASN
12	U8	51	GLN

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Mol	Chain	Res	Type
12	U8	89	HIS
12	U8	139	GLN
12	U8	238	ASN
12	U8	299	ASN
17	V8	21	ASN
17	V8	135	ASN
18	W8	45	ASN
18	W8	63	GLN
18	W8	111	ASN
18	W8	132	GLN
18	W8	143	ASN
18	W8	157	ASN
17	X8	21	ASN
17	X8	135	ASN
18	Y8	63	GLN
18	Y8	68	GLN
18	Y8	111	ASN
18	Y8	132	GLN
18	Y8	143	ASN
18	Y8	157	ASN
17	Z8	15	GLN
17	Z8	135	ASN
18	f9	63	GLN
18	f9	65	GLN
18	f9	72	ASN
18	f9	111	ASN
18	f9	118	GLN
18	f9	132	GLN
18	f9	143	ASN
18	f9	157	ASN
17	g9	21	ASN
17	g9	135	ASN
18	h9	35	ASN
18	h9	111	ASN
18	h9	132	GLN
18	h9	143	ASN
18	h9	157	ASN
17	i9	15	GLN
17	i9	21	ASN
17	i9	135	ASN
18	j9	21	ASN
18	j9	35	ASN

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Mol	Chain	Res	Type
18	j9	63	GLN
18	j9	111	ASN
18	j9	132	GLN
18	j9	143	ASN
18	j9	157	ASN
17	k9	21	ASN
17	k9	25	GLN
18	l9	63	GLN
18	l9	111	ASN
18	l9	132	GLN
18	l9	143	ASN
18	l9	157	ASN
10	m9	30	ASN
10	m9	121	ASN
10	m9	161	ASN
11	n9	35	ASN
11	n9	111	ASN
10	o9	30	ASN
10	o9	48	HIS
10	o9	121	ASN
10	o9	161	ASN
11	p9	47	ASN
11	p9	111	ASN
10	q9	30	ASN
10	q9	76	GLN
10	q9	121	ASN
10	q9	161	ASN
11	r9	47	ASN
11	r9	111	ASN
10	s9	30	ASN
10	s9	121	ASN
11	t9	35	ASN
11	t9	47	ASN
11	t9	111	ASN
10	u9	30	ASN
10	u9	48	HIS
10	u9	121	ASN
11	v9	35	ASN
11	v9	47	ASN
11	v9	111	ASN
10	w9	30	ASN
10	w9	121	ASN

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Mol	Chain	Res	Type
11	x9	35	ASN
11	x9	47	ASN
11	x9	76	ASN
11	x9	111	ASN
10	y9	30	ASN
10	y9	121	ASN
11	z9	47	ASN
11	z9	159	GLN
10	A9	30	ASN
10	A9	121	ASN
10	A9	147	GLN
11	B9	35	ASN
11	B9	47	ASN
11	B9	111	ASN
10	C9	30	ASN
10	C9	121	ASN
11	D9	35	ASN
11	D9	47	ASN
11	D9	111	ASN
10	E9	30	ASN
10	E9	94	ASN
10	E9	121	ASN
11	F9	35	ASN
11	F9	47	ASN
11	F9	111	ASN
10	G9	30	ASN
10	G9	121	ASN
11	H9	35	ASN
11	H9	47	ASN
11	H9	111	ASN
10	I9	30	ASN
10	I9	121	ASN
11	J9	35	ASN
11	J9	47	ASN
11	J9	111	ASN
10	K9	28	GLN
10	K9	30	ASN
10	K9	32	GLN
10	K9	121	ASN
11	L9	35	ASN
11	L9	111	ASN
10	M9	28	GLN

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Mol	Chain	Res	Type
10	M9	30	ASN
10	M9	121	ASN
10	M9	161	ASN
11	N9	35	ASN
11	N9	47	ASN
11	N9	111	ASN
10	O9	30	ASN
10	O9	121	ASN
10	O9	161	ASN
11	P9	35	ASN
11	P9	111	ASN
10	Q9	30	ASN
10	Q9	94	ASN
10	Q9	121	ASN
11	R9	111	ASN
10	S9	30	ASN
10	S9	94	ASN
10	S9	121	ASN
11	T9	47	ASN
11	T9	111	ASN
10	U9	28	GLN
10	U9	30	ASN
10	U9	32	GLN
10	U9	121	ASN
10	U9	161	ASN
11	V9	35	ASN
11	V9	42	ASN
11	V9	111	ASN
15	W9	76	ASN
16	X9	236	GLN
16	X9	241	GLN
16	X9	289	GLN
16	X9	317	GLN
16	X9	359	HIS
14	Y9	98	GLN
14	Y9	146	HIS
14	Y9	149	HIS
14	Y9	150	HIS
14	Y9	230	ASN
14	Y9	262	ASN
12	Z9	139	GLN
12	Z9	238	ASN

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Mol	Chain	Res	Type
12	Z9	299	ASN
17	aa	21	ASN
17	aa	135	ASN
18	ab	45	ASN
18	ab	63	GLN
18	ab	111	ASN
18	ab	132	GLN
18	ab	143	ASN
18	ab	157	ASN
17	ac	21	ASN
17	ac	135	ASN
18	ad	63	GLN
18	ad	68	GLN
18	ad	111	ASN
18	ad	132	GLN
18	ad	143	ASN
18	ad	157	ASN
17	ae	135	ASN
18	af	63	GLN
18	af	65	GLN
18	af	111	ASN
18	af	132	GLN
18	af	143	ASN
18	af	157	ASN
17	ag	21	ASN
17	ag	135	ASN
18	ah	132	GLN
18	ah	143	ASN
18	ah	157	ASN
17	ai	15	GLN
17	ai	21	ASN
17	ai	135	ASN
18	aj	63	GLN
18	aj	111	ASN
18	aj	132	GLN
18	aj	143	ASN
18	aj	157	ASN
17	ak	21	ASN
18	al	63	GLN
18	al	111	ASN
18	al	132	GLN
18	al	143	ASN

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Mol	Chain	Res	Type
18	al	157	ASN
10	am	30	ASN
10	am	121	ASN
11	an	35	ASN
11	an	111	ASN
10	ao	30	ASN
10	ao	121	ASN
11	ap	47	ASN
11	ap	111	ASN
11	ap	159	GLN
10	aq	30	ASN
10	aq	121	ASN
10	aq	161	ASN
11	ar	35	ASN
11	ar	47	ASN
11	ar	111	ASN
10	as	30	ASN
10	as	94	ASN
10	as	121	ASN
10	as	161	ASN
11	at	35	ASN
11	at	47	ASN
11	at	111	ASN
10	au	30	ASN
10	au	121	ASN
11	av	11	ASN
11	av	47	ASN
11	av	111	ASN
10	aw	30	ASN
10	aw	121	ASN
11	ax	35	ASN
11	ax	47	ASN
11	ax	111	ASN
10	ay	30	ASN
10	ay	121	ASN
11	az	47	ASN
11	az	111	ASN
10	aA	30	ASN
10	aA	121	ASN
11	aB	35	ASN
11	aB	47	ASN
11	aB	72	ASN

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Mol	Chain	Res	Type
11	aB	111	ASN
10	aC	28	GLN
10	aC	30	ASN
10	aC	47	ASN
10	aC	121	ASN
11	aD	35	ASN
11	aD	47	ASN
11	aD	72	ASN
11	aD	111	ASN
10	aE	28	GLN
10	aE	30	ASN
10	aE	94	ASN
10	aE	121	ASN
11	aF	35	ASN
11	aF	47	ASN
11	aF	72	ASN
11	aF	111	ASN
10	aG	28	GLN
10	aG	30	ASN
10	aG	94	ASN
11	aH	35	ASN
11	aH	47	ASN
11	aH	72	ASN
11	aH	111	ASN
10	aI	28	GLN
10	aI	30	ASN
10	aI	121	ASN
11	aJ	35	ASN
11	aJ	47	ASN
11	aJ	72	ASN
11	aJ	111	ASN
10	aK	30	ASN
10	aK	121	ASN
11	aL	47	ASN
11	aL	72	ASN
11	aL	111	ASN
10	aM	30	ASN
10	aM	147	GLN
10	aM	161	ASN
11	aN	47	ASN
11	aN	72	ASN
11	aN	111	ASN

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Mol	Chain	Res	Type
10	aO	28	GLN
10	aO	30	ASN
10	aO	121	ASN
11	aP	35	ASN
11	aP	47	ASN
11	aP	72	ASN
11	aP	111	ASN
10	aQ	30	ASN
10	aQ	121	ASN
11	aR	47	ASN
11	aR	72	ASN
11	aR	111	ASN
10	aS	30	ASN
10	aS	121	ASN
11	aT	47	ASN
11	aT	72	ASN
11	aT	111	ASN
10	aU	30	ASN
10	aU	121	ASN
10	aU	161	ASN
11	aV	47	ASN
11	aV	72	ASN
11	aV	111	ASN
15	aW	59	GLN
15	aW	66	GLN
15	aW	77	GLN
15	aW	97	ASN
15	aW	103	ASN
15	aW	121	ASN
15	aW	122	HIS
15	aW	153	ASN
15	aW	209	GLN
16	aX	160	HIS
16	aX	241	GLN
16	aX	285	HIS
16	aX	317	GLN
16	aX	341	ASN
12	aY	150	ASN
12	aY	238	ASN
12	aY	252	HIS
14	aZ	65	ASN
14	aZ	98	GLN

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Mol	Chain	Res	Type
14	aZ	149	HIS
14	aZ	150	HIS
14	aZ	213	ASN
14	aZ	259	HIS
14	aZ	269	ASN
17	ba	68	GLN
17	ba	148	ASN
18	bb	72	ASN
18	bb	132	GLN
17	bc	25	GLN
17	bc	119	ASN
17	bc	135	ASN
18	bd	68	GLN
18	bd	72	ASN
18	bd	132	GLN
17	be	21	ASN
17	be	57	GLN
17	be	119	ASN
17	be	135	ASN
17	be	159	ASN
18	bf	23	GLN
18	bf	45	ASN
18	bf	72	ASN
18	bf	132	GLN
17	bg	21	ASN
17	bg	25	GLN
17	bg	135	ASN
17	bg	159	ASN
18	bh	42	ASN
18	bh	132	GLN
17	bi	21	ASN
17	bi	32	GLN
17	bi	57	GLN
17	bi	135	ASN
18	bj	54	ASN
18	bj	72	ASN
18	bj	111	ASN
18	bj	132	GLN
17	bk	15	GLN
17	bk	21	ASN
17	bk	68	GLN
18	bl	42	ASN

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Mol	Chain	Res	Type
18	bl	132	GLN
10	bm	30	ASN
10	bm	76	GLN
10	bm	147	GLN
10	bm	161	ASN
11	bn	35	ASN
11	bn	47	ASN
11	bn	72	ASN
11	bo	35	ASN
11	bo	47	ASN
11	bo	63	ASN
11	bo	72	ASN
11	bo	111	ASN
11	bp	47	ASN
11	bp	72	ASN
11	bp	111	ASN
11	bq	35	ASN
11	bq	47	ASN
11	bq	72	ASN
11	bq	111	ASN
11	br	35	ASN
11	br	47	ASN
11	br	72	ASN
11	bs	35	ASN
11	bs	47	ASN
11	bs	72	ASN
11	bs	111	ASN
10	bt	28	GLN
10	bt	30	ASN
10	bt	94	ASN
10	bt	121	ASN
10	bu	28	GLN
10	bu	30	ASN
10	bu	48	HIS
10	bu	76	GLN
10	bu	121	ASN
10	bv	30	ASN
10	bv	121	ASN
10	bv	161	ASN
10	bw	30	ASN
10	bw	76	GLN
10	bw	94	ASN

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Mol	Chain	Res	Type
10	bw	121	ASN
10	bw	161	ASN
10	bx	30	ASN
10	bx	121	ASN
10	by	30	ASN
10	by	32	GLN
10	by	121	ASN
11	bz	47	ASN
11	bz	72	ASN
11	bz	111	ASN
10	bA	30	ASN
10	bA	121	ASN
11	bB	35	ASN
11	bB	47	ASN
11	bB	72	ASN
11	bB	111	ASN
10	bC	28	GLN
10	bC	30	ASN
10	bC	121	ASN
11	bD	35	ASN
11	bD	47	ASN
11	bD	72	ASN
11	bD	111	ASN
10	bE	28	GLN
10	bE	30	ASN
10	bE	94	ASN
10	bE	121	ASN
11	bF	35	ASN
11	bF	47	ASN
11	bF	72	ASN
11	bF	111	ASN
10	bG	28	GLN
10	bG	30	ASN
10	bG	121	ASN
11	bH	35	ASN
11	bH	47	ASN
11	bH	72	ASN
11	bH	111	ASN
10	bI	28	GLN
10	bI	30	ASN
10	bI	121	ASN
11	bJ	35	ASN

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Mol	Chain	Res	Type
11	bJ	47	ASN
11	bJ	72	ASN
11	bJ	111	ASN
10	bK	30	ASN
11	bL	47	ASN
11	bL	72	ASN
11	bL	111	ASN
10	bM	30	ASN
10	bM	121	ASN
10	bM	147	GLN
11	bN	47	ASN
11	bN	72	ASN
11	bN	111	ASN
10	bO	28	GLN
10	bO	30	ASN
10	bO	121	ASN
11	bP	35	ASN
11	bP	47	ASN
11	bP	72	ASN
11	bP	111	ASN
10	bQ	30	ASN
10	bQ	121	ASN
11	bR	35	ASN
11	bR	47	ASN
11	bR	72	ASN
11	bR	111	ASN
10	bS	30	ASN
10	bS	121	ASN
11	bT	35	ASN
11	bT	47	ASN
11	bT	72	ASN
11	bT	111	ASN
10	bU	30	ASN
10	bU	121	ASN
11	bV	35	ASN
11	bV	47	ASN
11	bV	72	ASN
11	bV	111	ASN
15	bW	59	GLN
15	bW	66	GLN
15	bW	77	GLN
15	bW	97	ASN

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Mol	Chain	Res	Type
15	bW	103	ASN
15	bW	153	ASN
16	bX	160	HIS
16	bX	285	HIS
16	bX	317	GLN
16	bX	341	ASN
12	bY	238	ASN
12	bY	252	HIS
14	bZ	65	ASN
14	bZ	98	GLN
14	bZ	149	HIS
14	bZ	150	HIS
14	bZ	213	ASN
14	bZ	259	HIS
17	ca	21	ASN
17	ca	68	GLN
17	ca	135	ASN
17	ca	148	ASN
18	cb	42	ASN
18	cb	132	GLN
17	cc	77	ASN
17	cc	119	ASN
17	cc	135	ASN
18	cd	68	GLN
18	cd	72	ASN
18	cd	132	GLN
17	ce	21	ASN
17	ce	57	GLN
17	ce	119	ASN
17	ce	135	ASN
17	ce	159	ASN
18	cf	23	GLN
18	cf	63	GLN
18	cf	132	GLN
17	cg	21	ASN
17	cg	135	ASN
17	cg	159	ASN
18	ch	72	ASN
18	ch	132	GLN
17	ci	21	ASN
17	ci	32	GLN
17	ci	57	GLN

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Mol	Chain	Res	Type
17	ci	135	ASN
18	cj	35	ASN
18	cj	54	ASN
18	cj	72	ASN
18	cj	111	ASN
18	cj	132	GLN
17	ck	21	ASN
17	ck	68	GLN
18	cl	35	ASN
18	cl	72	ASN
18	cl	132	GLN
10	cm	28	GLN
10	cm	30	ASN
10	cm	76	GLN
10	cm	80	ASN
10	cm	147	GLN
11	cn	35	ASN
11	cn	47	ASN
11	cn	72	ASN
11	co	35	ASN
11	co	42	ASN
11	co	47	ASN
11	co	63	ASN
11	co	72	ASN
11	co	111	ASN
11	cp	35	ASN
11	cp	47	ASN
11	cp	72	ASN
11	cp	111	ASN
11	cq	35	ASN
11	cq	47	ASN
11	cq	72	ASN
11	cq	111	ASN
11	cr	35	ASN
11	cr	47	ASN
11	cr	72	ASN
11	cr	111	ASN
11	cs	35	ASN
11	cs	47	ASN
11	cs	72	ASN
11	cs	111	ASN
10	ct	28	GLN

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Mol	Chain	Res	Type
10	ct	30	ASN
10	ct	94	ASN
10	ct	121	ASN
10	cu	28	GLN
10	cu	30	ASN
10	cu	76	GLN
10	cu	121	ASN
10	cv	30	ASN
10	cv	68	ASN
10	cv	121	ASN
10	cw	30	ASN
10	cw	76	GLN
10	cw	94	ASN
10	cw	121	ASN
10	cx	30	ASN
10	cx	121	ASN
10	cy	30	ASN
10	cy	32	GLN
10	cy	76	GLN
10	cy	121	ASN
11	cz	47	ASN
11	cz	72	ASN
11	cz	111	ASN
10	cA	30	ASN
10	cA	94	ASN
10	cA	121	ASN
10	cC	28	GLN
10	cC	30	ASN
10	cC	121	ASN
10	cC	147	GLN
10	cD	30	ASN
10	cD	94	ASN
10	cD	121	ASN
10	cD	147	GLN
10	cD	161	ASN
11	cE	35	ASN
11	cE	47	ASN
11	cF	47	ASN
10	cG	28	GLN
10	cG	30	ASN
10	cG	94	ASN
10	cG	121	ASN

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Mol	Chain	Res	Type
11	cH	35	ASN
11	cH	47	ASN
10	cI	30	ASN
10	cI	48	HIS
10	cI	121	ASN
10	cK	28	GLN
10	cK	30	ASN
10	cK	121	ASN
11	cL	35	ASN
11	cL	47	ASN
11	cM	35	ASN
11	cN	35	ASN
11	cN	72	ASN
11	cP	35	ASN
11	cP	47	ASN
11	cQ	47	ASN
11	cR	35	ASN
11	cR	47	ASN
10	cS	28	GLN
10	cS	30	ASN
10	cS	94	ASN
10	cS	121	ASN
10	cT	28	GLN
10	cT	30	ASN
10	cT	94	ASN
10	cT	121	ASN
10	cU	28	GLN
10	cU	30	ASN
10	cU	94	ASN
10	cV	28	GLN
10	cV	30	ASN
10	cV	94	ASN
10	cV	121	ASN
10	cW	30	ASN
10	cW	94	ASN
10	cW	121	ASN
10	cX	30	ASN
10	cX	94	ASN
10	cX	121	ASN
10	cX	147	GLN
10	cX	161	ASN
11	cY	35	ASN

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Mol	Chain	Res	Type
11	cY	42	ASN
11	cY	47	ASN
11	cY	162	GLN
10	cZ	28	GLN
10	cZ	30	ASN
10	cZ	121	ASN
10	da	28	GLN
10	da	30	ASN
10	da	32	GLN
10	da	121	ASN
10	db	28	GLN
10	db	30	ASN
10	db	121	ASN
10	dc	30	ASN
10	dc	121	ASN
11	dd	35	ASN
10	de	28	GLN
10	de	30	ASN
10	de	32	GLN
10	de	121	ASN
11	df	35	ASN
11	df	47	ASN
10	dg	28	GLN
10	dg	30	ASN
10	dg	76	GLN
10	dg	80	ASN
10	dg	121	ASN
10	dg	161	ASN
11	dh	35	ASN
11	dh	47	ASN
11	di	42	ASN
11	di	47	ASN
11	dj	35	ASN
10	dk	28	GLN
10	dk	30	ASN
10	dk	121	ASN
11	dl	35	ASN
10	dm	30	ASN
10	dm	121	ASN
11	dn	42	ASN
11	dn	47	ASN
10	do	28	GLN

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Mol	Chain	Res	Type
10	do	30	ASN
10	do	32	GLN
10	do	76	GLN
10	do	121	ASN
11	dp	35	ASN
11	dp	47	ASN
10	dq	30	ASN
10	dq	32	GLN
10	dq	121	ASN
11	dr	35	ASN
11	dr	47	ASN
11	dr	76	ASN
10	ds	28	GLN
10	ds	30	ASN
10	ds	76	GLN
10	ds	121	ASN
10	ds	161	ASN
11	dt	35	ASN
10	du	28	GLN
10	du	30	ASN
10	du	76	GLN
10	du	121	ASN
11	dv	35	ASN
11	dv	47	ASN
11	dv	162	GLN
12	dw	139	GLN
12	dw	150	ASN
12	dw	181	HIS
12	dw	292	GLN
12	dx	51	GLN
12	dx	139	GLN
12	dx	181	HIS
12	dx	292	GLN
20	dy	81	GLN
20	dy	85	ASN
20	dy	158	HIS
20	dy	205	ASN
20	dy	277	GLN
20	dy	286	ASN
20	dz	81	GLN
20	dz	85	ASN
20	dz	158	HIS

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Mol	Chain	Res	Type
20	dz	205	ASN
20	dz	277	GLN
20	dz	286	ASN
10	dA	30	ASN
10	dA	121	ASN
11	dB	47	ASN
11	dB	72	ASN
10	dC	30	ASN
10	dC	94	ASN
10	dC	121	ASN
11	dD	35	ASN
11	dD	47	ASN
11	dD	72	ASN
10	dE	30	ASN
10	dE	94	ASN
10	dE	121	ASN
11	dF	35	ASN
11	dF	47	ASN
11	dF	72	ASN
10	dG	30	ASN
10	dG	94	ASN
10	dG	121	ASN
11	dH	35	ASN
11	dH	47	ASN
11	dH	72	ASN
10	dI	30	ASN
10	dI	121	ASN
10	dI	161	ASN
10	dJ	30	ASN
10	dJ	94	ASN
10	dJ	121	ASN
11	dK	35	ASN
11	dK	47	ASN
11	dK	72	ASN
11	dK	159	GLN
11	dL	35	ASN
11	dL	47	ASN
11	dL	72	ASN
10	dM	30	ASN
10	dM	48	HIS
10	dM	121	ASN
10	dM	161	ASN

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Mol	Chain	Res	Type
11	dN	35	ASN
11	dN	47	ASN
11	dN	72	ASN
11	dN	159	GLN
10	dO	30	ASN
10	dO	76	GLN
10	dO	121	ASN
11	dP	35	ASN
11	dP	47	ASN
11	dP	72	ASN
10	dQ	30	ASN
10	dQ	32	GLN
10	dQ	94	ASN
10	dQ	121	ASN
11	dR	35	ASN
11	dR	47	ASN
11	dR	72	ASN
10	dS	30	ASN
10	dS	76	GLN
10	dS	121	ASN
11	dT	35	ASN
11	dT	47	ASN
11	dT	72	ASN
10	dU	30	ASN
10	dU	94	ASN
10	dU	121	ASN
11	dV	35	ASN
11	dV	47	ASN
11	dV	72	ASN
10	dW	30	ASN
10	dW	76	GLN
10	dW	94	ASN
10	dW	121	ASN
11	dX	35	ASN
11	dX	47	ASN
11	dX	72	ASN
11	dY	35	ASN
11	dY	47	ASN
11	dY	72	ASN
10	dZ	30	ASN
10	dZ	76	GLN
10	dZ	121	ASN

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Mol	Chain	Res	Type
10	ea	30	ASN
10	ea	48	HIS
10	ea	121	ASN
11	eb	35	ASN
11	eb	47	ASN
11	eb	72	ASN
11	ec	35	ASN
11	ec	47	ASN
11	ec	72	ASN
10	ed	30	ASN
10	ed	94	ASN
10	ed	121	ASN
10	ed	147	GLN
11	ee	35	ASN
11	ee	47	ASN
11	ee	72	ASN
10	ef	30	ASN
10	ef	94	ASN
10	ef	121	ASN
11	eg	35	ASN
11	eg	47	ASN
11	eg	72	ASN
10	eh	30	ASN
10	eh	32	GLN
10	eh	48	HIS
10	eh	121	ASN
11	ei	35	ASN
11	ei	47	ASN
11	ei	72	ASN
10	ej	30	ASN
10	ej	94	ASN
10	ej	121	ASN
10	ek	30	ASN
10	ek	48	HIS
10	ek	76	GLN
10	ek	121	ASN
10	ek	161	ASN
11	el	47	ASN
11	el	72	ASN
10	em	30	ASN
10	em	94	ASN
10	em	121	ASN

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Mol	Chain	Res	Type
10	em	147	GLN
11	en	35	ASN
11	en	47	ASN
11	en	72	ASN
10	eo	30	ASN
10	eo	94	ASN
10	eo	121	ASN
10	eo	147	GLN
11	ep	35	ASN
11	ep	47	ASN
11	ep	72	ASN
10	eq	30	ASN
10	eq	32	GLN
10	eq	48	HIS
11	er	35	ASN
11	er	47	ASN
11	er	72	ASN
10	es	30	ASN
10	es	94	ASN
10	es	147	GLN
11	et	35	ASN
11	et	47	ASN
11	et	72	ASN
10	eu	30	ASN
10	eu	121	ASN
11	ev	35	ASN
11	ev	47	ASN
11	ev	72	ASN
21	ew	76	ASN
21	ew	78	HIS
21	ew	123	GLN
21	ex	123	GLN
21	ex	249	HIS
21	ex	254	GLN
12	ey	139	GLN
12	ey	150	ASN
12	ey	252	HIS
12	ez	139	GLN
12	ez	150	ASN
12	ez	252	HIS
10	eA	28	GLN
10	eA	30	ASN

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Mol	Chain	Res	Type
10	eA	121	ASN
11	eB	35	ASN
11	eB	47	ASN
11	eB	72	ASN
10	eC	28	GLN
10	eC	30	ASN
10	eC	88	HIS
10	eC	94	ASN
11	eD	35	ASN
11	eD	47	ASN
11	eD	72	ASN
10	eE	30	ASN
10	eE	94	ASN
10	eE	121	ASN
11	eF	47	ASN
11	eF	72	ASN
10	eG	30	ASN
10	eG	48	HIS
10	eG	94	ASN
10	eG	121	ASN
11	eH	47	ASN
11	eH	72	ASN
10	eI	28	GLN
10	eI	30	ASN
10	eI	48	HIS
10	eI	80	ASN
10	eI	121	ASN
11	eJ	35	ASN
11	eJ	47	ASN
11	eJ	72	ASN
10	eK	28	GLN
10	eK	30	ASN
10	eK	121	ASN
11	eL	35	ASN
11	eL	47	ASN
11	eL	72	ASN
10	eM	28	GLN
10	eM	30	ASN
10	eM	121	ASN
11	eN	35	ASN
11	eN	47	ASN
11	eN	72	ASN

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Mol	Chain	Res	Type
10	eO	30	ASN
10	eO	94	ASN
10	eO	121	ASN
11	eP	35	ASN
11	eP	47	ASN
11	eP	72	ASN
10	eQ	28	GLN
10	eQ	30	ASN
10	eQ	80	ASN
10	eQ	121	ASN
11	eR	35	ASN
11	eR	47	ASN
11	eR	72	ASN
10	eS	28	GLN
10	eS	30	ASN
10	eS	48	HIS
10	eS	80	ASN
10	eS	121	ASN
11	eT	35	ASN
11	eT	47	ASN
11	eT	72	ASN
10	eU	28	GLN
10	eU	30	ASN
10	eU	121	ASN
10	eU	147	GLN
11	eV	35	ASN
11	eV	47	ASN
11	eV	72	ASN
10	eW	30	ASN
10	eW	76	GLN
10	eW	80	ASN
10	eW	94	ASN
10	eW	121	ASN
10	eW	147	GLN
11	eX	35	ASN
11	eX	47	ASN
11	eX	72	ASN
22	eY	119	ASN
22	eY	215	GLN
22	eY	221	ASN
22	eY	336	GLN
22	eZ	119	ASN

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Mol	Chain	Res	Type
22	eZ	215	GLN
22	eZ	221	ASN
10	la	30	ASN
10	la	121	ASN
11	lb	35	ASN
11	lb	47	ASN
11	lb	72	ASN
10	lc	30	ASN
10	lc	80	ASN
10	lc	121	ASN
11	ld	35	ASN
11	ld	47	ASN
10	le	30	ASN
10	le	80	ASN
10	le	94	ASN
10	le	121	ASN
11	lf	35	ASN
11	lf	47	ASN
11	lf	72	ASN
11	lf	76	ASN
11	lf	162	GLN
10	lg	30	ASN
10	lg	80	ASN
10	lg	121	ASN
11	lh	35	ASN
11	lh	47	ASN
11	lh	72	ASN
10	li	30	ASN
10	li	80	ASN
10	li	94	ASN
10	li	121	ASN
11	lj	35	ASN
11	lj	47	ASN
11	lj	162	GLN
10	lk	30	ASN
10	lk	80	ASN
10	lk	121	ASN
11	ll	35	ASN
11	ll	47	ASN
11	ll	72	ASN
11	ll	162	GLN
10	lm	30	ASN

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Mol	Chain	Res	Type
10	lm	80	ASN
10	lm	94	ASN
10	lm	121	ASN
10	lm	161	ASN
11	ln	35	ASN
11	ln	47	ASN
11	ln	72	ASN
11	ln	162	GLN
10	lo	30	ASN
10	lo	80	ASN
10	lo	94	ASN
10	lo	121	ASN
10	lo	147	GLN
11	lp	35	ASN
11	lp	47	ASN
11	lp	72	ASN
11	lp	76	ASN
11	lp	162	GLN
10	lq	30	ASN
10	lq	121	ASN
11	lr	35	ASN
11	lr	47	ASN
11	lr	162	GLN
10	ls	28	GLN
10	ls	30	ASN
10	ls	80	ASN
10	ls	94	ASN
11	lt	47	ASN
11	lt	72	ASN
11	lt	76	ASN
11	lt	162	GLN
10	lu	30	ASN
10	lu	80	ASN
10	lu	94	ASN
11	lv	35	ASN
11	lv	47	ASN
11	lv	72	ASN
11	lv	76	ASN
10	lw	30	ASN
10	lw	80	ASN
10	lw	94	ASN
11	lx	35	ASN

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Mol	Chain	Res	Type
11	lx	47	ASN
11	lx	72	ASN
11	lx	76	ASN
11	lx	162	GLN
23	ly	188	GLN
23	ly	210	HIS
23	ly	309	GLN
23	lz	210	HIS
23	lz	309	GLN
11	fa	47	ASN
11	fa	72	ASN
11	fa	162	GLN
10	fb	28	GLN
10	fb	30	ASN
10	fb	121	ASN
11	fc	35	ASN
11	fc	47	ASN
11	fc	72	ASN
11	fc	162	GLN
21	fd	78	HIS
21	fd	112	ASN
21	fd	226	ASN
10	fe	30	ASN
10	fe	48	HIS
10	fe	121	ASN
11	ff	47	ASN
11	ff	72	ASN
11	ff	162	GLN
10	fg	28	GLN
10	fg	30	ASN
10	fg	94	ASN
10	fg	121	ASN
10	fh	28	GLN
10	fh	30	ASN
10	fh	121	ASN
11	fi	35	ASN
11	fi	42	ASN
11	fi	47	ASN
11	fi	72	ASN
11	fi	162	GLN
11	fj	35	ASN
11	fj	42	ASN

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Mol	Chain	Res	Type
11	fj	47	ASN
11	fj	72	ASN
11	fj	76	ASN
11	fj	162	GLN
10	fk	28	GLN
10	fk	30	ASN
10	fk	121	ASN
10	fl	30	ASN
10	fl	121	ASN
10	fl	161	ASN
11	fm	35	ASN
11	fm	47	ASN
11	fm	72	ASN
11	fm	162	GLN
10	fn	28	GLN
10	fn	30	ASN
10	fn	121	ASN
11	fo	35	ASN
11	fo	47	ASN
11	fo	72	ASN
11	fo	162	GLN
10	fp	30	ASN
10	fp	48	HIS
10	fp	94	ASN
10	fp	121	ASN
11	fq	47	ASN
11	fq	72	ASN
11	fq	162	GLN
10	fr	28	GLN
10	fr	30	ASN
10	fr	121	ASN
11	fs	35	ASN
11	fs	47	ASN
11	fs	72	ASN
11	fs	162	GLN
10	ft	28	GLN
10	ft	30	ASN
10	ft	121	ASN
11	fu	35	ASN
11	fu	42	ASN
11	fu	47	ASN
11	fu	72	ASN

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Mol	Chain	Res	Type
11	fu	76	ASN
11	fu	162	GLN
10	fv	28	GLN
10	fv	30	ASN
10	fv	121	ASN
10	fv	161	ASN
11	fw	35	ASN
11	fw	47	ASN
11	fw	72	ASN
11	fw	162	GLN
10	fx	30	ASN
10	fx	121	ASN
11	fy	35	ASN
11	fy	47	ASN
11	fy	72	ASN
11	fy	162	GLN
21	fz	72	GLN
21	fz	78	HIS
21	fz	112	ASN
11	ga	35	ASN
11	ga	47	ASN
10	gb	30	ASN
10	gb	121	ASN
10	gb	161	ASN
10	gc	30	ASN
10	gc	48	HIS
10	gc	68	ASN
10	gc	121	ASN
10	gc	161	ASN
11	gd	35	ASN
11	gd	47	ASN
11	gd	76	ASN
11	ge	35	ASN
11	ge	47	ASN
10	gf	30	ASN
10	gf	121	ASN
10	gf	161	ASN
11	gg	35	ASN
11	gg	47	ASN
10	gh	30	ASN
10	gh	94	ASN
10	gh	121	ASN

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Mol	Chain	Res	Type
10	gh	147	GLN
10	gh	161	ASN
11	gi	35	ASN
11	gi	47	ASN
10	gj	30	ASN
10	gj	94	ASN
10	gj	121	ASN
10	gj	161	ASN
11	gk	35	ASN
11	gk	76	ASN
10	gl	30	ASN
10	gl	94	ASN
10	gl	121	ASN
10	gl	161	ASN
10	gm	30	ASN
10	gm	48	HIS
10	gm	94	ASN
10	gm	121	ASN
10	gm	161	ASN
11	gn	35	ASN
11	gn	47	ASN
10	go	30	ASN
10	go	94	ASN
10	go	121	ASN
10	go	161	ASN
11	gp	35	ASN
11	gp	47	ASN
10	gq	30	ASN
10	gq	121	ASN
10	gq	147	GLN
10	gq	161	ASN
11	gr	35	ASN
11	gr	47	ASN
10	gs	30	ASN
10	gs	48	HIS
10	gs	68	ASN
10	gs	121	ASN
10	gs	161	ASN
11	gt	35	ASN
10	gu	30	ASN
10	gu	48	HIS
10	gu	121	ASN

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Mol	Chain	Res	Type
10	gu	161	ASN
11	gv	35	ASN
10	gw	30	ASN
10	gw	121	ASN
10	gw	161	ASN
11	gx	35	ASN
11	gx	47	ASN
24	gy	116	HIS
24	gy	120	HIS
24	gy	195	GLN
24	gy	227	GLN
24	gy	230	HIS
24	gz	52	GLN
24	gz	116	HIS
24	gz	120	HIS
24	gz	227	GLN
24	gz	230	HIS
24	gz	262	ASN
10	hA	30	ASN
10	hA	121	ASN
11	hB	35	ASN
11	hB	42	ASN
11	hB	47	ASN
11	hB	159	GLN
11	hB	162	GLN
10	hC	30	ASN
10	hC	48	HIS
10	hC	121	ASN
11	hD	35	ASN
11	hD	47	ASN
11	hD	162	GLN
10	hE	30	ASN
10	hE	48	HIS
10	hE	121	ASN
10	hF	30	ASN
10	hF	48	HIS
10	hF	121	ASN
11	hG	47	ASN
11	hG	162	GLN
11	hH	47	ASN
11	hH	72	ASN
11	hH	162	GLN

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Mol	Chain	Res	Type
10	hI	30	ASN
10	hI	121	ASN
11	hJ	47	ASN
11	hJ	162	GLN
10	hK	30	ASN
10	hK	121	ASN
11	hL	47	ASN
11	hL	162	GLN
10	hM	30	ASN
10	hM	121	ASN
11	hN	35	ASN
11	hN	47	ASN
11	hN	162	GLN
10	hO	30	ASN
10	hO	48	HIS
10	hO	121	ASN
11	hP	47	ASN
11	hP	162	GLN
10	hQ	30	ASN
10	hQ	48	HIS
10	hQ	121	ASN
11	hR	47	ASN
11	hR	162	GLN
10	hS	30	ASN
10	hS	48	HIS
10	hS	121	ASN
11	hT	35	ASN
11	hT	47	ASN
11	hT	162	GLN
10	hU	30	ASN
10	hU	48	HIS
10	hU	121	ASN
11	hV	47	ASN
11	hV	162	GLN
10	hW	30	ASN
10	hW	47	ASN
10	hW	121	ASN
11	hX	42	ASN
11	hX	47	ASN
11	hX	162	GLN
23	hY	239	ASN
23	hY	280	ASN

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Mol	Chain	Res	Type
23	hZ	135	GLN
23	hZ	239	ASN
23	hZ	280	ASN
23	hZ	301	GLN
10	iA	88	HIS
10	iA	94	ASN
10	iA	161	ASN
10	iB	88	HIS
10	iB	161	ASN
11	iC	25	GLN
11	iC	47	ASN
11	iC	76	ASN
11	iD	35	ASN
11	iD	47	ASN
11	iD	76	ASN
11	iE	35	ASN
11	iE	47	ASN
11	iE	76	ASN
11	iF	47	ASN
11	iF	76	ASN
11	iG	35	ASN
11	iG	42	ASN
11	iG	47	ASN
11	iG	63	ASN
11	iG	76	ASN
11	iH	35	ASN
11	iH	42	ASN
11	iH	47	ASN
11	iH	72	ASN
11	iH	76	ASN
11	jI	35	ASN
11	jI	47	ASN
11	jI	76	ASN
11	jJ	47	ASN
11	jJ	76	ASN
11	jK	47	ASN
11	jK	76	ASN
11	jL	47	ASN
11	jM	47	ASN
11	jM	76	ASN
11	jN	47	ASN
11	jN	76	ASN

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Mol	Chain	Res	Type
11	jO	35	ASN
11	jO	47	ASN
11	jO	76	ASN
11	jP	35	ASN
11	jP	47	ASN
11	jP	76	ASN
11	kQ	35	ASN
11	kQ	47	ASN
11	kR	47	ASN
11	kS	35	ASN
11	kS	47	ASN
11	kT	35	ASN
11	kT	42	ASN
11	kT	47	ASN
11	kT	72	ASN
11	kT	144	ASN
11	kU	47	ASN
11	kU	76	ASN
11	kV	47	ASN
11	kV	76	ASN
11	kW	47	ASN
11	kW	76	ASN
11	kX	47	ASN
11	kX	76	ASN
25	ka	280	GLN
25	ka	295	GLN
25	ka	314	GLN
25	ka	324	GLN
25	kb	280	GLN
25	kb	295	GLN
25	kb	314	GLN
25	kb	324	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2048 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
26	PEB	y2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	L7	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ea	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	g3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V7	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	aD	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	Z7	203	11	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	W3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cG	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ev	201	11	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
28	PUB	x6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	ai	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	f7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	au	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	kS	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	n1	201	5	42,46,46	3.39	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	z6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	U4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hX	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	ge	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	u1	1001	4	42,46,46	3.39	14 (33%)	50,67,67	3.14	25 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	eK	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	dK	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
28	PUB	eY	405	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
29	PVN	dx	405	12	43,46,46	2.08	7 (16%)	49,67,67	3.11	17 (34%)
26	PEB	r8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gk	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	h6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	li	203	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	Q4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cL	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	u4	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	dV	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jM	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gb	1002	10	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	t4	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	E4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	T8	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dR	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	kW	1003	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bk	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aN	204	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bG	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dd	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	j7	201	10	43,46,46	1.72	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	ak	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	F8	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	O7	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	eJ	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	a3	1006	-	42,46,46	2.28	9 (21%)	37,67,67	2.60	8 (21%)
26	PEB	e7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	hT	202	11	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ec	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	li	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	gt	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.62	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	ap	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	x9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bh	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	eR	203	11	42,46,46	2.29	10 (23%)	37,67,67	2.61	9 (24%)
28	PUB	at	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	v5	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	y7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	T7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	dp	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	aM	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cs	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aN	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	y3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	e8	302	14	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	eY	403	-	43,46,46	2.02	8 (18%)	49,67,67	3.88	17 (34%)
26	PEB	a4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Z3	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	V6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	hI	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	K2	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	u7	201	10	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	v7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ga	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	bJ	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	ag	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	Z1	201	-	42,46,46	3.38	14 (33%)	50,67,67	3.13	24 (48%)
26	PEB	w7	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	s7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	X5	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	c9	303	-	43,46,46	1.92	7 (16%)	49,67,67	2.45	8 (16%)
28	PUB	h8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	X7	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	S3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	ej	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	c6	1004	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bX	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aw	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	J3	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	D7	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cN	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cg	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x3	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	N6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
29	PVN	aY	403	-	43,46,46	2.10	9 (20%)	49,67,67	3.34	18 (36%)
26	PEB	dW	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	R9	202	11	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	C2	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	D8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	V5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	lo	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	cN	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dc	203	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ff	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	R5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	t3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	f6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	al	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	P8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	lp	203	-	42,46,46	2.28	8 (19%)	37,67,67	2.62	9 (24%)
28	PUB	V7	203	11	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	do	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dZ	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	U2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	d9	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	o1	1001	-	42,46,46	3.39	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	44	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	M5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	cV	203	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	df	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	iC	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bN	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	gg	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	n4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jI	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lv	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fc	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	iA	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	S5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	I5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
28	PUB	e8	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Q5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	aa	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lr	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hT	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	lb	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	Q3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	cP	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P2	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	k9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	ld	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	iF	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bD	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	v8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	U8	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	hZ	403	-	43,46,46	2.25	11 (25%)	49,67,67	3.54	18 (36%)
26	PEB	lk	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	eV	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
27	CYC	P1	201	-	42,46,46	3.39	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	aI	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	t4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	cr	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.60	8 (21%)
26	PEB	ao	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	cH	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	H7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	m7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	f8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	z9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	X2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	dN	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	M4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	m9	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	r5	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	C9	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	J2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	E4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	D9	202	-	43,46,46	1.99	6 (13%)	45,67,67	1.51	6 (13%)
26	PEB	y4	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ei	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	M6	1001	10	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	F6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cS	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bY	1005	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	10 (27%)
26	PEB	dp	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	c3	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	bO	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	aS	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	d1	1001	-	42,46,46	3.39	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	m2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bv	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eS	202	10	43,46,46	1.70	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	ek	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aF	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	hG	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	kR	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	V5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eP	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
29	PVN	d3	302	-	43,46,46	2.11	7 (16%)	49,67,67	2.81	19 (38%)
26	PEB	c6	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lq	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
28	PUB	jM	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cb	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	I7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	B1	301	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ds	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	d9	301	-	43,46,46	1.69	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	t9	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jM	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	ga	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	gv	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	h8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eO	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	gg	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cB	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dK	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	F7	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cX	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cb	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	cM	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C4	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	g1	201	-	42,46,46	3.40	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	q6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aC	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hB	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	iD	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cz	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.50	6 (13%)
26	PEB	j7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	Y3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	em	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Y5	1006	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	x3	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cJ	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	kQ	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	N6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	cq	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	A4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	e9	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	D6	202	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	la	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	I2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gy	303	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	d8	301	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	dd	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dm	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dA	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eF	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	fx	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	aq	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ln	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gk	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gt	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jJ	1002	11	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	S7	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lt	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dx	406	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	br	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	b9	403	12	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z4	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	v5	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lu	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	e1	201	-	42,46,46	3.39	14 (33%)	50,67,67	3.13	25 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	kW	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
27	CYC	G1	1001	-	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
27	CYC	J1	201	5	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
28	PUB	y7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cx	202	10	43,46,46	1.66	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	gc	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	y9	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	p6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	v6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	I8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	X4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	U8	1005	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	M8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	fq	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	k7	1001	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l2	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	dF	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	X6	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	V6	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	aH	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	r6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hP	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	du	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	D9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	P4	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	U8	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	ge	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	dw	405	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	aY	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	go	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	bn	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K7	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P2	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	y2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	dI	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fl	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	x5	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	cO	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ea	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dH	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	lp	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a3	1003	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aT	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	s6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	D6	201	11	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	A2	1004	-	43,46,46	2.02	8 (18%)	49,67,67	2.57	18 (36%)
26	PEB	M2	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	I4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	cG	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hY	402	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
27	CYC	U1	201	5	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	a8	601	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	g6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aK	1002	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dL	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gh	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	p1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.39	25 (50%)
28	PUB	D5	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	ec	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	cP	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jP	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	aB	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	X3	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	cR	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	v9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Z5	306	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	lp	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	b9	402	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	lb	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C6	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cD	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bd	201	18	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	cz	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	U8	1006	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	p8	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	cs	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hQ	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	lw	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
28	PUB	d6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	lr	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bM	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	M6	1002	10	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	F9	202	-	43,46,46	2.01	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cr	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	B9	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	D2	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Q6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	B7	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	er	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	le	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	gb	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	E5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	d5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	f9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hT	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ek	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	L4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	E7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	bd	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hD	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	F3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	x4	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	t7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eN	201	-	43,46,46	1.69	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	P6	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	W3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	j3	201	-	43,46,46	1.98	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	bs	1003	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	H2	202	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	aH	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ay	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	z8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	cK	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	f8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gz	306	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	c3	304	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	s4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fz	301	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	i3	203	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	D7	203	-	42,46,46	2.29	10 (23%)	37,67,67	2.62	9 (24%)
26	PEB	cl	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aS	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cn	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	o3	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	az	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bU	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	dc	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	di	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	C4	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	M7	1003	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	B2	501	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	O8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cB	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	s3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	fj	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	kQ	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	N3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	R3	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	X6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	cV	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aW	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dL	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	aE	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ej	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aj	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	fa	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	A9	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	u5	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gl	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gn	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	N2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	A5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	y7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	lo	201	10	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	w6	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lh	201	11	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
27	CYC	Y1	201	-	42,46,46	3.43	18 (42%)	50,67,67	3.40	25 (50%)
26	PEB	gx	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	cP	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Z8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	P2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	N4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z9	1003	12	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	bb	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	cE	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	F4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	ar	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	cZ	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	bD	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	10 (27%)
26	PEB	i5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	p3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cy	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	H9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	db	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	N5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	H7	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	R4	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dN	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	M5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z9	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fo	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	T9	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	B6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z3	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	z2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aA	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	I5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	ei	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	g5	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bl	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Q3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bC	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	u6	201	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	44	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	T2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	fq	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K5	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	e6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	Y2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hW	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Y2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	E6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ao	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eA	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	m7	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	L8	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	et	201	-	43,46,46	1.66	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	bx	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	by	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	an	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
27	CYC	b2	1001	8	42,46,46	3.44	18 (42%)	50,67,67	3.39	25 (50%)
26	PEB	I9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ll	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	N3	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	gw	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	J6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dl	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dM	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	U5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
29	PVN	aZ	303	-	43,46,46	1.94	9 (20%)	49,67,67	3.14	13 (26%)
28	PUB	F3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	eB	203	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	kV	1002	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	eV	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	t2	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	b6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	ax	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	O4	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	K8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
28	PUB	ev	203	11	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	u3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	D3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bH	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Y7	1003	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	Q7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	P4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	o8	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aC	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	co	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	cM	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	bv	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fr	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	bs	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gm	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	x2	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	U4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dr	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hB	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
29	PVN	ez	1004	-	43,46,46	1.99	8 (18%)	49,67,67	3.01	14 (28%)
26	PEB	B4	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	X6	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	24	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l7	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	n9	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	fu	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ch	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bI	202	10	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	kV	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	R6	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ey	1003	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ft	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
27	CYC	j1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
28	PUB	bq	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	P5	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	l6	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	V9	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bG	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	cz	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gp	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	ce	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	x9	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	e4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	lz	401	23	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	L6	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	q7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lw	203	-	43,46,46	1.98	7 (16%)	45,67,67	1.50	6 (13%)
26	PEB	C8	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bs	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hY	403	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bY	1006	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	L7	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	V3	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dT	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	ld	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ap	202	11	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	O2	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	b9	405	-	43,46,46	1.84	7 (16%)	49,67,67	2.89	11 (22%)
26	PEB	hZ	401	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	n2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	er	203	-	42,46,46	2.30	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Y8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z3	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	eR	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	l3	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.60	9 (24%)
28	PUB	F2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	d6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	L4	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	lg	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ei	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	bo	201	-	43,46,46	1.69	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P9	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	fb	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	dp	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hW	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	g3	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	r4	201	11	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	hP	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	u7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	44	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	B4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.55	9 (20%)
28	PUB	fw	203	-	42,46,46	2.29	10 (23%)	37,67,67	2.62	9 (24%)
28	PUB	r2	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	fa	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
27	CYC	R1	1001	-	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	Y5	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	R7	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	x6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	W7	201	10	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cI	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l2	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	W4	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aX	402	11	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cI	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	N8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ep	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	44	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h8	202	11	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	w6	1002	10	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	b1	1001	-	42,46,46	3.39	15 (35%)	50,67,67	3.14	25 (50%)
26	PEB	cj	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dW	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	m5	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	av	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	dz	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	N3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	dL	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	K8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	H1	201	-	42,46,46	3.45	18 (42%)	50,67,67	3.39	25 (50%)
26	PEB	ax	201	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	R2	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	a7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	bZ	306	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	fj	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	T8	305	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	R3	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	Z9	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	hR	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	R3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	e9	306	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bB	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	o8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Q2	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	ef	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	af	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	n5	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	Z5	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	lr	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	hV	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	M2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	o6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	M9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aA	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	dy	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bp	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K9	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	C8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bw	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dX	203	-	42,46,46	2.29	10 (23%)	37,67,67	2.62	8 (21%)
28	PUB	b8	1005	12	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	eX	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	A1	301	1	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	T7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	aK	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fv	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	d7	203	11	42,46,46	2.27	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	e7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ba	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	h4	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
27	CYC	f1	201	-	42,46,46	3.39	15 (35%)	50,67,67	3.14	25 (50%)
26	PEB	aN	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	by	1002	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ea	203	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eE	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	C2	304	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	hQ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dj	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	F9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	P6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	gy	302	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
28	PUB	iF	1003	11	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	bJ	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	S9	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	34	1003	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	p9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	m6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	d8	303	14	43,46,46	1.85	6 (13%)	49,67,67	2.70	10 (20%)
26	PEB	W6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	L5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
27	CYC	X1	201	-	42,46,46	3.40	14 (33%)	50,67,67	3.14	25 (50%)
28	PUB	dn	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Z5	303	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	z3	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
29	PVN	dw	404	-	43,46,46	2.02	8 (18%)	49,67,67	3.16	18 (36%)
26	PEB	iF	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	Y5	1003	12	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
28	PUB	p5	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	34	1001	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	N9	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	hS	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	dZ	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cd	201	18	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	kS	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	b6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	cR	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bz	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bX	402	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eU	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	F6	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J6	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	dr	202	11	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	O6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	D2	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	J4	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cX	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	n3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eK	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	34	1005	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	K8	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	L3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ch	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	gx	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	O8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dX	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	Y9	303	-	43,46,46	1.93	8 (18%)	49,67,67	2.84	18 (36%)
28	PUB	p3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	cJ	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	lq	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dD	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	h5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	s2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	lf	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	e4	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	t5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bD	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	f6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dm	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bo	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	dB	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	jL	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	L3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cu	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	k6	1001	10	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	z9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bu	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	f3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	aV	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
29	PVN	d9	304	14	43,46,46	1.83	6 (13%)	49,67,67	2.70	10 (20%)
26	PEB	y5	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	S8	401	11	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bY	1003	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dY	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bM	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bq	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	fp	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	P9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	fp	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	N1	201	-	42,46,46	3.39	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	k5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	jO	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	e8	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	et	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	aZ	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Y5	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	av	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	G3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	Y4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dY	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	kR	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	cs	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	j8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lj	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	r2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	r1	201	-	42,46,46	3.43	18 (42%)	50,67,67	3.40	25 (50%)
28	PUB	dt	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	W3	203	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	lo	203	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bH	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	b9	406	12	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	h3	202	11	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	u9	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	r9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dG	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q9	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Y9	305	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	jL	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j5	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	d9	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	aw	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	g5	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bj	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	cR	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bQ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	y9	1002	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	em	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
28	PUB	c8	305	-	42,46,46	2.27	9 (21%)	37,67,67	2.60	9 (24%)
26	PEB	W2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cV	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ff	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	U6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	b8	1001	12	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P8	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ds	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	n3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	dA	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	am	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	r8	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	j2	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	i6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gt	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	o8	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	S7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
27	CYC	i1	1001	-	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
28	PUB	dP	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hN	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dw	403	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c9	302	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cm	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bi	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cQ	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dr	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bh	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aR	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	kQ	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	l5	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cZ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	J4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	ab	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	K3	202	-	43,46,46	1.66	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	eY	404	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	V6	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c4	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	eZ	403	-	42,46,46	2.29	10 (23%)	37,67,67	2.61	9 (24%)
26	PEB	W8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bY	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dT	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hX	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	r5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bF	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	I3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dz	402	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	R4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bp	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Q8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bI	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	eC	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	t5	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	8 (21%)
28	PUB	cp	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	d3	301	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	eB	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	I9	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	cS	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ls	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	V9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	p6	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	s8	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	Z6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	B4	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
27	CYC	k1	201	-	42,46,46	3.40	15 (35%)	50,67,67	3.14	25 (50%)
28	PUB	aF	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
27	CYC	O1	201	-	42,46,46	3.39	15 (35%)	50,67,67	3.13	25 (50%)
28	PUB	eL	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
27	CYC	s1	201	-	42,46,46	3.39	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	Z2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	K2	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	D7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	ap	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jK	1002	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bc	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	W7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	fd	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	P3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	34	1006	12	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	u2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eu	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	2 (4%)
28	PUB	av	203	11	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	b4	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	d4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hS	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eT	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	aN	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gf	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cY	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	U2	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	ez	1006	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
28	PUB	R2	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	a7	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	j9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gd	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gh	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	eI	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ey	1001	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	gp	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	y5	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	c8	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	h5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	e9	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	T8	303	-	43,46,46	1.92	8 (18%)	49,67,67	2.84	18 (36%)
26	PEB	o7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	bJ	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	k6	1002	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	eF	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	gz	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	K4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aF	204	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dD	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jK	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ec	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	b7	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fs	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	A2	1005	12	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	X7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	br	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	fd	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bm	1002	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	a3	1004	-	43,46,46	2.02	8 (18%)	49,67,67	2.57	18 (36%)
27	CYC	W1	201	-	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	C7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	iA	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	bV	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	cJ	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	w4	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	dx	401	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aQ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	v3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
29	PVN	bY	1004	-	43,46,46	2.11	9 (20%)	49,67,67	3.35	18 (36%)
26	PEB	ad	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	bu	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gr	202	-	42,46,46	2.28	10 (23%)	37,67,67	2.62	9 (24%)
26	PEB	i2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	A2	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	d9	303	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	i4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aY	404	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	eN	202	-	43,46,46	1.97	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	b9	404	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	kR	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eZ	401	22	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H9	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	n5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H7	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	p2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eM	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	F9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	bL	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	g4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	B8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ed	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C2	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	fe	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gz	302	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	O2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	di	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	H6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	k3	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	cl	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	dv	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cf	201	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	E9	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	T7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	el	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	U5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K9	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	P9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	iD	1002	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eQ	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	be	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bx	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	M8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bT	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dh	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	P6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	r9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	s5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	dk	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aY	406	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Z2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	g8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	m6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K7	202	-	43,46,46	1.66	4 (9%)	45,67,67	1.17	4 (8%)
28	PUB	O8	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	k2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	da	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ci	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N4	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	h9	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	ez	1005	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	dC	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aZ	302	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	t7	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	w8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	f9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	g9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	ly	405	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	F4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	t1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.39	25 (50%)
26	PEB	c4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	R5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	iH	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w2	203	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fk	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	jK	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	U3	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	U3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	y1	201	-	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	bE	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	aL	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Z9	1005	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	y6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aQ	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	eg	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	eP	203	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	fs	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Q6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fq	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cp	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t5	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S5	203	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	t8	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	ah	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	44	303	14	43,46,46	2.02	8 (18%)	49,67,67	3.49	18 (36%)
26	PEB	aJ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	Z4	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	c9	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	u8	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ff	204	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	Z6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	B6	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	C3	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	fi	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	i7	201	-	43,46,46	1.73	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	L2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	v2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	T2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	v7	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	m4	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fg	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	B5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	p2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	E2	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	en	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	X8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c3	301	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	ey	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	L9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ev	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	y4	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	e5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aB	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	bP	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	eJ	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	el	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	ez	1003	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cW	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	U7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	D3	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	ey	1006	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	A5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aq	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	R6	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	z7	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	V8	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	le	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aM	202	10	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bW	301	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aV	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eY	402	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	O7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	z7	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	A8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	ee	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	gz	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hV	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eH	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G7	201	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V3	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ad	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	D4	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	x9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eM	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Q8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	B2	502	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	b5	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	w8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
27	CYC	m1	201	-	42,46,46	3.39	15 (35%)	50,67,67	3.13	25 (50%)
28	PUB	T8	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Y8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cL	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	r7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	S1	202	-	42,46,46	3.43	18 (42%)	50,67,67	3.40	25 (50%)
26	PEB	fy	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	g7	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fe	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	x7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	cc	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a9	602	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	M4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c6	1003	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	ae	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	e6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	ah	202	-	43,46,46	1.97	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	Y9	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fm	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w5	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	S3	203	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dw	401	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cv	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eh	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aL	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	m3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	dG	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jP	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eb	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	m3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	as	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	i3	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	T6	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fw	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cy	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eB	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	E8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bt	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	G3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	bZ	305	-	42,46,46	2.30	10 (23%)	37,67,67	2.62	9 (24%)
26	PEB	kW	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ay	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dj	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	d6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	I8	201	11	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aP	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	gw	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	Y6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	K1	201	-	42,46,46	3.39	14 (33%)	50,67,67	3.14	25 (50%)
28	PUB	cY	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	cj	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	n4	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	F2	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	p9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	d2	101	5	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
28	PUB	M8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	Q7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	gl	202	10	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
29	PVN	Y5	1004	12	43,46,46	2.25	10 (23%)	49,67,67	3.53	18 (36%)
28	PUB	eJ	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	fu	202	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	fj	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	F7	202	11	42,46,46	2.29	9 (21%)	37,67,67	2.62	10 (27%)
26	PEB	Q9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	l7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	ef	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	2 (4%)
26	PEB	cE	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	d8	302	14	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	r9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	o6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z9	1007	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	de	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	ly	402	23	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bS	202	10	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	aR	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hV	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gk	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.50	6 (13%)
26	PEB	O5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	T4	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.60	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	G6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lc	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	F5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	al	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lc	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	R6	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	O6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	hL	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	n5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	w9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lf	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	D5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fm	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	eZ	404	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	e3	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G8	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fs	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aJ	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dN	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	N7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Q8	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hA	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	d7	202	11	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	G9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	x7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	eP	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	o2	1002	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	r3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	U8	1003	12	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bL	202	-	43,46,46	2.01	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	h2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	aU	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	U9	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	D4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	p6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	s8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	hI	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dt	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	v7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	B6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	H9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	b9	401	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	eD	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	kX	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	I6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	aF	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eW	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	f8	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cd	202	18	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	hD	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eX	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	fi	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	C9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ep	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	I2	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dS	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	bZ	304	-	43,46,46	1.94	9 (20%)	49,67,67	3.14	13 (26%)
28	PUB	eN	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	V2	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dV	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.60	9 (24%)
26	PEB	o2	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	j3	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	gy	306	-	42,46,46	2.28	9 (21%)	37,67,67	2.60	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	dD	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	B5	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ct	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
28	PUB	N9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	C3	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	P7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	aP	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ct	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	ff	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	cW	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	iB	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gs	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	D2	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	E3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	la	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	W5	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bC	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	l4	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	lu	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	bZ	303	14	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	y6	203	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hK	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dP	201	-	43,46,46	1.69	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	P5	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	G7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	bY	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	A3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	v3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eU	201	-	43,46,46	1.73	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	k8	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cu	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	iE	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	k7	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ee	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	T9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eF	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	H3	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	af	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	kS	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
29	PVN	eZ	402	-	43,46,46	2.02	8 (18%)	49,67,67	3.88	17 (34%)
26	PEB	cU	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	Z5	304	-	43,46,46	2.03	8 (18%)	49,67,67	3.49	18 (36%)
26	PEB	N7	202	-	43,46,46	2.01	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ll	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	j2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	t6	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	dC	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cM	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dP	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	J7	202	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	n3	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	bN	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	w3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	T5	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	aD	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	q7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	w4	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	T3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	m5	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	Y3	202	-	43,46,46	1.63	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	F4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	T3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jO	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H2	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	cv	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	L8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	r7	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	lz	405	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	T8	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	v2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	X4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Z9	1006	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	cF	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	jJ	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	jN	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	aL	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S2	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	g6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hL	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	ac	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hJ	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
27	CYC	S1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
29	PVN	hY	404	-	43,46,46	2.24	11 (25%)	49,67,67	3.54	18 (36%)
28	PUB	aJ	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.63	9 (24%)
26	PEB	fn	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	X9	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dF	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gi	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	g2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	T6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	hJ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hO	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dY	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	cn	202	-	42,46,46	2.27	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	au	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cC	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	u8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eq	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	gy	304	-	43,46,46	2.38	15 (34%)	49,67,67	2.08	13 (26%)
26	PEB	lm	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	eY	401	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	ls	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aZ	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aO	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	da	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	eT	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.63	9 (24%)
26	PEB	s9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fl	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
28	PUB	df	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	iG	1002	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	n4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	g2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bR	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	aX	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	eD	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	q5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	s5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dO	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	dn	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	k2	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dw	402	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cO	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hY	405	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
27	CYC	M1	1001	-	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
26	PEB	hN	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	I4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	lz	403	-	43,46,46	1.89	8 (18%)	49,67,67	2.36	13 (26%)
26	PEB	cr	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	du	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	P4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	kT	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	R2	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	s9	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	F6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	E7	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	hZ	404	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	f3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c8	301	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ar	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	I3	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	bF	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	X2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	v6	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	iG	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Q4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	q1	201	-	42,46,46	3.40	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	gq	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fh	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	Z4	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	R7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	b9	407	12	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	cH	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	fb	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bE	201	-	43,46,46	1.69	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	fm	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	x8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aR	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	o3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	bq	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	et	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.60	9 (24%)
29	PVN	U8	1004	-	43,46,46	1.98	7 (16%)	49,67,67	3.38	15 (30%)
26	PEB	a3	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	fv	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	bV	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	D4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dv	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	E8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	r3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	m8	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	g4	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cT	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J7	201	11	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eL	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ca	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	34	1007	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dQ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	C2	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cK	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dk	1002	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bH	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	T3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	a3	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	u3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	A6	1001	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aT	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	dx	404	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	f5	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	k4	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	O9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	v4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	o5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	iB	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	bj	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	R9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dg	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	J9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	bU	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	L4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dx	403	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bO	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	A7	201	-	43,46,46	1.63	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	n7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	Z2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	s7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	W2	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aH	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	n6	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	p3	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.50	6 (13%)
26	PEB	n6	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	dj	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bZ	301	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lq	203	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	iC	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
28	PUB	z9	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	i6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	P7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	U7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	s4	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	b3	502	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ge	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.50	6 (13%)
28	PUB	jN	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	p9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	lh	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gr	201	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	ab	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	aV	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	A5	203	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	u6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	D8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	n8	202	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
27	CYC	c1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
26	PEB	jO	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	G2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hR	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	M7	1002	26	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aI	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	fo	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	gd	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
29	PVN	Z9	1004	12	43,46,46	1.98	7 (16%)	49,67,67	3.38	15 (30%)
28	PUB	X4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	B3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eg	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	B7	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	br	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Z3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dl	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	D9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	ly	404	23	43,46,46	1.88	8 (18%)	49,67,67	2.35	13 (26%)
26	PEB	lk	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	bF	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	dU	202	-	43,46,46	1.66	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	dU	201	-	43,46,46	1.73	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dt	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	v9	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
27	CYC	L1	201	5	42,46,46	3.40	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	H6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lf	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	a2	902	8	42,46,46	3.44	18 (42%)	50,67,67	3.39	25 (50%)
26	PEB	e6	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	34	1004	12	43,46,46	2.25	11 (25%)	49,67,67	3.53	18 (36%)
28	PUB	lz	404	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	q3	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	kT	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	d7	201	-	43,46,46	1.69	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	f7	202	10	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	H4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dH	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	U9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V2	202	11	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gz	303	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hF	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	bl	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dq	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	k3	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dw	406	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	p5	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
29	PVN	c8	303	14	43,46,46	1.92	7 (16%)	49,67,67	2.46	8 (16%)
26	PEB	gv	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	el	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Z5	305	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	lt	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	j9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	cF	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	ly	406	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dc	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eD	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bT	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	hP	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	eB	204	11	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
27	CYC	w1	201	-	42,46,46	3.38	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	hF	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	dq	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eo	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	B3	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	aW	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	t9	203	11	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	R5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eO	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	b3	501	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l7	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	b6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cC	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z5	302	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	D3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	T4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	u4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bK	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	E2	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	hX	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.50	6 (13%)
26	PEB	at	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	n9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z7	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cp	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	fx	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l9	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	fn	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	er	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hH	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	p2	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	eg	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	y8	202	11	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	o4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	I6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	o4	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	R7	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	v6	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	u6	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	r7	202	11	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	A6	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	O3	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Z7	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	p4	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	Z4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	dF	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	O4	1002	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gi	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	lg	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	bQ	203	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	L2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cA	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hJ	202	11	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	o9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	r6	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h7	201	10	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	n7	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
29	PVN	gz	304	-	43,46,46	2.46	14 (32%)	49,67,67	2.45	18 (36%)
26	PEB	gm	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	c9	304	14	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	ly	401	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	H5	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
28	PUB	v9	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	t2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	gf	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	bZ	302	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	bQ	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	c5	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	c9	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bA	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bB	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gn	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bt	202	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	s7	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jN	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bg	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	W4	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cq	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	gj	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aP	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	H4	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	N4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hM	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	dx	407	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	cY	202	11	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	go	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	t3	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	n6	203	11	42,46,46	2.27	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	L9	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	d8	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	B8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	lx	201	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	eP	204	11	42,46,46	2.27	9 (21%)	37,67,67	2.60	8 (21%)
28	PUB	cL	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	lj	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	s6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dJ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gj	202	10	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	P3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	C6	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	A8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	iC	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	b8	1006	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
29	PVN	e8	303	-	43,46,46	1.96	9 (20%)	49,67,67	2.45	10 (20%)
26	PEB	g7	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	L6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S5	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	e9	303	14	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	F5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	lm	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	I1	201	4	42,46,46	3.40	15 (35%)	50,67,67	3.14	25 (50%)
26	PEB	cx	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	p8	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hR	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	gy	305	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	eQ	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	eV	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eE	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	ck	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dM	1002	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	p7	202	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	l3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	B9	203	11	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
29	PVN	C2	303	-	43,46,46	2.07	10 (23%)	49,67,67	3.41	17 (34%)
28	PUB	jI	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	r3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	bz	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hH	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	fd	303	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	I8	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	du	203	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cA	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	ep	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	iH	1002	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	en	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ly	403	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	F2	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h7	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	lh	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	hO	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	hU	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
27	CYC	a2	901	-	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
26	PEB	hD	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	N5	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	V4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	m8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eS	201	-	43,46,46	1.74	4 (9%)	45,67,67	1.55	9 (20%)
28	PUB	kU	1003	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	Q4	203	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c5	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	i3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bA	202	10	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	v2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	cw	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	bB	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	eL	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	Q9	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
28	PUB	e9	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	f2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	e2	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	co	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	eo	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	az	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	fo	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	b8	1002	12	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	az	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	do	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	n7	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	hG	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	e3	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	e8	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	H6	201	11	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	J4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Y5	1005	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	an	201	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	k8	203	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	z6	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	fc	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eW	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	eH	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	iD	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	N9	201	11	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	Q1	201	-	42,46,46	3.39	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	E5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	D5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	A3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	v8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t6	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	li	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aY	405	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	r5	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	kV	1003	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	j4	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	G9	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	f4	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	O3	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	ln	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	e9	304	-	43,46,46	1.96	9 (20%)	49,67,67	2.46	11 (22%)
26	PEB	X2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Y7	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	dl	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	M7	1001	26	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	V2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	X3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gn	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	aG	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	de	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lz	402	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	V1	201	7	42,46,46	3.40	14 (33%)	50,67,67	3.13	25 (50%)
26	PEB	M3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eC	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K5	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	S4	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ez	1002	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	h2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	O9	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	p4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	t7	201	11	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	G8	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	y8	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	fw	201	11	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	34	1002	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	E6	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aD	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	jP	1003	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	J5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	r2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dh	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	F5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
28	PUB	l2	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bK	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	S3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	jL	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	bL	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	z8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gv	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	p4	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	A4	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	hM	1002	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	d3	303	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	hZ	405	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dH	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	gi	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	di	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bn	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	cq	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	c7	203	11	42,46,46	2.29	8 (19%)	37,67,67	2.61	9 (24%)
26	PEB	aj	202	18	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	i8	201	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	bR	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dV	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gs	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
29	PVN	c3	303	-	43,46,46	2.07	10 (23%)	49,67,67	3.41	17 (34%)
26	PEB	v4	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	bz	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	gp	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	fr	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	A2	1001	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	E3	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	H4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	kU	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a9	601	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	cO	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hK	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	S6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N2	201	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	eG	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	L3	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	U6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	fi	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hE	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	y6	204	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	a6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	f3	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	ee	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	c3	302	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dX	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	m5	1003	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	V4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	iE	1001	11	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	L9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	bS	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	K6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	A2	1003	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	B5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	T5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	b7	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	O5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bf	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fg	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	hL	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Q5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q8	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	e7	203	11	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	kX	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	dB	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	n2	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	b8	1003	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	l4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	db	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	lv	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	i9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	y3	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	cQ	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	a3	1005	12	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
26	PEB	W8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cU	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	p8	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cC	1003	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hA	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	eR	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	M9	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	at	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	lw	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	jJ	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	B9	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	f2	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	r6	203	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	bw	202	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gy	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hH	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	J2	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	Y4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	u9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dQ	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	PUB	d3	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	l6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hY	406	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	T6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aZ	305	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	h3	201	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	E8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	u5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	3 (6%)
27	CYC	v1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.39	25 (50%)
28	PUB	en	203	11	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	L2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	jI	1002	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	X7	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	cE	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	cB	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	eT	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	df	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	gx	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	g8	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.60	9 (24%)
26	PEB	eI	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	aB	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	R9	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	ey	1004	-	43,46,46	1.99	9 (20%)	49,67,67	3.04	15 (30%)
26	PEB	v3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	N8	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gu	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	z5	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	gu	202	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	ar	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	o7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dR	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	hN	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	A9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	k8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Y9	301	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	G4	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	D2	302	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	w2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	gq	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	3 (6%)
26	PEB	bN	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q6	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	a6	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	aY	402	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x8	202	10	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	Y9	304	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	8 (21%)
28	PUB	R4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	s2	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G6	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	c6	1001	10	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	eA	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	T9	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	F8	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	A8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ew	301	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	cw	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ld	201	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	m2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	L5	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	y8	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	z3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	L5	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	iE	1002	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	I7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	ed	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hY	401	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dx	402	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	dT	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aU	202	10	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	dO	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	F3	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	x4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	o5	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	T2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	r4	202	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	hC	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	i2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hC	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cm	1002	10	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	dh	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	K6	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	kU	1002	-	43,46,46	2.00	7 (16%)	45,67,67	1.52	6 (13%)
26	PEB	v4	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	dK	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	f2	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	ga	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hZ	402	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c7	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	J9	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	s3	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	Y7	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	eh	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	hE	1002	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	A2	1006	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	eb	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	8 (21%)
26	PEB	l8	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	z1	201	-	42,46,46	3.44	18 (42%)	50,67,67	3.40	25 (50%)
26	PEB	dn	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	J5	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	eu	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	i7	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.16	4 (8%)
26	PEB	eG	202	10	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	hT	204	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dJ	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	aE	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	fk	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
26	PEB	fh	1001	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	gg	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dR	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dd	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	w7	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	E9	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bP	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	ez	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	fc	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	dE	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	aT	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	eH	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	dg	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H3	202	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	lt	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	V4	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H3	201	-	43,46,46	1.69	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	D2	303	14	43,46,46	2.12	7 (16%)	49,67,67	2.81	19 (38%)
26	PEB	W6	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	c8	302	14	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	G2	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	t3	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	v5	202	-	43,46,46	2.00	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	e2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	hB	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
29	PVN	b8	1004	-	43,46,46	1.84	7 (16%)	49,67,67	2.88	11 (22%)
26	PEB	bP	202	-	43,46,46	2.01	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	lb	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	cD	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.16	3 (6%)
28	PUB	bs	1004	11	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
28	PUB	ln	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	PEB	B3	202	-	43,46,46	1.98	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	z2	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	es	202	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	es	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	cT	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	V9	203	-	42,46,46	2.29	9 (21%)	37,67,67	2.62	9 (24%)
28	PUB	ey	1005	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	n8	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
28	PUB	z4	203	-	42,46,46	2.28	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	M3	202	-	43,46,46	1.64	4 (9%)	45,67,67	1.17	4 (8%)
26	PEB	n2	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bm	1001	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	ft	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	h1	201	-	42,46,46	3.43	18 (42%)	50,67,67	3.39	25 (50%)
26	PEB	a8	602	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	H8	202	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	y6	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	a9	603	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
28	PUB	fy	202	-	42,46,46	2.28	9 (21%)	37,67,67	2.62	9 (24%)
26	PEB	p7	201	-	43,46,46	1.99	7 (16%)	45,67,67	1.51	6 (13%)
26	PEB	u2	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	q4	202	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	eq	201	-	43,46,46	1.70	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	bV	201	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
27	CYC	a1	201	-	42,46,46	3.40	14 (33%)	50,67,67	3.14	25 (50%)
26	PEB	kT	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.53	9 (20%)
28	PUB	ll	203	-	42,46,46	2.27	9 (21%)	37,67,67	2.61	9 (24%)
26	PEB	gc	201	-	43,46,46	1.72	4 (9%)	45,67,67	1.53	9 (20%)
26	PEB	kX	1001	-	43,46,46	1.71	4 (9%)	45,67,67	1.54	9 (20%)
26	PEB	dI	1002	-	43,46,46	1.70	4 (9%)	45,67,67	1.55	9 (20%)
26	PEB	as	202	-	43,46,46	1.65	4 (9%)	45,67,67	1.17	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	y2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	L7	201	-	-	7/24/74/74	0/4/4/4
26	PEB	ea	202	-	-	8/24/74/74	0/4/4/4
26	PEB	g3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	V7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	aD	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J3	202	-	-	7/24/74/74	0/4/4/4
28	PUB	Z7	203	11	-	7/24/74/74	0/4/4/4
26	PEB	W3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cG	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ev	201	11	-	8/24/74/74	0/4/4/4
28	PUB	x6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ai	201	-	-	8/24/74/74	0/4/4/4
26	PEB	f7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	au	202	-	-	8/24/74/74	0/4/4/4
26	PEB	kS	1001	-	-	8/24/74/74	0/4/4/4
27	CYC	n1	201	5	-	9/25/74/74	0/4/4/4
26	PEB	z6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	U4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hX	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ge	201	-	-	8/24/74/74	0/4/4/4
27	CYC	u1	1001	4	-	9/25/74/74	0/4/4/4
26	PEB	eK	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dK	203	-	-	7/24/74/74	0/4/4/4
29	PVN	dx	405	12	1/1/14/18	13/24/74/74	0/4/4/4
28	PUB	eY	405	-	-	7/24/74/74	0/4/4/4
26	PEB	r8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	gk	203	-	-	7/24/74/74	0/4/4/4
26	PEB	h6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	li	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Q4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cL	201	-	-	8/24/74/74	0/4/4/4
26	PEB	u4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dV	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jM	1001	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	gb	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	t4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	E4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	T8	301	-	-	8/24/74/74	0/4/4/4
28	PUB	dR	203	-	-	7/24/74/74	0/4/4/4
28	PUB	kW	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	bk	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aN	204	-	-	8/24/74/74	0/4/4/4
26	PEB	bG	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dd	203	-	-	7/24/74/74	0/4/4/4
26	PEB	j7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	ak	201	-	-	8/24/74/74	0/4/4/4
26	PEB	F8	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	O7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	eJ	202	-	-	7/24/74/74	0/4/4/4
28	PUB	a3	1006	-	-	7/24/74/74	0/4/4/4
26	PEB	e7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	hT	202	11	-	7/24/74/74	0/4/4/4
26	PEB	ec	201	-	-	8/24/74/74	0/4/4/4
26	PEB	li	202	-	-	8/24/74/74	0/4/4/4
26	PEB	S4	202	-	-	8/24/74/74	0/4/4/4
28	PUB	gt	203	-	-	7/24/74/74	0/4/4/4
28	PUB	ap	203	-	-	7/24/74/74	0/4/4/4
26	PEB	x9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bh	201	-	-	8/24/74/74	0/4/4/4
28	PUB	eR	203	11	-	7/24/74/74	0/4/4/4
28	PUB	at	203	11	-	7/24/74/74	0/4/4/4
28	PUB	v5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	y7	201	-	-	8/24/74/74	0/4/4/4
28	PUB	T7	203	-	-	7/24/74/74	0/4/4/4
28	PUB	dp	203	-	-	7/24/74/74	0/4/4/4
26	PEB	aM	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cs	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q8	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	Z6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	aN	203	-	-	7/24/74/74	0/4/4/4
26	PEB	y3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	e8	302	14	-	8/24/74/74	0/4/4/4
29	PVN	eY	403	-	1/1/14/18	17/24/74/74	0/4/4/4
26	PEB	a4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	Z3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	V6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hI	202	-	-	8/24/74/74	0/4/4/4
26	PEB	K2	201	10	-	8/24/74/74	0/4/4/4
26	PEB	u7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	v7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ga	202	-	-	7/24/74/74	0/4/4/4
28	PUB	bJ	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ag	201	-	-	8/24/74/74	0/4/4/4
27	CYC	Z1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	w7	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	s7	202	-	-	8/24/74/74	0/4/4/4
29	PVN	c9	303	-	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	X5	401	-	-	8/24/74/74	0/4/4/4
28	PUB	h8	203	-	-	7/24/74/74	0/4/4/4
28	PUB	X7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	S3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ej	202	-	-	8/24/74/74	0/4/4/4
28	PUB	c6	1004	-	-	7/24/74/74	0/4/4/4
26	PEB	bX	401	-	-	8/24/74/74	0/4/4/4
26	PEB	aw	201	-	-	8/24/74/74	0/4/4/4
28	PUB	J3	203	11	-	7/24/74/74	0/4/4/4
26	PEB	D7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cN	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cg	201	-	-	8/24/74/74	0/4/4/4
26	PEB	x3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	N6	202	-	-	8/24/74/74	0/4/4/4
29	PVN	aY	403	-	1/1/14/18	14/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	dW	201	-	-	8/24/74/74	0/4/4/4
26	PEB	N6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	R9	202	11	-	7/24/74/74	0/4/4/4
26	PEB	C2	302	-	-	8/24/74/74	0/4/4/4
26	PEB	D8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	V5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	lo	202	-	-	8/24/74/74	0/4/4/4
28	PUB	cN	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dc	203	-	-	8/24/74/74	0/4/4/4
26	PEB	ff	201	-	-	8/24/74/74	0/4/4/4
28	PUB	R5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	t3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	f6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	al	202	-	-	7/24/74/74	0/4/4/4
26	PEB	P8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	lp	203	-	-	7/24/74/74	0/4/4/4
28	PUB	V7	203	11	-	7/24/74/74	0/4/4/4
26	PEB	do	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dZ	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	U2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	d9	302	-	-	8/24/74/74	0/4/4/4
27	CYC	o1	1001	-	-	9/25/74/74	0/4/4/4
26	PEB	44	302	-	-	8/24/74/74	0/4/4/4
26	PEB	M5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cV	203	-	-	8/24/74/74	0/4/4/4
26	PEB	df	201	-	-	8/24/74/74	0/4/4/4
26	PEB	iC	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	bN	203	-	-	7/24/74/74	0/4/4/4
26	PEB	gg	201	-	-	8/24/74/74	0/4/4/4
26	PEB	n4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jI	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	lv	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fc	202	-	-	7/24/74/74	0/4/4/4
26	PEB	iA	1002	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	S5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	I5	202	-	-	8/24/74/74	0/4/4/4
28	PUB	e8	304	-	-	7/24/74/74	0/4/4/4
26	PEB	Q5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aa	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	lr	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hT	203	-	-	7/24/74/74	0/4/4/4
28	PUB	lb	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Q3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cP	201	-	-	8/24/74/74	0/4/4/4
26	PEB	P2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	ld	203	-	-	7/24/74/74	0/4/4/4
26	PEB	iF	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	bD	201	-	-	8/24/74/74	0/4/4/4
26	PEB	v8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	U8	1001	-	-	8/24/74/74	0/4/4/4
29	PVN	hZ	403	-	1/1/14/18	12/24/74/74	0/4/4/4
26	PEB	lk	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eV	202	-	-	7/24/74/74	0/4/4/4
27	CYC	P1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	aI	202	10	-	8/24/74/74	0/4/4/4
28	PUB	t4	203	-	-	7/24/74/74	0/4/4/4
28	PUB	cr	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ao	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cH	201	-	-	7/24/74/74	0/4/4/4
26	PEB	H7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	m7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	f8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	X2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dN	201	-	-	8/24/74/74	0/4/4/4
26	PEB	M4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	m9	1001	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	r5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	C9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	J2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	E4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	j6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	D9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	y4	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	ei	201	-	-	8/24/74/74	0/4/4/4
26	PEB	M6	1001	10	-	8/24/74/74	0/4/4/4
26	PEB	F6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cS	202	-	-	8/24/74/74	0/4/4/4
28	PUB	bY	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	dp	201	-	-	8/24/74/74	0/4/4/4
28	PUB	c3	305	-	-	7/24/74/74	0/4/4/4
26	PEB	bO	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aS	202	10	-	8/24/74/74	0/4/4/4
27	CYC	d1	1001	-	-	9/25/74/74	0/4/4/4
26	PEB	m2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	N5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bv	202	10	-	8/24/74/74	0/4/4/4
26	PEB	eS	202	10	-	8/24/74/74	0/4/4/4
26	PEB	ek	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	aF	202	-	-	7/24/74/74	0/4/4/4
26	PEB	hG	201	-	-	7/24/74/74	0/4/4/4
28	PUB	kR	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	V5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eP	201	-	-	8/24/74/74	0/4/4/4
29	PVN	d3	302	-	1/1/14/18	18/24/74/74	0/4/4/4
26	PEB	c6	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	j6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	lq	202	-	-	8/24/74/74	0/4/4/4
28	PUB	jM	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	cb	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	I7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	B1	301	-	-	7/24/74/74	0/4/4/4
26	PEB	ds	202	-	-	8/24/74/74	0/4/4/4
26	PEB	J6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	d9	301	-	-	8/24/74/74	0/4/4/4
26	PEB	t9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	jM	1002	-	-	7/24/74/74	0/4/4/4
28	PUB	ga	203	-	-	7/24/74/74	0/4/4/4
26	PEB	gv	202	-	-	7/24/74/74	0/4/4/4
26	PEB	h8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eO	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gg	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cB	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dK	201	-	-	8/24/74/74	0/4/4/4
26	PEB	F7	201	-	-	7/24/74/74	0/4/4/4
26	PEB	cX	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cb	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cM	202	-	-	8/24/74/74	0/4/4/4
26	PEB	C4	1001	-	-	8/24/74/74	0/4/4/4
27	CYC	g1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	q6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aC	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hB	203	-	-	7/24/74/74	0/4/4/4
26	PEB	iD	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	cz	202	-	-	7/24/74/74	0/4/4/4
26	PEB	j7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Y3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	em	201	-	-	8/24/74/74	0/4/4/4
28	PUB	Y5	1006	-	-	7/24/74/74	0/4/4/4
28	PUB	x3	203	11	-	7/24/74/74	0/4/4/4
26	PEB	cJ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	kQ	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	N6	203	-	-	7/24/74/74	0/4/4/4
28	PUB	cq	203	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	A4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	e9	301	-	-	8/24/74/74	0/4/4/4
28	PUB	D6	202	11	-	7/24/74/74	0/4/4/4
26	PEB	la	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	I2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gy	303	-	-	8/24/74/74	0/4/4/4
26	PEB	d8	301	-	-	8/24/74/74	0/4/4/4
26	PEB	dd	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dm	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dA	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eF	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fx	202	10	-	8/24/74/74	0/4/4/4
26	PEB	aq	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ln	202	-	-	7/24/74/74	0/4/4/4
26	PEB	gk	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gt	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jJ	1002	11	-	7/24/74/74	0/4/4/4
26	PEB	S7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	lt	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dx	406	-	-	7/24/74/74	0/4/4/4
26	PEB	br	202	-	-	8/24/74/74	0/4/4/4
26	PEB	b9	403	12	-	8/24/74/74	0/4/4/4
26	PEB	z4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	w9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	v5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	a6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lu	201	-	-	8/24/74/74	0/4/4/4
27	CYC	e1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	kW	1002	-	-	7/24/74/74	0/4/4/4
27	CYC	G1	1001	-	-	9/25/74/74	0/4/4/4
27	CYC	J1	201	5	-	10/25/74/74	0/4/4/4
28	PUB	y7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cx	202	10	-	8/24/74/74	0/4/4/4
26	PEB	gc	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	y9	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	p6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	v6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	I8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	X4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	U8	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	M8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	fq	203	-	-	7/24/74/74	0/4/4/4
26	PEB	k7	1001	10	-	8/24/74/74	0/4/4/4
26	PEB	H8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dF	202	-	-	8/24/74/74	0/4/4/4
26	PEB	X6	202	-	-	7/24/74/74	0/4/4/4
28	PUB	V6	203	-	-	7/24/74/74	0/4/4/4
28	PUB	aH	203	-	-	7/24/74/74	0/4/4/4
26	PEB	r6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hP	201	-	-	8/24/74/74	0/4/4/4
26	PEB	du	202	-	-	8/24/74/74	0/4/4/4
28	PUB	D9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	P4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	U8	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	ge	203	-	-	7/24/74/74	0/4/4/4
28	PUB	dw	405	-	-	7/24/74/74	0/4/4/4
26	PEB	aY	401	-	-	8/24/74/74	0/4/4/4
26	PEB	go	202	10	-	8/24/74/74	0/4/4/4
26	PEB	bn	201	-	-	8/24/74/74	0/4/4/4
26	PEB	S2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	K7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	P2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	y2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dI	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	fl	201	-	-	8/24/74/74	0/4/4/4
28	PUB	x5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cO	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	ea	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dH	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lp	201	-	-	8/24/74/74	0/4/4/4
26	PEB	a3	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	aT	202	-	-	8/24/74/74	0/4/4/4
26	PEB	V7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	s6	202	-	-	8/24/74/74	0/4/4/4
29	PVN	A2	1004	-	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	D6	201	11	-	8/24/74/74	0/4/4/4
26	PEB	M2	202	10	-	8/24/74/74	0/4/4/4
26	PEB	I4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cG	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hY	402	-	-	8/24/74/74	0/4/4/4
27	CYC	U1	201	5	-	9/25/74/74	0/4/4/4
26	PEB	a8	601	-	-	8/24/74/74	0/4/4/4
26	PEB	g6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aK	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	dL	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gh	201	-	-	8/24/74/74	0/4/4/4
27	CYC	p1	201	-	-	10/25/74/74	0/4/4/4
28	PUB	D5	203	11	-	7/24/74/74	0/4/4/4
28	PUB	ec	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cP	202	-	-	8/24/74/74	0/4/4/4
26	PEB	jP	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	aB	202	-	-	8/24/74/74	0/4/4/4
28	PUB	X3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cR	201	-	-	8/24/74/74	0/4/4/4
26	PEB	v9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	Z5	306	-	-	7/24/74/74	0/4/4/4
26	PEB	lp	202	-	-	7/24/74/74	0/4/4/4
26	PEB	b9	402	-	-	8/24/74/74	0/4/4/4
26	PEB	lb	201	-	-	8/24/74/74	0/4/4/4
26	PEB	C6	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	h6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	cD	201	-	-	8/24/74/74	0/4/4/4
26	PEB	j2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bd	201	18	-	8/24/74/74	0/4/4/4
28	PUB	cz	203	-	-	7/24/74/74	0/4/4/4
28	PUB	U8	1006	-	-	7/24/74/74	0/4/4/4
26	PEB	p8	202	-	-	7/24/74/74	0/4/4/4
28	PUB	cs	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hQ	202	-	-	8/24/74/74	0/4/4/4
26	PEB	lw	202	-	-	8/24/74/74	0/4/4/4
28	PUB	d6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	lr	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bM	202	10	-	8/24/74/74	0/4/4/4
26	PEB	M6	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	F9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cr	201	-	-	8/24/74/74	0/4/4/4
26	PEB	B9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	D2	301	-	-	8/24/74/74	0/4/4/4
26	PEB	Q6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	B7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	er	202	-	-	7/24/74/74	0/4/4/4
26	PEB	le	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gb	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	E5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	d5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	f9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	G5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	w5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	C8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hT	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ek	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	L4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	E7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bd	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	hD	203	-	-	7/24/74/74	0/4/4/4
26	PEB	F3	202	-	-	7/24/74/74	0/4/4/4
28	PUB	x4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	t7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eN	201	-	-	8/24/74/74	0/4/4/4
28	PUB	P6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	W3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	j3	201	-	-	7/24/74/74	0/4/4/4
26	PEB	bs	1003	-	-	8/24/74/74	0/4/4/4
28	PUB	H2	202	11	-	7/24/74/74	0/4/4/4
26	PEB	aH	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ay	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	z8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cK	202	-	-	8/24/74/74	0/4/4/4
26	PEB	f8	202	-	-	8/24/74/74	0/4/4/4
28	PUB	gz	306	-	-	7/24/74/74	0/4/4/4
28	PUB	c3	304	-	-	7/24/74/74	0/4/4/4
26	PEB	s4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fz	301	-	-	8/24/74/74	0/4/4/4
26	PEB	i3	203	-	-	7/24/74/74	0/4/4/4
28	PUB	D7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cl	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aS	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cn	201	-	-	7/24/74/74	0/4/4/4
26	PEB	o3	202	10	-	8/24/74/74	0/4/4/4
26	PEB	az	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bU	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dc	202	-	-	8/24/74/74	0/4/4/4
26	PEB	di	202	-	-	7/24/74/74	0/4/4/4
26	PEB	C4	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	M7	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	B2	501	-	-	8/24/74/74	0/4/4/4
26	PEB	O8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cB	202	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	s3	202	-	-	8/24/74/74	0/4/4/4
28	PUB	fj	203	11	-	7/24/74/74	0/4/4/4
26	PEB	kQ	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	N3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	R3	203	-	-	7/24/74/74	0/4/4/4
28	PUB	X6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cV	202	10	-	8/24/74/74	0/4/4/4
26	PEB	aW	302	-	-	8/24/74/74	0/4/4/4
26	PEB	dL	202	-	-	7/24/74/74	0/4/4/4
26	PEB	aE	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ej	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aj	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fa	201	-	-	8/24/74/74	0/4/4/4
26	PEB	a7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	A9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	u5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gl	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gn	201	-	-	8/24/74/74	0/4/4/4
26	PEB	x3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	N2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	A5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	y7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	lo	201	10	-	8/24/74/74	0/4/4/4
26	PEB	w6	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	lh	201	11	-	8/24/74/74	0/4/4/4
27	CYC	Y1	201	-	-	10/25/74/74	0/4/4/4
26	PEB	gx	202	-	-	7/24/74/74	0/4/4/4
28	PUB	cP	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Z8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	P2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	N4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	h9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Z9	1003	12	-	8/24/74/74	0/4/4/4
26	PEB	bb	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	cE	203	-	-	7/24/74/74	0/4/4/4
28	PUB	F4	203	-	-	7/24/74/74	0/4/4/4
28	PUB	ar	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cZ	202	-	-	8/24/74/74	0/4/4/4
28	PUB	bD	203	-	-	7/24/74/74	0/4/4/4
26	PEB	i5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	p3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cy	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	H9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	db	201	-	-	8/24/74/74	0/4/4/4
28	PUB	N5	203	-	-	7/24/74/74	0/4/4/4
28	PUB	H7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	R4	202	-	-	8/24/74/74	0/4/4/4
28	PUB	dN	203	-	-	7/24/74/74	0/4/4/4
26	PEB	M5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Z9	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	fo	201	-	-	8/24/74/74	0/4/4/4
26	PEB	T9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	B6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Z3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	z2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aA	201	-	-	8/24/74/74	0/4/4/4
26	PEB	I5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	ei	203	-	-	7/24/74/74	0/4/4/4
26	PEB	g5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bl	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Q3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bC	202	-	-	8/24/74/74	0/4/4/4
26	PEB	u6	201	10	-	8/24/74/74	0/4/4/4
28	PUB	44	304	-	-	7/24/74/74	0/4/4/4
26	PEB	T2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	fq	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	K5	1001	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	e6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Y2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hW	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Y2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	E6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ao	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eA	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	m7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	L8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	c7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	et	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bx	201	-	-	8/24/74/74	0/4/4/4
26	PEB	by	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	an	202	-	-	7/24/74/74	0/4/4/4
27	CYC	b2	1001	8	-	10/25/74/74	0/4/4/4
26	PEB	I9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ll	202	-	-	7/24/74/74	0/4/4/4
26	PEB	N3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	gw	201	-	-	8/24/74/74	0/4/4/4
28	PUB	J6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dl	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dM	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	U5	202	-	-	8/24/74/74	0/4/4/4
29	PVN	aZ	303	-	1/1/14/18	14/24/74/74	0/4/4/4
28	PUB	F3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eB	203	-	-	7/24/74/74	0/4/4/4
26	PEB	kV	1002	-	-	7/24/74/74	0/4/4/4
28	PUB	eV	203	-	-	7/24/74/74	0/4/4/4
28	PUB	t2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	b6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	ax	202	-	-	7/24/74/74	0/4/4/4
26	PEB	O4	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	K8	203	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	ev	203	11	-	7/24/74/74	0/4/4/4
26	PEB	u3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	D3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bH	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Y7	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	Q7	201	-	-	8/24/74/74	0/4/4/4
28	PUB	P4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	o8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aC	202	-	-	8/24/74/74	0/4/4/4
26	PEB	co	201	-	-	7/24/74/74	0/4/4/4
28	PUB	cM	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bv	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fr	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bs	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	gm	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	x2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	U4	202	-	-	8/24/74/74	0/4/4/4
29	PVN	ez	1004	-	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	dr	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hB	202	-	-	7/24/74/74	0/4/4/4
26	PEB	B4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	X6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	24	401	-	-	8/24/74/74	0/4/4/4
26	PEB	l7	202	-	-	7/24/74/74	0/4/4/4
28	PUB	n9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	fu	201	-	-	7/24/74/74	0/4/4/4
26	PEB	ch	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bI	202	10	-	8/24/74/74	0/4/4/4
26	PEB	kV	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	R6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ey	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	w8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ft	202	-	-	8/24/74/74	0/4/4/4
27	CYC	j1	201	-	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	bq	203	11	-	7/24/74/74	0/4/4/4
28	PUB	P5	202	-	-	7/24/74/74	0/4/4/4
28	PUB	l6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	V9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bG	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cz	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gp	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ce	201	-	-	8/24/74/74	0/4/4/4
28	PUB	x9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	e4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lz	401	23	-	8/24/74/74	0/4/4/4
28	PUB	L6	202	-	-	7/24/74/74	0/4/4/4
26	PEB	q7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lw	203	-	-	7/24/74/74	0/4/4/4
26	PEB	C8	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bs	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	hY	403	-	-	8/24/74/74	0/4/4/4
28	PUB	bY	1006	-	-	7/24/74/74	0/4/4/4
28	PUB	L7	202	-	-	7/24/74/74	0/4/4/4
28	PUB	V3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dT	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ld	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ap	202	11	-	7/24/74/74	0/4/4/4
26	PEB	O2	202	-	-	8/24/74/74	0/4/4/4
29	PVN	b9	405	-	1/1/14/18	17/24/74/74	0/4/4/4
26	PEB	hZ	401	-	-	8/24/74/74	0/4/4/4
28	PUB	n2	203	-	-	7/24/74/74	0/4/4/4
28	PUB	er	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Y8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eR	202	-	-	8/24/74/74	0/4/4/4
28	PUB	l3	202	-	-	7/24/74/74	0/4/4/4
28	PUB	F2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	d6	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	L4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	lg	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ei	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bo	201	-	-	8/24/74/74	0/4/4/4
26	PEB	P9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	fb	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dp	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hW	202	-	-	8/24/74/74	0/4/4/4
26	PEB	g3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	r4	201	11	-	7/24/74/74	0/4/4/4
28	PUB	hP	203	-	-	7/24/74/74	0/4/4/4
26	PEB	u7	202	-	-	8/24/74/74	0/4/4/4
28	PUB	44	305	-	-	7/24/74/74	0/4/4/4
26	PEB	B4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	fw	203	-	-	7/24/74/74	0/4/4/4
28	PUB	r2	203	-	-	7/24/74/74	0/4/4/4
28	PUB	fa	202	-	-	7/24/74/74	0/4/4/4
27	CYC	R1	1001	-	-	9/25/74/74	0/4/4/4
26	PEB	Y5	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	R7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	x6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	K4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	W7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	cI	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	W4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aX	402	11	-	8/24/74/74	0/4/4/4
26	PEB	cI	202	-	-	8/24/74/74	0/4/4/4
26	PEB	N8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ep	202	-	-	7/24/74/74	0/4/4/4
26	PEB	44	301	-	-	8/24/74/74	0/4/4/4
26	PEB	h8	202	11	-	7/24/74/74	0/4/4/4
26	PEB	w6	1002	10	-	8/24/74/74	0/4/4/4
27	CYC	b1	1001	-	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	cj	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dW	202	-	-	8/24/74/74	0/4/4/4
26	PEB	m5	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	av	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dz	401	-	-	8/24/74/74	0/4/4/4
28	PUB	N3	203	-	-	7/24/74/74	0/4/4/4
28	PUB	dL	203	-	-	7/24/74/74	0/4/4/4
26	PEB	K8	201	-	-	8/24/74/74	0/4/4/4
27	CYC	H1	201	-	-	10/25/74/74	0/4/4/4
26	PEB	ax	201	-	-	7/24/74/74	0/4/4/4
26	PEB	R2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	a7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	w2	202	-	-	8/24/74/74	0/4/4/4
28	PUB	bZ	306	-	-	7/24/74/74	0/4/4/4
26	PEB	fj	201	-	-	8/24/74/74	0/4/4/4
28	PUB	T8	305	-	-	7/24/74/74	0/4/4/4
26	PEB	R3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	Z9	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	hR	201	-	-	8/24/74/74	0/4/4/4
26	PEB	R3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	e9	306	-	-	7/24/74/74	0/4/4/4
26	PEB	bB	202	-	-	7/24/74/74	0/4/4/4
28	PUB	o8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Q2	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	P3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ef	201	-	-	8/24/74/74	0/4/4/4
26	PEB	af	201	-	-	8/24/74/74	0/4/4/4
26	PEB	n5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	Z5	301	-	-	8/24/74/74	0/4/4/4
28	PUB	lr	203	-	-	7/24/74/74	0/4/4/4
28	PUB	hV	203	-	-	7/24/74/74	0/4/4/4
26	PEB	M2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	o6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	M9	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	aA	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dy	401	-	-	8/24/74/74	0/4/4/4
26	PEB	bp	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	K9	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	C8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bw	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dX	203	-	-	7/24/74/74	0/4/4/4
28	PUB	b8	1005	12	-	7/24/74/74	0/4/4/4
28	PUB	eX	202	-	-	7/24/74/74	0/4/4/4
26	PEB	A1	301	1	-	7/24/74/74	0/4/4/4
26	PEB	T7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	aK	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	K3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fv	201	-	-	8/24/74/74	0/4/4/4
28	PUB	d7	203	11	-	7/24/74/74	0/4/4/4
26	PEB	e7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ba	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	w3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	h4	201	-	-	8/24/74/74	0/4/4/4
27	CYC	f1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	aN	202	-	-	8/24/74/74	0/4/4/4
26	PEB	by	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	G8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ea	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eE	201	-	-	8/24/74/74	0/4/4/4
28	PUB	C2	304	-	-	7/24/74/74	0/4/4/4
26	PEB	hQ	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dj	203	-	-	7/24/74/74	0/4/4/4
26	PEB	F9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	P6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gy	302	-	-	8/24/74/74	0/4/4/4
28	PUB	iF	1003	11	-	7/24/74/74	0/4/4/4
26	PEB	bJ	202	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	S9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	34	1003	-	-	8/24/74/74	0/4/4/4
28	PUB	p9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	m6	202	-	-	8/24/74/74	0/4/4/4
29	PVN	d8	303	14	1/1/14/18	14/24/74/74	0/4/4/4
26	PEB	W6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	L5	203	-	-	7/24/74/74	0/4/4/4
27	CYC	X1	201	-	-	9/25/74/74	0/4/4/4
28	PUB	dn	203	-	-	7/24/74/74	0/4/4/4
29	PVN	dw	404	-	1/1/14/18	14/24/74/74	0/4/4/4
26	PEB	Z5	303	-	-	8/24/74/74	0/4/4/4
28	PUB	z3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	iF	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	Y5	1003	12	-	8/24/74/74	0/4/4/4
28	PUB	p5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	34	1001	-	-	7/24/74/74	0/4/4/4
26	PEB	N9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	hS	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dZ	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	x5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cd	201	18	-	8/24/74/74	0/4/4/4
28	PUB	kS	1003	-	-	7/24/74/74	0/4/4/4
28	PUB	b6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cR	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bz	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bX	402	-	-	8/24/74/74	0/4/4/4
26	PEB	eU	202	-	-	8/24/74/74	0/4/4/4
26	PEB	F6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J6	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dr	202	11	-	8/24/74/74	0/4/4/4
26	PEB	x2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	O6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	D2	304	-	-	7/24/74/74	0/4/4/4
26	PEB	J4	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	cX	202	-	-	8/24/74/74	0/4/4/4
26	PEB	n3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eK	202	-	-	8/24/74/74	0/4/4/4
28	PUB	34	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	K8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	L3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ch	202	-	-	7/24/74/74	0/4/4/4
28	PUB	gx	203	-	-	7/24/74/74	0/4/4/4
26	PEB	O8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dX	202	-	-	8/24/74/74	0/4/4/4
29	PVN	Y9	303	-	1/1/14/18	15/24/74/74	0/4/4/4
28	PUB	p3	203	-	-	7/24/74/74	0/4/4/4
28	PUB	cJ	203	-	-	7/24/74/74	0/4/4/4
26	PEB	lq	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dD	203	-	-	7/24/74/74	0/4/4/4
26	PEB	h5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	s2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	lf	203	-	-	7/24/74/74	0/4/4/4
26	PEB	e4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	t5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bD	202	-	-	7/24/74/74	0/4/4/4
26	PEB	f6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	dm	202	-	-	8/24/74/74	0/4/4/4
28	PUB	bo	202	-	-	7/24/74/74	0/4/4/4
28	PUB	dB	202	-	-	7/24/74/74	0/4/4/4
28	PUB	jL	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	L3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cu	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k6	1001	10	-	8/24/74/74	0/4/4/4
26	PEB	z9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bu	201	-	-	8/24/74/74	0/4/4/4
26	PEB	f3	202	-	-	7/24/74/74	0/4/4/4
28	PUB	aV	203	-	-	7/24/74/74	0/4/4/4
29	PVN	d9	304	14	1/1/14/18	14/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	y5	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	S8	401	11	-	8/24/74/74	0/4/4/4
26	PEB	N7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bY	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	dY	201	-	-	8/24/74/74	0/4/4/4
26	PEB	V3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bM	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bq	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fp	202	-	-	8/24/74/74	0/4/4/4
28	PUB	P9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	fp	201	-	-	8/24/74/74	0/4/4/4
27	CYC	N1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	k5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	jO	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	e8	301	-	-	8/24/74/74	0/4/4/4
26	PEB	et	202	-	-	7/24/74/74	0/4/4/4
28	PUB	aZ	304	-	-	7/24/74/74	0/4/4/4
26	PEB	Y5	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	av	202	-	-	7/24/74/74	0/4/4/4
26	PEB	G3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Y4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dY	202	-	-	7/24/74/74	0/4/4/4
26	PEB	kR	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	cs	202	-	-	7/24/74/74	0/4/4/4
26	PEB	j8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	lj	201	-	-	8/24/74/74	0/4/4/4
26	PEB	r2	201	-	-	8/24/74/74	0/4/4/4
27	CYC	r1	201	-	-	10/25/74/74	0/4/4/4
28	PUB	dt	203	-	-	7/24/74/74	0/4/4/4
26	PEB	W3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	lo	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bH	202	-	-	7/24/74/74	0/4/4/4
28	PUB	b9	406	12	-	7/24/74/74	0/4/4/4
28	PUB	h3	202	11	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	u9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	r9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dG	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q9	202	-	-	8/24/74/74	0/4/4/4
28	PUB	Y9	305	-	-	7/24/74/74	0/4/4/4
26	PEB	jL	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	j5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	j5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	d9	305	-	-	7/24/74/74	0/4/4/4
26	PEB	aw	202	-	-	8/24/74/74	0/4/4/4
26	PEB	g5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bj	202	-	-	8/24/74/74	0/4/4/4
28	PUB	cR	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bQ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	y9	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	em	202	-	-	8/24/74/74	0/4/4/4
28	PUB	c8	305	-	-	7/24/74/74	0/4/4/4
26	PEB	W2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cV	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ff	202	-	-	7/24/74/74	0/4/4/4
26	PEB	U6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	b8	1001	12	-	8/24/74/74	0/4/4/4
26	PEB	P8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ds	201	-	-	8/24/74/74	0/4/4/4
26	PEB	n3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dA	202	-	-	8/24/74/74	0/4/4/4
26	PEB	am	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	r8	202	-	-	8/24/74/74	0/4/4/4
28	PUB	j2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	i6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gt	202	-	-	7/24/74/74	0/4/4/4
26	PEB	o8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	S7	202	-	-	8/24/74/74	0/4/4/4
27	CYC	i1	1001	-	-	9/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	dP	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hN	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dw	403	-	-	8/24/74/74	0/4/4/4
26	PEB	c9	302	-	-	8/24/74/74	0/4/4/4
26	PEB	cm	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	bi	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cQ	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dr	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bh	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aR	201	-	-	8/24/74/74	0/4/4/4
28	PUB	kQ	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	l5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cZ	201	-	-	8/24/74/74	0/4/4/4
28	PUB	J4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ab	202	-	-	7/24/74/74	0/4/4/4
26	PEB	K3	202	-	-	8/24/74/74	0/4/4/4
28	PUB	eY	404	-	-	7/24/74/74	0/4/4/4
26	PEB	V6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	c4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	eZ	403	-	-	7/24/74/74	0/4/4/4
26	PEB	W8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bY	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	dT	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hX	201	-	-	8/24/74/74	0/4/4/4
26	PEB	r5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bF	201	-	-	8/24/74/74	0/4/4/4
26	PEB	I3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dz	402	-	-	8/24/74/74	0/4/4/4
26	PEB	R4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bp	202	-	-	7/24/74/74	0/4/4/4
26	PEB	Q8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bI	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eC	201	-	-	8/24/74/74	0/4/4/4
28	PUB	t5	203	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	cp	203	-	-	7/24/74/74	0/4/4/4
26	PEB	d3	301	-	-	8/24/74/74	0/4/4/4
26	PEB	eB	202	-	-	8/24/74/74	0/4/4/4
26	PEB	I9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cS	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ls	202	-	-	8/24/74/74	0/4/4/4
26	PEB	V9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	p6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	s8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Z6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	B4	203	11	-	7/24/74/74	0/4/4/4
27	CYC	k1	201	-	-	9/25/74/74	0/4/4/4
28	PUB	aF	203	-	-	7/24/74/74	0/4/4/4
27	CYC	O1	201	-	-	9/25/74/74	0/4/4/4
28	PUB	eL	203	-	-	7/24/74/74	0/4/4/4
27	CYC	s1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	Z2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	K2	202	10	-	8/24/74/74	0/4/4/4
26	PEB	D7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ap	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jK	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	bc	201	-	-	8/24/74/74	0/4/4/4
26	PEB	W7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fd	301	-	-	8/24/74/74	0/4/4/4
28	PUB	P3	203	-	-	7/24/74/74	0/4/4/4
28	PUB	34	1006	12	-	7/24/74/74	0/4/4/4
26	PEB	u2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eu	202	-	-	8/24/74/74	0/4/4/4
28	PUB	av	203	11	-	7/24/74/74	0/4/4/4
26	PEB	b4	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	d4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hS	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eT	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	aN	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gf	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cY	201	-	-	8/24/74/74	0/4/4/4
26	PEB	U2	202	-	-	8/24/74/74	0/4/4/4
28	PUB	ez	1006	-	-	7/24/74/74	0/4/4/4
28	PUB	R2	203	11	-	7/24/74/74	0/4/4/4
28	PUB	a7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	j9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gd	201	-	-	7/24/74/74	0/4/4/4
26	PEB	gh	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eI	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ey	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	gp	202	-	-	7/24/74/74	0/4/4/4
26	PEB	y5	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	c8	304	-	-	7/24/74/74	0/4/4/4
26	PEB	h5	202	-	-	8/24/74/74	0/4/4/4
29	PVN	T8	303	-	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	e9	302	-	-	8/24/74/74	0/4/4/4
26	PEB	o7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bJ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k6	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	eF	203	-	-	7/24/74/74	0/4/4/4
28	PUB	gz	305	-	-	7/24/74/74	0/4/4/4
26	PEB	K4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aF	204	-	-	8/24/74/74	0/4/4/4
26	PEB	dD	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jK	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	ec	202	-	-	7/24/74/74	0/4/4/4
26	PEB	b7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fs	202	-	-	7/24/74/74	0/4/4/4
28	PUB	A2	1005	12	-	7/24/74/74	0/4/4/4
26	PEB	X7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	br	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fd	302	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	bm	1002	10	-	8/24/74/74	0/4/4/4
29	PVN	a3	1004	-	1/1/14/18	15/24/74/74	0/4/4/4
27	CYC	W1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	C7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	iA	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	bV	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cJ	202	-	-	7/24/74/74	0/4/4/4
26	PEB	w4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dx	401	-	-	8/24/74/74	0/4/4/4
26	PEB	aQ	201	-	-	8/24/74/74	0/4/4/4
28	PUB	v3	203	-	-	7/24/74/74	0/4/4/4
29	PVN	bY	1004	-	1/1/14/18	14/24/74/74	0/4/4/4
26	PEB	ad	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bu	202	-	-	8/24/74/74	0/4/4/4
28	PUB	gr	202	-	-	7/24/74/74	0/4/4/4
26	PEB	i2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	A2	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	d9	303	-	-	8/24/74/74	0/4/4/4
26	PEB	i4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	aY	404	-	-	7/24/74/74	0/4/4/4
26	PEB	eN	202	-	-	7/24/74/74	0/4/4/4
26	PEB	b9	404	-	-	8/24/74/74	0/4/4/4
26	PEB	kR	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	eZ	401	22	-	8/24/74/74	0/4/4/4
26	PEB	H9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	n5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	H7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	p2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eM	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	F9	203	-	-	7/24/74/74	0/4/4/4
28	PUB	bL	203	-	-	7/24/74/74	0/4/4/4
26	PEB	g4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	B8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ed	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	C2	301	-	-	8/24/74/74	0/4/4/4
26	PEB	fe	201	-	-	8/24/74/74	0/4/4/4
26	PEB	x7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gz	302	-	-	8/24/74/74	0/4/4/4
26	PEB	O2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	di	203	-	-	7/24/74/74	0/4/4/4
28	PUB	H6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	k3	202	10	-	8/24/74/74	0/4/4/4
26	PEB	cl	202	-	-	7/24/74/74	0/4/4/4
28	PUB	dv	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cf	201	-	-	7/24/74/74	0/4/4/4
26	PEB	E9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	T7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	el	202	-	-	7/24/74/74	0/4/4/4
26	PEB	U5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	K9	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	P9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	P7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	iD	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	eQ	202	-	-	8/24/74/74	0/4/4/4
26	PEB	be	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bx	202	10	-	8/24/74/74	0/4/4/4
26	PEB	M8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	J8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bT	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dh	202	-	-	7/24/74/74	0/4/4/4
26	PEB	P6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	r9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	s5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dk	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	S9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aY	406	-	-	8/24/74/74	0/4/4/4
28	PUB	Z2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	g8	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	m6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	K7	202	-	-	8/24/74/74	0/4/4/4
28	PUB	O8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	k2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	da	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	ci	201	-	-	8/24/74/74	0/4/4/4
26	PEB	N4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	h9	202	-	-	8/24/74/74	0/4/4/4
28	PUB	ez	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	dC	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aZ	302	-	-	8/24/74/74	0/4/4/4
28	PUB	t7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	w8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	f9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	g9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	ly	405	-	-	7/24/74/74	0/4/4/4
26	PEB	F4	202	-	-	8/24/74/74	0/4/4/4
27	CYC	t1	201	-	-	10/25/74/74	0/4/4/4
26	PEB	c4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	R5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	iH	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	w2	203	-	-	8/24/74/74	0/4/4/4
26	PEB	fk	201	-	-	8/24/74/74	0/4/4/4
28	PUB	jK	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	U3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	U3	201	-	-	8/24/74/74	0/4/4/4
27	CYC	y1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	bE	202	10	-	8/24/74/74	0/4/4/4
26	PEB	aL	202	-	-	8/24/74/74	0/4/4/4
28	PUB	Z9	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	y6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aQ	202	-	-	8/24/74/74	0/4/4/4
28	PUB	eg	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eP	203	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	fs	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Q6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fq	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cp	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	S5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	t8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ah	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q4	201	-	-	8/24/74/74	0/4/4/4
29	PVN	44	303	14	1/1/14/18	17/24/74/74	0/4/4/4
26	PEB	aJ	201	-	-	8/24/74/74	0/4/4/4
28	PUB	Z4	203	-	-	7/24/74/74	0/4/4/4
28	PUB	c9	305	-	-	7/24/74/74	0/4/4/4
26	PEB	u8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ff	204	-	-	8/24/74/74	0/4/4/4
28	PUB	Z6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	B6	202	-	-	7/24/74/74	0/4/4/4
26	PEB	C3	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	fi	203	-	-	7/24/74/74	0/4/4/4
26	PEB	i7	201	-	-	8/24/74/74	0/4/4/4
28	PUB	L2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	v2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	T2	203	-	-	7/24/74/74	0/4/4/4
28	PUB	v7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	m4	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	fg	202	-	-	8/24/74/74	0/4/4/4
28	PUB	B5	203	-	-	7/24/74/74	0/4/4/4
28	PUB	p2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	E2	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	en	202	-	-	7/24/74/74	0/4/4/4
26	PEB	X8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	c3	301	-	-	8/24/74/74	0/4/4/4
26	PEB	ey	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	L9	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	ev	202	-	-	7/24/74/74	0/4/4/4
26	PEB	y4	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	e5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aB	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bP	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eJ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	j8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	el	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ez	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	S6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	cW	202	-	-	8/24/74/74	0/4/4/4
26	PEB	U7	202	-	-	8/24/74/74	0/4/4/4
28	PUB	D3	203	-	-	7/24/74/74	0/4/4/4
28	PUB	ey	1006	-	-	7/24/74/74	0/4/4/4
26	PEB	A5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aq	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	R6	202	-	-	7/24/74/74	0/4/4/4
28	PUB	z7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	V8	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	le	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aM	202	10	-	8/24/74/74	0/4/4/4
26	PEB	bW	301	-	-	8/24/74/74	0/4/4/4
26	PEB	aV	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eY	402	-	-	8/24/74/74	0/4/4/4
26	PEB	O7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	z7	201	-	-	8/24/74/74	0/4/4/4
28	PUB	A8	203	-	-	7/24/74/74	0/4/4/4
28	PUB	ee	203	-	-	7/24/74/74	0/4/4/4
26	PEB	gz	301	-	-	8/24/74/74	0/4/4/4
26	PEB	hV	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eH	202	-	-	8/24/74/74	0/4/4/4
26	PEB	G7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	V3	202	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	ad	202	-	-	7/24/74/74	0/4/4/4
26	PEB	D4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	x9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eM	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	N2	202	-	-	8/24/74/74	0/4/4/4
28	PUB	Q8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	B2	502	-	-	8/24/74/74	0/4/4/4
26	PEB	b5	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	w8	203	-	-	7/24/74/74	0/4/4/4
27	CYC	m1	201	-	-	9/25/74/74	0/4/4/4
28	PUB	T8	304	-	-	7/24/74/74	0/4/4/4
26	PEB	Y8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cL	202	-	-	7/24/74/74	0/4/4/4
26	PEB	r7	201	-	-	8/24/74/74	0/4/4/4
27	CYC	S1	202	-	-	10/25/74/74	0/4/4/4
26	PEB	fy	201	-	-	7/24/74/74	0/4/4/4
26	PEB	g7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fe	202	-	-	8/24/74/74	0/4/4/4
26	PEB	x7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cc	201	-	-	8/24/74/74	0/4/4/4
26	PEB	a9	602	-	-	8/24/74/74	0/4/4/4
26	PEB	M4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	c6	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	ae	201	-	-	8/24/74/74	0/4/4/4
28	PUB	e6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ah	202	-	-	7/24/74/74	0/4/4/4
26	PEB	Y9	302	-	-	8/24/74/74	0/4/4/4
26	PEB	fm	201	-	-	8/24/74/74	0/4/4/4
26	PEB	w5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	S3	203	-	-	8/24/74/74	0/4/4/4
26	PEB	dw	401	-	-	8/24/74/74	0/4/4/4
26	PEB	cv	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eh	201	-	-	8/24/74/74	0/4/4/4
28	PUB	aL	203	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	m3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dG	202	-	-	8/24/74/74	0/4/4/4
26	PEB	jP	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	eb	201	-	-	8/24/74/74	0/4/4/4
26	PEB	m3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	as	201	-	-	8/24/74/74	0/4/4/4
26	PEB	i3	202	10	-	8/24/74/74	0/4/4/4
26	PEB	T6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fw	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cy	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	eB	201	-	-	8/24/74/74	0/4/4/4
26	PEB	E8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bt	201	-	-	8/24/74/74	0/4/4/4
26	PEB	G3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bZ	305	-	-	7/24/74/74	0/4/4/4
26	PEB	kW	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	ay	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	dj	202	-	-	7/24/74/74	0/4/4/4
26	PEB	d6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	I8	201	11	-	8/24/74/74	0/4/4/4
28	PUB	aP	203	-	-	7/24/74/74	0/4/4/4
26	PEB	gw	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Y6	201	-	-	8/24/74/74	0/4/4/4
27	CYC	K1	201	-	-	9/25/74/74	0/4/4/4
28	PUB	cY	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cj	202	-	-	7/24/74/74	0/4/4/4
26	PEB	n4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	F2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	p9	202	-	-	8/24/74/74	0/4/4/4
27	CYC	d2	101	5	-	9/25/74/74	0/4/4/4
28	PUB	M8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Q7	202	-	-	8/24/74/74	0/4/4/4
29	PVN	Y5	1004	12	1/1/14/18	12/24/74/74	0/4/4/4
26	PEB	gl	202	10	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	eJ	203	-	-	7/24/74/74	0/4/4/4
28	PUB	fu	202	-	-	7/24/74/74	0/4/4/4
26	PEB	fj	202	-	-	7/24/74/74	0/4/4/4
28	PUB	F7	202	11	-	7/24/74/74	0/4/4/4
26	PEB	Q9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	l7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ef	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cE	202	-	-	7/24/74/74	0/4/4/4
26	PEB	d8	302	14	-	8/24/74/74	0/4/4/4
26	PEB	r9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	o6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	Z9	1007	-	-	8/24/74/74	0/4/4/4
26	PEB	de	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ly	402	23	-	8/24/74/74	0/4/4/4
26	PEB	bS	202	10	-	8/24/74/74	0/4/4/4
28	PUB	aR	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hV	202	-	-	7/24/74/74	0/4/4/4
26	PEB	gk	202	-	-	7/24/74/74	0/4/4/4
26	PEB	O5	202	-	-	8/24/74/74	0/4/4/4
28	PUB	T4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	G6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lc	202	-	-	8/24/74/74	0/4/4/4
26	PEB	F5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	al	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lc	201	-	-	8/24/74/74	0/4/4/4
26	PEB	G4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	R6	203	11	-	7/24/74/74	0/4/4/4
26	PEB	O6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	hL	202	-	-	7/24/74/74	0/4/4/4
28	PUB	n5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	w9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	h4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	lf	202	-	-	7/24/74/74	0/4/4/4
26	PEB	D5	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	j4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fm	202	-	-	7/24/74/74	0/4/4/4
28	PUB	eZ	404	-	-	7/24/74/74	0/4/4/4
26	PEB	e3	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	G8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fs	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aJ	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dN	202	-	-	8/24/74/74	0/4/4/4
28	PUB	N7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Q8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hA	201	10	-	8/24/74/74	0/4/4/4
26	PEB	d7	202	11	-	7/24/74/74	0/4/4/4
26	PEB	G9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	x7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eP	202	-	-	8/24/74/74	0/4/4/4
26	PEB	o2	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	r3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	U8	1003	12	-	8/24/74/74	0/4/4/4
26	PEB	bL	202	-	-	7/24/74/74	0/4/4/4
28	PUB	h2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	aU	201	-	-	8/24/74/74	0/4/4/4
26	PEB	U9	202	-	-	8/24/74/74	0/4/4/4
28	PUB	D4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	p6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	s8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	h2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hI	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dt	201	-	-	8/24/74/74	0/4/4/4
26	PEB	v7	201	-	-	8/24/74/74	0/4/4/4
28	PUB	B6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	H9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	b9	401	-	-	8/24/74/74	0/4/4/4
26	PEB	eD	202	-	-	8/24/74/74	0/4/4/4
28	PUB	kX	1003	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	I6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Z7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	x6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aF	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eW	202	10	-	8/24/74/74	0/4/4/4
28	PUB	f8	203	11	-	7/24/74/74	0/4/4/4
26	PEB	cd	202	18	-	7/24/74/74	0/4/4/4
26	PEB	hD	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eX	201	-	-	7/24/74/74	0/4/4/4
26	PEB	fi	202	-	-	7/24/74/74	0/4/4/4
26	PEB	C9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ep	201	-	-	8/24/74/74	0/4/4/4
26	PEB	I2	202	10	-	8/24/74/74	0/4/4/4
26	PEB	dS	201	-	-	8/24/74/74	0/4/4/4
29	PVN	bZ	304	-	1/1/14/18	14/24/74/74	0/4/4/4
28	PUB	eN	203	-	-	7/24/74/74	0/4/4/4
26	PEB	V2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dV	203	-	-	7/24/74/74	0/4/4/4
26	PEB	o2	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	a5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	j3	202	-	-	7/24/74/74	0/4/4/4
28	PUB	gy	306	-	-	7/24/74/74	0/4/4/4
26	PEB	dD	202	-	-	8/24/74/74	0/4/4/4
26	PEB	B5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ct	202	-	-	8/24/74/74	0/4/4/4
28	PUB	N9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	C3	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	C5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	P7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aP	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ct	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	ff	203	-	-	7/24/74/74	0/4/4/4
26	PEB	cW	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	iB	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	gs	201	-	-	8/24/74/74	0/4/4/4
28	PUB	D2	305	-	-	7/24/74/74	0/4/4/4
26	PEB	E3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	la	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	W5	301	-	-	8/24/74/74	0/4/4/4
26	PEB	bC	201	-	-	8/24/74/74	0/4/4/4
26	PEB	V5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	l4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	lu	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bZ	303	14	-	8/24/74/74	0/4/4/4
26	PEB	y6	203	-	-	8/24/74/74	0/4/4/4
26	PEB	hK	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dP	201	-	-	8/24/74/74	0/4/4/4
26	PEB	P5	201	-	-	7/24/74/74	0/4/4/4
26	PEB	G7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bY	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	A3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	v3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eU	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cu	202	10	-	8/24/74/74	0/4/4/4
28	PUB	iE	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	k7	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	ee	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	T9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eF	201	-	-	8/24/74/74	0/4/4/4
28	PUB	H3	203	11	-	7/24/74/74	0/4/4/4
26	PEB	af	202	-	-	7/24/74/74	0/4/4/4
26	PEB	kS	1002	-	-	7/24/74/74	0/4/4/4
29	PVN	eZ	402	-	1/1/14/18	17/24/74/74	0/4/4/4
26	PEB	cU	202	-	-	8/24/74/74	0/4/4/4
29	PVN	Z5	304	-	1/1/14/18	17/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	N7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ll	201	-	-	8/24/74/74	0/4/4/4
26	PEB	j2	202	-	-	7/24/74/74	0/4/4/4
28	PUB	t6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dC	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cM	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dP	202	-	-	8/24/74/74	0/4/4/4
28	PUB	J7	202	-	-	7/24/74/74	0/4/4/4
28	PUB	n3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bN	202	-	-	7/24/74/74	0/4/4/4
26	PEB	w3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	T5	202	-	-	7/24/74/74	0/4/4/4
28	PUB	aD	203	-	-	7/24/74/74	0/4/4/4
26	PEB	q7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	w4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	T3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	m5	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	Y3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	F4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	T3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jO	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	H2	201	-	-	7/24/74/74	0/4/4/4
26	PEB	cv	202	10	-	8/24/74/74	0/4/4/4
26	PEB	L8	201	-	-	8/24/74/74	0/4/4/4
28	PUB	r7	203	-	-	7/24/74/74	0/4/4/4
28	PUB	lz	405	-	-	7/24/74/74	0/4/4/4
26	PEB	T8	302	-	-	8/24/74/74	0/4/4/4
28	PUB	v2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	X4	202	-	-	8/24/74/74	0/4/4/4
28	PUB	Z9	1006	-	-	7/24/74/74	0/4/4/4
26	PEB	cF	201	-	-	7/24/74/74	0/4/4/4
28	PUB	jJ	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	jN	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	aL	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	S2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	g6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hL	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ac	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hJ	203	-	-	7/24/74/74	0/4/4/4
29	PVN	hY	404	-	1/1/14/18	12/24/74/74	0/4/4/4
27	CYC	S1	201	-	-	10/25/74/74	0/4/4/4
28	PUB	aJ	203	-	-	7/24/74/74	0/4/4/4
26	PEB	fn	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	X9	401	-	-	8/24/74/74	0/4/4/4
26	PEB	dF	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gi	201	-	-	8/24/74/74	0/4/4/4
26	PEB	g2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	T6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hJ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hO	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dY	203	-	-	7/24/74/74	0/4/4/4
28	PUB	cn	202	-	-	7/24/74/74	0/4/4/4
26	PEB	au	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cC	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	u8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eq	202	-	-	8/24/74/74	0/4/4/4
29	PVN	gy	304	-	-	13/24/74/74	0/4/4/4
26	PEB	lm	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	eY	401	-	-	8/24/74/74	0/4/4/4
26	PEB	ls	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aZ	301	-	-	8/24/74/74	0/4/4/4
26	PEB	aO	201	-	-	8/24/74/74	0/4/4/4
26	PEB	da	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	eT	203	-	-	7/24/74/74	0/4/4/4
26	PEB	s9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fl	202	-	-	8/24/74/74	0/4/4/4
28	PUB	df	203	-	-	7/24/74/74	0/4/4/4
28	PUB	iG	1002	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	n4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	g2	202	-	-	8/24/74/74	0/4/4/4
28	PUB	bR	202	-	-	7/24/74/74	0/4/4/4
26	PEB	aX	401	-	-	8/24/74/74	0/4/4/4
28	PUB	eD	203	-	-	7/24/74/74	0/4/4/4
26	PEB	q5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	s5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dO	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dn	202	-	-	8/24/74/74	0/4/4/4
26	PEB	k2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dw	402	-	-	8/24/74/74	0/4/4/4
26	PEB	cO	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hY	405	-	-	7/24/74/74	0/4/4/4
27	CYC	M1	1001	-	-	10/25/74/74	0/4/4/4
26	PEB	hN	202	-	-	7/24/74/74	0/4/4/4
26	PEB	I4	202	-	-	8/24/74/74	0/4/4/4
29	PVN	lz	403	-	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	cr	202	-	-	7/24/74/74	0/4/4/4
26	PEB	du	201	-	-	8/24/74/74	0/4/4/4
26	PEB	P4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	kT	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	R2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	s9	202	-	-	8/24/74/74	0/4/4/4
28	PUB	F6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	E7	201	10	-	8/24/74/74	0/4/4/4
28	PUB	hZ	404	-	-	7/24/74/74	0/4/4/4
26	PEB	f3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	c8	301	-	-	8/24/74/74	0/4/4/4
26	PEB	ar	201	-	-	8/24/74/74	0/4/4/4
26	PEB	I3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bF	202	-	-	7/24/74/74	0/4/4/4
28	PUB	X2	203	-	-	7/24/74/74	0/4/4/4
28	PUB	v6	203	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	iG	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	Q4	202	-	-	8/24/74/74	0/4/4/4
27	CYC	q1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	gq	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fh	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	Z4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	C7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	R7	201	-	-	8/24/74/74	0/4/4/4
28	PUB	b9	407	12	-	7/24/74/74	0/4/4/4
28	PUB	cH	202	-	-	7/24/74/74	0/4/4/4
26	PEB	fb	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bE	201	-	-	8/24/74/74	0/4/4/4
28	PUB	fm	203	-	-	7/24/74/74	0/4/4/4
26	PEB	x8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aR	202	-	-	8/24/74/74	0/4/4/4
26	PEB	o3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	G5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bq	201	-	-	8/24/74/74	0/4/4/4
28	PUB	et	203	-	-	7/24/74/74	0/4/4/4
29	PVN	U8	1004	-	1/1/14/18	10/24/74/74	0/4/4/4
26	PEB	a3	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	fv	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bV	202	-	-	7/24/74/74	0/4/4/4
26	PEB	D4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dv	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	E8	203	-	-	7/24/74/74	0/4/4/4
28	PUB	r3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	m8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	g4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cT	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	J7	201	11	-	7/24/74/74	0/4/4/4
26	PEB	eL	202	-	-	7/24/74/74	0/4/4/4
26	PEB	ca	1001	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	34	1007	-	-	8/24/74/74	0/4/4/4
26	PEB	dQ	201	-	-	8/24/74/74	0/4/4/4
28	PUB	C2	305	-	-	7/24/74/74	0/4/4/4
26	PEB	cK	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dk	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	bH	203	-	-	7/24/74/74	0/4/4/4
28	PUB	T3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	a3	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	u3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	A6	1001	10	-	8/24/74/74	0/4/4/4
28	PUB	aT	203	11	-	7/24/74/74	0/4/4/4
26	PEB	dx	404	-	-	8/24/74/74	0/4/4/4
26	PEB	f5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	O9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	v4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	o5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	iB	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	bj	201	-	-	8/24/74/74	0/4/4/4
28	PUB	R9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dg	202	10	-	8/24/74/74	0/4/4/4
28	PUB	J9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bU	201	-	-	8/24/74/74	0/4/4/4
26	PEB	L4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dx	403	-	-	8/24/74/74	0/4/4/4
26	PEB	bO	202	-	-	8/24/74/74	0/4/4/4
26	PEB	A7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	n7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Z2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	s7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	W2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aH	202	-	-	8/24/74/74	0/4/4/4
26	PEB	n6	202	-	-	7/24/74/74	0/4/4/4
26	PEB	p3	202	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	n6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dj	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bZ	301	-	-	8/24/74/74	0/4/4/4
26	PEB	lq	203	-	-	8/24/74/74	0/4/4/4
26	PEB	iC	1002	-	-	7/24/74/74	0/4/4/4
28	PUB	z9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	i6	201	10	-	8/24/74/74	0/4/4/4
28	PUB	P7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	U7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	s4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	b3	502	-	-	8/24/74/74	0/4/4/4
26	PEB	ge	202	-	-	7/24/74/74	0/4/4/4
28	PUB	jN	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	p9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	H5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lh	202	-	-	7/24/74/74	0/4/4/4
26	PEB	gr	201	-	-	7/24/74/74	0/4/4/4
26	PEB	ab	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aV	201	-	-	8/24/74/74	0/4/4/4
26	PEB	A5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	u6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	D8	202	-	-	8/24/74/74	0/4/4/4
28	PUB	n8	202	-	-	7/24/74/74	0/4/4/4
27	CYC	c1	201	-	-	10/25/74/74	0/4/4/4
26	PEB	jO	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	G2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	hR	203	-	-	7/24/74/74	0/4/4/4
26	PEB	M7	1002	26	-	8/24/74/74	0/4/4/4
26	PEB	aI	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fo	202	-	-	7/24/74/74	0/4/4/4
28	PUB	gd	202	-	-	7/24/74/74	0/4/4/4
29	PVN	Z9	1004	12	1/1/14/18	10/24/74/74	0/4/4/4
28	PUB	X4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	B3	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	eg	201	-	-	8/24/74/74	0/4/4/4
26	PEB	B7	201	-	-	7/24/74/74	0/4/4/4
28	PUB	br	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Z3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dl	202	-	-	7/24/74/74	0/4/4/4
29	PVN	ly	404	23	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	D9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lk	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bF	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dU	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dU	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dt	202	-	-	8/24/74/74	0/4/4/4
26	PEB	v9	202	-	-	7/24/74/74	0/4/4/4
27	CYC	L1	201	5	-	9/25/74/74	0/4/4/4
26	PEB	H6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	lf	201	-	-	8/24/74/74	0/4/4/4
27	CYC	a2	902	8	-	10/25/74/74	0/4/4/4
26	PEB	e6	201	-	-	8/24/74/74	0/4/4/4
29	PVN	34	1004	12	1/1/14/18	12/24/74/74	0/4/4/4
28	PUB	lz	404	-	-	7/24/74/74	0/4/4/4
26	PEB	q3	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	kT	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	d7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	f7	202	10	-	8/24/74/74	0/4/4/4
26	PEB	H4	202	-	-	8/24/74/74	0/4/4/4
28	PUB	dH	203	-	-	7/24/74/74	0/4/4/4
26	PEB	U9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	V2	202	11	-	7/24/74/74	0/4/4/4
26	PEB	gz	303	-	-	8/24/74/74	0/4/4/4
26	PEB	hF	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bl	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dq	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k3	201	10	-	8/24/74/74	0/4/4/4
28	PUB	dw	406	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	p5	201	-	-	7/24/74/74	0/4/4/4
29	PVN	c8	303	14	1/1/14/18	15/24/74/74	0/4/4/4
26	PEB	gv	201	-	-	8/24/74/74	0/4/4/4
26	PEB	el	201	-	-	8/24/74/74	0/4/4/4
28	PUB	Z5	305	-	-	7/24/74/74	0/4/4/4
28	PUB	lt	203	11	-	7/24/74/74	0/4/4/4
26	PEB	j9	201	-	-	8/24/74/74	0/4/4/4
28	PUB	cF	202	-	-	7/24/74/74	0/4/4/4
28	PUB	ly	406	-	-	7/24/74/74	0/4/4/4
26	PEB	dc	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eD	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bT	201	-	-	7/24/74/74	0/4/4/4
26	PEB	hP	202	-	-	7/24/74/74	0/4/4/4
28	PUB	eB	204	11	-	7/24/74/74	0/4/4/4
27	CYC	w1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	hF	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dq	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eo	201	-	-	8/24/74/74	0/4/4/4
28	PUB	B3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	aW	301	-	-	8/24/74/74	0/4/4/4
28	PUB	t9	203	11	-	7/24/74/74	0/4/4/4
26	PEB	R5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eO	201	-	-	8/24/74/74	0/4/4/4
26	PEB	b3	501	-	-	8/24/74/74	0/4/4/4
26	PEB	l9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	b6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cC	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	Z5	302	-	-	8/24/74/74	0/4/4/4
26	PEB	D3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	C5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	T4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	u4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bK	1002	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	E2	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	hX	202	-	-	7/24/74/74	0/4/4/4
26	PEB	at	202	-	-	7/24/74/74	0/4/4/4
26	PEB	n9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cp	202	-	-	7/24/74/74	0/4/4/4
26	PEB	fx	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fn	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	er	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hH	202	-	-	7/24/74/74	0/4/4/4
26	PEB	p2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eg	202	-	-	7/24/74/74	0/4/4/4
26	PEB	y8	202	11	-	7/24/74/74	0/4/4/4
26	PEB	o4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	I6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	o4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	R7	203	-	-	7/24/74/74	0/4/4/4
26	PEB	v6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	u6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	r7	202	11	-	7/24/74/74	0/4/4/4
26	PEB	A6	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	O3	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	Z7	202	-	-	7/24/74/74	0/4/4/4
28	PUB	p4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	Z4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	dF	203	-	-	7/24/74/74	0/4/4/4
26	PEB	O4	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	gi	203	-	-	7/24/74/74	0/4/4/4
26	PEB	lg	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bQ	203	-	-	7/24/74/74	0/4/4/4
26	PEB	L2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cA	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	hJ	202	11	-	7/24/74/74	0/4/4/4
26	PEB	o9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	r6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	h7	201	10	-	8/24/74/74	0/4/4/4
26	PEB	n7	202	-	-	7/24/74/74	0/4/4/4
29	PVN	gz	304	-	-	10/24/74/74	0/4/4/4
26	PEB	gm	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	c9	304	14	-	7/24/74/74	0/4/4/4
26	PEB	ly	401	-	-	8/24/74/74	0/4/4/4
28	PUB	H5	202	-	-	7/24/74/74	0/4/4/4
28	PUB	v9	203	11	-	7/24/74/74	0/4/4/4
26	PEB	t2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gf	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bZ	302	-	-	8/24/74/74	0/4/4/4
26	PEB	bQ	202	-	-	8/24/74/74	0/4/4/4
26	PEB	c5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	c9	301	-	-	8/24/74/74	0/4/4/4
26	PEB	bA	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bB	201	-	-	8/24/74/74	0/4/4/4
28	PUB	gn	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bt	202	10	-	8/24/74/74	0/4/4/4
26	PEB	s7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jN	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	bg	201	-	-	8/24/74/74	0/4/4/4
26	PEB	W4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cq	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gj	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aP	202	-	-	8/24/74/74	0/4/4/4
28	PUB	H4	203	-	-	7/24/74/74	0/4/4/4
28	PUB	N4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hM	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	dx	407	-	-	7/24/74/74	0/4/4/4
26	PEB	cY	202	11	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	go	201	-	-	8/24/74/74	0/4/4/4
28	PUB	t3	203	11	-	7/24/74/74	0/4/4/4
28	PUB	n6	203	11	-	7/24/74/74	0/4/4/4
26	PEB	L9	202	-	-	7/24/74/74	0/4/4/4
28	PUB	d8	304	-	-	7/24/74/74	0/4/4/4
26	PEB	B8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	l5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	lx	201	-	-	7/24/74/74	0/4/4/4
28	PUB	eP	204	11	-	7/24/74/74	0/4/4/4
28	PUB	cL	203	-	-	7/24/74/74	0/4/4/4
28	PUB	lj	202	-	-	7/24/74/74	0/4/4/4
26	PEB	s6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	dJ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gj	202	10	-	8/24/74/74	0/4/4/4
26	PEB	P3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	C6	201	10	-	8/24/74/74	0/4/4/4
26	PEB	A8	202	-	-	8/24/74/74	0/4/4/4
28	PUB	iC	1003	-	-	7/24/74/74	0/4/4/4
28	PUB	b8	1006	-	-	7/24/74/74	0/4/4/4
29	PVN	e8	303	-	1/1/14/18	14/24/74/74	0/4/4/4
26	PEB	g7	202	10	-	8/24/74/74	0/4/4/4
26	PEB	L6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	S5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	e9	303	14	-	8/24/74/74	0/4/4/4
26	PEB	F5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	lm	1001	-	-	8/24/74/74	0/4/4/4
27	CYC	I1	201	4	-	9/25/74/74	0/4/4/4
26	PEB	cx	201	-	-	8/24/74/74	0/4/4/4
28	PUB	p8	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hR	202	-	-	7/24/74/74	0/4/4/4
28	PUB	gy	305	-	-	7/24/74/74	0/4/4/4
26	PEB	eQ	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eV	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eE	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	ck	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dM	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	p7	202	11	-	7/24/74/74	0/4/4/4
26	PEB	l3	201	-	-	8/24/74/74	0/4/4/4
28	PUB	B9	203	11	-	7/24/74/74	0/4/4/4
29	PVN	C2	303	-	1/1/14/18	17/24/74/74	0/4/4/4
28	PUB	jI	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	r3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	bz	202	-	-	8/24/74/74	0/4/4/4
28	PUB	hH	203	-	-	7/24/74/74	0/4/4/4
26	PEB	fd	303	-	-	8/24/74/74	0/4/4/4
26	PEB	I8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	du	203	-	-	8/24/74/74	0/4/4/4
26	PEB	cA	202	-	-	8/24/74/74	0/4/4/4
28	PUB	ep	203	-	-	7/24/74/74	0/4/4/4
28	PUB	iH	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	en	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ly	403	-	-	8/24/74/74	0/4/4/4
26	PEB	F2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	h7	202	-	-	8/24/74/74	0/4/4/4
28	PUB	lh	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hO	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hU	201	-	-	8/24/74/74	0/4/4/4
27	CYC	a2	901	-	-	10/25/74/74	0/4/4/4
26	PEB	hD	202	-	-	7/24/74/74	0/4/4/4
26	PEB	N5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	V4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	m8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eS	201	-	-	8/24/74/74	0/4/4/4
28	PUB	kU	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	Q4	203	-	-	8/24/74/74	0/4/4/4
26	PEB	c5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	i3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bA	202	10	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	v2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cw	202	10	-	8/24/74/74	0/4/4/4
28	PUB	bB	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eL	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Q9	202	-	-	8/24/74/74	0/4/4/4
28	PUB	e9	305	-	-	7/24/74/74	0/4/4/4
26	PEB	f2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	e2	202	-	-	8/24/74/74	0/4/4/4
28	PUB	co	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eo	202	-	-	8/24/74/74	0/4/4/4
26	PEB	az	201	-	-	8/24/74/74	0/4/4/4
28	PUB	fo	203	-	-	7/24/74/74	0/4/4/4
26	PEB	b8	1002	12	-	8/24/74/74	0/4/4/4
28	PUB	az	203	-	-	7/24/74/74	0/4/4/4
26	PEB	do	201	-	-	8/24/74/74	0/4/4/4
28	PUB	n7	203	-	-	7/24/74/74	0/4/4/4
28	PUB	hG	202	-	-	7/24/74/74	0/4/4/4
26	PEB	e3	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	e8	305	-	-	7/24/74/74	0/4/4/4
26	PEB	H6	201	11	-	8/24/74/74	0/4/4/4
26	PEB	J4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	Y5	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	an	201	-	-	7/24/74/74	0/4/4/4
26	PEB	k8	203	-	-	8/24/74/74	0/4/4/4
28	PUB	z6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	fc	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eW	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eH	201	-	-	8/24/74/74	0/4/4/4
28	PUB	iD	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	N9	201	11	-	8/24/74/74	0/4/4/4
27	CYC	Q1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	E5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	D5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	A3	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	v8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	li	201	-	-	8/24/74/74	0/4/4/4
28	PUB	aY	405	-	-	7/24/74/74	0/4/4/4
28	PUB	r5	203	11	-	7/24/74/74	0/4/4/4
28	PUB	kV	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	j4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	G9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	f4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	O3	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	ln	201	-	-	8/24/74/74	0/4/4/4
29	PVN	e9	304	-	1/1/14/18	14/24/74/74	0/4/4/4
26	PEB	X2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Y7	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	dl	203	-	-	7/24/74/74	0/4/4/4
26	PEB	M7	1001	26	-	8/24/74/74	0/4/4/4
28	PUB	V2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	X3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gn	202	-	-	7/24/74/74	0/4/4/4
26	PEB	aG	201	-	-	8/24/74/74	0/4/4/4
26	PEB	de	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lz	402	-	-	8/24/74/74	0/4/4/4
27	CYC	V1	201	7	-	9/25/74/74	0/4/4/4
26	PEB	M3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eC	202	10	-	8/24/74/74	0/4/4/4
26	PEB	K5	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	S4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ez	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	h2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	O9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	p4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t7	201	11	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	G8	203	-	-	7/24/74/74	0/4/4/4
28	PUB	y8	203	11	-	7/24/74/74	0/4/4/4
26	PEB	fw	201	11	-	8/24/74/74	0/4/4/4
26	PEB	34	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	E6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aD	202	-	-	7/24/74/74	0/4/4/4
28	PUB	jP	1003	-	-	7/24/74/74	0/4/4/4
28	PUB	J5	203	-	-	7/24/74/74	0/4/4/4
26	PEB	r2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	dh	201	-	-	8/24/74/74	0/4/4/4
28	PUB	F5	203	-	-	7/24/74/74	0/4/4/4
28	PUB	l2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bK	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	S3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	jL	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	bL	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z8	202	-	-	8/24/74/74	0/4/4/4
28	PUB	gv	203	-	-	7/24/74/74	0/4/4/4
26	PEB	p4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	A4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hM	1002	-	-	8/24/74/74	0/4/4/4
28	PUB	d3	303	-	-	7/24/74/74	0/4/4/4
28	PUB	hZ	405	-	-	7/24/74/74	0/4/4/4
26	PEB	dH	202	-	-	8/24/74/74	0/4/4/4
26	PEB	gi	202	-	-	7/24/74/74	0/4/4/4
26	PEB	di	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bn	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cq	202	-	-	7/24/74/74	0/4/4/4
28	PUB	c7	203	11	-	7/24/74/74	0/4/4/4
26	PEB	aj	202	18	-	7/24/74/74	0/4/4/4
26	PEB	i8	201	10	-	8/24/74/74	0/4/4/4
26	PEB	z5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bR	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dV	202	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PVN	c3	303	-	1/1/14/18	17/24/74/74	0/4/4/4
26	PEB	gs	202	-	-	8/24/74/74	0/4/4/4
26	PEB	v4	201	-	-	8/24/74/74	0/4/4/4
28	PUB	bz	203	-	-	7/24/74/74	0/4/4/4
28	PUB	gp	203	-	-	7/24/74/74	0/4/4/4
26	PEB	fr	201	-	-	8/24/74/74	0/4/4/4
26	PEB	A2	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	E3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	H4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	kU	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	a9	601	-	-	8/24/74/74	0/4/4/4
28	PUB	cO	203	-	-	7/24/74/74	0/4/4/4
26	PEB	hK	202	-	-	8/24/74/74	0/4/4/4
26	PEB	S6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	N2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	eG	201	-	-	8/24/74/74	0/4/4/4
28	PUB	L3	203	-	-	7/24/74/74	0/4/4/4
26	PEB	U6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fi	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hE	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	y6	204	-	-	7/24/74/74	0/4/4/4
26	PEB	a6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	f3	203	11	-	7/24/74/74	0/4/4/4
26	PEB	ee	202	-	-	7/24/74/74	0/4/4/4
26	PEB	c3	302	-	-	8/24/74/74	0/4/4/4
26	PEB	dX	201	-	-	8/24/74/74	0/4/4/4
26	PEB	m5	1003	-	-	7/24/74/74	0/4/4/4
28	PUB	V4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	iE	1001	11	-	8/24/74/74	0/4/4/4
28	PUB	L9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	bS	201	-	-	8/24/74/74	0/4/4/4
26	PEB	K6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	A2	1003	-	-	7/24/74/74	0/4/4/4
26	PEB	B5	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	T5	201	-	-	8/24/74/74	0/4/4/4
28	PUB	b7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	O5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bf	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fg	201	-	-	7/24/74/74	0/4/4/4
26	PEB	hL	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Q5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q8	202	-	-	8/24/74/74	0/4/4/4
28	PUB	e7	203	11	-	7/24/74/74	0/4/4/4
26	PEB	kX	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	dB	201	-	-	8/24/74/74	0/4/4/4
26	PEB	n2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	b8	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	l4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	db	202	-	-	8/24/74/74	0/4/4/4
28	PUB	lv	202	-	-	7/24/74/74	0/4/4/4
26	PEB	i9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	y3	202	-	-	8/24/74/74	0/4/4/4
28	PUB	cQ	202	-	-	7/24/74/74	0/4/4/4
28	PUB	a3	1005	12	-	7/24/74/74	0/4/4/4
26	PEB	W8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cU	201	-	-	8/24/74/74	0/4/4/4
26	PEB	p8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cC	1003	-	-	8/24/74/74	0/4/4/4
26	PEB	hA	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eR	201	-	-	8/24/74/74	0/4/4/4
26	PEB	M9	202	-	-	8/24/74/74	0/4/4/4
26	PEB	at	201	-	-	8/24/74/74	0/4/4/4
26	PEB	lw	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jJ	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	B9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	f2	202	-	-	7/24/74/74	0/4/4/4
28	PUB	r6	203	11	-	7/24/74/74	0/4/4/4
26	PEB	bw	202	10	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	gy	301	-	-	8/24/74/74	0/4/4/4
26	PEB	hH	201	-	-	8/24/74/74	0/4/4/4
28	PUB	J2	202	-	-	7/24/74/74	0/4/4/4
26	PEB	Y4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	u9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dQ	202	-	-	8/24/74/74	0/4/4/4
28	PUB	d3	304	-	-	7/24/74/74	0/4/4/4
26	PEB	l6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	hY	406	-	-	7/24/74/74	0/4/4/4
26	PEB	T6	202	-	-	8/24/74/74	0/4/4/4
28	PUB	aZ	305	-	-	7/24/74/74	0/4/4/4
26	PEB	h3	201	-	-	7/24/74/74	0/4/4/4
26	PEB	E8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	u5	202	-	-	8/24/74/74	0/4/4/4
27	CYC	v1	201	-	-	10/25/74/74	0/4/4/4
28	PUB	en	203	11	-	7/24/74/74	0/4/4/4
26	PEB	L2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	jI	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	X7	202	-	-	7/24/74/74	0/4/4/4
26	PEB	cE	201	-	-	8/24/74/74	0/4/4/4
28	PUB	cB	203	-	-	7/24/74/74	0/4/4/4
26	PEB	eT	202	-	-	8/24/74/74	0/4/4/4
26	PEB	df	202	-	-	7/24/74/74	0/4/4/4
26	PEB	gx	201	-	-	8/24/74/74	0/4/4/4
28	PUB	g8	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eI	202	-	-	8/24/74/74	0/4/4/4
28	PUB	aB	203	-	-	7/24/74/74	0/4/4/4
26	PEB	R9	201	-	-	8/24/74/74	0/4/4/4
29	PVN	ey	1004	-	1/1/14/18	13/24/74/74	0/4/4/4
26	PEB	v3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	N8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gu	201	-	-	8/24/74/74	0/4/4/4
26	PEB	z6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	z5	203	-	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	gu	202	10	-	8/24/74/74	0/4/4/4
26	PEB	ar	202	-	-	7/24/74/74	0/4/4/4
26	PEB	o7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dR	202	-	-	8/24/74/74	0/4/4/4
28	PUB	hN	203	-	-	7/24/74/74	0/4/4/4
26	PEB	A9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	k8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Y9	301	-	-	8/24/74/74	0/4/4/4
26	PEB	G4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	D2	302	-	-	8/24/74/74	0/4/4/4
26	PEB	w2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	gq	202	-	-	8/24/74/74	0/4/4/4
26	PEB	bN	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q6	201	-	-	8/24/74/74	0/4/4/4
28	PUB	a6	203	-	-	7/24/74/74	0/4/4/4
26	PEB	aY	402	-	-	8/24/74/74	0/4/4/4
26	PEB	x8	202	10	-	8/24/74/74	0/4/4/4
28	PUB	Y9	304	-	-	7/24/74/74	0/4/4/4
28	PUB	R4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	s2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	G6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	c6	1001	10	-	8/24/74/74	0/4/4/4
26	PEB	eA	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	T9	203	-	-	7/24/74/74	0/4/4/4
26	PEB	F8	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	A8	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ew	301	-	-	8/24/74/74	0/4/4/4
26	PEB	cw	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ld	201	-	-	8/24/74/74	0/4/4/4
26	PEB	m2	202	-	-	8/24/74/74	0/4/4/4
26	PEB	L5	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	y8	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	z3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	t4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	L5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	iE	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	I7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	ed	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hY	401	-	-	8/24/74/74	0/4/4/4
26	PEB	dx	402	-	-	8/24/74/74	0/4/4/4
26	PEB	dT	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aU	202	10	-	8/24/74/74	0/4/4/4
26	PEB	dO	202	-	-	8/24/74/74	0/4/4/4
26	PEB	F3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	x4	201	-	-	8/24/74/74	0/4/4/4
26	PEB	o5	202	-	-	8/24/74/74	0/4/4/4
26	PEB	T2	201	-	-	8/24/74/74	0/4/4/4
28	PUB	r4	202	11	-	7/24/74/74	0/4/4/4
26	PEB	hC	202	-	-	8/24/74/74	0/4/4/4
26	PEB	i2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hC	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cm	1002	10	-	8/24/74/74	0/4/4/4
28	PUB	dh	203	-	-	7/24/74/74	0/4/4/4
26	PEB	K6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	kU	1002	-	-	7/24/74/74	0/4/4/4
26	PEB	v4	202	-	-	7/24/74/74	0/4/4/4
26	PEB	dK	202	-	-	8/24/74/74	0/4/4/4
28	PUB	f2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	ga	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hZ	402	-	-	8/24/74/74	0/4/4/4
26	PEB	c7	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J9	202	-	-	7/24/74/74	0/4/4/4
26	PEB	s3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	Y7	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	eh	202	-	-	8/24/74/74	0/4/4/4
26	PEB	hE	1002	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PUB	A2	1006	-	-	7/24/74/74	0/4/4/4
28	PUB	eb	202	-	-	7/24/74/74	0/4/4/4
26	PEB	l8	202	-	-	8/24/74/74	0/4/4/4
27	CYC	z1	201	-	-	10/25/74/74	0/4/4/4
26	PEB	dn	201	-	-	8/24/74/74	0/4/4/4
26	PEB	J5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	eu	201	-	-	8/24/74/74	0/4/4/4
26	PEB	i7	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eG	202	10	-	8/24/74/74	0/4/4/4
26	PEB	hT	204	-	-	8/24/74/74	0/4/4/4
26	PEB	dJ	202	-	-	8/24/74/74	0/4/4/4
26	PEB	aE	201	-	-	8/24/74/74	0/4/4/4
26	PEB	fk	202	-	-	8/24/74/74	0/4/4/4
26	PEB	fh	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	gg	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dR	201	-	-	8/24/74/74	0/4/4/4
26	PEB	dd	202	-	-	7/24/74/74	0/4/4/4
26	PEB	w7	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	E9	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bP	201	-	-	8/24/74/74	0/4/4/4
26	PEB	ez	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	fc	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dE	201	-	-	8/24/74/74	0/4/4/4
26	PEB	aT	201	-	-	8/24/74/74	0/4/4/4
28	PUB	eH	203	-	-	7/24/74/74	0/4/4/4
26	PEB	dg	201	-	-	8/24/74/74	0/4/4/4
26	PEB	H3	202	-	-	7/24/74/74	0/4/4/4
26	PEB	lt	202	-	-	8/24/74/74	0/4/4/4
26	PEB	V4	201	-	-	8/24/74/74	0/4/4/4
29	PVN	D2	303	14	1/1/14/18	18/24/74/74	0/4/4/4
26	PEB	H3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	W6	202	-	-	8/24/74/74	0/4/4/4
26	PEB	c8	302	14	-	8/24/74/74	0/4/4/4
26	PEB	G2	202	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	t3	201	-	-	8/24/74/74	0/4/4/4
26	PEB	v5	202	-	-	7/24/74/74	0/4/4/4
26	PEB	e2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	hB	201	-	-	8/24/74/74	0/4/4/4
29	PVN	b8	1004	-	1/1/14/18	17/24/74/74	0/4/4/4
26	PEB	bP	202	-	-	7/24/74/74	0/4/4/4
26	PEB	lb	202	-	-	8/24/74/74	0/4/4/4
26	PEB	cD	202	-	-	8/24/74/74	0/4/4/4
28	PUB	bs	1004	11	-	7/24/74/74	0/4/4/4
28	PUB	ln	203	-	-	7/24/74/74	0/4/4/4
26	PEB	B3	202	-	-	7/24/74/74	0/4/4/4
28	PUB	z2	203	-	-	7/24/74/74	0/4/4/4
26	PEB	es	202	-	-	8/24/74/74	0/4/4/4
26	PEB	es	201	-	-	8/24/74/74	0/4/4/4
26	PEB	cT	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	V9	203	-	-	7/24/74/74	0/4/4/4
28	PUB	ey	1005	-	-	7/24/74/74	0/4/4/4
26	PEB	n8	201	-	-	7/24/74/74	0/4/4/4
28	PUB	z4	203	-	-	7/24/74/74	0/4/4/4
26	PEB	M3	202	-	-	8/24/74/74	0/4/4/4
26	PEB	n2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bm	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	ft	201	-	-	8/24/74/74	0/4/4/4
27	CYC	h1	201	-	-	10/25/74/74	0/4/4/4
26	PEB	a8	602	-	-	8/24/74/74	0/4/4/4
26	PEB	H8	202	-	-	8/24/74/74	0/4/4/4
26	PEB	y6	201	-	-	8/24/74/74	0/4/4/4
26	PEB	a9	603	-	-	8/24/74/74	0/4/4/4
28	PUB	fy	202	-	-	7/24/74/74	0/4/4/4
26	PEB	p7	201	-	-	7/24/74/74	0/4/4/4
26	PEB	u2	201	-	-	8/24/74/74	0/4/4/4
26	PEB	q4	202	-	-	8/24/74/74	0/4/4/4
26	PEB	eq	201	-	-	8/24/74/74	0/4/4/4
26	PEB	bV	201	-	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CYC	a1	201	-	-	9/25/74/74	0/4/4/4
26	PEB	kT	1001	-	-	8/24/74/74	0/4/4/4
28	PUB	ll	203	-	-	7/24/74/74	0/4/4/4
26	PEB	gc	201	-	-	8/24/74/74	0/4/4/4
26	PEB	kX	1001	-	-	8/24/74/74	0/4/4/4
26	PEB	dI	1002	-	-	8/24/74/74	0/4/4/4
26	PEB	as	202	-	-	8/24/74/74	0/4/4/4

All (11802) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X1	201	CYC	CHA-C1A	15.87	1.48	1.35
27	V1	201	CYC	CHA-C1A	15.86	1.48	1.35
27	R1	1001	CYC	CHA-C1A	15.85	1.48	1.35
27	i1	1001	CYC	CHA-C1A	15.85	1.48	1.35
27	I1	201	CYC	CHA-C1A	15.84	1.48	1.35
27	q1	201	CYC	CHA-C1A	15.83	1.48	1.35
27	G1	1001	CYC	CHA-C1A	15.81	1.48	1.35
27	L1	201	CYC	CHA-C1A	15.81	1.48	1.35
27	a1	201	CYC	CHA-C1A	15.81	1.48	1.35
27	P1	201	CYC	CHA-C1A	15.80	1.48	1.35
27	U1	201	CYC	CHA-C1A	15.80	1.48	1.35
27	d2	101	CYC	CHA-C1A	15.80	1.48	1.35
27	y1	201	CYC	CHA-C1A	15.79	1.48	1.35
27	W1	201	CYC	CHA-C1A	15.78	1.48	1.35
27	k1	201	CYC	CHA-C1A	15.78	1.48	1.35
27	g1	201	CYC	CHA-C1A	15.77	1.48	1.35
27	s1	201	CYC	CHA-C1A	15.77	1.48	1.35
27	n1	201	CYC	CHA-C1A	15.77	1.48	1.35
27	m1	201	CYC	CHA-C1A	15.76	1.48	1.35
27	u1	1001	CYC	CHA-C1A	15.76	1.48	1.35
27	Q1	201	CYC	CHA-C1A	15.75	1.48	1.35
27	d1	1001	CYC	CHA-C1A	15.75	1.48	1.35
27	o1	1001	CYC	CHA-C1A	15.74	1.48	1.35
27	O1	201	CYC	CHA-C1A	15.72	1.48	1.35
27	K1	201	CYC	CHA-C1A	15.71	1.48	1.35
27	b1	1001	CYC	CHA-C1A	15.71	1.48	1.35
27	e1	201	CYC	CHA-C1A	15.71	1.48	1.35
27	Z1	201	CYC	CHA-C1A	15.71	1.48	1.35
27	f1	201	CYC	CHA-C1A	15.71	1.48	1.35
27	N1	201	CYC	CHA-C1A	15.70	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	w1	201	CYC	CHA-C1A	15.67	1.48	1.35
27	H1	201	CYC	CHA-C1A	15.62	1.48	1.35
27	v1	201	CYC	CHA-C1A	15.61	1.48	1.35
27	t1	201	CYC	CHA-C1A	15.59	1.48	1.35
27	z1	201	CYC	CHA-C1A	15.57	1.48	1.35
27	S1	201	CYC	CHA-C1A	15.56	1.48	1.35
27	j1	201	CYC	CHA-C1A	15.56	1.48	1.35
27	M1	1001	CYC	CHA-C1A	15.56	1.48	1.35
27	S1	202	CYC	CHA-C1A	15.56	1.48	1.35
27	a2	901	CYC	CHA-C1A	15.55	1.48	1.35
27	h1	201	CYC	CHA-C1A	15.54	1.48	1.35
27	r1	201	CYC	CHA-C1A	15.54	1.48	1.35
27	p1	201	CYC	CHA-C1A	15.53	1.48	1.35
27	a2	902	CYC	CHA-C1A	15.53	1.48	1.35
27	b2	1001	CYC	CHA-C1A	15.53	1.48	1.35
27	c1	201	CYC	CHA-C1A	15.52	1.48	1.35
27	J1	201	CYC	CHA-C1A	15.51	1.48	1.35
27	Y1	201	CYC	CHA-C1A	15.51	1.48	1.35
28	eX	202	PUB	C3A-C2A	10.61	1.46	1.34
28	er	203	PUB	C3A-C2A	10.58	1.46	1.34
28	34	1005	PUB	C3A-C2A	10.55	1.46	1.34
28	J3	203	PUB	C3A-C2A	10.54	1.46	1.34
28	az	203	PUB	C3A-C2A	10.54	1.46	1.34
28	en	203	PUB	C3A-C2A	10.54	1.46	1.34
28	av	203	PUB	C3A-C2A	10.54	1.46	1.34
28	bJ	203	PUB	C3A-C2A	10.53	1.46	1.34
28	fi	203	PUB	C3A-C2A	10.53	1.46	1.34
28	fs	203	PUB	C3A-C2A	10.53	1.46	1.34
28	cL	203	PUB	C3A-C2A	10.53	1.46	1.34
28	F7	202	PUB	C3A-C2A	10.52	1.46	1.34
28	gz	306	PUB	C3A-C2A	10.52	1.46	1.34
28	dw	405	PUB	C3A-C2A	10.52	1.46	1.34
28	V7	203	PUB	C3A-C2A	10.52	1.46	1.34
28	eF	203	PUB	C3A-C2A	10.52	1.46	1.34
28	ly	405	PUB	C3A-C2A	10.52	1.46	1.34
28	ly	406	PUB	C3A-C2A	10.52	1.46	1.34
28	lz	404	PUB	C3A-C2A	10.52	1.46	1.34
28	lz	405	PUB	C3A-C2A	10.52	1.46	1.34
28	ff	203	PUB	C3A-C2A	10.52	1.46	1.34
28	v4	203	PUB	C3A-C2A	10.51	1.46	1.34
28	v5	203	PUB	C3A-C2A	10.51	1.46	1.34
28	c6	1004	PUB	C3A-C2A	10.51	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	eT	203	PUB	C3A-C2A	10.51	1.46	1.34
28	f2	203	PUB	C3A-C2A	10.51	1.46	1.34
28	l6	203	PUB	C3A-C2A	10.51	1.46	1.34
28	cR	203	PUB	C3A-C2A	10.51	1.46	1.34
28	ee	203	PUB	C3A-C2A	10.51	1.46	1.34
28	e9	306	PUB	C3A-C2A	10.51	1.46	1.34
28	H7	203	PUB	C3A-C2A	10.51	1.46	1.34
28	fc	203	PUB	C3A-C2A	10.51	1.46	1.34
28	c3	304	PUB	C3A-C2A	10.51	1.46	1.34
28	V6	203	PUB	C3A-C2A	10.51	1.46	1.34
28	T7	203	PUB	C3A-C2A	10.51	1.46	1.34
28	Z9	1006	PUB	C3A-C2A	10.51	1.46	1.34
28	bY	1005	PUB	C3A-C2A	10.51	1.46	1.34
28	bZ	305	PUB	C3A-C2A	10.51	1.46	1.34
28	bn	202	PUB	C3A-C2A	10.51	1.46	1.34
28	iF	1003	PUB	C3A-C2A	10.51	1.46	1.34
28	iG	1002	PUB	C3A-C2A	10.51	1.46	1.34
28	dj	203	PUB	C3A-C2A	10.51	1.46	1.34
28	dt	203	PUB	C3A-C2A	10.51	1.46	1.34
28	hZ	405	PUB	C3A-C2A	10.51	1.46	1.34
28	c7	203	PUB	C3A-C2A	10.50	1.46	1.34
28	fm	203	PUB	C3A-C2A	10.50	1.46	1.34
28	V9	203	PUB	C3A-C2A	10.50	1.46	1.34
28	iC	1003	PUB	C3A-C2A	10.50	1.46	1.34
28	iD	1003	PUB	C3A-C2A	10.50	1.46	1.34
28	x5	202	PUB	C3A-C2A	10.50	1.46	1.34
28	kX	1003	PUB	C3A-C2A	10.50	1.46	1.34
28	B5	203	PUB	C3A-C2A	10.50	1.46	1.34
28	jL	1003	PUB	C3A-C2A	10.50	1.46	1.34
28	p7	202	PUB	C3A-C2A	10.50	1.46	1.34
28	ep	203	PUB	C3A-C2A	10.50	1.46	1.34
28	fa	202	PUB	C3A-C2A	10.50	1.46	1.34
28	gy	305	PUB	C3A-C2A	10.50	1.46	1.34
28	cF	202	PUB	C3A-C2A	10.50	1.46	1.34
28	cO	203	PUB	C3A-C2A	10.50	1.46	1.34
28	fo	203	PUB	C3A-C2A	10.50	1.46	1.34
28	z9	203	PUB	C3A-C2A	10.50	1.46	1.34
28	h3	202	PUB	C3A-C2A	10.50	1.46	1.34
28	dF	203	PUB	C3A-C2A	10.50	1.46	1.34
28	P2	203	PUB	C3A-C2A	10.50	1.46	1.34
28	p3	203	PUB	C3A-C2A	10.50	1.46	1.34
28	P5	202	PUB	C3A-C2A	10.49	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	ap	203	PUB	C3A-C2A	10.49	1.46	1.34
28	dN	203	PUB	C3A-C2A	10.49	1.46	1.34
28	jM	1003	PUB	C3A-C2A	10.49	1.46	1.34
28	H9	203	PUB	C3A-C2A	10.49	1.46	1.34
28	r2	203	PUB	C3A-C2A	10.49	1.46	1.34
28	R3	203	PUB	C3A-C2A	10.49	1.46	1.34
28	d3	303	PUB	C3A-C2A	10.49	1.46	1.34
28	34	1006	PUB	C3A-C2A	10.49	1.46	1.34
28	n4	203	PUB	C3A-C2A	10.49	1.46	1.34
28	aY	405	PUB	C3A-C2A	10.49	1.46	1.34
28	bY	1006	PUB	C3A-C2A	10.49	1.46	1.34
28	ez	1005	PUB	C3A-C2A	10.49	1.46	1.34
28	lp	203	PUB	C3A-C2A	10.49	1.46	1.34
28	hT	203	PUB	C3A-C2A	10.49	1.46	1.34
28	p2	203	PUB	C3A-C2A	10.49	1.46	1.34
28	F6	203	PUB	C3A-C2A	10.49	1.46	1.34
28	X7	203	PUB	C3A-C2A	10.49	1.46	1.34
28	dL	203	PUB	C3A-C2A	10.49	1.46	1.34
28	V2	203	PUB	C3A-C2A	10.49	1.46	1.34
28	J5	203	PUB	C3A-C2A	10.49	1.46	1.34
28	e8	304	PUB	C3A-C2A	10.49	1.46	1.34
28	N2	203	PUB	C3A-C2A	10.49	1.46	1.34
28	br	203	PUB	C3A-C2A	10.49	1.46	1.34
28	eL	203	PUB	C3A-C2A	10.49	1.46	1.34
28	bH	203	PUB	C3A-C2A	10.49	1.46	1.34
28	ge	203	PUB	C3A-C2A	10.49	1.46	1.34
28	P4	203	PUB	C3A-C2A	10.49	1.46	1.34
28	L5	203	PUB	C3A-C2A	10.49	1.46	1.34
28	p9	203	PUB	C3A-C2A	10.49	1.46	1.34
28	bD	203	PUB	C3A-C2A	10.49	1.46	1.34
28	hL	203	PUB	C3A-C2A	10.49	1.46	1.34
28	hN	203	PUB	C3A-C2A	10.49	1.46	1.34
28	A8	203	PUB	C3A-C2A	10.48	1.46	1.34
28	ld	203	PUB	C3A-C2A	10.48	1.46	1.34
28	ln	203	PUB	C3A-C2A	10.48	1.46	1.34
28	cq	203	PUB	C3A-C2A	10.48	1.46	1.34
28	x6	203	PUB	C3A-C2A	10.48	1.46	1.34
28	n2	203	PUB	C3A-C2A	10.48	1.46	1.34
28	lv	202	PUB	C3A-C2A	10.48	1.46	1.34
28	n3	203	PUB	C3A-C2A	10.48	1.46	1.34
28	C8	203	PUB	C3A-C2A	10.48	1.46	1.34
28	Y9	305	PUB	C3A-C2A	10.48	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	aZ	305	PUB	C3A-C2A	10.48	1.46	1.34
28	t2	203	PUB	C3A-C2A	10.48	1.46	1.34
28	B3	203	PUB	C3A-C2A	10.48	1.46	1.34
28	eY	405	PUB	C3A-C2A	10.48	1.46	1.34
28	eZ	404	PUB	C3A-C2A	10.48	1.46	1.34
28	Q8	203	PUB	C3A-C2A	10.48	1.46	1.34
28	aB	203	PUB	C3A-C2A	10.48	1.46	1.34
28	V5	203	PUB	C3A-C2A	10.48	1.46	1.34
28	aZ	304	PUB	C3A-C2A	10.48	1.46	1.34
28	F2	203	PUB	C3A-C2A	10.48	1.46	1.34
28	v9	203	PUB	C3A-C2A	10.48	1.46	1.34
28	bp	202	PUB	C3A-C2A	10.48	1.46	1.34
28	bz	203	PUB	C3A-C2A	10.48	1.46	1.34
28	cN	202	PUB	C3A-C2A	10.48	1.46	1.34
28	lt	203	PUB	C3A-C2A	10.48	1.46	1.34
28	l2	203	PUB	C3A-C2A	10.48	1.46	1.34
28	n9	202	PUB	C3A-C2A	10.48	1.46	1.34
28	kS	1003	PUB	C3A-C2A	10.48	1.46	1.34
28	Z6	203	PUB	C3A-C2A	10.47	1.46	1.34
28	g8	202	PUB	C3A-C2A	10.47	1.46	1.34
28	cM	203	PUB	C3A-C2A	10.47	1.46	1.34
28	lf	203	PUB	C3A-C2A	10.47	1.46	1.34
28	hR	203	PUB	C3A-C2A	10.47	1.46	1.34
28	F3	203	PUB	C3A-C2A	10.47	1.46	1.34
28	B4	203	PUB	C3A-C2A	10.47	1.46	1.34
28	n5	203	PUB	C3A-C2A	10.47	1.46	1.34
28	J7	202	PUB	C3A-C2A	10.47	1.46	1.34
28	h8	203	PUB	C3A-C2A	10.47	1.46	1.34
28	T8	304	PUB	C3A-C2A	10.47	1.46	1.34
28	bL	203	PUB	C3A-C2A	10.47	1.46	1.34
28	ey	1006	PUB	C3A-C2A	10.47	1.46	1.34
28	Z5	306	PUB	C3A-C2A	10.47	1.46	1.34
28	H6	203	PUB	C3A-C2A	10.47	1.46	1.34
28	dl	203	PUB	C3A-C2A	10.47	1.46	1.34
28	dB	202	PUB	C3A-C2A	10.47	1.46	1.34
28	lh	203	PUB	C3A-C2A	10.47	1.46	1.34
28	kU	1003	PUB	C3A-C2A	10.47	1.46	1.34
28	f8	203	PUB	C3A-C2A	10.47	1.46	1.34
28	bo	202	PUB	C3A-C2A	10.47	1.46	1.34
28	eJ	203	PUB	C3A-C2A	10.47	1.46	1.34
28	p4	203	PUB	C3A-C2A	10.47	1.46	1.34
28	B9	203	PUB	C3A-C2A	10.47	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dX	203	PUB	C3A-C2A	10.47	1.46	1.34
28	V3	203	PUB	C3A-C2A	10.47	1.46	1.34
28	z4	203	PUB	C3A-C2A	10.47	1.46	1.34
28	z5	203	PUB	C3A-C2A	10.47	1.46	1.34
28	B7	202	PUB	C3A-C2A	10.47	1.46	1.34
28	G8	203	PUB	C3A-C2A	10.47	1.46	1.34
28	bN	203	PUB	C3A-C2A	10.47	1.46	1.34
28	dR	203	PUB	C3A-C2A	10.47	1.46	1.34
28	fy	202	PUB	C3A-C2A	10.47	1.46	1.34
28	D6	202	PUB	C3A-C2A	10.47	1.46	1.34
28	p5	202	PUB	C3A-C2A	10.47	1.46	1.34
28	x7	203	PUB	C3A-C2A	10.47	1.46	1.34
28	U8	1005	PUB	C3A-C2A	10.47	1.46	1.34
28	R2	203	PUB	C3A-C2A	10.47	1.46	1.34
28	df	203	PUB	C3A-C2A	10.47	1.46	1.34
28	D4	203	PUB	C3A-C2A	10.46	1.46	1.34
28	bR	202	PUB	C3A-C2A	10.46	1.46	1.34
28	hV	203	PUB	C3A-C2A	10.46	1.46	1.34
28	T3	203	PUB	C3A-C2A	10.46	1.46	1.34
28	j3	202	PUB	C3A-C2A	10.46	1.46	1.34
28	T4	202	PUB	C3A-C2A	10.46	1.46	1.34
28	44	304	PUB	C3A-C2A	10.46	1.46	1.34
28	Z5	305	PUB	C3A-C2A	10.46	1.46	1.34
28	t5	203	PUB	C3A-C2A	10.46	1.46	1.34
28	a7	203	PUB	C3A-C2A	10.46	1.46	1.34
28	r9	203	PUB	C3A-C2A	10.46	1.46	1.34
28	eR	203	PUB	C3A-C2A	10.46	1.46	1.34
28	T6	203	PUB	C3A-C2A	10.46	1.46	1.34
28	bs	1004	PUB	C3A-C2A	10.46	1.46	1.34
28	lj	202	PUB	C3A-C2A	10.46	1.46	1.34
28	lx	201	PUB	C3A-C2A	10.46	1.46	1.34
28	A2	1006	PUB	C3A-C2A	10.46	1.46	1.34
28	r4	202	PUB	C3A-C2A	10.46	1.46	1.34
28	r5	203	PUB	C3A-C2A	10.46	1.46	1.34
28	b8	1006	PUB	C3A-C2A	10.46	1.46	1.34
28	b9	407	PUB	C3A-C2A	10.46	1.46	1.34
28	J2	202	PUB	C3A-C2A	10.46	1.46	1.34
28	aD	203	PUB	C3A-C2A	10.46	1.46	1.34
28	bq	203	PUB	C3A-C2A	10.46	1.46	1.34
28	et	203	PUB	C3A-C2A	10.46	1.46	1.34
28	jO	1003	PUB	C3A-C2A	10.46	1.46	1.34
28	z7	203	PUB	C3A-C2A	10.46	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z9	1005	PUB	C3A-C2A	10.46	1.46	1.34
28	aL	203	PUB	C3A-C2A	10.46	1.46	1.34
28	gi	203	PUB	C3A-C2A	10.46	1.46	1.34
28	jJ	1003	PUB	C3A-C2A	10.46	1.46	1.34
28	X4	203	PUB	C3A-C2A	10.46	1.46	1.34
28	T5	202	PUB	C3A-C2A	10.46	1.46	1.34
28	B6	203	PUB	C3A-C2A	10.46	1.46	1.34
28	D7	203	PUB	C3A-C2A	10.46	1.46	1.34
28	L7	202	PUB	C3A-C2A	10.46	1.46	1.34
28	e8	305	PUB	C3A-C2A	10.46	1.46	1.34
28	ga	203	PUB	C3A-C2A	10.46	1.46	1.34
28	gn	203	PUB	C3A-C2A	10.46	1.46	1.34
28	gr	202	PUB	C3A-C2A	10.46	1.46	1.34
28	aN	203	PUB	C3A-C2A	10.46	1.46	1.34
28	hH	203	PUB	C3A-C2A	10.46	1.46	1.34
28	e6	203	PUB	C3A-C2A	10.46	1.46	1.34
28	o8	203	PUB	C3A-C2A	10.46	1.46	1.34
28	b8	1005	PUB	C3A-C2A	10.46	1.46	1.34
28	d6	203	PUB	C3A-C2A	10.46	1.46	1.34
28	N7	203	PUB	C3A-C2A	10.46	1.46	1.34
28	cB	203	PUB	C3A-C2A	10.46	1.46	1.34
28	eV	203	PUB	C3A-C2A	10.46	1.46	1.34
28	fj	203	PUB	C3A-C2A	10.46	1.46	1.34
28	T2	203	PUB	C3A-C2A	10.46	1.46	1.34
28	t3	203	PUB	C3A-C2A	10.46	1.46	1.34
28	aT	203	PUB	C3A-C2A	10.46	1.46	1.34
28	gx	203	PUB	C3A-C2A	10.46	1.46	1.34
28	di	203	PUB	C3A-C2A	10.45	1.46	1.34
28	L2	203	PUB	C3A-C2A	10.45	1.46	1.34
28	l3	202	PUB	C3A-C2A	10.45	1.46	1.34
28	a6	203	PUB	C3A-C2A	10.45	1.46	1.34
28	l7	203	PUB	C3A-C2A	10.45	1.46	1.34
28	t4	203	PUB	C3A-C2A	10.45	1.46	1.34
28	x2	202	PUB	C3A-C2A	10.45	1.46	1.34
28	X3	202	PUB	C3A-C2A	10.45	1.46	1.34
28	c8	304	PUB	C3A-C2A	10.45	1.46	1.34
28	c9	304	PUB	C3A-C2A	10.45	1.46	1.34
28	E8	203	PUB	C3A-C2A	10.45	1.46	1.34
28	M8	203	PUB	C3A-C2A	10.45	1.46	1.34
28	cs	203	PUB	C3A-C2A	10.45	1.46	1.34
28	T8	305	PUB	C3A-C2A	10.45	1.46	1.34
28	bB	203	PUB	C3A-C2A	10.45	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	cQ	202	PUB	C3A-C2A	10.45	1.46	1.34
28	bT	202	PUB	C3A-C2A	10.45	1.46	1.34
28	D2	305	PUB	C3A-C2A	10.45	1.46	1.34
28	d3	304	PUB	C3A-C2A	10.45	1.46	1.34
28	d8	304	PUB	C3A-C2A	10.45	1.46	1.34
28	eH	203	PUB	C3A-C2A	10.45	1.46	1.34
28	eY	404	PUB	C3A-C2A	10.45	1.46	1.34
28	eZ	403	PUB	C3A-C2A	10.45	1.46	1.34
28	kT	1003	PUB	C3A-C2A	10.45	1.46	1.34
28	J4	203	PUB	C3A-C2A	10.45	1.46	1.34
28	n7	203	PUB	C3A-C2A	10.45	1.46	1.34
28	dn	203	PUB	C3A-C2A	10.45	1.46	1.34
28	dr	203	PUB	C3A-C2A	10.45	1.46	1.34
28	dK	203	PUB	C3A-C2A	10.45	1.46	1.34
28	jK	1003	PUB	C3A-C2A	10.45	1.46	1.34
28	Y5	1005	PUB	C3A-C2A	10.45	1.46	1.34
28	lb	203	PUB	C3A-C2A	10.45	1.46	1.34
28	J6	203	PUB	C3A-C2A	10.45	1.46	1.34
28	N6	203	PUB	C3A-C2A	10.45	1.46	1.34
28	e9	305	PUB	C3A-C2A	10.45	1.46	1.34
28	gk	203	PUB	C3A-C2A	10.45	1.46	1.34
28	A2	1005	PUB	C3A-C2A	10.45	1.46	1.34
28	a3	1005	PUB	C3A-C2A	10.45	1.46	1.34
28	dv	202	PUB	C3A-C2A	10.45	1.46	1.34
28	fw	203	PUB	C3A-C2A	10.45	1.46	1.34
28	V4	203	PUB	C3A-C2A	10.44	1.46	1.34
28	R5	203	PUB	C3A-C2A	10.44	1.46	1.34
28	cn	202	PUB	C3A-C2A	10.44	1.46	1.34
28	dY	203	PUB	C3A-C2A	10.44	1.46	1.34
28	Z2	203	PUB	C3A-C2A	10.44	1.46	1.34
28	bF	203	PUB	C3A-C2A	10.44	1.46	1.34
28	cY	203	PUB	C3A-C2A	10.44	1.46	1.34
28	hP	203	PUB	C3A-C2A	10.44	1.46	1.34
28	X2	203	PUB	C3A-C2A	10.44	1.46	1.34
28	x3	203	PUB	C3A-C2A	10.44	1.46	1.34
28	bZ	306	PUB	C3A-C2A	10.44	1.46	1.34
28	gg	203	PUB	C3A-C2A	10.44	1.46	1.34
28	H2	202	PUB	C3A-C2A	10.44	1.46	1.34
28	v3	203	PUB	C3A-C2A	10.44	1.46	1.34
28	r6	203	PUB	C3A-C2A	10.44	1.46	1.34
28	y8	203	PUB	C3A-C2A	10.44	1.46	1.34
28	aR	203	PUB	C3A-C2A	10.44	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dd	203	PUB	C3A-C2A	10.44	1.46	1.34
28	dx	406	PUB	C3A-C2A	10.44	1.46	1.34
28	ey	1005	PUB	C3A-C2A	10.44	1.46	1.34
28	F5	203	PUB	C3A-C2A	10.44	1.46	1.34
28	p8	203	PUB	C3A-C2A	10.44	1.46	1.34
28	cE	203	PUB	C3A-C2A	10.44	1.46	1.34
28	y6	204	PUB	C3A-C2A	10.44	1.46	1.34
28	O8	203	PUB	C3A-C2A	10.44	1.46	1.34
28	T9	203	PUB	C3A-C2A	10.44	1.46	1.34
28	gd	202	PUB	C3A-C2A	10.44	1.46	1.34
28	N3	203	PUB	C3A-C2A	10.44	1.46	1.34
28	an	202	PUB	C3A-C2A	10.44	1.46	1.34
28	jN	1003	PUB	C3A-C2A	10.44	1.46	1.34
28	kQ	1003	PUB	C3A-C2A	10.44	1.46	1.34
28	F4	203	PUB	C3A-C2A	10.44	1.46	1.34
28	P7	203	PUB	C3A-C2A	10.44	1.46	1.34
28	aJ	203	PUB	C3A-C2A	10.44	1.46	1.34
28	bV	203	PUB	C3A-C2A	10.44	1.46	1.34
28	ez	1006	PUB	C3A-C2A	10.44	1.46	1.34
28	aY	404	PUB	C3A-C2A	10.44	1.46	1.34
28	cH	202	PUB	C3A-C2A	10.44	1.46	1.34
28	hD	203	PUB	C3A-C2A	10.44	1.46	1.34
28	jP	1003	PUB	C3A-C2A	10.44	1.46	1.34
28	n8	202	PUB	C3A-C2A	10.44	1.46	1.34
28	c8	305	PUB	C3A-C2A	10.44	1.46	1.34
28	eb	202	PUB	C3A-C2A	10.44	1.46	1.34
28	hJ	203	PUB	C3A-C2A	10.44	1.46	1.34
28	C2	305	PUB	C3A-C2A	10.44	1.46	1.34
28	H3	203	PUB	C3A-C2A	10.44	1.46	1.34
28	a3	1006	PUB	C3A-C2A	10.44	1.46	1.34
28	c3	305	PUB	C3A-C2A	10.44	1.46	1.34
28	d9	305	PUB	C3A-C2A	10.44	1.46	1.34
28	F9	203	PUB	C3A-C2A	10.44	1.46	1.34
28	R9	203	PUB	C3A-C2A	10.44	1.46	1.34
28	cz	203	PUB	C3A-C2A	10.44	1.46	1.34
28	dV	203	PUB	C3A-C2A	10.44	1.46	1.34
28	hB	203	PUB	C3A-C2A	10.44	1.46	1.34
28	x4	202	PUB	C3A-C2A	10.43	1.46	1.34
28	H5	202	PUB	C3A-C2A	10.43	1.46	1.34
28	ec	203	PUB	C3A-C2A	10.43	1.46	1.34
28	hZ	404	PUB	C3A-C2A	10.43	1.46	1.34
28	Y5	1006	PUB	C3A-C2A	10.43	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b9	406	PUB	C3A-C2A	10.43	1.46	1.34
28	K8	203	PUB	C3A-C2A	10.43	1.46	1.34
28	iH	1002	PUB	C3A-C2A	10.43	1.46	1.34
28	jI	1003	PUB	C3A-C2A	10.43	1.46	1.34
28	b7	202	PUB	C3A-C2A	10.43	1.46	1.34
28	dp	203	PUB	C3A-C2A	10.43	1.46	1.34
28	f3	203	PUB	C3A-C2A	10.43	1.46	1.34
28	e7	203	PUB	C3A-C2A	10.43	1.46	1.34
28	h2	203	PUB	C3A-C2A	10.43	1.46	1.34
28	D3	203	PUB	C3A-C2A	10.43	1.46	1.34
28	N4	203	PUB	C3A-C2A	10.43	1.46	1.34
28	hY	405	PUB	C3A-C2A	10.43	1.46	1.34
28	R4	203	PUB	C3A-C2A	10.43	1.46	1.34
28	N5	203	PUB	C3A-C2A	10.43	1.46	1.34
28	aV	203	PUB	C3A-C2A	10.43	1.46	1.34
28	cJ	203	PUB	C3A-C2A	10.43	1.46	1.34
28	dH	203	PUB	C3A-C2A	10.43	1.46	1.34
28	kW	1003	PUB	C3A-C2A	10.43	1.46	1.34
28	I8	203	PUB	C3A-C2A	10.43	1.46	1.34
28	N9	203	PUB	C3A-C2A	10.43	1.46	1.34
28	Y9	304	PUB	C3A-C2A	10.43	1.46	1.34
28	Z7	203	PUB	C3A-C2A	10.43	1.46	1.34
28	P9	203	PUB	C3A-C2A	10.43	1.46	1.34
28	kV	1003	PUB	C3A-C2A	10.43	1.46	1.34
28	R7	203	PUB	C3A-C2A	10.43	1.46	1.34
28	gp	203	PUB	C3A-C2A	10.43	1.46	1.34
28	D9	203	PUB	C3A-C2A	10.43	1.46	1.34
28	L6	202	PUB	C3A-C2A	10.43	1.46	1.34
28	iE	1003	PUB	C3A-C2A	10.43	1.46	1.34
28	D2	304	PUB	C3A-C2A	10.42	1.46	1.34
28	H4	203	PUB	C3A-C2A	10.42	1.46	1.34
28	D5	203	PUB	C3A-C2A	10.42	1.46	1.34
28	p6	203	PUB	C3A-C2A	10.42	1.46	1.34
28	aP	203	PUB	C3A-C2A	10.42	1.46	1.34
28	dx	407	PUB	C3A-C2A	10.42	1.46	1.34
28	ll	203	PUB	C3A-C2A	10.42	1.46	1.34
28	dP	203	PUB	C3A-C2A	10.42	1.46	1.34
28	eD	203	PUB	C3A-C2A	10.42	1.46	1.34
28	C2	304	PUB	C3A-C2A	10.42	1.46	1.34
28	y7	203	PUB	C3A-C2A	10.42	1.46	1.34
28	dD	203	PUB	C3A-C2A	10.42	1.46	1.34
28	ei	203	PUB	C3A-C2A	10.42	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P3	203	PUB	C3A-C2A	10.42	1.46	1.34
28	w8	203	PUB	C3A-C2A	10.42	1.46	1.34
28	dT	203	PUB	C3A-C2A	10.42	1.46	1.34
28	b6	203	PUB	C3A-C2A	10.42	1.46	1.34
28	fq	203	PUB	C3A-C2A	10.42	1.46	1.34
28	r3	203	PUB	C3A-C2A	10.42	1.46	1.34
28	el	203	PUB	C3A-C2A	10.42	1.46	1.34
28	v2	203	PUB	C3A-C2A	10.41	1.46	1.34
28	r7	203	PUB	C3A-C2A	10.41	1.46	1.34
28	aH	203	PUB	C3A-C2A	10.41	1.46	1.34
28	c9	305	PUB	C3A-C2A	10.41	1.46	1.34
28	hY	406	PUB	C3A-C2A	10.41	1.46	1.34
28	co	202	PUB	C3A-C2A	10.41	1.46	1.34
28	cP	203	PUB	C3A-C2A	10.41	1.46	1.34
28	R6	203	PUB	C3A-C2A	10.41	1.46	1.34
28	v6	203	PUB	C3A-C2A	10.41	1.46	1.34
28	L3	203	PUB	C3A-C2A	10.41	1.46	1.34
28	J9	203	PUB	C3A-C2A	10.41	1.46	1.34
28	P6	203	PUB	C3A-C2A	10.41	1.46	1.34
28	hG	202	PUB	C3A-C2A	10.41	1.46	1.34
28	hX	203	PUB	C3A-C2A	10.41	1.46	1.34
28	d7	203	PUB	C3A-C2A	10.41	1.46	1.34
28	s7	203	PUB	C3A-C2A	10.41	1.46	1.34
28	L9	203	PUB	C3A-C2A	10.41	1.46	1.34
28	j2	203	PUB	C3A-C2A	10.41	1.46	1.34
28	gz	305	PUB	C3A-C2A	10.41	1.46	1.34
28	X6	203	PUB	C3A-C2A	10.40	1.46	1.34
28	gv	203	PUB	C3A-C2A	10.40	1.46	1.34
28	gy	306	PUB	C3A-C2A	10.40	1.46	1.34
28	n6	203	PUB	C3A-C2A	10.40	1.46	1.34
28	z6	203	PUB	C3A-C2A	10.40	1.46	1.34
28	dw	406	PUB	C3A-C2A	10.40	1.46	1.34
28	44	305	PUB	C3A-C2A	10.40	1.46	1.34
28	U8	1006	PUB	C3A-C2A	10.40	1.46	1.34
28	t9	203	PUB	C3A-C2A	10.40	1.46	1.34
28	z2	203	PUB	C3A-C2A	10.40	1.46	1.34
28	Z3	203	PUB	C3A-C2A	10.40	1.46	1.34
28	u6	203	PUB	C3A-C2A	10.40	1.46	1.34
28	dh	203	PUB	C3A-C2A	10.40	1.46	1.34
28	v7	203	PUB	C3A-C2A	10.40	1.46	1.34
28	eB	204	PUB	C3A-C2A	10.40	1.46	1.34
28	eN	203	PUB	C3A-C2A	10.40	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	kR	1003	PUB	C3A-C2A	10.40	1.46	1.34
28	aF	203	PUB	C3A-C2A	10.40	1.46	1.34
28	Z4	203	PUB	C3A-C2A	10.39	1.46	1.34
28	cp	203	PUB	C3A-C2A	10.39	1.46	1.34
28	ar	203	PUB	C3A-C2A	10.39	1.46	1.34
28	z3	203	PUB	C3A-C2A	10.39	1.46	1.34
28	t7	203	PUB	C3A-C2A	10.39	1.46	1.34
28	x9	203	PUB	C3A-C2A	10.39	1.46	1.34
28	ax	202	PUB	C3A-C2A	10.39	1.46	1.34
28	fu	202	PUB	C3A-C2A	10.39	1.46	1.34
28	L4	203	PUB	C3A-C2A	10.39	1.46	1.34
28	bP	203	PUB	C3A-C2A	10.38	1.46	1.34
28	eg	203	PUB	C3A-C2A	10.38	1.46	1.34
28	t6	203	PUB	C3A-C2A	10.38	1.46	1.34
28	at	203	PUB	C3A-C2A	10.38	1.46	1.34
28	cr	203	PUB	C3A-C2A	10.38	1.46	1.34
28	lr	203	PUB	C3A-C2A	10.38	1.46	1.34
28	gt	203	PUB	C3A-C2A	10.37	1.46	1.34
28	ev	203	PUB	C3A-C2A	10.33	1.46	1.34
28	eP	204	PUB	C3A-C2A	10.32	1.46	1.34
26	bL	202	PEB	C2D-C3D	9.49	1.46	1.34
26	cp	202	PEB	C2D-C3D	9.48	1.46	1.34
26	ax	201	PEB	C2D-C3D	9.46	1.46	1.34
26	bP	202	PEB	C2D-C3D	9.46	1.46	1.34
26	en	202	PEB	C2D-C3D	9.44	1.46	1.34
26	eL	202	PEB	C2D-C3D	9.44	1.46	1.34
26	at	202	PEB	C2D-C3D	9.44	1.46	1.34
26	t7	202	PEB	C2D-C3D	9.44	1.46	1.34
26	N7	202	PEB	C2D-C3D	9.43	1.46	1.34
26	v5	202	PEB	C2D-C3D	9.43	1.46	1.34
26	cE	202	PEB	C2D-C3D	9.43	1.46	1.34
26	g5	202	PEB	C2D-C3D	9.43	1.46	1.34
26	i3	203	PEB	C2D-C3D	9.42	1.46	1.34
26	N3	202	PEB	C2D-C3D	9.42	1.46	1.34
26	F9	202	PEB	C2D-C3D	9.42	1.46	1.34
26	er	202	PEB	C2D-C3D	9.42	1.46	1.34
26	r4	201	PEB	C2D-C3D	9.42	1.46	1.34
26	p8	202	PEB	C2D-C3D	9.42	1.46	1.34
26	C8	202	PEB	C2D-C3D	9.42	1.46	1.34
26	H2	201	PEB	C2D-C3D	9.42	1.46	1.34
26	Z7	202	PEB	C2D-C3D	9.42	1.46	1.34
26	di	202	PEB	C2D-C3D	9.42	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	jI	1002	PEB	C2D-C3D	9.42	1.46	1.34
26	H9	202	PEB	C2D-C3D	9.42	1.46	1.34
26	bN	202	PEB	C2D-C3D	9.42	1.46	1.34
26	bH	202	PEB	C2D-C3D	9.42	1.46	1.34
26	r7	202	PEB	C2D-C3D	9.41	1.46	1.34
26	dd	202	PEB	C2D-C3D	9.41	1.46	1.34
26	gv	202	PEB	C2D-C3D	9.41	1.46	1.34
26	cL	202	PEB	C2D-C3D	9.41	1.46	1.34
26	m5	1003	PEB	C2D-C3D	9.41	1.46	1.34
26	dl	202	PEB	C2D-C3D	9.41	1.46	1.34
26	B4	202	PEB	C2D-C3D	9.41	1.46	1.34
26	r3	202	PEB	C2D-C3D	9.41	1.46	1.34
26	ar	202	PEB	C2D-C3D	9.41	1.46	1.34
26	l2	202	PEB	C2D-C3D	9.41	1.46	1.34
26	cb	202	PEB	C2D-C3D	9.41	1.46	1.34
26	bB	202	PEB	C2D-C3D	9.41	1.46	1.34
26	eV	202	PEB	C2D-C3D	9.41	1.46	1.34
26	t3	202	PEB	C2D-C3D	9.40	1.46	1.34
26	cj	202	PEB	C2D-C3D	9.40	1.46	1.34
26	ab	202	PEB	C2D-C3D	9.40	1.46	1.34
26	fs	202	PEB	C2D-C3D	9.40	1.46	1.34
26	h2	202	PEB	C2D-C3D	9.40	1.46	1.34
26	X7	202	PEB	C2D-C3D	9.40	1.46	1.34
26	h3	201	PEB	C2D-C3D	9.40	1.46	1.34
26	34	1001	PEB	C2D-C3D	9.40	1.46	1.34
26	av	202	PEB	C2D-C3D	9.40	1.46	1.34
26	hR	202	PEB	C2D-C3D	9.40	1.46	1.34
26	z3	202	PEB	C2D-C3D	9.40	1.46	1.34
26	e4	202	PEB	C2D-C3D	9.40	1.46	1.34
26	jK	1002	PEB	C2D-C3D	9.40	1.46	1.34
26	34	1002	PEB	C2D-C3D	9.40	1.46	1.34
26	j2	202	PEB	C2D-C3D	9.40	1.46	1.34
26	j4	202	PEB	C2D-C3D	9.40	1.46	1.34
26	H7	202	PEB	C2D-C3D	9.40	1.46	1.34
26	fw	202	PEB	C2D-C3D	9.40	1.46	1.34
26	r5	202	PEB	C2D-C3D	9.39	1.46	1.34
26	R3	202	PEB	C2D-C3D	9.39	1.46	1.34
26	N9	202	PEB	C2D-C3D	9.39	1.46	1.34
26	ch	202	PEB	C2D-C3D	9.39	1.46	1.34
26	eg	202	PEB	C2D-C3D	9.39	1.46	1.34
26	cr	202	PEB	C2D-C3D	9.39	1.46	1.34
26	fo	202	PEB	C2D-C3D	9.39	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bV	202	PEB	C2D-C3D	9.39	1.46	1.34
26	ec	202	PEB	C2D-C3D	9.39	1.46	1.34
26	lf	202	PEB	C2D-C3D	9.39	1.46	1.34
26	dY	202	PEB	C2D-C3D	9.39	1.46	1.34
26	fq	202	PEB	C2D-C3D	9.39	1.46	1.34
26	L5	202	PEB	C2D-C3D	9.39	1.46	1.34
26	df	202	PEB	C2D-C3D	9.39	1.46	1.34
26	gt	202	PEB	C2D-C3D	9.39	1.46	1.34
26	kV	1002	PEB	C2D-C3D	9.39	1.46	1.34
26	x7	202	PEB	C2D-C3D	9.39	1.46	1.34
26	hH	202	PEB	C2D-C3D	9.39	1.46	1.34
26	f2	202	PEB	C2D-C3D	9.38	1.46	1.34
26	z5	202	PEB	C2D-C3D	9.38	1.46	1.34
26	d7	202	PEB	C2D-C3D	9.38	1.46	1.34
26	li	203	PEB	C2D-C3D	9.38	1.46	1.34
26	ga	202	PEB	C2D-C3D	9.38	1.46	1.34
26	kU	1002	PEB	C2D-C3D	9.38	1.46	1.34
26	B5	202	PEB	C2D-C3D	9.38	1.46	1.34
26	n7	202	PEB	C2D-C3D	9.38	1.46	1.34
26	A1	301	PEB	C2D-C3D	9.38	1.46	1.34
26	B1	301	PEB	C2D-C3D	9.38	1.46	1.34
26	P7	202	PEB	C2D-C3D	9.38	1.46	1.34
26	ei	202	PEB	C2D-C3D	9.38	1.46	1.34
26	J5	202	PEB	C2D-C3D	9.38	1.46	1.34
26	al	202	PEB	C2D-C3D	9.38	1.46	1.34
26	R5	202	PEB	C2D-C3D	9.38	1.46	1.34
26	bJ	202	PEB	C2D-C3D	9.38	1.46	1.34
26	v9	202	PEB	C2D-C3D	9.38	1.46	1.34
26	X2	202	PEB	C2D-C3D	9.38	1.46	1.34
26	y8	202	PEB	C2D-C3D	9.38	1.46	1.34
26	D9	202	PEB	C2D-C3D	9.38	1.46	1.34
26	el	202	PEB	C2D-C3D	9.38	1.46	1.34
26	p2	202	PEB	C2D-C3D	9.38	1.46	1.34
26	y7	202	PEB	C2D-C3D	9.38	1.46	1.34
26	B9	202	PEB	C2D-C3D	9.38	1.46	1.34
26	gg	202	PEB	C2D-C3D	9.37	1.46	1.34
26	V3	202	PEB	C2D-C3D	9.37	1.46	1.34
26	V5	202	PEB	C2D-C3D	9.37	1.46	1.34
26	B6	202	PEB	C2D-C3D	9.37	1.46	1.34
26	D7	202	PEB	C2D-C3D	9.37	1.46	1.34
26	et	202	PEB	C2D-C3D	9.37	1.46	1.34
26	ev	202	PEB	C2D-C3D	9.37	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hP	202	PEB	C2D-C3D	9.37	1.46	1.34
26	iE	1002	PEB	C2D-C3D	9.37	1.46	1.34
26	jL	1002	PEB	C2D-C3D	9.37	1.46	1.34
26	hV	202	PEB	C2D-C3D	9.37	1.46	1.34
26	c7	202	PEB	C2D-C3D	9.37	1.46	1.34
26	iC	1002	PEB	C2D-C3D	9.37	1.46	1.34
26	e7	202	PEB	C2D-C3D	9.37	1.46	1.34
26	an	201	PEB	C2D-C3D	9.37	1.46	1.34
26	aF	202	PEB	C2D-C3D	9.37	1.46	1.34
26	bF	202	PEB	C2D-C3D	9.37	1.46	1.34
26	kT	1002	PEB	C2D-C3D	9.37	1.46	1.34
26	D3	202	PEB	C2D-C3D	9.37	1.46	1.34
26	D4	202	PEB	C2D-C3D	9.37	1.46	1.34
26	R6	202	PEB	C2D-C3D	9.37	1.46	1.34
26	ea	203	PEB	C2D-C3D	9.37	1.46	1.34
26	jP	1002	PEB	C2D-C3D	9.37	1.46	1.34
26	P5	201	PEB	C2D-C3D	9.37	1.46	1.34
26	n6	202	PEB	C2D-C3D	9.37	1.46	1.34
26	lr	202	PEB	C2D-C3D	9.36	1.46	1.34
26	J3	202	PEB	C2D-C3D	9.36	1.46	1.34
26	P3	202	PEB	C2D-C3D	9.36	1.46	1.34
26	X6	202	PEB	C2D-C3D	9.36	1.46	1.34
26	cd	202	PEB	C2D-C3D	9.36	1.46	1.34
26	cz	202	PEB	C2D-C3D	9.36	1.46	1.34
26	cB	202	PEB	C2D-C3D	9.36	1.46	1.34
26	F3	202	PEB	C2D-C3D	9.36	1.46	1.34
26	p4	202	PEB	C2D-C3D	9.36	1.46	1.34
26	p5	201	PEB	C2D-C3D	9.36	1.46	1.34
26	n3	202	PEB	C2D-C3D	9.36	1.46	1.34
26	L7	201	PEB	C2D-C3D	9.36	1.46	1.34
26	hB	202	PEB	C2D-C3D	9.36	1.46	1.34
26	hN	202	PEB	C2D-C3D	9.36	1.46	1.34
26	V2	202	PEB	C2D-C3D	9.36	1.46	1.34
26	v7	202	PEB	C2D-C3D	9.36	1.46	1.34
26	af	202	PEB	C2D-C3D	9.36	1.46	1.34
26	hL	202	PEB	C2D-C3D	9.36	1.46	1.34
26	kQ	1002	PEB	C2D-C3D	9.36	1.46	1.34
26	L3	202	PEB	C2D-C3D	9.36	1.46	1.34
26	cq	202	PEB	C2D-C3D	9.36	1.46	1.34
26	fi	202	PEB	C2D-C3D	9.36	1.46	1.34
26	gd	201	PEB	C2D-C3D	9.36	1.46	1.34
26	lp	202	PEB	C2D-C3D	9.35	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ln	202	PEB	C2D-C3D	9.35	1.46	1.34
26	B7	201	PEB	C2D-C3D	9.35	1.46	1.34
26	cJ	202	PEB	C2D-C3D	9.35	1.46	1.34
26	n8	201	PEB	C2D-C3D	9.35	1.46	1.34
26	v4	202	PEB	C2D-C3D	9.35	1.46	1.34
26	ad	202	PEB	C2D-C3D	9.35	1.46	1.34
26	fc	202	PEB	C2D-C3D	9.35	1.46	1.34
26	l7	202	PEB	C2D-C3D	9.35	1.46	1.34
26	aD	202	PEB	C2D-C3D	9.35	1.46	1.34
26	bD	202	PEB	C2D-C3D	9.35	1.46	1.34
26	ll	202	PEB	C2D-C3D	9.35	1.46	1.34
26	L2	202	PEB	C2D-C3D	9.35	1.46	1.34
26	ap	202	PEB	C2D-C3D	9.35	1.46	1.34
26	fj	202	PEB	C2D-C3D	9.35	1.46	1.34
26	f3	202	PEB	C2D-C3D	9.35	1.46	1.34
26	L9	202	PEB	C2D-C3D	9.35	1.46	1.34
26	lh	202	PEB	C2D-C3D	9.35	1.46	1.34
26	kR	1002	PEB	C2D-C3D	9.35	1.46	1.34
26	N5	202	PEB	C2D-C3D	9.35	1.46	1.34
26	cH	201	PEB	C2D-C3D	9.35	1.46	1.34
26	hX	202	PEB	C2D-C3D	9.35	1.46	1.34
26	n2	202	PEB	C2D-C3D	9.35	1.46	1.34
26	dh	202	PEB	C2D-C3D	9.35	1.46	1.34
26	jO	1002	PEB	C2D-C3D	9.35	1.46	1.34
26	V9	202	PEB	C2D-C3D	9.34	1.46	1.34
26	cY	202	PEB	C2D-C3D	9.34	1.46	1.34
26	dL	202	PEB	C2D-C3D	9.34	1.46	1.34
26	eJ	202	PEB	C2D-C3D	9.34	1.46	1.34
26	kS	1002	PEB	C2D-C3D	9.34	1.46	1.34
26	gp	202	PEB	C2D-C3D	9.34	1.46	1.34
26	H3	202	PEB	C2D-C3D	9.34	1.46	1.34
26	gi	202	PEB	C2D-C3D	9.34	1.46	1.34
26	gk	202	PEB	C2D-C3D	9.34	1.46	1.34
26	T7	202	PEB	C2D-C3D	9.34	1.46	1.34
26	A2	1003	PEB	C2D-C3D	9.34	1.46	1.34
26	D5	202	PEB	C2D-C3D	9.34	1.46	1.34
26	cn	201	PEB	C2D-C3D	9.34	1.46	1.34
26	co	201	PEB	C2D-C3D	9.34	1.46	1.34
26	ep	202	PEB	C2D-C3D	9.34	1.46	1.34
26	fm	202	PEB	C2D-C3D	9.34	1.46	1.34
26	jJ	1002	PEB	C2D-C3D	9.34	1.46	1.34
26	ge	202	PEB	C2D-C3D	9.34	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g4	202	PEB	C2D-C3D	9.34	1.46	1.34
26	lo	203	PEB	C2D-C3D	9.34	1.46	1.34
26	l4	202	PEB	C2D-C3D	9.34	1.46	1.34
26	p7	201	PEB	C2D-C3D	9.34	1.46	1.34
26	cs	202	PEB	C2D-C3D	9.34	1.46	1.34
26	fy	201	PEB	C2D-C3D	9.34	1.46	1.34
26	R9	202	PEB	C2D-C3D	9.34	1.46	1.34
26	fg	201	PEB	C2D-C3D	9.34	1.46	1.34
26	fu	201	PEB	C2D-C3D	9.34	1.46	1.34
26	A5	203	PEB	C2D-C3D	9.34	1.46	1.34
26	n4	202	PEB	C2D-C3D	9.33	1.46	1.34
26	F5	202	PEB	C2D-C3D	9.33	1.46	1.34
26	hJ	202	PEB	C2D-C3D	9.33	1.46	1.34
26	jN	1002	PEB	C2D-C3D	9.33	1.46	1.34
26	T9	202	PEB	C2D-C3D	9.33	1.46	1.34
26	F7	201	PEB	C2D-C3D	9.33	1.46	1.34
26	bT	201	PEB	C2D-C3D	9.33	1.46	1.34
26	hT	202	PEB	C2D-C3D	9.33	1.46	1.34
26	gx	202	PEB	C2D-C3D	9.33	1.46	1.34
26	B3	202	PEB	C2D-C3D	9.33	1.46	1.34
26	ff	202	PEB	C2D-C3D	9.33	1.46	1.34
26	W3	203	PEB	C2D-C3D	9.32	1.46	1.34
26	P9	202	PEB	C2D-C3D	9.32	1.46	1.34
26	ld	202	PEB	C2D-C3D	9.32	1.46	1.34
26	eX	201	PEB	C2D-C3D	9.32	1.46	1.34
26	J9	202	PEB	C2D-C3D	9.32	1.46	1.34
26	hG	201	PEB	C2D-C3D	9.32	1.46	1.34
26	T2	202	PEB	C2D-C3D	9.32	1.46	1.34
26	Z2	202	PEB	C2D-C3D	9.32	1.46	1.34
26	dj	202	PEB	C2D-C3D	9.32	1.46	1.34
26	J7	201	PEB	C2D-C3D	9.32	1.46	1.34
26	x3	202	PEB	C2D-C3D	9.32	1.46	1.34
26	cF	201	PEB	C2D-C3D	9.32	1.46	1.34
26	t5	202	PEB	C2D-C3D	9.32	1.46	1.34
26	kW	1002	PEB	C2D-C3D	9.32	1.46	1.34
26	hD	202	PEB	C2D-C3D	9.32	1.46	1.34
26	J6	202	PEB	C2D-C3D	9.32	1.46	1.34
26	cl	202	PEB	C2D-C3D	9.32	1.46	1.34
26	jM	1002	PEB	C2D-C3D	9.32	1.46	1.34
26	S5	203	PEB	C2D-C3D	9.31	1.46	1.34
26	gn	202	PEB	C2D-C3D	9.31	1.46	1.34
26	cf	201	PEB	C2D-C3D	9.31	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a7	202	PEB	C2D-C3D	9.31	1.46	1.34
26	kX	1002	PEB	C2D-C3D	9.31	1.46	1.34
26	h8	202	PEB	C2D-C3D	9.31	1.46	1.34
26	T3	202	PEB	C2D-C3D	9.30	1.46	1.34
26	j3	201	PEB	C2D-C3D	9.30	1.46	1.34
26	dV	202	PEB	C2D-C3D	9.30	1.46	1.34
26	Z3	202	PEB	C2D-C3D	9.30	1.46	1.34
26	iD	1002	PEB	C2D-C3D	9.30	1.46	1.34
26	z7	202	PEB	C2D-C3D	9.30	1.46	1.34
26	ee	202	PEB	C2D-C3D	9.30	1.46	1.34
26	bQ	203	PEB	C2D-C3D	9.30	1.46	1.34
26	v3	202	PEB	C2D-C3D	9.29	1.46	1.34
26	n5	202	PEB	C2D-C3D	9.29	1.46	1.34
26	gr	201	PEB	C2D-C3D	9.29	1.46	1.34
26	aj	202	PEB	C2D-C3D	9.28	1.46	1.34
26	lw	203	PEB	C2D-C3D	9.28	1.46	1.34
26	eB	203	PEB	C2D-C3D	9.28	1.46	1.34
26	R7	202	PEB	C2D-C3D	9.28	1.46	1.34
26	p3	202	PEB	C2D-C3D	9.28	1.46	1.34
26	Y7	1003	PEB	C2D-C3D	9.27	1.46	1.34
26	V7	202	PEB	C2D-C3D	9.26	1.46	1.34
26	eN	202	PEB	C2D-C3D	9.24	1.46	1.34
26	az	202	PEB	C2D-C3D	9.23	1.46	1.34
26	ah	202	PEB	C2D-C3D	9.22	1.46	1.34
29	dx	405	PVN	C10-C11	9.17	1.42	1.35
29	D2	303	PVN	C10-C11	9.15	1.42	1.35
29	d3	302	PVN	C10-C11	9.09	1.42	1.35
29	bY	1004	PVN	C10-C11	9.06	1.42	1.35
29	aY	403	PVN	C10-C11	9.02	1.42	1.35
29	dw	404	PVN	C10-C11	8.81	1.42	1.35
29	Z5	304	PVN	C10-C11	8.48	1.42	1.35
29	44	303	PVN	C10-C11	8.39	1.42	1.35
29	e8	303	PVN	C10-C11	8.35	1.42	1.35
29	e9	304	PVN	C10-C11	8.30	1.42	1.35
29	Z9	1004	PVN	C10-C11	8.26	1.42	1.35
29	U8	1004	PVN	C10-C11	8.20	1.42	1.35
29	34	1004	PVN	C10-C11	7.99	1.41	1.35
29	Y5	1004	PVN	C10-C11	7.99	1.41	1.35
29	hZ	403	PVN	C10-C11	7.93	1.41	1.35
29	aZ	303	PVN	C10-C11	7.91	1.41	1.35
29	bZ	304	PVN	C10-C11	7.91	1.41	1.35
29	hY	404	PVN	C10-C11	7.89	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ez	1004	PVN	C10-C11	7.73	1.41	1.35
29	d8	303	PVN	C10-C11	7.72	1.41	1.35
29	b8	1004	PVN	C10-C11	7.71	1.41	1.35
29	b9	405	PVN	C10-C11	7.71	1.41	1.35
29	C2	303	PVN	C10-C11	7.67	1.41	1.35
29	c3	303	PVN	C10-C11	7.67	1.41	1.35
29	Y9	303	PVN	C10-C11	7.66	1.41	1.35
26	K7	202	PEB	C2D-C3D	7.65	1.44	1.34
26	K3	202	PEB	C2D-C3D	7.63	1.44	1.34
29	T8	303	PVN	C10-C11	7.63	1.41	1.35
26	o8	201	PEB	C2D-C3D	7.62	1.44	1.34
29	A2	1004	PVN	C10-C11	7.62	1.41	1.35
29	a3	1004	PVN	C10-C11	7.62	1.41	1.35
26	u5	202	PEB	C2D-C3D	7.62	1.44	1.34
26	cx	202	PEB	C2D-C3D	7.61	1.44	1.34
29	d9	304	PVN	C10-C11	7.60	1.41	1.35
26	hW	202	PEB	C2D-C3D	7.60	1.44	1.34
26	eu	202	PEB	C2D-C3D	7.60	1.44	1.34
26	dU	202	PEB	C2D-C3D	7.59	1.44	1.34
26	lq	203	PEB	C2D-C3D	7.59	1.44	1.34
26	O7	202	PEB	C2D-C3D	7.59	1.44	1.34
26	A5	202	PEB	C2D-C3D	7.59	1.44	1.34
26	bC	202	PEB	C2D-C3D	7.59	1.44	1.34
26	bA	202	PEB	C2D-C3D	7.59	1.44	1.34
26	P2	202	PEB	C2D-C3D	7.59	1.44	1.34
26	lo	201	PEB	C2D-C3D	7.59	1.44	1.34
26	f7	202	PEB	C2D-C3D	7.59	1.44	1.34
26	as	202	PEB	C2D-C3D	7.59	1.44	1.34
26	S9	202	PEB	C2D-C3D	7.58	1.44	1.34
26	eB	201	PEB	C2D-C3D	7.58	1.44	1.34
26	gb	1002	PEB	C2D-C3D	7.58	1.44	1.34
26	hZ	401	PEB	C2D-C3D	7.58	1.44	1.34
26	Z5	302	PEB	C2D-C3D	7.58	1.44	1.34
26	lg	201	PEB	C2D-C3D	7.58	1.44	1.34
26	lw	202	PEB	C2D-C3D	7.58	1.44	1.34
26	hA	202	PEB	C2D-C3D	7.58	1.44	1.34
26	i7	202	PEB	C2D-C3D	7.58	1.44	1.34
26	W7	202	PEB	C2D-C3D	7.58	1.44	1.34
26	hY	402	PEB	C2D-C3D	7.58	1.44	1.34
26	bK	1002	PEB	C2D-C3D	7.58	1.44	1.34
26	C5	202	PEB	C2D-C3D	7.58	1.44	1.34
26	hQ	202	PEB	C2D-C3D	7.58	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hS	202	PEB	C2D-C3D	7.58	1.44	1.34
26	Q5	202	PEB	C2D-C3D	7.57	1.44	1.34
26	lh	201	PEB	C2D-C3D	7.57	1.44	1.34
26	h4	201	PEB	C2D-C3D	7.57	1.44	1.34
26	C7	202	PEB	C2D-C3D	7.57	1.44	1.34
26	cK	202	PEB	C2D-C3D	7.57	1.44	1.34
26	hC	202	PEB	C2D-C3D	7.57	1.44	1.34
26	de	202	PEB	C2D-C3D	7.57	1.44	1.34
26	lm	1002	PEB	C2D-C3D	7.57	1.44	1.34
26	gl	202	PEB	C2D-C3D	7.57	1.44	1.34
26	w3	202	PEB	C2D-C3D	7.57	1.44	1.34
26	q5	202	PEB	C2D-C3D	7.57	1.44	1.34
26	C4	1002	PEB	C2D-C3D	7.57	1.44	1.34
26	o5	202	PEB	C2D-C3D	7.57	1.44	1.34
26	I7	202	PEB	C2D-C3D	7.57	1.44	1.34
26	hK	202	PEB	C2D-C3D	7.57	1.44	1.34
26	Z9	1002	PEB	C2D-C3D	7.57	1.44	1.34
26	fh	1002	PEB	C2D-C3D	7.56	1.44	1.34
26	S3	202	PEB	C2D-C3D	7.56	1.44	1.34
26	c5	201	PEB	C2D-C3D	7.56	1.44	1.34
26	o7	202	PEB	C2D-C3D	7.56	1.44	1.34
26	bO	202	PEB	C2D-C3D	7.56	1.44	1.34
26	gj	202	PEB	C2D-C3D	7.56	1.44	1.34
26	cD	202	PEB	C2D-C3D	7.56	1.44	1.34
26	gz	302	PEB	C2D-C3D	7.56	1.44	1.34
26	w7	1002	PEB	C2D-C3D	7.56	1.44	1.34
26	lo	202	PEB	C2D-C3D	7.56	1.44	1.34
26	A3	202	PEB	C2D-C3D	7.56	1.44	1.34
26	W3	202	PEB	C2D-C3D	7.56	1.44	1.34
26	A4	202	PEB	C2D-C3D	7.56	1.44	1.34
26	Y7	1002	PEB	C2D-C3D	7.56	1.44	1.34
26	em	202	PEB	C2D-C3D	7.56	1.44	1.34
26	iF	1002	PEB	C2D-C3D	7.56	1.44	1.34
26	eL	201	PEB	C2D-C3D	7.56	1.44	1.34
26	hE	1002	PEB	C2D-C3D	7.56	1.44	1.34
26	y3	202	PEB	C2D-C3D	7.56	1.44	1.34
26	fb	202	PEB	C2D-C3D	7.56	1.44	1.34
26	M9	202	PEB	C2D-C3D	7.55	1.44	1.34
26	gf	202	PEB	C2D-C3D	7.55	1.44	1.34
26	U3	202	PEB	C2D-C3D	7.55	1.44	1.34
26	O5	202	PEB	C2D-C3D	7.55	1.44	1.34
26	s8	202	PEB	C2D-C3D	7.55	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E7	202	PEB	C2D-C3D	7.55	1.44	1.34
26	cA	202	PEB	C2D-C3D	7.55	1.44	1.34
26	eA	1002	PEB	C2D-C3D	7.55	1.44	1.34
26	m3	202	PEB	C2D-C3D	7.55	1.44	1.34
26	c8	301	PEB	C2D-C3D	7.55	1.44	1.34
26	O9	202	PEB	C2D-C3D	7.55	1.44	1.34
26	au	202	PEB	C2D-C3D	7.55	1.44	1.34
26	w4	202	PEB	C2D-C3D	7.55	1.44	1.34
26	d8	301	PEB	C2D-C3D	7.55	1.44	1.34
26	I5	202	PEB	C2D-C3D	7.55	1.44	1.34
26	j7	202	PEB	C2D-C3D	7.55	1.44	1.34
26	hM	1002	PEB	C2D-C3D	7.55	1.44	1.34
26	U5	202	PEB	C2D-C3D	7.55	1.44	1.34
26	a6	202	PEB	C2D-C3D	7.55	1.44	1.34
26	u8	202	PEB	C2D-C3D	7.55	1.44	1.34
26	ld	201	PEB	C2D-C3D	7.55	1.44	1.34
26	A2	1001	PEB	C2D-C3D	7.55	1.44	1.34
26	G6	202	PEB	C2D-C3D	7.55	1.44	1.34
26	ec	201	PEB	C2D-C3D	7.55	1.44	1.34
26	gy	302	PEB	C2D-C3D	7.55	1.44	1.34
26	lw	201	PEB	C2D-C3D	7.55	1.44	1.34
26	M7	1003	PEB	C2D-C3D	7.54	1.44	1.34
26	s7	202	PEB	C2D-C3D	7.54	1.44	1.34
26	lk	202	PEB	C2D-C3D	7.54	1.44	1.34
26	hI	202	PEB	C2D-C3D	7.54	1.44	1.34
26	bS	202	PEB	C2D-C3D	7.54	1.44	1.34
26	u3	202	PEB	C2D-C3D	7.54	1.44	1.34
26	p6	202	PEB	C2D-C3D	7.54	1.44	1.34
26	bU	202	PEB	C2D-C3D	7.54	1.44	1.34
26	aw	202	PEB	C2D-C3D	7.54	1.44	1.34
26	U2	202	PEB	C2D-C3D	7.54	1.44	1.34
26	M3	202	PEB	C2D-C3D	7.54	1.44	1.34
26	c3	301	PEB	C2D-C3D	7.54	1.44	1.34
26	Y5	1002	PEB	C2D-C3D	7.54	1.44	1.34
26	V6	202	PEB	C2D-C3D	7.54	1.44	1.34
26	G7	202	PEB	C2D-C3D	7.54	1.44	1.34
26	E9	202	PEB	C2D-C3D	7.54	1.44	1.34
26	h5	202	PEB	C2D-C3D	7.54	1.44	1.34
29	c9	303	PVN	C10-C11	7.54	1.41	1.35
26	A9	202	PEB	C2D-C3D	7.54	1.44	1.34
26	cC	1002	PEB	C2D-C3D	7.54	1.44	1.34
26	ei	201	PEB	C2D-C3D	7.54	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	lc	202	PEB	C2D-C3D	7.54	1.44	1.34
26	hF	202	PEB	C2D-C3D	7.54	1.44	1.34
26	hU	201	PEB	C2D-C3D	7.54	1.44	1.34
26	C3	1002	PEB	C2D-C3D	7.54	1.44	1.34
26	i3	202	PEB	C2D-C3D	7.54	1.44	1.34
26	S5	202	PEB	C2D-C3D	7.54	1.44	1.34
26	cI	202	PEB	C2D-C3D	7.53	1.44	1.34
26	Q3	202	PEB	C2D-C3D	7.53	1.44	1.34
26	s4	202	PEB	C2D-C3D	7.53	1.44	1.34
26	K5	1002	PEB	C2D-C3D	7.53	1.44	1.34
26	bE	202	PEB	C2D-C3D	7.53	1.44	1.34
26	dZ	1002	PEB	C2D-C3D	7.53	1.44	1.34
26	ft	202	PEB	C2D-C3D	7.53	1.44	1.34
26	M5	202	PEB	C2D-C3D	7.53	1.44	1.34
26	Y9	301	PEB	C2D-C3D	7.53	1.44	1.34
26	le	202	PEB	C2D-C3D	7.53	1.44	1.34
26	gc	202	PEB	C2D-C3D	7.53	1.44	1.34
26	w5	202	PEB	C2D-C3D	7.53	1.44	1.34
26	dJ	202	PEB	C2D-C3D	7.53	1.44	1.34
26	G3	202	PEB	C2D-C3D	7.53	1.44	1.34
26	bM	202	PEB	C2D-C3D	7.53	1.44	1.34
26	N6	202	PEB	C2D-C3D	7.53	1.44	1.34
26	O3	1002	PEB	C2D-C3D	7.53	1.44	1.34
26	e3	1002	PEB	C2D-C3D	7.53	1.44	1.34
26	f6	202	PEB	C2D-C3D	7.53	1.44	1.34
26	C9	202	PEB	C2D-C3D	7.53	1.44	1.34
26	d3	301	PEB	C2D-C3D	7.53	1.44	1.34
26	lt	202	PEB	C2D-C3D	7.53	1.44	1.34
26	iB	1002	PEB	C2D-C3D	7.53	1.44	1.34
26	s5	202	PEB	C2D-C3D	7.53	1.44	1.34
26	y5	1002	PEB	C2D-C3D	7.53	1.44	1.34
26	U9	202	PEB	C2D-C3D	7.53	1.44	1.34
26	bG	202	PEB	C2D-C3D	7.53	1.44	1.34
26	u7	202	PEB	C2D-C3D	7.52	1.44	1.34
26	G5	202	PEB	C2D-C3D	7.52	1.44	1.34
26	ev	201	PEB	C2D-C3D	7.52	1.44	1.34
26	g3	202	PEB	C2D-C3D	7.52	1.44	1.34
26	g7	202	PEB	C2D-C3D	7.52	1.44	1.34
26	m7	202	PEB	C2D-C3D	7.52	1.44	1.34
26	bQ	202	PEB	C2D-C3D	7.52	1.44	1.34
26	eY	401	PEB	C2D-C3D	7.52	1.44	1.34
26	s3	202	PEB	C2D-C3D	7.52	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q7	202	PEB	C2D-C3D	7.52	1.44	1.34
26	ay	1002	PEB	C2D-C3D	7.52	1.44	1.34
26	ey	1001	PEB	C2D-C3D	7.52	1.44	1.34
26	ls	202	PEB	C2D-C3D	7.52	1.44	1.34
26	I9	202	PEB	C2D-C3D	7.52	1.44	1.34
26	et	201	PEB	C2D-C3D	7.52	1.44	1.34
26	fp	202	PEB	C2D-C3D	7.52	1.44	1.34
26	k3	202	PEB	C2D-C3D	7.52	1.44	1.34
26	gq	202	PEB	C2D-C3D	7.52	1.44	1.34
26	d6	202	PEB	C2D-C3D	7.52	1.44	1.34
26	t6	201	PEB	C2D-C3D	7.52	1.44	1.34
26	h7	202	PEB	C2D-C3D	7.52	1.44	1.34
26	cy	1002	PEB	C2D-C3D	7.52	1.44	1.34
26	lg	202	PEB	C2D-C3D	7.52	1.44	1.34
26	S2	202	PEB	C2D-C3D	7.52	1.44	1.34
26	U6	202	PEB	C2D-C3D	7.52	1.44	1.34
26	fv	202	PEB	C2D-C3D	7.52	1.44	1.34
26	E2	1002	PEB	C2D-C3D	7.51	1.44	1.34
26	S7	202	PEB	C2D-C3D	7.51	1.44	1.34
26	c4	201	PEB	C2D-C3D	7.51	1.44	1.34
26	lj	201	PEB	C2D-C3D	7.51	1.44	1.34
26	cu	202	PEB	C2D-C3D	7.51	1.44	1.34
26	N4	202	PEB	C2D-C3D	7.51	1.44	1.34
26	k7	1002	PEB	C2D-C3D	7.51	1.44	1.34
26	Q9	202	PEB	C2D-C3D	7.51	1.44	1.34
26	eh	202	PEB	C2D-C3D	7.51	1.44	1.34
26	gs	202	PEB	C2D-C3D	7.51	1.44	1.34
26	cm	1002	PEB	C2D-C3D	7.51	1.44	1.34
26	lu	202	PEB	C2D-C3D	7.51	1.44	1.34
26	fk	202	PEB	C2D-C3D	7.51	1.44	1.34
26	fr	202	PEB	C2D-C3D	7.51	1.44	1.34
26	aq	202	PEB	C2D-C3D	7.51	1.44	1.34
26	G9	202	PEB	C2D-C3D	7.51	1.44	1.34
29	c8	303	PVN	C10-C11	7.51	1.41	1.35
26	m5	1002	PEB	C2D-C3D	7.51	1.44	1.34
26	cw	202	PEB	C2D-C3D	7.51	1.44	1.34
26	gw	202	PEB	C2D-C3D	7.51	1.44	1.34
26	cZ	202	PEB	C2D-C3D	7.51	1.44	1.34
26	da	1002	PEB	C2D-C3D	7.51	1.44	1.34
26	hO	202	PEB	C2D-C3D	7.51	1.44	1.34
26	K9	1002	PEB	C2D-C3D	7.50	1.44	1.34
26	ek	1002	PEB	C2D-C3D	7.50	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fg	202	PEB	C2D-C3D	7.50	1.44	1.34
26	E3	202	PEB	C2D-C3D	7.50	1.44	1.34
26	fx	202	PEB	C2D-C3D	7.50	1.44	1.34
26	iA	1002	PEB	C2D-C3D	7.50	1.44	1.34
26	ct	202	PEB	C2D-C3D	7.50	1.44	1.34
26	cG	202	PEB	C2D-C3D	7.50	1.44	1.34
26	gh	202	PEB	C2D-C3D	7.50	1.44	1.34
26	bI	202	PEB	C2D-C3D	7.50	1.44	1.34
26	fl	202	PEB	C2D-C3D	7.50	1.44	1.34
26	o3	202	PEB	C2D-C3D	7.50	1.44	1.34
26	ef	202	PEB	C2D-C3D	7.50	1.44	1.34
26	ao	202	PEB	C2D-C3D	7.50	1.44	1.34
26	gm	1002	PEB	C2D-C3D	7.50	1.44	1.34
26	db	202	PEB	C2D-C3D	7.50	1.44	1.34
26	N2	201	PEB	C2D-C3D	7.50	1.44	1.34
26	H6	201	PEB	C2D-C3D	7.50	1.44	1.34
26	eP	201	PEB	C2D-C3D	7.50	1.44	1.34
26	dc	202	PEB	C2D-C3D	7.49	1.44	1.34
26	I3	202	PEB	C2D-C3D	7.49	1.44	1.34
26	r8	202	PEB	C2D-C3D	7.49	1.44	1.34
26	cv	202	PEB	C2D-C3D	7.49	1.44	1.34
26	fe	202	PEB	C2D-C3D	7.49	1.44	1.34
26	fn	1002	PEB	C2D-C3D	7.49	1.44	1.34
26	go	202	PEB	C2D-C3D	7.49	1.44	1.34
26	E5	202	PEB	C2D-C3D	7.49	1.44	1.34
26	n6	201	PEB	C2D-C3D	7.49	1.44	1.34
26	fz	301	PEB	C2D-C3D	7.49	1.44	1.34
26	dg	202	PEB	C2D-C3D	7.49	1.44	1.34
26	R2	201	PEB	C2D-C3D	7.49	1.44	1.34
26	gu	202	PEB	C2D-C3D	7.49	1.44	1.34
26	q8	202	PEB	C2D-C3D	7.49	1.44	1.34
26	U7	202	PEB	C2D-C3D	7.48	1.44	1.34
26	t8	202	PEB	C2D-C3D	7.48	1.44	1.34
26	f5	201	PEB	C2D-C3D	7.48	1.44	1.34
26	A7	201	PEB	C2D-C3D	7.47	1.44	1.34
26	e6	202	PEB	C2D-C3D	7.47	1.44	1.34
26	bZ	302	PEB	C2D-C3D	7.47	1.44	1.34
26	bY	1002	PEB	C2D-C3D	7.47	1.44	1.34
26	Q7	202	PEB	C2D-C3D	7.46	1.44	1.34
26	a3	1002	PEB	C2D-C3D	7.44	1.44	1.34
26	Y3	202	PEB	C2D-C3D	7.42	1.44	1.34
29	ey	1004	PVN	C10-C11	7.32	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	lz	403	PVN	C10-C11	6.92	1.40	1.35
26	ep	201	PEB	C2D-C3D	6.83	1.43	1.34
26	eS	201	PEB	C2D-C3D	6.82	1.43	1.34
26	a7	201	PEB	C2D-C3D	6.80	1.43	1.34
29	eZ	402	PVN	C10-C11	6.79	1.40	1.35
26	dU	201	PEB	C2D-C3D	6.79	1.43	1.34
26	eU	201	PEB	C2D-C3D	6.79	1.43	1.34
29	ly	404	PVN	C10-C11	6.78	1.40	1.35
26	g5	201	PEB	C2D-C3D	6.78	1.43	1.34
26	V6	201	PEB	C2D-C3D	6.78	1.43	1.34
26	U7	201	PEB	C2D-C3D	6.78	1.43	1.34
26	dQ	202	PEB	C2D-C3D	6.78	1.43	1.34
26	aA	201	PEB	C2D-C3D	6.77	1.43	1.34
26	X7	201	PEB	C2D-C3D	6.77	1.43	1.34
26	ai	201	PEB	C2D-C3D	6.77	1.43	1.34
26	es	201	PEB	C2D-C3D	6.77	1.43	1.34
26	t2	201	PEB	C2D-C3D	6.77	1.43	1.34
26	W7	201	PEB	C2D-C3D	6.77	1.43	1.34
26	t5	201	PEB	C2D-C3D	6.77	1.43	1.34
26	H7	201	PEB	C2D-C3D	6.77	1.43	1.34
26	en	201	PEB	C2D-C3D	6.77	1.43	1.34
26	E6	201	PEB	C2D-C3D	6.77	1.43	1.34
26	eM	1001	PEB	C2D-C3D	6.77	1.43	1.34
26	eQ	202	PEB	C2D-C3D	6.76	1.43	1.34
29	eY	403	PVN	C10-C11	6.76	1.40	1.35
26	M3	201	PEB	C2D-C3D	6.76	1.43	1.34
26	dg	201	PEB	C2D-C3D	6.76	1.43	1.34
26	eD	201	PEB	C2D-C3D	6.76	1.43	1.34
26	bZ	301	PEB	C2D-C3D	6.76	1.43	1.34
26	Q5	201	PEB	C2D-C3D	6.76	1.43	1.34
26	k8	201	PEB	C2D-C3D	6.76	1.43	1.34
26	K2	201	PEB	C2D-C3D	6.76	1.43	1.34
26	M6	1002	PEB	C2D-C3D	6.76	1.43	1.34
26	dN	201	PEB	C2D-C3D	6.76	1.43	1.34
26	aH	201	PEB	C2D-C3D	6.76	1.43	1.34
26	gg	201	PEB	C2D-C3D	6.76	1.43	1.34
26	G9	201	PEB	C2D-C3D	6.75	1.43	1.34
26	ck	201	PEB	C2D-C3D	6.75	1.43	1.34
26	eu	201	PEB	C2D-C3D	6.75	1.43	1.34
26	D9	201	PEB	C2D-C3D	6.75	1.43	1.34
26	ad	201	PEB	C2D-C3D	6.75	1.43	1.34
26	B4	201	PEB	C2D-C3D	6.75	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ee	201	PEB	C2D-C3D	6.75	1.43	1.34
26	ez	1001	PEB	C2D-C3D	6.75	1.43	1.34
26	c6	1003	PEB	C2D-C3D	6.75	1.43	1.34
26	cD	201	PEB	C2D-C3D	6.75	1.43	1.34
26	cQ	201	PEB	C2D-C3D	6.75	1.43	1.34
26	G8	202	PEB	C2D-C3D	6.75	1.43	1.34
26	dM	1001	PEB	C2D-C3D	6.75	1.43	1.34
26	D8	202	PEB	C2D-C3D	6.75	1.43	1.34
26	eo	202	PEB	C2D-C3D	6.75	1.43	1.34
26	ly	401	PEB	C2D-C3D	6.75	1.43	1.34
26	eG	201	PEB	C2D-C3D	6.75	1.43	1.34
26	J4	202	PEB	C2D-C3D	6.75	1.43	1.34
26	f7	201	PEB	C2D-C3D	6.75	1.43	1.34
26	f3	201	PEB	C2D-C3D	6.75	1.43	1.34
26	u5	201	PEB	C2D-C3D	6.75	1.43	1.34
26	w2	201	PEB	C2D-C3D	6.75	1.43	1.34
26	bJ	201	PEB	C2D-C3D	6.75	1.43	1.34
26	ea	201	PEB	C2D-C3D	6.75	1.43	1.34
26	U2	201	PEB	C2D-C3D	6.74	1.43	1.34
26	Y4	201	PEB	C2D-C3D	6.74	1.43	1.34
26	S5	201	PEB	C2D-C3D	6.74	1.43	1.34
26	o8	202	PEB	C2D-C3D	6.74	1.43	1.34
26	be	201	PEB	C2D-C3D	6.74	1.43	1.34
26	v5	201	PEB	C2D-C3D	6.74	1.43	1.34
26	M6	1001	PEB	C2D-C3D	6.74	1.43	1.34
26	x8	201	PEB	C2D-C3D	6.74	1.43	1.34
26	dW	201	PEB	C2D-C3D	6.74	1.43	1.34
26	gy	303	PEB	C2D-C3D	6.74	1.43	1.34
26	ci	201	PEB	C2D-C3D	6.74	1.43	1.34
26	i4	201	PEB	C2D-C3D	6.74	1.43	1.34
26	C2	302	PEB	C2D-C3D	6.74	1.43	1.34
26	l8	201	PEB	C2D-C3D	6.74	1.43	1.34
26	i6	201	PEB	C2D-C3D	6.74	1.43	1.34
26	aw	201	PEB	C2D-C3D	6.74	1.43	1.34
26	aK	1002	PEB	C2D-C3D	6.74	1.43	1.34
26	E4	201	PEB	C2D-C3D	6.74	1.43	1.34
26	i9	201	PEB	C2D-C3D	6.74	1.43	1.34
26	bm	1001	PEB	C2D-C3D	6.74	1.43	1.34
26	eD	202	PEB	C2D-C3D	6.74	1.43	1.34
26	K3	201	PEB	C2D-C3D	6.74	1.43	1.34
26	s6	201	PEB	C2D-C3D	6.74	1.43	1.34
26	cO	202	PEB	C2D-C3D	6.74	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eg	201	PEB	C2D-C3D	6.74	1.43	1.34
26	gc	201	PEB	C2D-C3D	6.74	1.43	1.34
26	e6	201	PEB	C2D-C3D	6.74	1.43	1.34
26	i7	201	PEB	C2D-C3D	6.74	1.43	1.34
26	C9	201	PEB	C2D-C3D	6.74	1.43	1.34
26	gz	301	PEB	C2D-C3D	6.74	1.43	1.34
26	s2	202	PEB	C2D-C3D	6.74	1.43	1.34
26	N6	201	PEB	C2D-C3D	6.74	1.43	1.34
26	t8	201	PEB	C2D-C3D	6.74	1.43	1.34
26	gz	303	PEB	C2D-C3D	6.74	1.43	1.34
26	m8	201	PEB	C2D-C3D	6.74	1.43	1.34
26	cT	1002	PEB	C2D-C3D	6.74	1.43	1.34
26	eK	201	PEB	C2D-C3D	6.74	1.43	1.34
26	q6	202	PEB	C2D-C3D	6.74	1.43	1.34
26	u7	201	PEB	C2D-C3D	6.74	1.43	1.34
26	aC	202	PEB	C2D-C3D	6.74	1.43	1.34
26	eS	202	PEB	C2D-C3D	6.74	1.43	1.34
26	H9	201	PEB	C2D-C3D	6.74	1.43	1.34
26	aM	202	PEB	C2D-C3D	6.74	1.43	1.34
26	j8	201	PEB	C2D-C3D	6.73	1.43	1.34
26	S7	201	PEB	C2D-C3D	6.73	1.43	1.34
26	aL	201	PEB	C2D-C3D	6.73	1.43	1.34
26	Q4	201	PEB	C2D-C3D	6.73	1.43	1.34
26	aL	202	PEB	C2D-C3D	6.73	1.43	1.34
26	bG	201	PEB	C2D-C3D	6.73	1.43	1.34
26	bL	201	PEB	C2D-C3D	6.73	1.43	1.34
26	fd	301	PEB	C2D-C3D	6.73	1.43	1.34
26	B2	501	PEB	C2D-C3D	6.73	1.43	1.34
26	q4	202	PEB	C2D-C3D	6.73	1.43	1.34
26	b9	404	PEB	C2D-C3D	6.73	1.43	1.34
26	I8	201	PEB	C2D-C3D	6.73	1.43	1.34
26	u9	202	PEB	C2D-C3D	6.73	1.43	1.34
26	bg	201	PEB	C2D-C3D	6.73	1.43	1.34
26	bK	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	cp	201	PEB	C2D-C3D	6.73	1.43	1.34
26	cG	201	PEB	C2D-C3D	6.73	1.43	1.34
26	da	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	dq	202	PEB	C2D-C3D	6.73	1.43	1.34
26	dA	202	PEB	C2D-C3D	6.73	1.43	1.34
26	al	201	PEB	C2D-C3D	6.73	1.43	1.34
26	dD	201	PEB	C2D-C3D	6.73	1.43	1.34
26	O5	201	PEB	C2D-C3D	6.73	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c6	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	g9	201	PEB	C2D-C3D	6.73	1.43	1.34
26	ag	201	PEB	C2D-C3D	6.73	1.43	1.34
26	aR	202	PEB	C2D-C3D	6.73	1.43	1.34
26	bj	201	PEB	C2D-C3D	6.73	1.43	1.34
26	bs	1002	PEB	C2D-C3D	6.73	1.43	1.34
26	hF	201	PEB	C2D-C3D	6.73	1.43	1.34
26	jP	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	n3	201	PEB	C2D-C3D	6.73	1.43	1.34
26	H5	201	PEB	C2D-C3D	6.73	1.43	1.34
26	k7	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	u9	201	PEB	C2D-C3D	6.73	1.43	1.34
26	Z9	1007	PEB	C2D-C3D	6.73	1.43	1.34
26	lr	201	PEB	C2D-C3D	6.73	1.43	1.34
26	gb	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	C3	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	aU	202	PEB	C2D-C3D	6.73	1.43	1.34
26	hL	201	PEB	C2D-C3D	6.73	1.43	1.34
26	bd	202	PEB	C2D-C3D	6.73	1.43	1.34
26	bB	201	PEB	C2D-C3D	6.73	1.43	1.34
26	s2	201	PEB	C2D-C3D	6.73	1.43	1.34
26	w3	201	PEB	C2D-C3D	6.73	1.43	1.34
26	D8	201	PEB	C2D-C3D	6.73	1.43	1.34
26	cY	201	PEB	C2D-C3D	6.73	1.43	1.34
26	ds	202	PEB	C2D-C3D	6.73	1.43	1.34
26	dK	202	PEB	C2D-C3D	6.73	1.43	1.34
26	dN	202	PEB	C2D-C3D	6.73	1.43	1.34
26	v3	201	PEB	C2D-C3D	6.73	1.43	1.34
26	w6	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	z9	201	PEB	C2D-C3D	6.73	1.43	1.34
26	eW	201	PEB	C2D-C3D	6.73	1.43	1.34
26	Z4	202	PEB	C2D-C3D	6.73	1.43	1.34
26	b6	202	PEB	C2D-C3D	6.73	1.43	1.34
26	j7	201	PEB	C2D-C3D	6.73	1.43	1.34
26	E8	201	PEB	C2D-C3D	6.73	1.43	1.34
26	I9	201	PEB	C2D-C3D	6.73	1.43	1.34
26	aQ	201	PEB	C2D-C3D	6.73	1.43	1.34
26	cU	201	PEB	C2D-C3D	6.73	1.43	1.34
26	n2	201	PEB	C2D-C3D	6.73	1.43	1.34
26	O4	1001	PEB	C2D-C3D	6.73	1.43	1.34
26	q7	201	PEB	C2D-C3D	6.73	1.43	1.34
26	V9	201	PEB	C2D-C3D	6.73	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aC	201	PEB	C2D-C3D	6.73	1.43	1.34
26	bc	201	PEB	C2D-C3D	6.73	1.43	1.34
26	eP	203	PEB	C2D-C3D	6.73	1.43	1.34
26	lp	201	PEB	C2D-C3D	6.73	1.43	1.34
26	I3	201	PEB	C2D-C3D	6.72	1.43	1.34
26	X5	401	PEB	C2D-C3D	6.72	1.43	1.34
26	e5	201	PEB	C2D-C3D	6.72	1.43	1.34
26	m6	201	PEB	C2D-C3D	6.72	1.43	1.34
26	eb	201	PEB	C2D-C3D	6.72	1.43	1.34
26	el	201	PEB	C2D-C3D	6.72	1.43	1.34
26	eU	202	PEB	C2D-C3D	6.72	1.43	1.34
26	K4	202	PEB	C2D-C3D	6.72	1.43	1.34
26	E8	202	PEB	C2D-C3D	6.72	1.43	1.34
26	E9	201	PEB	C2D-C3D	6.72	1.43	1.34
26	bD	201	PEB	C2D-C3D	6.72	1.43	1.34
26	cT	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	dd	201	PEB	C2D-C3D	6.72	1.43	1.34
26	A2	1002	PEB	C2D-C3D	6.72	1.43	1.34
26	C8	201	PEB	C2D-C3D	6.72	1.43	1.34
26	M8	202	PEB	C2D-C3D	6.72	1.43	1.34
26	az	201	PEB	C2D-C3D	6.72	1.43	1.34
26	cR	202	PEB	C2D-C3D	6.72	1.43	1.34
26	dP	202	PEB	C2D-C3D	6.72	1.43	1.34
26	eE	202	PEB	C2D-C3D	6.72	1.43	1.34
26	fc	201	PEB	C2D-C3D	6.72	1.43	1.34
26	hK	201	PEB	C2D-C3D	6.72	1.43	1.34
26	hT	201	PEB	C2D-C3D	6.72	1.43	1.34
26	m3	201	PEB	C2D-C3D	6.72	1.43	1.34
26	R4	202	PEB	C2D-C3D	6.72	1.43	1.34
26	b8	1003	PEB	C2D-C3D	6.72	1.43	1.34
26	Q8	202	PEB	C2D-C3D	6.72	1.43	1.34
26	bu	201	PEB	C2D-C3D	6.72	1.43	1.34
26	bH	201	PEB	C2D-C3D	6.72	1.43	1.34
26	cq	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dj	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dn	202	PEB	C2D-C3D	6.72	1.43	1.34
26	dC	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dJ	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dQ	201	PEB	C2D-C3D	6.72	1.43	1.34
26	eI	201	PEB	C2D-C3D	6.72	1.43	1.34
26	jJ	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	e2	201	PEB	C2D-C3D	6.72	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r2	202	PEB	C2D-C3D	6.72	1.43	1.34
26	E4	202	PEB	C2D-C3D	6.72	1.43	1.34
26	V8	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	Y8	201	PEB	C2D-C3D	6.72	1.43	1.34
26	eA	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	eK	202	PEB	C2D-C3D	6.72	1.43	1.34
26	iD	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	b4	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	q4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dB	201	PEB	C2D-C3D	6.72	1.43	1.34
26	eE	201	PEB	C2D-C3D	6.72	1.43	1.34
26	b8	1002	PEB	C2D-C3D	6.72	1.43	1.34
26	dh	201	PEB	C2D-C3D	6.72	1.43	1.34
26	hI	201	PEB	C2D-C3D	6.72	1.43	1.34
26	u2	201	PEB	C2D-C3D	6.72	1.43	1.34
26	J4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	Q4	202	PEB	C2D-C3D	6.72	1.43	1.34
26	Z4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	r9	202	PEB	C2D-C3D	6.72	1.43	1.34
26	bl	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dX	202	PEB	C2D-C3D	6.72	1.43	1.34
26	hC	201	PEB	C2D-C3D	6.72	1.43	1.34
26	hX	201	PEB	C2D-C3D	6.72	1.43	1.34
26	jN	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	j2	201	PEB	C2D-C3D	6.72	1.43	1.34
26	x2	201	PEB	C2D-C3D	6.72	1.43	1.34
26	Y5	1003	PEB	C2D-C3D	6.72	1.43	1.34
26	K6	201	PEB	C2D-C3D	6.72	1.43	1.34
26	T8	302	PEB	C2D-C3D	6.72	1.43	1.34
26	q9	202	PEB	C2D-C3D	6.72	1.43	1.34
26	cC	1003	PEB	C2D-C3D	6.72	1.43	1.34
26	dr	201	PEB	C2D-C3D	6.72	1.43	1.34
26	dW	202	PEB	C2D-C3D	6.72	1.43	1.34
26	B2	502	PEB	C2D-C3D	6.72	1.43	1.34
26	P8	202	PEB	C2D-C3D	6.72	1.43	1.34
26	aV	202	PEB	C2D-C3D	6.72	1.43	1.34
26	dk	1002	PEB	C2D-C3D	6.72	1.43	1.34
26	F2	202	PEB	C2D-C3D	6.72	1.43	1.34
26	A4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	H4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	cP	201	PEB	C2D-C3D	6.72	1.43	1.34
26	eh	201	PEB	C2D-C3D	6.72	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p2	201	PEB	C2D-C3D	6.72	1.43	1.34
26	M4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	P6	202	PEB	C2D-C3D	6.72	1.43	1.34
26	t9	201	PEB	C2D-C3D	6.72	1.43	1.34
26	af	201	PEB	C2D-C3D	6.72	1.43	1.34
26	bx	201	PEB	C2D-C3D	6.72	1.43	1.34
26	cx	201	PEB	C2D-C3D	6.72	1.43	1.34
26	cS	202	PEB	C2D-C3D	6.72	1.43	1.34
26	lk	201	PEB	C2D-C3D	6.72	1.43	1.34
26	lv	201	PEB	C2D-C3D	6.72	1.43	1.34
26	gl	201	PEB	C2D-C3D	6.72	1.43	1.34
26	o2	1001	PEB	C2D-C3D	6.72	1.43	1.34
26	F4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	a4	201	PEB	C2D-C3D	6.72	1.43	1.34
26	bA	201	PEB	C2D-C3D	6.72	1.43	1.34
26	gv	201	PEB	C2D-C3D	6.72	1.43	1.34
26	hO	201	PEB	C2D-C3D	6.72	1.43	1.34
26	J3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	m5	1001	PEB	C2D-C3D	6.71	1.43	1.34
26	h6	202	PEB	C2D-C3D	6.71	1.43	1.34
26	K7	201	PEB	C2D-C3D	6.71	1.43	1.34
26	aD	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bn	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bS	201	PEB	C2D-C3D	6.71	1.43	1.34
26	t3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bh	202	PEB	C2D-C3D	6.71	1.43	1.34
26	by	1002	PEB	C2D-C3D	6.71	1.43	1.34
26	ds	201	PEB	C2D-C3D	6.71	1.43	1.34
26	G3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	e3	1001	PEB	C2D-C3D	6.71	1.43	1.34
26	E5	201	PEB	C2D-C3D	6.71	1.43	1.34
26	k8	202	PEB	C2D-C3D	6.71	1.43	1.34
26	B9	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bM	201	PEB	C2D-C3D	6.71	1.43	1.34
26	dF	202	PEB	C2D-C3D	6.71	1.43	1.34
26	dT	202	PEB	C2D-C3D	6.71	1.43	1.34
26	jL	1001	PEB	C2D-C3D	6.71	1.43	1.34
26	z2	202	PEB	C2D-C3D	6.71	1.43	1.34
26	T3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	G8	201	PEB	C2D-C3D	6.71	1.43	1.34
26	M9	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bI	201	PEB	C2D-C3D	6.71	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dR	202	PEB	C2D-C3D	6.71	1.43	1.34
26	ea	202	PEB	C2D-C3D	6.71	1.43	1.34
26	g2	202	PEB	C2D-C3D	6.71	1.43	1.34
26	i5	201	PEB	C2D-C3D	6.71	1.43	1.34
26	Q7	201	PEB	C2D-C3D	6.71	1.43	1.34
26	B8	202	PEB	C2D-C3D	6.71	1.43	1.34
26	as	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bv	201	PEB	C2D-C3D	6.71	1.43	1.34
26	dy	401	PEB	C2D-C3D	6.71	1.43	1.34
26	dz	402	PEB	C2D-C3D	6.71	1.43	1.34
26	k2	201	PEB	C2D-C3D	6.71	1.43	1.34
26	K6	202	PEB	C2D-C3D	6.71	1.43	1.34
26	ef	201	PEB	C2D-C3D	6.71	1.43	1.34
26	eo	201	PEB	C2D-C3D	6.71	1.43	1.34
26	gw	201	PEB	C2D-C3D	6.71	1.43	1.34
26	kV	1001	PEB	C2D-C3D	6.71	1.43	1.34
26	z2	201	PEB	C2D-C3D	6.71	1.43	1.34
26	Q3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	o6	201	PEB	C2D-C3D	6.71	1.43	1.34
26	U8	1003	PEB	C2D-C3D	6.71	1.43	1.34
26	dq	201	PEB	C2D-C3D	6.71	1.43	1.34
26	e4	201	PEB	C2D-C3D	6.71	1.43	1.34
26	a5	201	PEB	C2D-C3D	6.71	1.43	1.34
26	x9	202	PEB	C2D-C3D	6.71	1.43	1.34
26	bQ	201	PEB	C2D-C3D	6.71	1.43	1.34
26	cA	201	PEB	C2D-C3D	6.71	1.43	1.34
26	dw	401	PEB	C2D-C3D	6.71	1.43	1.34
26	dz	401	PEB	C2D-C3D	6.71	1.43	1.34
26	dL	201	PEB	C2D-C3D	6.71	1.43	1.34
26	eP	202	PEB	C2D-C3D	6.71	1.43	1.34
26	w2	203	PEB	C2D-C3D	6.71	1.43	1.34
26	o3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	f4	201	PEB	C2D-C3D	6.71	1.43	1.34
26	y6	203	PEB	C2D-C3D	6.71	1.43	1.34
26	E7	201	PEB	C2D-C3D	6.71	1.43	1.34
26	N9	201	PEB	C2D-C3D	6.71	1.43	1.34
26	z3	201	PEB	C2D-C3D	6.71	1.43	1.34
26	W6	201	PEB	C2D-C3D	6.71	1.43	1.34
26	N8	201	PEB	C2D-C3D	6.71	1.43	1.34
26	j9	202	PEB	C2D-C3D	6.71	1.43	1.34
26	aT	201	PEB	C2D-C3D	6.71	1.43	1.34
26	bv	202	PEB	C2D-C3D	6.71	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	lu	201	PEB	C2D-C3D	6.71	1.43	1.34
26	P7	201	PEB	C2D-C3D	6.71	1.43	1.34
26	ae	201	PEB	C2D-C3D	6.71	1.43	1.34
26	aQ	202	PEB	C2D-C3D	6.71	1.43	1.34
26	cN	201	PEB	C2D-C3D	6.71	1.43	1.34
26	cX	201	PEB	C2D-C3D	6.71	1.43	1.34
26	lt	201	PEB	C2D-C3D	6.71	1.43	1.34
26	kS	1001	PEB	C2D-C3D	6.71	1.43	1.34
26	G2	202	PEB	C2D-C3D	6.71	1.43	1.34
26	G4	202	PEB	C2D-C3D	6.71	1.43	1.34
26	e8	302	PEB	C2D-C3D	6.71	1.43	1.34
26	f9	201	PEB	C2D-C3D	6.71	1.43	1.34
26	p9	201	PEB	C2D-C3D	6.71	1.43	1.34
26	aE	202	PEB	C2D-C3D	6.71	1.43	1.34
26	fn	1001	PEB	C2D-C3D	6.71	1.43	1.34
26	ft	201	PEB	C2D-C3D	6.71	1.43	1.34
26	b3	501	PEB	C2D-C3D	6.70	1.43	1.34
26	Q4	203	PEB	C2D-C3D	6.70	1.43	1.34
26	y4	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	c6	1002	PEB	C2D-C3D	6.70	1.43	1.34
26	b9	403	PEB	C2D-C3D	6.70	1.43	1.34
26	cB	201	PEB	C2D-C3D	6.70	1.43	1.34
26	eq	202	PEB	C2D-C3D	6.70	1.43	1.34
26	ln	201	PEB	C2D-C3D	6.70	1.43	1.34
26	fk	201	PEB	C2D-C3D	6.70	1.43	1.34
26	ga	201	PEB	C2D-C3D	6.70	1.43	1.34
26	jI	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	A5	201	PEB	C2D-C3D	6.70	1.43	1.34
26	M7	1002	PEB	C2D-C3D	6.70	1.43	1.34
26	x7	201	PEB	C2D-C3D	6.70	1.43	1.34
26	dr	202	PEB	C2D-C3D	6.70	1.43	1.34
26	fm	201	PEB	C2D-C3D	6.70	1.43	1.34
26	I2	202	PEB	C2D-C3D	6.70	1.43	1.34
26	u3	201	PEB	C2D-C3D	6.70	1.43	1.34
26	F6	202	PEB	C2D-C3D	6.70	1.43	1.34
26	Q6	201	PEB	C2D-C3D	6.70	1.43	1.34
26	q8	201	PEB	C2D-C3D	6.70	1.43	1.34
26	M7	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	W8	201	PEB	C2D-C3D	6.70	1.43	1.34
26	Y9	302	PEB	C2D-C3D	6.70	1.43	1.34
26	ab	201	PEB	C2D-C3D	6.70	1.43	1.34
26	aB	201	PEB	C2D-C3D	6.70	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bz	201	PEB	C2D-C3D	6.70	1.43	1.34
26	dH	202	PEB	C2D-C3D	6.70	1.43	1.34
26	ez	1003	PEB	C2D-C3D	6.70	1.43	1.34
26	g2	201	PEB	C2D-C3D	6.70	1.43	1.34
26	W3	201	PEB	C2D-C3D	6.70	1.43	1.34
26	ao	201	PEB	C2D-C3D	6.70	1.43	1.34
26	aJ	202	PEB	C2D-C3D	6.70	1.43	1.34
26	ew	301	PEB	C2D-C3D	6.70	1.43	1.34
26	gs	201	PEB	C2D-C3D	6.70	1.43	1.34
26	gt	201	PEB	C2D-C3D	6.70	1.43	1.34
26	e2	202	PEB	C2D-C3D	6.70	1.43	1.34
26	i2	202	PEB	C2D-C3D	6.70	1.43	1.34
26	b3	502	PEB	C2D-C3D	6.70	1.43	1.34
26	U4	202	PEB	C2D-C3D	6.70	1.43	1.34
26	m8	202	PEB	C2D-C3D	6.70	1.43	1.34
26	aM	201	PEB	C2D-C3D	6.70	1.43	1.34
26	di	201	PEB	C2D-C3D	6.70	1.43	1.34
26	fl	201	PEB	C2D-C3D	6.70	1.43	1.34
26	fp	201	PEB	C2D-C3D	6.70	1.43	1.34
26	fv	201	PEB	C2D-C3D	6.70	1.43	1.34
26	N3	201	PEB	C2D-C3D	6.70	1.43	1.34
26	Z3	201	PEB	C2D-C3D	6.70	1.43	1.34
26	w8	202	PEB	C2D-C3D	6.70	1.43	1.34
26	aF	201	PEB	C2D-C3D	6.70	1.43	1.34
26	bf	201	PEB	C2D-C3D	6.70	1.43	1.34
26	bl	202	PEB	C2D-C3D	6.70	1.43	1.34
26	cJ	201	PEB	C2D-C3D	6.70	1.43	1.34
26	dc	203	PEB	C2D-C3D	6.70	1.43	1.34
26	B5	201	PEB	C2D-C3D	6.70	1.43	1.34
26	T5	201	PEB	C2D-C3D	6.70	1.43	1.34
26	h9	202	PEB	C2D-C3D	6.70	1.43	1.34
26	p9	202	PEB	C2D-C3D	6.70	1.43	1.34
26	dm	201	PEB	C2D-C3D	6.70	1.43	1.34
26	dn	201	PEB	C2D-C3D	6.70	1.43	1.34
26	gk	201	PEB	C2D-C3D	6.70	1.43	1.34
26	24	401	PEB	C2D-C3D	6.70	1.43	1.34
26	p4	201	PEB	C2D-C3D	6.70	1.43	1.34
26	U5	201	PEB	C2D-C3D	6.70	1.43	1.34
26	G6	201	PEB	C2D-C3D	6.70	1.43	1.34
26	g6	202	PEB	C2D-C3D	6.70	1.43	1.34
26	r6	201	PEB	C2D-C3D	6.70	1.43	1.34
26	aX	402	PEB	C2D-C3D	6.70	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bX	402	PEB	C2D-C3D	6.70	1.43	1.34
26	dD	202	PEB	C2D-C3D	6.70	1.43	1.34
26	eR	201	PEB	C2D-C3D	6.70	1.43	1.34
26	o4	201	PEB	C2D-C3D	6.70	1.43	1.34
26	x4	201	PEB	C2D-C3D	6.70	1.43	1.34
26	Z6	201	PEB	C2D-C3D	6.70	1.43	1.34
26	c7	201	PEB	C2D-C3D	6.70	1.43	1.34
26	bq	202	PEB	C2D-C3D	6.70	1.43	1.34
26	cU	202	PEB	C2D-C3D	6.70	1.43	1.34
26	ed	201	PEB	C2D-C3D	6.70	1.43	1.34
26	ed	202	PEB	C2D-C3D	6.70	1.43	1.34
26	hM	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	iB	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	V2	201	PEB	C2D-C3D	6.70	1.43	1.34
26	y3	201	PEB	C2D-C3D	6.70	1.43	1.34
26	V5	201	PEB	C2D-C3D	6.70	1.43	1.34
26	l5	202	PEB	C2D-C3D	6.70	1.43	1.34
26	y5	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	C6	202	PEB	C2D-C3D	6.70	1.43	1.34
26	w6	1002	PEB	C2D-C3D	6.70	1.43	1.34
26	s8	201	PEB	C2D-C3D	6.70	1.43	1.34
26	br	202	PEB	C2D-C3D	6.70	1.43	1.34
26	cM	202	PEB	C2D-C3D	6.70	1.43	1.34
26	dx	402	PEB	C2D-C3D	6.70	1.43	1.34
26	hJ	201	PEB	C2D-C3D	6.70	1.43	1.34
26	iH	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	O7	201	PEB	C2D-C3D	6.70	1.43	1.34
26	f9	202	PEB	C2D-C3D	6.70	1.43	1.34
26	fa	201	PEB	C2D-C3D	6.70	1.43	1.34
26	o2	1002	PEB	C2D-C3D	6.70	1.43	1.34
26	R4	201	PEB	C2D-C3D	6.70	1.43	1.34
26	b6	201	PEB	C2D-C3D	6.70	1.43	1.34
26	r6	202	PEB	C2D-C3D	6.70	1.43	1.34
26	P9	201	PEB	C2D-C3D	6.70	1.43	1.34
26	fr	201	PEB	C2D-C3D	6.70	1.43	1.34
26	hP	201	PEB	C2D-C3D	6.70	1.43	1.34
26	l4	201	PEB	C2D-C3D	6.70	1.43	1.34
26	T6	201	PEB	C2D-C3D	6.70	1.43	1.34
26	e9	301	PEB	C2D-C3D	6.70	1.43	1.34
26	dR	201	PEB	C2D-C3D	6.70	1.43	1.34
26	ff	201	PEB	C2D-C3D	6.70	1.43	1.34
26	fo	201	PEB	C2D-C3D	6.70	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ge	201	PEB	C2D-C3D	6.70	1.43	1.34
26	jK	1001	PEB	C2D-C3D	6.70	1.43	1.34
26	Z2	201	PEB	C2D-C3D	6.69	1.43	1.34
26	E3	201	PEB	C2D-C3D	6.69	1.43	1.34
26	h6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	cL	201	PEB	C2D-C3D	6.69	1.43	1.34
26	cR	201	PEB	C2D-C3D	6.69	1.43	1.34
26	er	201	PEB	C2D-C3D	6.69	1.43	1.34
26	eH	202	PEB	C2D-C3D	6.69	1.43	1.34
26	d6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	y7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	N8	202	PEB	C2D-C3D	6.69	1.43	1.34
26	dY	201	PEB	C2D-C3D	6.69	1.43	1.34
26	gx	201	PEB	C2D-C3D	6.69	1.43	1.34
26	w4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	I6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	k9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	bd	201	PEB	C2D-C3D	6.69	1.43	1.34
26	bq	201	PEB	C2D-C3D	6.69	1.43	1.34
26	S2	201	PEB	C2D-C3D	6.69	1.43	1.34
26	g3	201	PEB	C2D-C3D	6.69	1.43	1.34
26	A6	1002	PEB	C2D-C3D	6.69	1.43	1.34
26	bX	401	PEB	C2D-C3D	6.69	1.43	1.34
26	eY	402	PEB	C2D-C3D	6.69	1.43	1.34
26	fs	201	PEB	C2D-C3D	6.69	1.43	1.34
26	hD	201	PEB	C2D-C3D	6.69	1.43	1.34
26	X2	201	PEB	C2D-C3D	6.69	1.43	1.34
26	D3	201	PEB	C2D-C3D	6.69	1.43	1.34
26	a3	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	x3	201	PEB	C2D-C3D	6.69	1.43	1.34
26	z9	202	PEB	C2D-C3D	6.69	1.43	1.34
26	X4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	o4	202	PEB	C2D-C3D	6.69	1.43	1.34
26	s4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	z6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	z8	202	PEB	C2D-C3D	6.69	1.43	1.34
26	aF	204	PEB	C2D-C3D	6.69	1.43	1.34
26	aG	201	PEB	C2D-C3D	6.69	1.43	1.34
26	cZ	201	PEB	C2D-C3D	6.69	1.43	1.34
26	du	201	PEB	C2D-C3D	6.69	1.43	1.34
26	dx	404	PEB	C2D-C3D	6.69	1.43	1.34
26	iF	1001	PEB	C2D-C3D	6.69	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C2	301	PEB	C2D-C3D	6.69	1.43	1.34
26	Y2	201	PEB	C2D-C3D	6.69	1.43	1.34
26	T4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	h8	201	PEB	C2D-C3D	6.69	1.43	1.34
26	g7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	b8	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	b9	402	PEB	C2D-C3D	6.69	1.43	1.34
26	S9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	br	201	PEB	C2D-C3D	6.69	1.43	1.34
26	cg	201	PEB	C2D-C3D	6.69	1.43	1.34
26	cV	203	PEB	C2D-C3D	6.69	1.43	1.34
26	iE	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	kU	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	L4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	O4	1002	PEB	C2D-C3D	6.69	1.43	1.34
26	P4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	L5	201	PEB	C2D-C3D	6.69	1.43	1.34
26	s9	202	PEB	C2D-C3D	6.69	1.43	1.34
26	Q9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	am	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	aP	202	PEB	C2D-C3D	6.69	1.43	1.34
26	cC	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	fj	201	PEB	C2D-C3D	6.69	1.43	1.34
26	r2	201	PEB	C2D-C3D	6.69	1.43	1.34
26	W2	202	PEB	C2D-C3D	6.69	1.43	1.34
26	m7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	n9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	o9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	O9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	ah	201	PEB	C2D-C3D	6.69	1.43	1.34
26	cc	201	PEB	C2D-C3D	6.69	1.43	1.34
26	44	301	PEB	C2D-C3D	6.69	1.43	1.34
26	F6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	o7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	L8	201	PEB	C2D-C3D	6.69	1.43	1.34
26	P8	201	PEB	C2D-C3D	6.69	1.43	1.34
26	U8	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	Z9	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	aN	201	PEB	C2D-C3D	6.69	1.43	1.34
26	aU	201	PEB	C2D-C3D	6.69	1.43	1.34
26	ej	202	PEB	C2D-C3D	6.69	1.43	1.34
26	H4	202	PEB	C2D-C3D	6.69	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d4	201	PEB	C2D-C3D	6.69	1.43	1.34
26	u4	202	PEB	C2D-C3D	6.69	1.43	1.34
26	K5	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	E6	202	PEB	C2D-C3D	6.69	1.43	1.34
26	U6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	l6	202	PEB	C2D-C3D	6.69	1.43	1.34
26	u6	202	PEB	C2D-C3D	6.69	1.43	1.34
26	l7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	aE	201	PEB	C2D-C3D	6.69	1.43	1.34
26	ca	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	du	202	PEB	C2D-C3D	6.69	1.43	1.34
26	hN	201	PEB	C2D-C3D	6.69	1.43	1.34
26	M2	201	PEB	C2D-C3D	6.69	1.43	1.34
26	Y6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	v7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	U9	201	PEB	C2D-C3D	6.69	1.43	1.34
26	bp	201	PEB	C2D-C3D	6.69	1.43	1.34
26	j8	202	PEB	C2D-C3D	6.69	1.43	1.34
26	D6	201	PEB	C2D-C3D	6.69	1.43	1.34
26	t6	202	PEB	C2D-C3D	6.69	1.43	1.34
26	y6	202	PEB	C2D-C3D	6.69	1.43	1.34
26	T7	201	PEB	C2D-C3D	6.69	1.43	1.34
26	aI	201	PEB	C2D-C3D	6.69	1.43	1.34
26	bs	1001	PEB	C2D-C3D	6.69	1.43	1.34
26	G2	201	PEB	C2D-C3D	6.68	1.43	1.34
26	K2	202	PEB	C2D-C3D	6.68	1.43	1.34
26	O8	202	PEB	C2D-C3D	6.68	1.43	1.34
26	T9	201	PEB	C2D-C3D	6.68	1.43	1.34
26	aK	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	aV	201	PEB	C2D-C3D	6.68	1.43	1.34
26	bw	202	PEB	C2D-C3D	6.68	1.43	1.34
26	dm	202	PEB	C2D-C3D	6.68	1.43	1.34
26	gn	201	PEB	C2D-C3D	6.68	1.43	1.34
26	gy	301	PEB	C2D-C3D	6.68	1.43	1.34
26	E2	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	r5	201	PEB	C2D-C3D	6.68	1.43	1.34
26	M8	201	PEB	C2D-C3D	6.68	1.43	1.34
26	J9	201	PEB	C2D-C3D	6.68	1.43	1.34
26	dH	201	PEB	C2D-C3D	6.68	1.43	1.34
26	dK	201	PEB	C2D-C3D	6.68	1.43	1.34
26	hY	403	PEB	C2D-C3D	6.68	1.43	1.34
26	I2	201	PEB	C2D-C3D	6.68	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W4	201	PEB	C2D-C3D	6.68	1.43	1.34
26	34	1007	PEB	C2D-C3D	6.68	1.43	1.34
26	y4	1002	PEB	C2D-C3D	6.68	1.43	1.34
26	K8	201	PEB	C2D-C3D	6.68	1.43	1.34
26	q9	201	PEB	C2D-C3D	6.68	1.43	1.34
26	ct	201	PEB	C2D-C3D	6.68	1.43	1.34
26	fq	201	PEB	C2D-C3D	6.68	1.43	1.34
26	hA	201	PEB	C2D-C3D	6.68	1.43	1.34
26	hZ	402	PEB	C2D-C3D	6.68	1.43	1.34
26	v8	202	PEB	C2D-C3D	6.68	1.43	1.34
26	x8	202	PEB	C2D-C3D	6.68	1.43	1.34
26	dI	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	em	201	PEB	C2D-C3D	6.68	1.43	1.34
26	lf	201	PEB	C2D-C3D	6.68	1.43	1.34
26	fh	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	gj	201	PEB	C2D-C3D	6.68	1.43	1.34
26	iC	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	kT	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	i3	201	PEB	C2D-C3D	6.68	1.43	1.34
26	c8	302	PEB	C2D-C3D	6.68	1.43	1.34
26	bW	301	PEB	C2D-C3D	6.68	1.43	1.34
26	cX	202	PEB	C2D-C3D	6.68	1.43	1.34
26	dV	201	PEB	C2D-C3D	6.68	1.43	1.34
26	lc	201	PEB	C2D-C3D	6.68	1.43	1.34
26	gi	201	PEB	C2D-C3D	6.68	1.43	1.34
26	m2	202	PEB	C2D-C3D	6.68	1.43	1.34
26	q2	201	PEB	C2D-C3D	6.68	1.43	1.34
26	v2	202	PEB	C2D-C3D	6.68	1.43	1.34
26	p6	201	PEB	C2D-C3D	6.68	1.43	1.34
26	c9	301	PEB	C2D-C3D	6.68	1.43	1.34
26	d9	303	PEB	C2D-C3D	6.68	1.43	1.34
26	w9	202	PEB	C2D-C3D	6.68	1.43	1.34
26	aY	406	PEB	C2D-C3D	6.68	1.43	1.34
26	cS	201	PEB	C2D-C3D	6.68	1.43	1.34
26	cV	202	PEB	C2D-C3D	6.68	1.43	1.34
26	dw	403	PEB	C2D-C3D	6.68	1.43	1.34
26	dX	201	PEB	C2D-C3D	6.68	1.43	1.34
26	eC	202	PEB	C2D-C3D	6.68	1.43	1.34
26	eG	202	PEB	C2D-C3D	6.68	1.43	1.34
26	hV	201	PEB	C2D-C3D	6.68	1.43	1.34
26	j4	201	PEB	C2D-C3D	6.68	1.43	1.34
26	j5	201	PEB	C2D-C3D	6.68	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	x6	202	PEB	C2D-C3D	6.68	1.43	1.34
26	s7	201	PEB	C2D-C3D	6.68	1.43	1.34
26	bN	201	PEB	C2D-C3D	6.68	1.43	1.34
26	kR	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	B3	201	PEB	C2D-C3D	6.68	1.43	1.34
26	S4	202	PEB	C2D-C3D	6.68	1.43	1.34
26	d9	302	PEB	C2D-C3D	6.68	1.43	1.34
26	dI	1002	PEB	C2D-C3D	6.68	1.43	1.34
26	dM	1002	PEB	C2D-C3D	6.68	1.43	1.34
26	cb	201	PEB	C2D-C3D	6.68	1.43	1.34
26	cu	201	PEB	C2D-C3D	6.68	1.43	1.34
26	eF	202	PEB	C2D-C3D	6.68	1.43	1.34
26	lq	201	PEB	C2D-C3D	6.68	1.43	1.34
26	ls	201	PEB	C2D-C3D	6.68	1.43	1.34
26	j5	202	PEB	C2D-C3D	6.68	1.43	1.34
26	J6	201	PEB	C2D-C3D	6.68	1.43	1.34
26	n7	201	PEB	C2D-C3D	6.68	1.43	1.34
26	aW	301	PEB	C2D-C3D	6.68	1.43	1.34
26	bi	201	PEB	C2D-C3D	6.68	1.43	1.34
26	do	202	PEB	C2D-C3D	6.68	1.43	1.34
26	ly	403	PEB	C2D-C3D	6.68	1.43	1.34
26	lz	402	PEB	C2D-C3D	6.68	1.43	1.34
26	fb	201	PEB	C2D-C3D	6.68	1.43	1.34
26	l2	201	PEB	C2D-C3D	6.68	1.43	1.34
26	u2	202	PEB	C2D-C3D	6.68	1.43	1.34
26	C5	201	PEB	C2D-C3D	6.68	1.43	1.34
26	x5	201	PEB	C2D-C3D	6.68	1.43	1.34
26	f8	201	PEB	C2D-C3D	6.68	1.43	1.34
26	aq	201	PEB	C2D-C3D	6.68	1.43	1.34
26	aJ	201	PEB	C2D-C3D	6.68	1.43	1.34
26	dv	201	PEB	C2D-C3D	6.68	1.43	1.34
26	eH	201	PEB	C2D-C3D	6.68	1.43	1.34
26	fe	201	PEB	C2D-C3D	6.68	1.43	1.34
26	hE	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	e7	201	PEB	C2D-C3D	6.68	1.43	1.34
26	dp	201	PEB	C2D-C3D	6.68	1.43	1.34
26	dC	202	PEB	C2D-C3D	6.68	1.43	1.34
26	dS	201	PEB	C2D-C3D	6.68	1.43	1.34
26	gq	201	PEB	C2D-C3D	6.68	1.43	1.34
26	z4	201	PEB	C2D-C3D	6.68	1.43	1.34
26	w8	201	PEB	C2D-C3D	6.68	1.43	1.34
26	bk	201	PEB	C2D-C3D	6.68	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bu	202	PEB	C2D-C3D	6.68	1.43	1.34
26	dk	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	dA	201	PEB	C2D-C3D	6.68	1.43	1.34
26	gm	1001	PEB	C2D-C3D	6.68	1.43	1.34
26	hW	201	PEB	C2D-C3D	6.68	1.43	1.34
26	D2	302	PEB	C2D-C3D	6.67	1.43	1.34
26	S3	203	PEB	C2D-C3D	6.67	1.43	1.34
26	l5	201	PEB	C2D-C3D	6.67	1.43	1.34
26	I7	201	PEB	C2D-C3D	6.67	1.43	1.34
26	Z7	201	PEB	C2D-C3D	6.67	1.43	1.34
26	O8	201	PEB	C2D-C3D	6.67	1.43	1.34
26	K9	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	cW	201	PEB	C2D-C3D	6.67	1.43	1.34
26	ey	1002	PEB	C2D-C3D	6.67	1.43	1.34
26	i8	201	PEB	C2D-C3D	6.67	1.43	1.34
26	m6	202	PEB	C2D-C3D	6.67	1.43	1.34
26	y9	1002	PEB	C2D-C3D	6.67	1.43	1.34
26	L9	201	PEB	C2D-C3D	6.67	1.43	1.34
26	av	201	PEB	C2D-C3D	6.67	1.43	1.34
26	aA	202	PEB	C2D-C3D	6.67	1.43	1.34
26	L2	201	PEB	C2D-C3D	6.67	1.43	1.34
26	A8	202	PEB	C2D-C3D	6.67	1.43	1.34
26	t9	202	PEB	C2D-C3D	6.67	1.43	1.34
26	aI	202	PEB	C2D-C3D	6.67	1.43	1.34
26	dZ	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	ek	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	li	202	PEB	C2D-C3D	6.67	1.43	1.34
26	gh	201	PEB	C2D-C3D	6.67	1.43	1.34
26	t4	201	PEB	C2D-C3D	6.67	1.43	1.34
26	y6	201	PEB	C2D-C3D	6.67	1.43	1.34
26	Q8	201	PEB	C2D-C3D	6.67	1.43	1.34
26	Z9	1003	PEB	C2D-C3D	6.67	1.43	1.34
26	bU	201	PEB	C2D-C3D	6.67	1.43	1.34
26	bZ	303	PEB	C2D-C3D	6.67	1.43	1.34
26	hB	201	PEB	C2D-C3D	6.67	1.43	1.34
26	dl	201	PEB	C2D-C3D	6.67	1.43	1.34
26	gu	201	PEB	C2D-C3D	6.67	1.43	1.34
26	kW	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	kX	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	y2	202	PEB	C2D-C3D	6.67	1.43	1.34
26	cl	201	PEB	C2D-C3D	6.67	1.43	1.34
26	dx	403	PEB	C2D-C3D	6.67	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	w2	202	PEB	C2D-C3D	6.67	1.43	1.34
26	O2	201	PEB	C2D-C3D	6.67	1.43	1.34
26	T2	201	PEB	C2D-C3D	6.67	1.43	1.34
26	a3	1003	PEB	C2D-C3D	6.67	1.43	1.34
26	V4	201	PEB	C2D-C3D	6.67	1.43	1.34
26	Z5	303	PEB	C2D-C3D	6.67	1.43	1.34
26	I6	202	PEB	C2D-C3D	6.67	1.43	1.34
26	j6	201	PEB	C2D-C3D	6.67	1.43	1.34
26	a9	602	PEB	C2D-C3D	6.67	1.43	1.34
26	A9	201	PEB	C2D-C3D	6.67	1.43	1.34
26	do	201	PEB	C2D-C3D	6.67	1.43	1.34
26	le	201	PEB	C2D-C3D	6.67	1.43	1.34
26	C7	201	PEB	C2D-C3D	6.67	1.43	1.34
26	e9	303	PEB	C2D-C3D	6.67	1.43	1.34
26	A8	201	PEB	C2D-C3D	6.67	1.43	1.34
26	S8	401	PEB	C2D-C3D	6.67	1.43	1.34
26	X9	401	PEB	C2D-C3D	6.67	1.43	1.34
26	au	201	PEB	C2D-C3D	6.67	1.43	1.34
26	la	1002	PEB	C2D-C3D	6.67	1.43	1.34
26	k4	201	PEB	C2D-C3D	6.67	1.43	1.34
26	m4	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	w5	201	PEB	C2D-C3D	6.67	1.43	1.34
26	O6	202	PEB	C2D-C3D	6.67	1.43	1.34
26	aR	201	PEB	C2D-C3D	6.67	1.43	1.34
26	cw	201	PEB	C2D-C3D	6.67	1.43	1.34
26	li	201	PEB	C2D-C3D	6.67	1.43	1.34
26	hY	401	PEB	C2D-C3D	6.67	1.43	1.34
26	F2	201	PEB	C2D-C3D	6.67	1.43	1.34
26	F4	202	PEB	C2D-C3D	6.67	1.43	1.34
26	U4	201	PEB	C2D-C3D	6.67	1.43	1.34
26	Y4	202	PEB	C2D-C3D	6.67	1.43	1.34
26	h4	202	PEB	C2D-C3D	6.67	1.43	1.34
26	k8	203	PEB	C2D-C3D	6.67	1.43	1.34
26	S6	201	PEB	C2D-C3D	6.67	1.43	1.34
26	S6	202	PEB	C2D-C3D	6.67	1.43	1.34
26	o6	202	PEB	C2D-C3D	6.67	1.43	1.34
26	aS	201	PEB	C2D-C3D	6.67	1.43	1.34
26	dO	201	PEB	C2D-C3D	6.67	1.43	1.34
26	eI	202	PEB	C2D-C3D	6.67	1.43	1.34
26	ll	201	PEB	C2D-C3D	6.67	1.43	1.34
26	hQ	201	PEB	C2D-C3D	6.67	1.43	1.34
26	S4	201	PEB	C2D-C3D	6.67	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F8	1001	PEB	C2D-C3D	6.67	1.43	1.34
26	w9	201	PEB	C2D-C3D	6.67	1.43	1.34
26	aN	204	PEB	C2D-C3D	6.67	1.43	1.34
26	aS	202	PEB	C2D-C3D	6.67	1.43	1.34
26	bw	201	PEB	C2D-C3D	6.67	1.43	1.34
26	dc	201	PEB	C2D-C3D	6.67	1.43	1.34
26	es	202	PEB	C2D-C3D	6.67	1.43	1.34
26	c3	302	PEB	C2D-C3D	6.67	1.43	1.34
26	a6	201	PEB	C2D-C3D	6.67	1.43	1.34
26	p8	201	PEB	C2D-C3D	6.67	1.43	1.34
26	T8	301	PEB	C2D-C3D	6.67	1.43	1.34
26	eF	201	PEB	C2D-C3D	6.67	1.43	1.34
26	v2	201	PEB	C2D-C3D	6.66	1.43	1.34
26	C4	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	c5	202	PEB	C2D-C3D	6.66	1.43	1.34
26	I8	202	PEB	C2D-C3D	6.66	1.43	1.34
26	v9	201	PEB	C2D-C3D	6.66	1.43	1.34
26	at	201	PEB	C2D-C3D	6.66	1.43	1.34
26	cV	201	PEB	C2D-C3D	6.66	1.43	1.34
26	iG	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	X3	201	PEB	C2D-C3D	6.66	1.43	1.34
26	f8	202	PEB	C2D-C3D	6.66	1.43	1.34
26	w7	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	aY	401	PEB	C2D-C3D	6.66	1.43	1.34
26	aZ	301	PEB	C2D-C3D	6.66	1.43	1.34
26	bt	202	PEB	C2D-C3D	6.66	1.43	1.34
26	ly	402	PEB	C2D-C3D	6.66	1.43	1.34
26	lz	401	PEB	C2D-C3D	6.66	1.43	1.34
26	u4	201	PEB	C2D-C3D	6.66	1.43	1.34
26	v4	201	PEB	C2D-C3D	6.66	1.43	1.34
26	z7	201	PEB	C2D-C3D	6.66	1.43	1.34
26	F8	1002	PEB	C2D-C3D	6.66	1.43	1.34
26	W8	202	PEB	C2D-C3D	6.66	1.43	1.34
26	bb	201	PEB	C2D-C3D	6.66	1.43	1.34
26	dp	202	PEB	C2D-C3D	6.66	1.43	1.34
26	fd	302	PEB	C2D-C3D	6.66	1.43	1.34
26	H3	201	PEB	C2D-C3D	6.66	1.43	1.34
26	k6	1002	PEB	C2D-C3D	6.66	1.43	1.34
26	aX	401	PEB	C2D-C3D	6.66	1.43	1.34
26	gf	201	PEB	C2D-C3D	6.66	1.43	1.34
26	q2	202	PEB	C2D-C3D	6.66	1.43	1.34
26	G5	201	PEB	C2D-C3D	6.66	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bx	202	PEB	C2D-C3D	6.66	1.43	1.34
26	bC	201	PEB	C2D-C3D	6.66	1.43	1.34
26	eB	202	PEB	C2D-C3D	6.66	1.43	1.34
26	O2	202	PEB	C2D-C3D	6.66	1.43	1.34
26	s3	201	PEB	C2D-C3D	6.66	1.43	1.34
26	W6	202	PEB	C2D-C3D	6.66	1.43	1.34
26	y8	201	PEB	C2D-C3D	6.66	1.43	1.34
26	ay	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	cr	201	PEB	C2D-C3D	6.66	1.43	1.34
26	fd	303	PEB	C2D-C3D	6.66	1.43	1.34
26	hT	204	PEB	C2D-C3D	6.66	1.43	1.34
26	F3	201	PEB	C2D-C3D	6.66	1.43	1.34
26	B6	201	PEB	C2D-C3D	6.66	1.43	1.34
26	dt	202	PEB	C2D-C3D	6.66	1.43	1.34
26	eW	202	PEB	C2D-C3D	6.66	1.43	1.34
26	bz	202	PEB	C2D-C3D	6.66	1.43	1.34
26	cd	201	PEB	C2D-C3D	6.66	1.43	1.34
26	ce	201	PEB	C2D-C3D	6.66	1.43	1.34
26	lq	202	PEB	C2D-C3D	6.66	1.43	1.34
26	gp	201	PEB	C2D-C3D	6.66	1.43	1.34
26	N5	201	PEB	C2D-C3D	6.66	1.43	1.34
26	z5	201	PEB	C2D-C3D	6.66	1.43	1.34
26	s6	202	PEB	C2D-C3D	6.66	1.43	1.34
26	L8	202	PEB	C2D-C3D	6.66	1.43	1.34
26	m9	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	O3	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	R5	201	PEB	C2D-C3D	6.66	1.43	1.34
26	bO	201	PEB	C2D-C3D	6.66	1.43	1.34
26	f2	201	PEB	C2D-C3D	6.66	1.43	1.34
26	M2	202	PEB	C2D-C3D	6.66	1.43	1.34
26	X4	202	PEB	C2D-C3D	6.66	1.43	1.34
26	44	302	PEB	C2D-C3D	6.66	1.43	1.34
26	M5	201	PEB	C2D-C3D	6.66	1.43	1.34
26	d5	201	PEB	C2D-C3D	6.66	1.43	1.34
26	Z6	202	PEB	C2D-C3D	6.66	1.43	1.34
26	r7	201	PEB	C2D-C3D	6.66	1.43	1.34
26	B8	201	PEB	C2D-C3D	6.66	1.43	1.34
26	bt	201	PEB	C2D-C3D	6.66	1.43	1.34
26	go	201	PEB	C2D-C3D	6.66	1.43	1.34
26	i2	201	PEB	C2D-C3D	6.66	1.43	1.34
26	l3	201	PEB	C2D-C3D	6.66	1.43	1.34
26	K4	201	PEB	C2D-C3D	6.66	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y8	202	PEB	C2D-C3D	6.66	1.43	1.34
26	x9	201	PEB	C2D-C3D	6.66	1.43	1.34
26	kQ	1001	PEB	C2D-C3D	6.66	1.43	1.34
26	l9	202	PEB	C2D-C3D	6.66	1.43	1.34
26	fw	201	PEB	C2D-C3D	6.66	1.43	1.34
26	I4	202	PEB	C2D-C3D	6.65	1.43	1.34
26	t4	202	PEB	C2D-C3D	6.65	1.43	1.34
26	x6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	aT	202	PEB	C2D-C3D	6.65	1.43	1.34
26	dE	201	PEB	C2D-C3D	6.65	1.43	1.34
26	hH	201	PEB	C2D-C3D	6.65	1.43	1.34
26	jO	1001	PEB	C2D-C3D	6.65	1.43	1.34
26	J8	201	PEB	C2D-C3D	6.65	1.43	1.34
26	J2	201	PEB	C2D-C3D	6.65	1.43	1.34
26	q5	201	PEB	C2D-C3D	6.65	1.43	1.34
26	C6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	P6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	D7	201	PEB	C2D-C3D	6.65	1.43	1.34
26	R7	201	PEB	C2D-C3D	6.65	1.43	1.34
26	bs	1003	PEB	C2D-C3D	6.65	1.43	1.34
26	bR	201	PEB	C2D-C3D	6.65	1.43	1.34
26	eC	201	PEB	C2D-C3D	6.65	1.43	1.34
26	p3	201	PEB	C2D-C3D	6.65	1.43	1.34
26	g6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	u6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	Y7	1001	PEB	C2D-C3D	6.65	1.43	1.34
26	eR	202	PEB	C2D-C3D	6.65	1.43	1.34
26	W2	201	PEB	C2D-C3D	6.65	1.43	1.34
26	c4	202	PEB	C2D-C3D	6.65	1.43	1.34
26	n4	201	PEB	C2D-C3D	6.65	1.43	1.34
26	n5	201	PEB	C2D-C3D	6.65	1.43	1.34
26	T6	202	PEB	C2D-C3D	6.65	1.43	1.34
26	X6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	q6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	u8	201	PEB	C2D-C3D	6.65	1.43	1.34
26	e8	301	PEB	C2D-C3D	6.65	1.43	1.34
26	e9	302	PEB	C2D-C3D	6.65	1.43	1.34
26	R9	201	PEB	C2D-C3D	6.65	1.43	1.34
26	aj	201	PEB	C2D-C3D	6.65	1.43	1.34
26	cI	201	PEB	C2D-C3D	6.65	1.43	1.34
26	cK	201	PEB	C2D-C3D	6.65	1.43	1.34
26	dG	201	PEB	C2D-C3D	6.65	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dO	202	PEB	C2D-C3D	6.65	1.43	1.34
26	Y2	202	PEB	C2D-C3D	6.65	1.43	1.34
26	i6	202	PEB	C2D-C3D	6.65	1.43	1.34
26	R2	202	PEB	C2D-C3D	6.65	1.43	1.34
26	F5	201	PEB	C2D-C3D	6.65	1.43	1.34
26	k5	201	PEB	C2D-C3D	6.65	1.43	1.34
26	q3	1001	PEB	C2D-C3D	6.65	1.43	1.34
26	r8	201	PEB	C2D-C3D	6.65	1.43	1.34
26	df	201	PEB	C2D-C3D	6.65	1.43	1.34
26	la	1001	PEB	C2D-C3D	6.65	1.43	1.34
26	l6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	b7	201	PEB	C2D-C3D	6.65	1.43	1.34
26	a9	603	PEB	C2D-C3D	6.65	1.43	1.34
26	cO	201	PEB	C2D-C3D	6.65	1.43	1.34
26	db	201	PEB	C2D-C3D	6.65	1.43	1.34
26	du	203	PEB	C2D-C3D	6.65	1.43	1.34
26	D2	301	PEB	C2D-C3D	6.65	1.43	1.34
26	U3	201	PEB	C2D-C3D	6.65	1.43	1.34
26	ez	1002	PEB	C2D-C3D	6.65	1.43	1.34
26	eM	1002	PEB	C2D-C3D	6.65	1.43	1.34
26	eQ	201	PEB	C2D-C3D	6.65	1.43	1.34
26	P2	201	PEB	C2D-C3D	6.65	1.43	1.34
26	I4	201	PEB	C2D-C3D	6.65	1.43	1.34
26	z4	202	PEB	C2D-C3D	6.65	1.43	1.34
26	Q6	202	PEB	C2D-C3D	6.65	1.43	1.34
26	bh	201	PEB	C2D-C3D	6.65	1.43	1.34
26	f6	201	PEB	C2D-C3D	6.65	1.43	1.34
26	r9	201	PEB	C2D-C3D	6.65	1.43	1.34
26	aO	201	PEB	C2D-C3D	6.65	1.43	1.34
26	W5	301	PEB	C2D-C3D	6.65	1.43	1.34
26	j6	202	PEB	C2D-C3D	6.65	1.43	1.34
26	j9	201	PEB	C2D-C3D	6.65	1.43	1.34
26	aN	202	PEB	C2D-C3D	6.65	1.43	1.34
26	aW	302	PEB	C2D-C3D	6.65	1.43	1.34
26	cW	202	PEB	C2D-C3D	6.65	1.43	1.34
26	h2	201	PEB	C2D-C3D	6.64	1.43	1.34
26	l8	202	PEB	C2D-C3D	6.64	1.43	1.34
26	a9	601	PEB	C2D-C3D	6.64	1.43	1.34
26	H8	202	PEB	C2D-C3D	6.64	1.43	1.34
26	aB	202	PEB	C2D-C3D	6.64	1.43	1.34
26	ch	201	PEB	C2D-C3D	6.64	1.43	1.34
26	dF	201	PEB	C2D-C3D	6.64	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ey	1003	PEB	C2D-C3D	6.64	1.43	1.34
26	lb	201	PEB	C2D-C3D	6.64	1.43	1.34
26	ff	204	PEB	C2D-C3D	6.64	1.43	1.34
26	Q2	1001	PEB	C2D-C3D	6.64	1.43	1.34
26	V3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	L4	202	PEB	C2D-C3D	6.64	1.43	1.34
26	g4	201	PEB	C2D-C3D	6.64	1.43	1.34
26	Y5	1001	PEB	C2D-C3D	6.64	1.43	1.34
26	s5	201	PEB	C2D-C3D	6.64	1.43	1.34
26	U8	1002	PEB	C2D-C3D	6.64	1.43	1.34
26	bV	201	PEB	C2D-C3D	6.64	1.43	1.34
26	eO	201	PEB	C2D-C3D	6.64	1.43	1.34
26	g8	201	PEB	C2D-C3D	6.64	1.43	1.34
26	a8	602	PEB	C2D-C3D	6.64	1.43	1.34
26	ar	201	PEB	C2D-C3D	6.64	1.43	1.34
26	bY	1003	PEB	C2D-C3D	6.64	1.43	1.34
26	G4	201	PEB	C2D-C3D	6.64	1.43	1.34
26	dx	401	PEB	C2D-C3D	6.64	1.43	1.34
26	eJ	201	PEB	C2D-C3D	6.64	1.43	1.34
26	k3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	h9	201	PEB	C2D-C3D	6.64	1.43	1.34
26	y9	1001	PEB	C2D-C3D	6.64	1.43	1.34
26	aY	402	PEB	C2D-C3D	6.64	1.43	1.34
26	cy	1001	PEB	C2D-C3D	6.64	1.43	1.34
26	eT	201	PEB	C2D-C3D	6.64	1.43	1.34
26	L3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	R3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	aH	202	PEB	C2D-C3D	6.64	1.43	1.34
26	dt	201	PEB	C2D-C3D	6.64	1.43	1.34
26	k2	202	PEB	C2D-C3D	6.64	1.43	1.34
26	Z5	301	PEB	C2D-C3D	6.64	1.43	1.34
26	H8	201	PEB	C2D-C3D	6.64	1.43	1.34
26	fi	201	PEB	C2D-C3D	6.64	1.43	1.34
26	z8	201	PEB	C2D-C3D	6.64	1.43	1.34
26	cM	201	PEB	C2D-C3D	6.64	1.43	1.34
26	eZ	401	PEB	C2D-C3D	6.64	1.43	1.34
26	D4	201	PEB	C2D-C3D	6.64	1.43	1.34
26	dT	201	PEB	C2D-C3D	6.64	1.43	1.34
26	eO	202	PEB	C2D-C3D	6.64	1.43	1.34
26	t2	202	PEB	C2D-C3D	6.64	1.43	1.34
26	s9	201	PEB	C2D-C3D	6.64	1.43	1.34
26	cv	201	PEB	C2D-C3D	6.64	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	Y3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	P3	201	PEB	C2D-C3D	6.64	1.43	1.34
26	t7	201	PEB	C2D-C3D	6.64	1.43	1.34
26	X8	201	PEB	C2D-C3D	6.64	1.43	1.34
26	v8	201	PEB	C2D-C3D	6.63	1.43	1.34
26	Z8	201	PEB	C2D-C3D	6.63	1.43	1.34
26	bj	202	PEB	C2D-C3D	6.63	1.43	1.34
26	dG	202	PEB	C2D-C3D	6.63	1.43	1.34
26	m2	201	PEB	C2D-C3D	6.63	1.43	1.34
26	V4	202	PEB	C2D-C3D	6.63	1.43	1.34
26	L6	201	PEB	C2D-C3D	6.63	1.43	1.34
26	V7	201	PEB	C2D-C3D	6.63	1.43	1.34
26	bE	201	PEB	C2D-C3D	6.63	1.43	1.34
26	cm	1001	PEB	C2D-C3D	6.63	1.43	1.34
26	I5	201	PEB	C2D-C3D	6.63	1.43	1.34
26	R6	201	PEB	C2D-C3D	6.63	1.43	1.34
26	G7	201	PEB	C2D-C3D	6.63	1.43	1.34
26	O6	201	PEB	C2D-C3D	6.63	1.43	1.34
26	c9	302	PEB	C2D-C3D	6.63	1.43	1.34
26	aP	201	PEB	C2D-C3D	6.63	1.43	1.34
26	A6	1001	PEB	C2D-C3D	6.63	1.43	1.34
26	dw	402	PEB	C2D-C3D	6.63	1.43	1.34
26	v6	202	PEB	C2D-C3D	6.63	1.43	1.34
26	bY	1001	PEB	C2D-C3D	6.63	1.43	1.34
26	ej	201	PEB	C2D-C3D	6.63	1.43	1.34
26	l9	201	PEB	C2D-C3D	6.63	1.43	1.34
26	iA	1001	PEB	C2D-C3D	6.63	1.43	1.34
26	N2	202	PEB	C2D-C3D	6.63	1.43	1.34
26	r3	201	PEB	C2D-C3D	6.63	1.43	1.34
26	M4	202	PEB	C2D-C3D	6.63	1.43	1.34
26	P4	202	PEB	C2D-C3D	6.63	1.43	1.34
26	W4	202	PEB	C2D-C3D	6.63	1.43	1.34
26	bP	201	PEB	C2D-C3D	6.63	1.43	1.34
26	cz	201	PEB	C2D-C3D	6.63	1.43	1.34
26	hS	201	PEB	C2D-C3D	6.63	1.43	1.34
26	a8	601	PEB	C2D-C3D	6.63	1.43	1.34
26	D5	201	PEB	C2D-C3D	6.62	1.43	1.34
26	J5	201	PEB	C2D-C3D	6.62	1.43	1.34
26	ap	201	PEB	C2D-C3D	6.62	1.43	1.34
26	by	1001	PEB	C2D-C3D	6.62	1.43	1.34
26	H6	202	PEB	C2D-C3D	6.62	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eT	202	PEB	C2D-C3D	6.62	1.43	1.34
26	jM	1001	PEB	C2D-C3D	6.62	1.43	1.34
26	k6	1001	PEB	C2D-C3D	6.62	1.43	1.34
26	v6	201	PEB	C2D-C3D	6.62	1.43	1.34
26	S3	201	PEB	C2D-C3D	6.62	1.43	1.34
26	y2	201	PEB	C2D-C3D	6.62	1.43	1.34
26	34	1003	PEB	C2D-C3D	6.62	1.43	1.34
26	h7	201	PEB	C2D-C3D	6.62	1.43	1.34
26	ba	1001	PEB	C2D-C3D	6.62	1.43	1.34
26	bF	201	PEB	C2D-C3D	6.62	1.43	1.34
26	cP	202	PEB	C2D-C3D	6.62	1.43	1.34
26	aa	1001	PEB	C2D-C3D	6.62	1.43	1.34
26	ak	201	PEB	C2D-C3D	6.62	1.43	1.34
26	fx	201	PEB	C2D-C3D	6.62	1.43	1.34
26	dP	201	PEB	C2D-C3D	6.61	1.43	1.34
26	J8	202	PEB	C2D-C3D	6.61	1.43	1.34
26	K8	202	PEB	C2D-C3D	6.61	1.43	1.34
26	cj	201	PEB	C2D-C3D	6.61	1.43	1.34
26	de	201	PEB	C2D-C3D	6.61	1.43	1.34
26	N4	201	PEB	C2D-C3D	6.61	1.43	1.34
26	bm	1002	PEB	C2D-C3D	6.61	1.43	1.34
26	cs	201	PEB	C2D-C3D	6.61	1.43	1.34
26	h5	201	PEB	C2D-C3D	6.61	1.43	1.34
26	z6	202	PEB	C2D-C3D	6.61	1.43	1.34
26	lb	202	PEB	C2D-C3D	6.61	1.43	1.34
26	hR	201	PEB	C2D-C3D	6.61	1.43	1.34
26	lm	1001	PEB	C2D-C3D	6.61	1.43	1.34
26	b5	1001	PEB	C2D-C3D	6.61	1.43	1.34
26	d9	301	PEB	C2D-C3D	6.61	1.43	1.34
26	ac	201	PEB	C2D-C3D	6.61	1.43	1.34
26	d8	302	PEB	C2D-C3D	6.61	1.43	1.34
26	N7	201	PEB	C2D-C3D	6.60	1.43	1.34
26	aZ	302	PEB	C2D-C3D	6.60	1.43	1.34
26	bo	201	PEB	C2D-C3D	6.60	1.43	1.34
26	F9	201	PEB	C2D-C3D	6.60	1.43	1.34
26	cE	201	PEB	C2D-C3D	6.60	1.43	1.34
26	o5	201	PEB	C2D-C3D	6.60	1.43	1.34
26	d7	201	PEB	C2D-C3D	6.59	1.43	1.34
26	eV	201	PEB	C2D-C3D	6.58	1.43	1.34
26	b9	401	PEB	C2D-C3D	6.58	1.43	1.34
26	eq	201	PEB	C2D-C3D	6.56	1.43	1.34
26	eN	201	PEB	C2D-C3D	6.55	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gy	304	PVN	C19-C18	-6.05	1.36	1.48
29	gz	304	PVN	C1-N1	5.86	1.43	1.35
27	k1	201	CYC	C2A-C3A	5.80	1.49	1.36
29	gz	304	PVN	C11-C12	-5.80	1.36	1.45
27	u1	1001	CYC	C2A-C3A	5.79	1.49	1.36
27	Z1	201	CYC	C2A-C3A	5.79	1.49	1.36
27	K1	201	CYC	C2A-C3A	5.78	1.49	1.36
27	R1	1001	CYC	C2A-C3A	5.78	1.49	1.36
27	i1	1001	CYC	C2A-C3A	5.78	1.49	1.36
27	G1	1001	CYC	C2A-C3A	5.78	1.49	1.36
27	n1	201	CYC	C2A-C3A	5.78	1.49	1.36
27	a2	901	CYC	CHB-C1B	5.77	1.51	1.38
29	gz	304	PVN	C19-C18	-5.77	1.37	1.48
27	g1	201	CYC	C2A-C3A	5.77	1.49	1.36
27	q1	201	CYC	C2A-C3A	5.77	1.49	1.36
27	I1	201	CYC	C2A-C3A	5.77	1.49	1.36
27	w1	201	CYC	C2A-C3A	5.76	1.49	1.36
27	N1	201	CYC	C2A-C3A	5.76	1.49	1.36
27	V1	201	CYC	C2A-C3A	5.76	1.49	1.36
27	U1	201	CYC	C2A-C3A	5.76	1.49	1.36
27	d2	101	CYC	C2A-C3A	5.76	1.49	1.36
27	s1	201	CYC	C2A-C3A	5.76	1.49	1.36
27	b1	1001	CYC	C2A-C3A	5.75	1.49	1.36
27	y1	201	CYC	C2A-C3A	5.75	1.49	1.36
27	f1	201	CYC	C2A-C3A	5.75	1.49	1.36
27	r1	201	CYC	CHB-C1B	5.75	1.51	1.38
27	P1	201	CYC	C2A-C3A	5.75	1.48	1.36
27	X1	201	CYC	C2A-C3A	5.75	1.48	1.36
27	O1	201	CYC	C2A-C3A	5.74	1.48	1.36
27	o1	1001	CYC	C2A-C3A	5.74	1.48	1.36
27	W1	201	CYC	C2A-C3A	5.74	1.48	1.36
27	J1	201	CYC	CHB-C1B	5.74	1.51	1.38
27	Y1	201	CYC	CHB-C1B	5.74	1.51	1.38
27	t1	201	CYC	CHB-C1B	5.74	1.51	1.38
27	a2	902	CYC	CHB-C1B	5.74	1.51	1.38
27	b2	1001	CYC	CHB-C1B	5.74	1.51	1.38
27	e1	201	CYC	C2A-C3A	5.74	1.48	1.36
27	S1	201	CYC	CHB-C1B	5.73	1.51	1.38
27	j1	201	CYC	CHB-C1B	5.73	1.51	1.38
27	Q1	201	CYC	C2A-C3A	5.73	1.48	1.36
27	d1	1001	CYC	C2A-C3A	5.73	1.48	1.36
27	v1	201	CYC	CHB-C1B	5.73	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	L1	201	CYC	C2A-C3A	5.72	1.48	1.36
27	a1	201	CYC	C2A-C3A	5.72	1.48	1.36
27	p1	201	CYC	CHB-C1B	5.72	1.51	1.38
27	m1	201	CYC	C2A-C3A	5.72	1.48	1.36
27	S1	202	CYC	CHB-C1B	5.72	1.51	1.38
27	H1	201	CYC	CHB-C1B	5.72	1.51	1.38
27	c1	201	CYC	CHB-C1B	5.72	1.51	1.38
27	M1	1001	CYC	CHB-C1B	5.70	1.51	1.38
27	h1	201	CYC	CHB-C1B	5.70	1.51	1.38
27	z1	201	CYC	CHB-C1B	5.70	1.51	1.38
27	z1	201	CYC	CHB-C4A	5.69	1.53	1.40
27	r1	201	CYC	CHB-C4A	5.69	1.53	1.40
27	S1	201	CYC	CHB-C4A	5.67	1.53	1.40
27	j1	201	CYC	CHB-C4A	5.67	1.53	1.40
27	H1	201	CYC	CHB-C4A	5.67	1.53	1.40
27	p1	201	CYC	CHB-C4A	5.67	1.53	1.40
27	M1	1001	CYC	CHB-C4A	5.67	1.53	1.40
27	a2	902	CYC	CHB-C4A	5.66	1.53	1.40
27	b2	1001	CYC	CHB-C4A	5.66	1.53	1.40
27	c1	201	CYC	CHB-C4A	5.66	1.53	1.40
27	a2	901	CYC	CHB-C4A	5.66	1.53	1.40
27	h1	201	CYC	CHB-C4A	5.65	1.53	1.40
27	v1	201	CYC	CHB-C4A	5.65	1.53	1.40
27	J1	201	CYC	CHB-C4A	5.65	1.53	1.40
27	Y1	201	CYC	CHB-C4A	5.65	1.53	1.40
27	S1	202	CYC	CHB-C4A	5.64	1.53	1.40
27	t1	201	CYC	CHB-C4A	5.63	1.53	1.40
27	u1	1001	CYC	C3B-C2B	5.55	1.48	1.36
27	K1	201	CYC	C3B-C2B	5.54	1.48	1.36
27	g1	201	CYC	C3B-C2B	5.54	1.48	1.36
27	L1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	a1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	z1	201	CYC	C2C-C1C	-5.53	1.47	1.52
27	I1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	a2	901	CYC	C2C-C1C	-5.53	1.47	1.52
27	X1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	s1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	P1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	k1	201	CYC	C3B-C2B	5.53	1.48	1.36
27	O1	201	CYC	C3B-C2B	5.52	1.48	1.36
27	R1	1001	CYC	C3B-C2B	5.52	1.48	1.36
27	i1	1001	CYC	C3B-C2B	5.52	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	f1	201	CYC	C3B-C2B	5.52	1.48	1.36
27	q1	201	CYC	C3B-C2B	5.52	1.48	1.36
27	b1	1001	CYC	C3B-C2B	5.51	1.48	1.36
27	e1	201	CYC	C3B-C2B	5.51	1.48	1.36
27	H1	201	CYC	C2C-C1C	-5.51	1.47	1.52
27	S1	201	CYC	C2C-C1C	-5.51	1.47	1.52
27	j1	201	CYC	C2C-C1C	-5.51	1.47	1.52
27	V1	201	CYC	C3B-C2B	5.51	1.48	1.36
27	o1	1001	CYC	C3B-C2B	5.50	1.48	1.36
27	w1	201	CYC	C3B-C2B	5.50	1.48	1.36
27	c1	201	CYC	C2C-C1C	-5.50	1.47	1.52
27	N1	201	CYC	C3B-C2B	5.50	1.48	1.36
27	m1	201	CYC	C3B-C2B	5.50	1.48	1.36
27	W1	201	CYC	C3B-C2B	5.50	1.48	1.36
27	U1	201	CYC	C3B-C2B	5.50	1.48	1.36
27	d2	101	CYC	C3B-C2B	5.50	1.48	1.36
27	M1	1001	CYC	C2C-C1C	-5.50	1.47	1.52
27	Q1	201	CYC	C3B-C2B	5.50	1.48	1.36
27	a2	902	CYC	C2C-C1C	-5.50	1.47	1.52
27	b2	1001	CYC	C2C-C1C	-5.50	1.47	1.52
27	d1	1001	CYC	C3B-C2B	5.49	1.48	1.36
27	y1	201	CYC	C3B-C2B	5.49	1.48	1.36
27	n1	201	CYC	C3B-C2B	5.49	1.48	1.36
27	p1	201	CYC	C2C-C1C	-5.48	1.47	1.52
27	Z1	201	CYC	C3B-C2B	5.48	1.48	1.36
27	G1	1001	CYC	C3B-C2B	5.48	1.48	1.36
27	t1	201	CYC	C2C-C1C	-5.47	1.47	1.52
27	J1	201	CYC	C2C-C1C	-5.46	1.47	1.52
27	Y1	201	CYC	C2C-C1C	-5.46	1.47	1.52
27	v1	201	CYC	C2C-C1C	-5.45	1.47	1.52
27	h1	201	CYC	C2C-C1C	-5.45	1.47	1.52
27	r1	201	CYC	C2C-C1C	-5.42	1.47	1.52
29	A2	1004	PVN	C4-N1	-5.42	1.37	1.45
29	a3	1004	PVN	C4-N1	-5.42	1.37	1.45
27	e1	201	CYC	CHB-C4A	5.40	1.53	1.40
27	S1	202	CYC	C2C-C1C	-5.39	1.47	1.52
27	q1	201	CYC	CHB-C4A	5.38	1.53	1.40
27	N1	201	CYC	CHB-C4A	5.38	1.53	1.40
27	P1	201	CYC	CHB-C4A	5.38	1.53	1.40
27	Z1	201	CYC	CHB-C4A	5.38	1.53	1.40
27	u1	1001	CYC	CHB-C4A	5.37	1.53	1.40
27	R1	1001	CYC	CHB-C4A	5.37	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	i1	1001	CYC	CHB-C4A	5.37	1.53	1.40
27	O1	201	CYC	CHB-C4A	5.37	1.53	1.40
27	o1	1001	CYC	CHB-C4A	5.37	1.53	1.40
27	s1	201	CYC	CHB-C4A	5.37	1.53	1.40
27	W1	201	CYC	CHB-C4A	5.37	1.53	1.40
27	G1	1001	CYC	CHB-C4A	5.37	1.53	1.40
27	V1	201	CYC	CHB-C4A	5.36	1.53	1.40
27	d1	1001	CYC	CHB-C4A	5.36	1.53	1.40
27	w1	201	CYC	CHB-C4A	5.36	1.53	1.40
27	n1	201	CYC	CHB-C4A	5.36	1.53	1.40
27	k1	201	CYC	CHB-C4A	5.36	1.53	1.40
27	K1	201	CYC	CHB-C4A	5.36	1.53	1.40
27	g1	201	CYC	CHB-C4A	5.36	1.53	1.40
27	L1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	a1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	X1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	m1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	U1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	d2	101	CYC	CHB-C4A	5.35	1.52	1.40
27	f1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	y1	201	CYC	CHB-C4A	5.35	1.52	1.40
27	Q1	201	CYC	CHB-C4A	5.34	1.52	1.40
27	I1	201	CYC	CHB-C4A	5.34	1.52	1.40
27	b1	1001	CYC	CHB-C4A	5.34	1.52	1.40
29	C2	303	PVN	C4-N1	-5.29	1.37	1.45
29	c3	303	PVN	C4-N1	-5.29	1.37	1.45
29	gz	304	PVN	C14-C13	-5.28	1.34	1.45
29	gy	304	PVN	C1-N1	5.24	1.42	1.35
29	gy	304	PVN	C14-C13	-5.18	1.34	1.45
29	ey	1004	PVN	C4-N1	-5.17	1.38	1.45
29	hZ	403	PVN	C3-C2	5.09	1.40	1.34
29	hY	404	PVN	C3-C2	5.08	1.39	1.34
29	gz	304	PVN	C15-C14	5.07	1.52	1.40
29	34	1004	PVN	C3-C2	5.05	1.39	1.34
26	dP	202	PEB	C2A-C1A	-5.03	1.47	1.52
26	cs	201	PEB	C2A-C1A	-5.02	1.47	1.52
26	N7	201	PEB	C2A-C1A	-5.00	1.47	1.52
26	iG	1001	PEB	C2A-C1A	-5.00	1.47	1.52
26	B4	201	PEB	C2A-C1A	-5.00	1.47	1.52
26	v2	201	PEB	C2A-C1A	-4.99	1.47	1.52
26	eJ	201	PEB	C2A-C1A	-4.99	1.47	1.52
26	cJ	201	PEB	C2A-C1A	-4.98	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y5	1004	PVN	C3-C2	4.98	1.39	1.34
26	dG	201	PEB	C2A-C1A	-4.98	1.47	1.52
29	Y5	1004	PVN	C4-N1	-4.97	1.38	1.45
26	em	201	PEB	C2A-C1A	-4.97	1.47	1.52
26	cO	201	PEB	C2A-C1A	-4.97	1.47	1.52
26	P4	201	PEB	C2A-C1A	-4.97	1.47	1.52
26	r2	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	q9	202	PEB	C2A-C1A	-4.96	1.47	1.52
26	dK	202	PEB	C2A-C1A	-4.96	1.47	1.52
26	bc	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	cG	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	G3	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	I4	202	PEB	C2A-C1A	-4.96	1.47	1.52
26	ak	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	bC	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	M6	1001	PEB	C2A-C1A	-4.96	1.47	1.52
26	A8	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	F9	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	cL	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	eS	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	aB	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	iB	1001	PEB	C2A-C1A	-4.96	1.47	1.52
26	t3	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	s9	202	PEB	C2A-C1A	-4.96	1.47	1.52
26	az	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	dr	202	PEB	C2A-C1A	-4.96	1.47	1.52
26	G4	201	PEB	C2A-C1A	-4.96	1.47	1.52
26	lb	202	PEB	C2A-C1A	-4.96	1.47	1.52
26	n3	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	C6	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	jN	1001	PEB	C2A-C1A	-4.95	1.47	1.52
26	es	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	eP	203	PEB	C2A-C1A	-4.95	1.47	1.52
26	eT	202	PEB	C2A-C1A	-4.95	1.47	1.52
26	eU	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	hK	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	Q8	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	kR	1001	PEB	C2A-C1A	-4.95	1.47	1.52
26	R4	202	PEB	C2A-C1A	-4.95	1.47	1.52
26	z6	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	df	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	lq	202	PEB	C2A-C1A	-4.95	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O6	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	dr	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	dU	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	k9	201	PEB	C2A-C1A	-4.95	1.47	1.52
26	aH	202	PEB	C2A-C1A	-4.94	1.47	1.52
26	w3	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	aQ	202	PEB	C2A-C1A	-4.94	1.47	1.52
26	aY	401	PEB	C2A-C1A	-4.94	1.47	1.52
26	gb	1001	PEB	C2A-C1A	-4.94	1.47	1.52
26	hY	403	PEB	C2A-C1A	-4.94	1.47	1.52
26	kQ	1001	PEB	C2A-C1A	-4.94	1.47	1.52
26	g3	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	j8	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	T9	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	la	1001	PEB	C2A-C1A	-4.94	1.47	1.52
26	gp	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	m8	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	ea	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	h2	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	A8	202	PEB	C2A-C1A	-4.94	1.47	1.52
26	eu	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	eO	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	I6	202	PEB	C2A-C1A	-4.94	1.47	1.52
26	ds	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	i8	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	cV	203	PEB	C2A-C1A	-4.94	1.47	1.52
26	dH	201	PEB	C2A-C1A	-4.94	1.47	1.52
26	G2	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	ll	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	iC	1001	PEB	C2A-C1A	-4.93	1.47	1.52
26	A4	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	m3	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	dT	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	Q4	202	PEB	C2A-C1A	-4.93	1.47	1.52
26	m4	1001	PEB	C2A-C1A	-4.93	1.47	1.52
26	u4	202	PEB	C2A-C1A	-4.93	1.47	1.52
26	w6	1002	PEB	C2A-C1A	-4.93	1.47	1.52
26	r9	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	cm	1001	PEB	C2A-C1A	-4.93	1.47	1.52
26	gz	303	PEB	C2A-C1A	-4.93	1.47	1.52
26	a3	1001	PEB	C2A-C1A	-4.93	1.47	1.52
26	Z5	301	PEB	C2A-C1A	-4.93	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dX	202	PEB	C2A-C1A	-4.93	1.47	1.52
26	hZ	402	PEB	C2A-C1A	-4.93	1.47	1.52
26	t8	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	F8	1001	PEB	C2A-C1A	-4.93	1.47	1.52
26	x9	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	aT	202	PEB	C2A-C1A	-4.93	1.47	1.52
26	bR	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	dS	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	u5	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	N8	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	aE	202	PEB	C2A-C1A	-4.93	1.47	1.52
26	cN	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	hY	401	PEB	C2A-C1A	-4.93	1.47	1.52
26	t2	201	PEB	C2A-C1A	-4.93	1.47	1.52
26	dN	202	PEB	C2A-C1A	-4.93	1.47	1.52
26	D6	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	cl	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	hB	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	kX	1001	PEB	C2A-C1A	-4.92	1.47	1.52
26	M2	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	C5	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	U8	1002	PEB	C2A-C1A	-4.92	1.47	1.52
26	z9	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	bZ	301	PEB	C2A-C1A	-4.92	1.47	1.52
26	O8	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	cK	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	w2	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	Q7	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	jM	1001	PEB	C2A-C1A	-4.92	1.47	1.52
26	z5	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	y2	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	i4	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	Z9	1001	PEB	C2A-C1A	-4.92	1.47	1.52
26	B2	501	PEB	C2A-C1A	-4.92	1.47	1.52
26	b3	501	PEB	C2A-C1A	-4.92	1.47	1.52
26	T5	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	B6	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	Q8	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	aX	402	PEB	C2A-C1A	-4.92	1.47	1.52
26	gs	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	S4	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	J5	201	PEB	C2A-C1A	-4.92	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bm	1001	PEB	C2A-C1A	-4.92	1.47	1.52
26	dj	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	gu	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	K2	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	k8	202	PEB	C2A-C1A	-4.92	1.47	1.52
26	B9	201	PEB	C2A-C1A	-4.92	1.47	1.52
26	fd	303	PEB	C2A-C1A	-4.91	1.47	1.52
26	N3	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	T8	301	PEB	C2A-C1A	-4.91	1.47	1.52
26	N9	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	cV	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	dH	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	dM	1002	PEB	C2A-C1A	-4.91	1.47	1.52
26	o2	1001	PEB	C2A-C1A	-4.91	1.47	1.52
26	W2	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	D4	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	E6	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	z8	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	E8	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	cc	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	fj	201	PEB	C2A-C1A	-4.91	1.47	1.52
29	34	1004	PVN	C4-N1	-4.91	1.38	1.45
26	g2	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	b8	1002	PEB	C2A-C1A	-4.91	1.47	1.52
26	g9	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	aS	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	bF	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	eH	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	eW	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	o3	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	j9	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	R9	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	ai	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	aR	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	cb	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	ge	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	gw	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	M4	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	q8	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	cQ	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	cX	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	lb	201	PEB	C2A-C1A	-4.91	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hJ	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	s2	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	t2	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	F2	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	m8	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	u6	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	U8	1001	PEB	C2A-C1A	-4.91	1.47	1.52
26	Y9	302	PEB	C2A-C1A	-4.91	1.47	1.52
26	aX	401	PEB	C2A-C1A	-4.91	1.47	1.52
26	bX	401	PEB	C2A-C1A	-4.91	1.47	1.52
26	hS	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	o4	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	j5	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	y5	1001	PEB	C2A-C1A	-4.91	1.47	1.52
26	J8	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	l9	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	X9	401	PEB	C2A-C1A	-4.91	1.47	1.52
26	aI	202	PEB	C2A-C1A	-4.91	1.47	1.52
26	dE	201	PEB	C2A-C1A	-4.91	1.47	1.52
26	lm	1001	PEB	C2A-C1A	-4.91	1.47	1.52
26	m2	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	q5	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	t9	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	aA	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	ef	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	eK	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	o2	1002	PEB	C2A-C1A	-4.90	1.47	1.52
26	b8	1001	PEB	C2A-C1A	-4.90	1.47	1.52
26	b9	402	PEB	C2A-C1A	-4.90	1.47	1.52
26	G8	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	W8	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	dn	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	hN	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	kU	1001	PEB	C2A-C1A	-4.90	1.47	1.52
26	g6	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	v6	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	J8	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	Q9	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	aL	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	dq	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	dx	404	PEB	C2A-C1A	-4.90	1.47	1.52
26	dD	202	PEB	C2A-C1A	-4.90	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U4	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	E5	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	j7	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	w8	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	aZ	302	PEB	C2A-C1A	-4.90	1.47	1.52
26	dk	1002	PEB	C2A-C1A	-4.90	1.47	1.52
26	ds	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	dz	402	PEB	C2A-C1A	-4.90	1.47	1.52
26	eE	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	jP	1001	PEB	C2A-C1A	-4.90	1.47	1.52
26	N2	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	g4	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	T6	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	i7	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	n7	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	r7	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	U8	1003	PEB	C2A-C1A	-4.90	1.47	1.52
26	W8	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	Z8	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	P9	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	aS	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	dc	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	dm	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	lk	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	fe	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	y2	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	y6	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	aV	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	bl	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	bP	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	eP	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	g5	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	cB	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	dW	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	hX	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	iH	1001	PEB	C2A-C1A	-4.90	1.47	1.52
26	x2	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	M2	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	h8	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	o8	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	C7	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	e8	301	PEB	C2A-C1A	-4.90	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v9	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	aJ	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	bj	202	PEB	C2A-C1A	-4.90	1.47	1.52
26	eG	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	k3	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	K4	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	N4	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	b4	1001	PEB	C2A-C1A	-4.90	1.47	1.52
26	p4	201	PEB	C2A-C1A	-4.90	1.47	1.52
26	da	1001	PEB	C2A-C1A	-4.90	1.47	1.52
29	hZ	403	PVN	C4-N1	-4.90	1.38	1.45
26	T3	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	f4	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	t4	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	w5	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	c7	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	x9	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	bx	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	hA	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	44	301	PEB	C2A-C1A	-4.89	1.47	1.52
26	l4	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	f6	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	be	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	ce	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	dp	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	gj	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	jJ	1001	PEB	C2A-C1A	-4.89	1.47	1.52
26	T4	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	x6	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	l7	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	y7	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	l9	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	al	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	cW	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	i3	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	u4	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	z4	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	U5	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	P6	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	x8	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	C8	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	K8	201	PEB	C2A-C1A	-4.89	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hC	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	f2	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	m2	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	aQ	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	O3	1001	PEB	C2A-C1A	-4.89	1.47	1.52
26	L5	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	bG	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	cj	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	dq	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	dX	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	ea	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	eV	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	ly	401	PEB	C2A-C1A	-4.89	1.47	1.52
26	S2	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	F3	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	o9	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	aj	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	aO	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	bV	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	do	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	v3	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	c4	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	l5	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	l8	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	I6	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	w6	1001	PEB	C2A-C1A	-4.89	1.47	1.52
26	dA	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	q4	202	PEB	C2A-C1A	-4.89	1.47	1.52
26	E6	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	Y7	1001	PEB	C2A-C1A	-4.89	1.47	1.52
26	H8	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	bL	201	PEB	C2A-C1A	-4.89	1.47	1.52
26	ft	201	PEB	C2A-C1A	-4.89	1.47	1.52
29	ez	1004	PVN	C4-N1	-4.88	1.38	1.45
26	O2	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	d5	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	i6	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	h7	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	D8	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	cY	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	ly	402	PEB	C2A-C1A	-4.88	1.47	1.52
26	C2	301	PEB	C2A-C1A	-4.88	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z4	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	b5	1001	PEB	C2A-C1A	-4.88	1.47	1.52
26	aB	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	aK	1002	PEB	C2A-C1A	-4.88	1.47	1.52
26	aM	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	aU	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	dQ	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	gq	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	34	1003	PEB	C2A-C1A	-4.88	1.47	1.52
26	c5	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	bb	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	cM	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	de	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	lf	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	q3	1001	PEB	C2A-C1A	-4.88	1.47	1.52
26	E4	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	A5	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	S6	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	D8	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	ay	1001	PEB	C2A-C1A	-4.88	1.47	1.52
26	do	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	eR	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	hQ	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	hV	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	X4	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	h5	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	X6	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	v8	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	B8	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	F8	1002	PEB	C2A-C1A	-4.88	1.47	1.52
26	cV	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	dR	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	fw	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	w2	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	A2	1002	PEB	C2A-C1A	-4.88	1.47	1.52
26	O6	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	S7	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	h9	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	w9	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	ah	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	aC	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	ey	1002	PEB	C2A-C1A	-4.88	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	u2	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	H4	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	Q4	203	PEB	C2A-C1A	-4.88	1.47	1.52
26	s6	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	I7	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	q7	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	bs	1002	PEB	C2A-C1A	-4.88	1.47	1.52
26	bv	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	bw	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	bZ	303	PEB	C2A-C1A	-4.88	1.47	1.52
26	eA	1001	PEB	C2A-C1A	-4.88	1.47	1.52
26	Y2	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	A3	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	S5	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	m5	1001	PEB	C2A-C1A	-4.88	1.47	1.52
26	f7	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	c8	302	PEB	C2A-C1A	-4.88	1.47	1.52
26	w8	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	h9	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	V9	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	at	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	aA	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	ez	1003	PEB	C2A-C1A	-4.88	1.47	1.52
26	gy	301	PEB	C2A-C1A	-4.88	1.47	1.52
26	Y4	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	O5	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	e5	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	M6	1002	PEB	C2A-C1A	-4.88	1.47	1.52
26	l6	202	PEB	C2A-C1A	-4.88	1.47	1.52
26	li	201	PEB	C2A-C1A	-4.88	1.47	1.52
26	iF	1001	PEB	C2A-C1A	-4.88	1.47	1.52
29	hY	404	PVN	C4-N1	-4.88	1.38	1.45
26	I4	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	L4	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	X4	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	e4	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	H5	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	W5	301	PEB	C2A-C1A	-4.87	1.47	1.52
26	o7	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	ao	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	by	1001	PEB	C2A-C1A	-4.87	1.47	1.52
26	dv	201	PEB	C2A-C1A	-4.87	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eW	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	P6	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	Y6	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	p8	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	B8	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	cR	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	dm	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	dB	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	el	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	jO	1001	PEB	C2A-C1A	-4.87	1.47	1.52
26	f3	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	s4	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	j6	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	Z7	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	Y8	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	f9	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	p9	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	w9	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	Z9	1003	PEB	C2A-C1A	-4.87	1.47	1.52
26	ae	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	aw	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	bJ	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	bM	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	dw	401	PEB	C2A-C1A	-4.87	1.47	1.52
26	dx	401	PEB	C2A-C1A	-4.87	1.47	1.52
26	eF	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	lr	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	g2	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	S3	203	PEB	C2A-C1A	-4.87	1.47	1.52
26	R4	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	y6	203	PEB	C2A-C1A	-4.87	1.47	1.52
26	a9	602	PEB	C2A-C1A	-4.87	1.47	1.52
26	ag	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	eC	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	Y2	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	a3	1003	PEB	C2A-C1A	-4.87	1.47	1.52
26	r3	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	e6	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	b8	1003	PEB	C2A-C1A	-4.87	1.47	1.52
26	b9	404	PEB	C2A-C1A	-4.87	1.47	1.52
26	s9	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	as	201	PEB	C2A-C1A	-4.87	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aM	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	aN	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	aW	301	PEB	C2A-C1A	-4.87	1.47	1.52
26	aY	406	PEB	C2A-C1A	-4.87	1.47	1.52
26	cI	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	cP	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	dt	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	dx	402	PEB	C2A-C1A	-4.87	1.47	1.52
26	dJ	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	eF	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	eY	402	PEB	C2A-C1A	-4.87	1.47	1.52
26	x3	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	r8	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	J9	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	aD	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	ff	204	PEB	C2A-C1A	-4.87	1.47	1.52
26	V4	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	k8	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	r6	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	r9	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	eo	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	gg	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	F6	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	q9	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	aq	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	bA	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	cx	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	dC	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	eK	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	eS	202	PEB	C2A-C1A	-4.87	1.47	1.52
26	M5	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	m6	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	x8	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	O9	201	PEB	C2A-C1A	-4.87	1.47	1.52
26	q2	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	G8	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	aN	204	PEB	C2A-C1A	-4.86	1.47	1.52
26	dG	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	ga	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	X2	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	J6	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	q6	201	PEB	C2A-C1A	-4.86	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H7	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	a9	601	PEB	C2A-C1A	-4.86	1.47	1.52
26	m9	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	aV	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	aW	302	PEB	C2A-C1A	-4.86	1.47	1.52
26	bg	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	br	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	cO	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	dM	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	gy	303	PEB	C2A-C1A	-4.86	1.47	1.52
26	hR	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	kT	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	Z4	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	44	302	PEB	C2A-C1A	-4.86	1.47	1.52
26	Z5	303	PEB	C2A-C1A	-4.86	1.47	1.52
26	j8	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	M8	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	S8	401	PEB	C2A-C1A	-4.86	1.47	1.52
26	M9	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	aH	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	aJ	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	cq	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	eH	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	D3	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	F5	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	a8	601	PEB	C2A-C1A	-4.86	1.47	1.52
26	c9	302	PEB	C2A-C1A	-4.86	1.47	1.52
26	bp	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	ct	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	ed	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	H4	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	v5	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	w7	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	C9	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	bj	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	dK	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	ly	403	PEB	C2A-C1A	-4.86	1.47	1.52
26	lz	402	PEB	C2A-C1A	-4.86	1.47	1.52
26	hT	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	s2	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	W3	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	L6	201	PEB	C2A-C1A	-4.86	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m6	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	y8	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	cy	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	gk	201	PEB	C2A-C1A	-4.86	1.47	1.52
29	44	303	PVN	C4-N1	-4.86	1.38	1.45
29	Z5	304	PVN	C4-N1	-4.86	1.38	1.45
26	T2	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	Z2	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	C6	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	c6	1002	PEB	C2A-C1A	-4.86	1.47	1.52
26	v7	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	e9	301	PEB	C2A-C1A	-4.86	1.47	1.52
26	T8	302	PEB	C2A-C1A	-4.86	1.47	1.52
26	L9	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	eq	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	k2	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	z3	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	U4	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	D5	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	s8	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	bh	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	bs	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	bY	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	ch	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	dF	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	ey	1003	PEB	C2A-C1A	-4.86	1.47	1.52
26	lp	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	fv	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	e9	302	PEB	C2A-C1A	-4.86	1.47	1.52
26	e9	303	PEB	C2A-C1A	-4.86	1.47	1.52
26	aF	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	cP	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	du	202	PEB	C2A-C1A	-4.86	1.47	1.52
26	lc	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	fb	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	gi	201	PEB	C2A-C1A	-4.86	1.47	1.52
26	iD	1001	PEB	C2A-C1A	-4.86	1.47	1.52
26	R6	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	O8	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	u9	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	H9	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	S9	201	PEB	C2A-C1A	-4.85	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dz	401	PEB	C2A-C1A	-4.85	1.47	1.52
26	jK	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	C4	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	i9	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	dN	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	es	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	fd	302	PEB	C2A-C1A	-4.85	1.47	1.52
26	kV	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	W2	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	U3	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	24	401	PEB	C2A-C1A	-4.85	1.47	1.52
26	K7	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	P8	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	G9	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	aG	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	aY	402	PEB	C2A-C1A	-4.85	1.47	1.52
26	lq	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	ls	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	S3	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	aP	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	bw	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	cT	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	dk	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	gh	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	kS	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	i2	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	I2	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	W4	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	y4	1002	PEB	C2A-C1A	-4.85	1.47	1.52
26	A6	1002	PEB	C2A-C1A	-4.85	1.47	1.52
26	bI	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	eh	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	eq	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	gm	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	gt	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	hL	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	I2	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	v6	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	b9	403	PEB	C2A-C1A	-4.85	1.47	1.52
26	M8	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	ac	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	av	201	PEB	C2A-C1A	-4.85	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aI	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	ci	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	la	1002	PEB	C2A-C1A	-4.85	1.47	1.52
26	s5	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	x6	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	x7	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	z9	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	aC	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	bK	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	eI	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	J4	202	PEB	C2A-C1A	-4.85	1.47	1.52
26	a6	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	gc	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	hE	1001	PEB	C2A-C1A	-4.85	1.47	1.52
26	B5	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	D7	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	M7	1002	PEB	C2A-C1A	-4.85	1.47	1.52
26	X7	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	cu	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	dD	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	dV	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	ej	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	fa	201	PEB	C2A-C1A	-4.85	1.47	1.52
26	w2	203	PEB	C2A-C1A	-4.84	1.47	1.52
26	z2	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	U2	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	d6	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	o6	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	E7	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	g7	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	I8	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	bf	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	bz	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	cd	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	eo	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	ew	301	PEB	C2A-C1A	-4.84	1.47	1.52
26	fd	301	PEB	C2A-C1A	-4.84	1.47	1.52
26	ff	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	J3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	N5	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	R5	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	o5	201	PEB	C2A-C1A	-4.84	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g6	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	a9	603	PEB	C2A-C1A	-4.84	1.47	1.52
26	V8	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	aZ	301	PEB	C2A-C1A	-4.84	1.47	1.52
26	br	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	eM	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	R2	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	R3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	V5	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	K6	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	l6	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	u7	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	c9	301	PEB	C2A-C1A	-4.84	1.47	1.52
26	bi	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	du	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	u3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	d4	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	x4	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	c6	1003	PEB	C2A-C1A	-4.84	1.47	1.52
26	cM	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	dy	401	PEB	C2A-C1A	-4.84	1.47	1.52
26	eg	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	B2	502	PEB	C2A-C1A	-4.84	1.47	1.52
26	Q3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	Q6	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	V7	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	j9	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	cv	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	dR	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	fc	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	iA	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	L4	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	a4	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	aP	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	bs	1003	PEB	C2A-C1A	-4.84	1.47	1.52
26	hO	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	q2	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	K3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	k8	203	PEB	C2A-C1A	-4.84	1.47	1.52
26	c6	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	d8	302	PEB	C2A-C1A	-4.84	1.47	1.52
26	eD	201	PEB	C2A-C1A	-4.84	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eO	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	e3	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	j4	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	j5	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	U6	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	j6	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	s6	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	z6	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	z7	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	a8	602	PEB	C2A-C1A	-4.84	1.47	1.52
26	au	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	bD	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	bH	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	cC	1003	PEB	C2A-C1A	-4.84	1.47	1.52
26	fk	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	fr	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	hM	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	K2	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	B3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	Y3	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	K5	1001	PEB	C2A-C1A	-4.84	1.47	1.52
26	H6	202	PEB	C2A-C1A	-4.84	1.47	1.52
26	bv	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	cr	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	cR	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	db	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	lu	201	PEB	C2A-C1A	-4.84	1.47	1.52
26	M3	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	P4	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	k4	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	Y5	1001	PEB	C2A-C1A	-4.83	1.47	1.52
26	Y8	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	dc	203	PEB	C2A-C1A	-4.83	1.47	1.52
26	eQ	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	gn	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	u6	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	L8	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	bq	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	cW	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	li	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	jI	1001	PEB	C2A-C1A	-4.83	1.47	1.52
26	l3	201	PEB	C2A-C1A	-4.83	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W6	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	U7	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	y9	1002	PEB	C2A-C1A	-4.83	1.47	1.52
26	di	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	dC	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	r2	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	a5	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	g8	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	o6	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	bh	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	J4	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	K4	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	v4	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	y4	1001	PEB	C2A-C1A	-4.83	1.47	1.52
26	k5	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	r6	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	bt	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	bx	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	dw	402	PEB	C2A-C1A	-4.83	1.47	1.52
26	dP	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	eC	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	jL	1001	PEB	C2A-C1A	-4.83	1.47	1.52
29	aZ	303	PVN	C4-N1	-4.83	1.38	1.45
29	bZ	304	PVN	C4-N1	-4.83	1.38	1.45
26	b6	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	L8	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	gv	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	O2	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	n4	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	n5	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	l8	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	K6	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	d9	303	PEB	C2A-C1A	-4.83	1.47	1.52
26	bu	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	cS	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	n2	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	u2	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	P3	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	Z6	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	M7	1001	PEB	C2A-C1A	-4.83	1.47	1.52
26	Z9	1007	PEB	C2A-C1A	-4.83	1.47	1.52
26	dI	1001	PEB	C2A-C1A	-4.83	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fm	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	fn	1001	PEB	C2A-C1A	-4.83	1.47	1.52
26	E2	1001	PEB	C2A-C1A	-4.83	1.47	1.52
26	G4	202	PEB	C2A-C1A	-4.83	1.47	1.52
26	Z6	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	ez	1002	PEB	C2A-C1A	-4.83	1.47	1.52
26	ln	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	go	201	PEB	C2A-C1A	-4.83	1.47	1.52
26	s3	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	Q4	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	e8	302	PEB	C2A-C1A	-4.82	1.47	1.52
26	aL	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	dn	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	gl	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	k2	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	F4	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	F4	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	l5	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	t6	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	dd	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	i2	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	J2	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	z8	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	u9	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	aK	1001	PEB	C2A-C1A	-4.82	1.47	1.52
26	ck	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	cU	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	dF	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	dZ	1001	PEB	C2A-C1A	-4.82	1.47	1.52
26	eB	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	L3	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	X3	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	q4	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	H8	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	bd	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	bq	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	cX	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	hD	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	F2	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	ar	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	bk	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	cT	1002	PEB	C2A-C1A	-4.82	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dt	202	PEB	C2A-C1A	-4.82	1.47	1.52
29	gy	304	PVN	C15-C14	4.82	1.51	1.40
26	l2	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	h6	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	bd	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	cD	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	dL	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	v2	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	I3	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	h4	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	z4	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	b6	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	K9	1001	PEB	C2A-C1A	-4.82	1.47	1.52
26	bO	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	fq	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	M4	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	I5	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	r5	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	Q6	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	N8	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	ed	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	fi	201	PEB	C2A-C1A	-4.82	1.47	1.52
29	D2	303	PVN	C4-N1	-4.82	1.38	1.45
29	d3	302	PVN	C4-N1	-4.82	1.38	1.45
26	dO	202	PEB	C2A-C1A	-4.82	1.47	1.52
26	fo	201	PEB	C2A-C1A	-4.82	1.47	1.52
26	p2	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	G6	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	T7	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	bX	402	PEB	C2A-C1A	-4.81	1.47	1.52
26	dw	403	PEB	C2A-C1A	-4.81	1.47	1.52
26	p6	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	v8	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	bS	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	du	203	PEB	C2A-C1A	-4.81	1.47	1.52
26	lz	401	PEB	C2A-C1A	-4.81	1.47	1.52
26	hP	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	R7	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	bl	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	cC	1001	PEB	C2A-C1A	-4.81	1.47	1.52
26	dI	1002	PEB	C2A-C1A	-4.81	1.47	1.52
26	q6	202	PEB	C2A-C1A	-4.81	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b7	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	am	1001	PEB	C2A-C1A	-4.81	1.47	1.52
26	dO	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	iE	1001	PEB	C2A-C1A	-4.81	1.47	1.52
26	G2	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	L2	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	i6	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	I8	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	ba	1001	PEB	C2A-C1A	-4.81	1.47	1.52
26	hH	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	m7	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	E8	202	PEB	C2A-C1A	-4.81	1.47	1.52
28	B9	203	PUB	C4D-ND	4.81	1.41	1.35
26	e2	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	E3	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	h6	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	e7	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	K8	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	y9	1001	PEB	C2A-C1A	-4.81	1.47	1.52
26	aE	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	bE	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	kW	1001	PEB	C2A-C1A	-4.81	1.47	1.52
26	E4	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	x5	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	f8	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	bQ	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	eI	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	hI	201	PEB	C2A-C1A	-4.81	1.47	1.52
26	e2	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	c3	302	PEB	C2A-C1A	-4.81	1.47	1.52
26	eR	202	PEB	C2A-C1A	-4.81	1.47	1.52
26	eZ	401	PEB	C2A-C1A	-4.81	1.47	1.52
26	P2	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	p3	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	V6	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	dg	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	dx	403	PEB	C2A-C1A	-4.80	1.47	1.52
26	ee	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	y6	202	PEB	C2A-C1A	-4.80	1.47	1.52
26	W7	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	aT	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	ca	1001	PEB	C2A-C1A	-4.80	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O4	1001	PEB	C2A-C1A	-4.80	1.47	1.52
26	G7	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	t7	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	A9	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	fs	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	y3	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	k6	1001	PEB	C2A-C1A	-4.80	1.47	1.52
26	n9	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	ep	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	Y5	1003	PEB	C2A-C1A	-4.80	1.47	1.52
26	dQ	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	ez	1001	PEB	C2A-C1A	-4.80	1.47	1.52
26	f8	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	aU	202	PEB	C2A-C1A	-4.80	1.47	1.52
26	u8	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	eE	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	z2	202	PEB	C2A-C1A	-4.80	1.47	1.52
26	V3	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	A6	1001	PEB	C2A-C1A	-4.80	1.47	1.52
26	bB	201	PEB	C2A-C1A	-4.80	1.47	1.52
26	hT	204	PEB	C2A-C1A	-4.80	1.47	1.52
26	I9	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	ej	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	D2	301	PEB	C2A-C1A	-4.79	1.47	1.52
26	t4	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	O7	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	d9	302	PEB	C2A-C1A	-4.79	1.47	1.52
26	eG	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	34	1007	PEB	C2A-C1A	-4.79	1.47	1.52
26	w4	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	X5	401	PEB	C2A-C1A	-4.79	1.47	1.52
26	cp	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	dT	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	eU	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	S6	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	bn	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	cg	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	fx	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	j2	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	D2	302	PEB	C2A-C1A	-4.79	1.47	1.52
26	O4	1002	PEB	C2A-C1A	-4.79	1.47	1.52
26	bm	1002	PEB	C2A-C1A	-4.79	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dW	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	k6	1002	PEB	C2A-C1A	-4.79	1.47	1.52
26	aN	202	PEB	C2A-C1A	-4.79	1.47	1.52
26	le	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	bY	1003	PEB	C2A-C1A	-4.79	1.47	1.52
26	eM	1002	PEB	C2A-C1A	-4.79	1.47	1.52
26	fp	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	ab	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	aR	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	dh	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	lt	201	PEB	C2A-C1A	-4.79	1.47	1.52
26	Q2	1001	PEB	C2A-C1A	-4.78	1.47	1.52
26	aa	1001	PEB	C2A-C1A	-4.78	1.47	1.52
26	en	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	eN	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	V2	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	s7	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	aF	204	PEB	C2A-C1A	-4.78	1.47	1.52
26	bt	202	PEB	C2A-C1A	-4.78	1.47	1.52
26	bu	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	cw	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	dY	201	PEB	C2A-C1A	-4.78	1.47	1.52
28	dV	203	PUB	C4D-ND	4.78	1.41	1.35
26	P8	202	PEB	C2A-C1A	-4.78	1.47	1.52
26	S4	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	o4	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	N6	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	P7	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	bz	201	PEB	C2A-C1A	-4.78	1.47	1.52
28	eP	204	PUB	C4D-ND	4.78	1.41	1.35
26	bU	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	t9	202	PEB	C2A-C1A	-4.78	1.47	1.52
26	hW	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	Q5	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	W6	202	PEB	C2A-C1A	-4.78	1.47	1.52
26	dA	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	fl	201	PEB	C2A-C1A	-4.78	1.47	1.52
26	C3	1001	PEB	C2A-C1A	-4.78	1.47	1.52
26	k7	1001	PEB	C2A-C1A	-4.78	1.47	1.52
26	b9	401	PEB	C2A-C1A	-4.78	1.47	1.52
26	T6	202	PEB	C2A-C1A	-4.78	1.47	1.52
26	cZ	201	PEB	C2A-C1A	-4.78	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z3	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	G5	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	eQ	202	PEB	C2A-C1A	-4.77	1.47	1.52
26	F6	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	ek	1001	PEB	C2A-C1A	-4.77	1.47	1.52
26	V4	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	f9	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	cE	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	U9	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	p9	202	PEB	C2A-C1A	-4.77	1.47	1.52
26	cz	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	gf	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	gz	301	PEB	C2A-C1A	-4.77	1.47	1.52
26	W4	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	dp	202	PEB	C2A-C1A	-4.77	1.47	1.52
26	gx	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	ap	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	eD	202	PEB	C2A-C1A	-4.77	1.47	1.52
28	lv	202	PUB	C4D-ND	4.77	1.41	1.35
26	X8	201	PEB	C2A-C1A	-4.77	1.47	1.52
26	a7	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	by	1002	PEB	C2A-C1A	-4.76	1.47	1.52
28	P5	202	PUB	C4D-ND	4.76	1.41	1.35
26	C2	302	PEB	C2A-C1A	-4.76	1.47	1.52
26	cU	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	dl	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	eb	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	fh	1001	PEB	C2A-C1A	-4.76	1.47	1.52
26	Y4	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	ad	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	af	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	bN	201	PEB	C2A-C1A	-4.76	1.47	1.52
28	eN	203	PUB	C4D-ND	4.76	1.41	1.35
26	er	201	PEB	C2A-C1A	-4.76	1.47	1.52
28	av	203	PUB	C4D-ND	4.76	1.41	1.35
28	X4	203	PUB	C4D-ND	4.76	1.41	1.35
28	b9	407	PUB	C4D-ND	4.76	1.41	1.35
29	hY	404	PVN	C31-C3	4.76	1.61	1.51
26	t5	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	cA	201	PEB	C2A-C1A	-4.76	1.47	1.52
26	lv	201	PEB	C2A-C1A	-4.76	1.47	1.52
28	B7	202	PUB	C4D-ND	4.75	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	V4	203	PUB	C4D-ND	4.75	1.41	1.35
28	et	203	PUB	C4D-ND	4.75	1.41	1.35
26	eT	201	PEB	C2A-C1A	-4.75	1.47	1.52
26	b3	502	PEB	C2A-C1A	-4.75	1.47	1.52
26	d7	201	PEB	C2A-C1A	-4.75	1.47	1.52
28	a7	203	PUB	C4D-ND	4.75	1.41	1.35
28	eJ	203	PUB	C4D-ND	4.75	1.41	1.35
26	H3	201	PEB	C2A-C1A	-4.75	1.47	1.52
26	bo	201	PEB	C2A-C1A	-4.75	1.47	1.52
26	cS	201	PEB	C2A-C1A	-4.75	1.47	1.52
26	hF	201	PEB	C2A-C1A	-4.75	1.47	1.52
29	34	1004	PVN	C31-C3	4.75	1.61	1.51
29	Y5	1004	PVN	C31-C3	4.75	1.61	1.51
28	er	203	PUB	C4D-ND	4.75	1.41	1.35
27	d1	1001	CYC	CHB-C1B	4.75	1.49	1.38
28	Z9	1005	PUB	C4D-ND	4.75	1.41	1.35
28	jP	1003	PUB	C4D-ND	4.75	1.41	1.35
27	X1	201	CYC	CHB-C1B	4.75	1.49	1.38
28	aD	203	PUB	C4D-ND	4.75	1.41	1.35
27	W1	201	CYC	CHB-C1B	4.75	1.49	1.38
27	y1	201	CYC	CHB-C1B	4.74	1.49	1.38
28	an	202	PUB	C4D-ND	4.74	1.41	1.35
28	Z2	203	PUB	C4D-ND	4.74	1.41	1.35
28	eD	203	PUB	C4D-ND	4.74	1.41	1.35
28	iF	1003	PUB	C4D-ND	4.74	1.41	1.35
28	J7	202	PUB	C4D-ND	4.74	1.41	1.35
28	cO	203	PUB	C4D-ND	4.74	1.41	1.35
28	ez	1006	PUB	C4D-ND	4.74	1.41	1.35
27	w1	201	CYC	CHB-C1B	4.74	1.49	1.38
27	b1	1001	CYC	CHB-C1B	4.74	1.49	1.38
28	F5	203	PUB	C4D-ND	4.74	1.41	1.35
28	c8	304	PUB	C4D-ND	4.74	1.41	1.35
28	bF	203	PUB	C4D-ND	4.74	1.41	1.35
28	dd	203	PUB	C4D-ND	4.74	1.41	1.35
29	hZ	403	PVN	C31-C3	4.74	1.61	1.51
28	N6	203	PUB	C4D-ND	4.74	1.41	1.35
28	cY	203	PUB	C4D-ND	4.74	1.41	1.35
28	v4	203	PUB	C4D-ND	4.74	1.41	1.35
28	v5	203	PUB	C4D-ND	4.74	1.41	1.35
28	aZ	305	PUB	C4D-ND	4.74	1.41	1.35
28	gz	305	PUB	C4D-ND	4.74	1.41	1.35
27	k1	201	CYC	CHB-C1B	4.73	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	n1	201	CYC	CHB-C1B	4.73	1.49	1.38
28	c9	305	PUB	C4D-ND	4.73	1.41	1.35
28	Y9	304	PUB	C4D-ND	4.73	1.41	1.35
26	bW	301	PEB	C2A-C1A	-4.73	1.47	1.52
27	V1	201	CYC	CHB-C1B	4.73	1.49	1.38
28	fy	202	PUB	C4D-ND	4.73	1.41	1.35
28	G8	203	PUB	C4D-ND	4.73	1.41	1.35
27	I1	201	CYC	CHB-C1B	4.73	1.49	1.38
27	K1	201	CYC	CHB-C1B	4.73	1.49	1.38
28	y6	204	PUB	C4D-ND	4.73	1.41	1.35
28	aY	405	PUB	C4D-ND	4.73	1.41	1.35
28	bs	1004	PUB	C4D-ND	4.73	1.41	1.35
28	hX	203	PUB	C4D-ND	4.73	1.41	1.35
27	P1	201	CYC	CHB-C1B	4.73	1.49	1.38
28	dB	202	PUB	C4D-ND	4.73	1.41	1.35
28	fc	203	PUB	C4D-ND	4.73	1.41	1.35
28	hP	203	PUB	C4D-ND	4.73	1.41	1.35
28	T2	203	PUB	C4D-ND	4.73	1.41	1.35
28	d8	304	PUB	C4D-ND	4.73	1.41	1.35
28	bV	203	PUB	C4D-ND	4.73	1.41	1.35
28	z7	203	PUB	C4D-ND	4.73	1.41	1.35
28	bT	202	PUB	C4D-ND	4.73	1.41	1.35
28	dx	407	PUB	C4D-ND	4.73	1.41	1.35
26	d9	301	PEB	C2A-C1A	-4.73	1.47	1.52
28	t6	203	PUB	C4D-ND	4.73	1.41	1.35
27	R1	1001	CYC	CHB-C1B	4.73	1.49	1.38
27	i1	1001	CYC	CHB-C1B	4.73	1.49	1.38
28	E8	203	PUB	C4D-ND	4.73	1.41	1.35
28	dF	203	PUB	C4D-ND	4.73	1.41	1.35
28	gv	203	PUB	C4D-ND	4.73	1.41	1.35
27	L1	201	CYC	CHB-C1B	4.72	1.49	1.38
27	a1	201	CYC	CHB-C1B	4.72	1.49	1.38
27	g1	201	CYC	CHB-C1B	4.72	1.49	1.38
28	ly	406	PUB	C4D-ND	4.72	1.41	1.35
28	lz	405	PUB	C4D-ND	4.72	1.41	1.35
27	Z1	201	CYC	CHB-C1B	4.72	1.49	1.38
27	f1	201	CYC	CHB-C1B	4.72	1.49	1.38
28	L2	203	PUB	C4D-ND	4.72	1.41	1.35
28	l3	202	PUB	C4D-ND	4.72	1.41	1.35
28	44	305	PUB	C4D-ND	4.72	1.41	1.35
28	aY	404	PUB	C4D-ND	4.72	1.41	1.35
28	kU	1003	PUB	C4D-ND	4.72	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	aT	203	PUB	C4D-ND	4.72	1.41	1.35
28	v2	203	PUB	C4D-ND	4.72	1.41	1.35
28	V3	203	PUB	C4D-ND	4.72	1.41	1.35
28	H5	202	PUB	C4D-ND	4.72	1.41	1.35
28	J6	203	PUB	C4D-ND	4.72	1.41	1.35
28	l6	203	PUB	C4D-ND	4.72	1.41	1.35
28	H7	203	PUB	C4D-ND	4.72	1.41	1.35
28	br	203	PUB	C4D-ND	4.72	1.41	1.35
28	dY	203	PUB	C4D-ND	4.72	1.41	1.35
28	eY	404	PUB	C4D-ND	4.72	1.41	1.35
28	eZ	403	PUB	C4D-ND	4.72	1.41	1.35
26	D9	201	PEB	C2A-C1A	-4.72	1.47	1.52
28	N3	203	PUB	C4D-ND	4.72	1.41	1.35
28	T9	203	PUB	C4D-ND	4.72	1.41	1.35
28	e8	305	PUB	C4D-ND	4.72	1.41	1.35
28	U8	1005	PUB	C4D-ND	4.72	1.41	1.35
28	H9	203	PUB	C4D-ND	4.72	1.41	1.35
28	hH	203	PUB	C4D-ND	4.72	1.41	1.35
28	r9	203	PUB	C4D-ND	4.72	1.41	1.35
28	aV	203	PUB	C4D-ND	4.72	1.41	1.35
28	cs	203	PUB	C4D-ND	4.72	1.41	1.35
27	Q1	201	CYC	CHB-C1B	4.72	1.49	1.38
27	o1	1001	CYC	CHB-C1B	4.72	1.49	1.38
28	D2	304	PUB	C4D-ND	4.72	1.41	1.35
28	B3	203	PUB	C4D-ND	4.72	1.41	1.35
28	d3	303	PUB	C4D-ND	4.72	1.41	1.35
28	b9	406	PUB	C4D-ND	4.72	1.41	1.35
28	el	203	PUB	C4D-ND	4.72	1.41	1.35
27	G1	1001	CYC	CHB-C1B	4.72	1.49	1.38
28	t4	203	PUB	C4D-ND	4.72	1.41	1.35
28	t5	203	PUB	C4D-ND	4.72	1.41	1.35
28	eB	204	PUB	C4D-ND	4.72	1.41	1.35
28	f3	203	PUB	C4D-ND	4.72	1.41	1.35
28	N5	203	PUB	C4D-ND	4.72	1.41	1.35
28	P7	203	PUB	C4D-ND	4.72	1.41	1.35
28	A8	203	PUB	C4D-ND	4.72	1.41	1.35
28	aZ	304	PUB	C4D-ND	4.72	1.41	1.35
28	bN	203	PUB	C4D-ND	4.72	1.41	1.35
28	bZ	305	PUB	C4D-ND	4.72	1.41	1.35
28	lr	203	PUB	C4D-ND	4.72	1.41	1.35
28	F2	203	PUB	C4D-ND	4.72	1.41	1.35
28	c3	305	PUB	C4D-ND	4.72	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D9	203	PUB	C4D-ND	4.72	1.41	1.35
28	P9	203	PUB	C4D-ND	4.72	1.41	1.35
28	p3	203	PUB	C4D-ND	4.71	1.41	1.35
28	bq	203	PUB	C4D-ND	4.71	1.41	1.35
27	u1	1001	CYC	CHB-C1B	4.71	1.49	1.38
28	ar	203	PUB	C4D-ND	4.71	1.41	1.35
28	bZ	306	PUB	C4D-ND	4.71	1.41	1.35
28	co	202	PUB	C4D-ND	4.71	1.41	1.35
28	V6	203	PUB	C4D-ND	4.71	1.41	1.35
28	X7	203	PUB	C4D-ND	4.71	1.41	1.35
28	bY	1005	PUB	C4D-ND	4.71	1.41	1.35
28	gp	203	PUB	C4D-ND	4.71	1.41	1.35
28	A2	1005	PUB	C4D-ND	4.71	1.41	1.35
28	a3	1005	PUB	C4D-ND	4.71	1.41	1.35
28	44	304	PUB	C4D-ND	4.71	1.41	1.35
28	aP	203	PUB	C4D-ND	4.71	1.41	1.35
28	kT	1003	PUB	C4D-ND	4.71	1.41	1.35
28	c3	304	PUB	C4D-ND	4.71	1.41	1.35
28	dn	203	PUB	C4D-ND	4.71	1.41	1.35
28	fw	203	PUB	C4D-ND	4.71	1.41	1.35
28	v9	203	PUB	C4D-ND	4.71	1.41	1.35
28	bJ	203	PUB	C4D-ND	4.71	1.41	1.35
28	f2	203	PUB	C4D-ND	4.71	1.41	1.35
28	F3	203	PUB	C4D-ND	4.71	1.41	1.35
28	a3	1006	PUB	C4D-ND	4.71	1.41	1.35
28	bp	202	PUB	C4D-ND	4.71	1.41	1.35
28	cL	203	PUB	C4D-ND	4.71	1.41	1.35
28	dh	203	PUB	C4D-ND	4.71	1.41	1.35
27	q1	201	CYC	CHB-C1B	4.71	1.49	1.38
28	R4	203	PUB	C4D-ND	4.71	1.41	1.35
28	dL	203	PUB	C4D-ND	4.71	1.41	1.35
28	p9	203	PUB	C4D-ND	4.71	1.41	1.35
28	ap	203	PUB	C4D-ND	4.71	1.41	1.35
28	bH	203	PUB	C4D-ND	4.71	1.41	1.35
27	U1	201	CYC	CHB-C1B	4.71	1.49	1.38
27	m1	201	CYC	CHB-C1B	4.71	1.49	1.38
27	d2	101	CYC	CHB-C1B	4.71	1.49	1.38
28	z9	203	PUB	C4D-ND	4.71	1.41	1.35
28	L4	203	PUB	C4D-ND	4.71	1.41	1.35
28	J3	203	PUB	C4D-ND	4.71	1.41	1.35
28	X3	202	PUB	C4D-ND	4.71	1.41	1.35
28	D4	203	PUB	C4D-ND	4.71	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C8	203	PUB	C4D-ND	4.71	1.41	1.35
28	bR	202	PUB	C4D-ND	4.71	1.41	1.35
28	cF	202	PUB	C4D-ND	4.71	1.41	1.35
28	ei	203	PUB	C4D-ND	4.71	1.41	1.35
28	ld	203	PUB	C4D-ND	4.71	1.41	1.35
28	gn	203	PUB	C4D-ND	4.71	1.41	1.35
28	hZ	405	PUB	C4D-ND	4.71	1.41	1.35
28	l2	203	PUB	C4D-ND	4.70	1.41	1.35
28	L3	203	PUB	C4D-ND	4.70	1.41	1.35
28	p6	203	PUB	C4D-ND	4.70	1.41	1.35
28	bz	203	PUB	C4D-ND	4.70	1.41	1.35
28	ec	203	PUB	C4D-ND	4.70	1.41	1.35
28	n8	202	PUB	C4D-ND	4.70	1.41	1.35
28	x7	203	PUB	C4D-ND	4.70	1.41	1.35
28	cJ	203	PUB	C4D-ND	4.70	1.41	1.35
28	dp	203	PUB	C4D-ND	4.70	1.41	1.35
28	dX	203	PUB	C4D-ND	4.70	1.41	1.35
28	h3	202	PUB	C4D-ND	4.70	1.41	1.35
28	34	1005	PUB	C4D-ND	4.70	1.41	1.35
28	F7	202	PUB	C4D-ND	4.70	1.41	1.35
28	ey	1006	PUB	C4D-ND	4.70	1.41	1.35
28	fo	203	PUB	C4D-ND	4.70	1.41	1.35
28	d7	203	PUB	C4D-ND	4.70	1.41	1.35
28	ev	203	PUB	C4D-ND	4.70	1.41	1.35
28	gi	203	PUB	C4D-ND	4.70	1.41	1.35
28	gy	306	PUB	C4D-ND	4.70	1.41	1.35
28	j2	203	PUB	C4D-ND	4.70	1.41	1.35
28	H3	203	PUB	C4D-ND	4.70	1.41	1.35
28	z5	203	PUB	C4D-ND	4.70	1.41	1.35
28	g8	202	PUB	C4D-ND	4.70	1.41	1.35
28	aJ	203	PUB	C4D-ND	4.70	1.41	1.35
28	cH	202	PUB	C4D-ND	4.70	1.41	1.35
28	iH	1002	PUB	C4D-ND	4.70	1.41	1.35
28	e8	304	PUB	C4D-ND	4.70	1.41	1.35
28	e9	305	PUB	C4D-ND	4.70	1.41	1.35
28	aN	203	PUB	C4D-ND	4.70	1.41	1.35
28	cR	203	PUB	C4D-ND	4.70	1.41	1.35
28	eR	203	PUB	C4D-ND	4.70	1.41	1.35
28	fs	203	PUB	C4D-ND	4.70	1.41	1.35
28	jL	1003	PUB	C4D-ND	4.70	1.41	1.35
28	kQ	1003	PUB	C4D-ND	4.70	1.41	1.35
26	i5	201	PEB	C2A-C1A	-4.70	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n2	203	PUB	C4D-ND	4.70	1.41	1.35
28	J2	202	PUB	C4D-ND	4.70	1.41	1.35
28	p5	202	PUB	C4D-ND	4.70	1.41	1.35
28	c7	203	PUB	C4D-ND	4.70	1.41	1.35
28	cE	203	PUB	C4D-ND	4.70	1.41	1.35
28	hD	203	PUB	C4D-ND	4.70	1.41	1.35
27	s1	201	CYC	CHB-C1B	4.70	1.49	1.38
28	p4	203	PUB	C4D-ND	4.70	1.41	1.35
28	P4	203	PUB	C4D-ND	4.70	1.41	1.35
28	e9	306	PUB	C4D-ND	4.70	1.41	1.35
28	df	203	PUB	C4D-ND	4.70	1.41	1.35
28	J4	203	PUB	C4D-ND	4.70	1.41	1.35
28	u6	203	PUB	C4D-ND	4.70	1.41	1.35
28	p8	203	PUB	C4D-ND	4.70	1.41	1.35
28	s7	203	PUB	C4D-ND	4.70	1.41	1.35
28	cr	203	PUB	C4D-ND	4.70	1.41	1.35
28	hY	406	PUB	C4D-ND	4.70	1.41	1.35
28	T5	202	PUB	C4D-ND	4.70	1.41	1.35
28	eZ	404	PUB	C4D-ND	4.70	1.41	1.35
28	lt	203	PUB	C4D-ND	4.70	1.41	1.35
28	kX	1003	PUB	C4D-ND	4.70	1.41	1.35
28	z2	203	PUB	C4D-ND	4.69	1.41	1.35
28	Z3	203	PUB	C4D-ND	4.69	1.41	1.35
28	r2	203	PUB	C4D-ND	4.69	1.41	1.35
28	R3	203	PUB	C4D-ND	4.69	1.41	1.35
28	c6	1004	PUB	C4D-ND	4.69	1.41	1.35
28	r7	203	PUB	C4D-ND	4.69	1.41	1.35
28	aR	203	PUB	C4D-ND	4.69	1.41	1.35
28	dD	203	PUB	C4D-ND	4.69	1.41	1.35
28	dN	203	PUB	C4D-ND	4.69	1.41	1.35
28	dj	203	PUB	C4D-ND	4.69	1.41	1.35
28	dt	203	PUB	C4D-ND	4.69	1.41	1.35
28	fa	202	PUB	C4D-ND	4.69	1.41	1.35
27	N1	201	CYC	CHB-C1B	4.69	1.49	1.38
28	B6	203	PUB	C4D-ND	4.69	1.41	1.35
28	R6	203	PUB	C4D-ND	4.69	1.41	1.35
28	D7	203	PUB	C4D-ND	4.69	1.41	1.35
28	w8	203	PUB	C4D-ND	4.69	1.41	1.35
28	r6	203	PUB	C4D-ND	4.69	1.41	1.35
28	z6	203	PUB	C4D-ND	4.69	1.41	1.35
28	t7	203	PUB	C4D-ND	4.69	1.41	1.35
28	ax	202	PUB	C4D-ND	4.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	cP	203	PUB	C4D-ND	4.69	1.41	1.35
28	ey	1005	PUB	C4D-ND	4.69	1.41	1.35
28	jM	1003	PUB	C4D-ND	4.69	1.41	1.35
26	E9	201	PEB	C2A-C1A	-4.69	1.47	1.52
28	M8	203	PUB	C4D-ND	4.69	1.41	1.35
28	cq	203	PUB	C4D-ND	4.69	1.41	1.35
28	cB	203	PUB	C4D-ND	4.69	1.41	1.35
28	N4	203	PUB	C4D-ND	4.69	1.41	1.35
28	n7	203	PUB	C4D-ND	4.69	1.41	1.35
28	dl	203	PUB	C4D-ND	4.69	1.41	1.35
28	x6	203	PUB	C4D-ND	4.69	1.41	1.35
28	iC	1003	PUB	C4D-ND	4.69	1.41	1.35
28	iD	1003	PUB	C4D-ND	4.69	1.41	1.35
27	e1	201	CYC	CHB-C1B	4.69	1.49	1.38
28	B4	203	PUB	C4D-ND	4.69	1.41	1.35
28	F6	203	PUB	C4D-ND	4.69	1.41	1.35
28	kR	1003	PUB	C4D-ND	4.69	1.41	1.35
28	R2	203	PUB	C4D-ND	4.69	1.41	1.35
28	o8	203	PUB	C4D-ND	4.69	1.41	1.35
28	dw	406	PUB	C4D-ND	4.69	1.41	1.35
28	lb	203	PUB	C4D-ND	4.69	1.41	1.35
28	ga	203	PUB	C4D-ND	4.69	1.41	1.35
28	n9	202	PUB	C4D-ND	4.69	1.41	1.35
28	L9	203	PUB	C4D-ND	4.69	1.41	1.35
28	az	203	PUB	C4D-ND	4.69	1.41	1.35
28	hR	203	PUB	C4D-ND	4.69	1.41	1.35
28	bo	202	PUB	C4D-ND	4.69	1.41	1.35
28	bL	203	PUB	C4D-ND	4.69	1.41	1.35
28	gz	306	PUB	C4D-ND	4.69	1.41	1.35
28	x4	202	PUB	C4D-ND	4.69	1.41	1.35
28	x5	202	PUB	C4D-ND	4.69	1.41	1.35
28	O8	203	PUB	C4D-ND	4.69	1.41	1.35
28	J9	203	PUB	C4D-ND	4.69	1.41	1.35
28	jI	1003	PUB	C4D-ND	4.69	1.41	1.35
28	C2	304	PUB	C4D-ND	4.69	1.41	1.35
28	r3	203	PUB	C4D-ND	4.69	1.41	1.35
28	h8	203	PUB	C4D-ND	4.69	1.41	1.35
28	L6	202	PUB	C4D-ND	4.69	1.41	1.35
28	I8	203	PUB	C4D-ND	4.69	1.41	1.35
28	ff	203	PUB	C4D-ND	4.69	1.41	1.35
28	N9	203	PUB	C4D-ND	4.68	1.41	1.35
28	hL	203	PUB	C4D-ND	4.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	hN	203	PUB	C4D-ND	4.68	1.41	1.35
28	jK	1003	PUB	C4D-ND	4.68	1.41	1.35
28	t2	203	PUB	C4D-ND	4.68	1.41	1.35
28	T3	203	PUB	C4D-ND	4.68	1.41	1.35
28	t9	203	PUB	C4D-ND	4.68	1.41	1.35
28	x9	203	PUB	C4D-ND	4.68	1.41	1.35
28	V9	203	PUB	C4D-ND	4.68	1.41	1.35
28	aL	203	PUB	C4D-ND	4.68	1.41	1.35
28	lf	203	PUB	C4D-ND	4.68	1.41	1.35
28	lj	202	PUB	C4D-ND	4.68	1.41	1.35
28	lx	201	PUB	C4D-ND	4.68	1.41	1.35
28	jJ	1003	PUB	C4D-ND	4.68	1.41	1.35
28	aF	203	PUB	C4D-ND	4.68	1.41	1.35
28	cp	203	PUB	C4D-ND	4.68	1.41	1.35
28	F4	203	PUB	C4D-ND	4.68	1.41	1.35
28	B5	203	PUB	C4D-ND	4.68	1.41	1.35
28	l7	203	PUB	C4D-ND	4.68	1.41	1.35
28	F9	203	PUB	C4D-ND	4.68	1.41	1.35
28	hG	202	PUB	C4D-ND	4.68	1.41	1.35
29	dx	405	PVN	C4-N1	-4.68	1.38	1.45
28	X2	203	PUB	C4D-ND	4.68	1.41	1.35
28	aB	203	PUB	C4D-ND	4.68	1.41	1.35
28	ly	405	PUB	C4D-ND	4.68	1.41	1.35
28	lz	404	PUB	C4D-ND	4.68	1.41	1.35
28	hV	203	PUB	C4D-ND	4.68	1.41	1.35
28	e7	203	PUB	C4D-ND	4.68	1.41	1.35
27	O1	201	CYC	CHB-C1B	4.68	1.49	1.38
28	eH	203	PUB	C4D-ND	4.68	1.41	1.35
28	D6	202	PUB	C4D-ND	4.68	1.41	1.35
28	Y9	305	PUB	C4D-ND	4.68	1.41	1.35
28	n3	203	PUB	C4D-ND	4.68	1.41	1.35
28	b7	202	PUB	C4D-ND	4.68	1.41	1.35
28	34	1006	PUB	C4D-ND	4.68	1.41	1.35
28	r4	202	PUB	C4D-ND	4.68	1.41	1.35
28	Y5	1006	PUB	C4D-ND	4.68	1.41	1.35
28	r5	203	PUB	C4D-ND	4.68	1.41	1.35
28	b6	203	PUB	C4D-ND	4.68	1.41	1.35
28	Z4	203	PUB	C4D-ND	4.68	1.41	1.35
28	V5	203	PUB	C4D-ND	4.68	1.41	1.35
28	P6	203	PUB	C4D-ND	4.68	1.41	1.35
28	v6	203	PUB	C4D-ND	4.68	1.41	1.35
28	U8	1006	PUB	C4D-ND	4.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z9	1006	PUB	C4D-ND	4.68	1.41	1.35
28	dx	406	PUB	C4D-ND	4.68	1.41	1.35
28	ee	203	PUB	C4D-ND	4.68	1.41	1.35
28	ez	1005	PUB	C4D-ND	4.68	1.41	1.35
28	fu	202	PUB	C4D-ND	4.68	1.41	1.35
28	h2	203	PUB	C4D-ND	4.68	1.41	1.35
28	x2	202	PUB	C4D-ND	4.68	1.41	1.35
28	D2	305	PUB	C4D-ND	4.68	1.41	1.35
28	d3	304	PUB	C4D-ND	4.68	1.41	1.35
28	x3	203	PUB	C4D-ND	4.68	1.41	1.35
28	lp	203	PUB	C4D-ND	4.68	1.41	1.35
28	z4	203	PUB	C4D-ND	4.67	1.41	1.35
28	eV	203	PUB	C4D-ND	4.67	1.41	1.35
28	ln	203	PUB	C4D-ND	4.67	1.41	1.35
28	e6	203	PUB	C4D-ND	4.67	1.41	1.35
28	eg	203	PUB	C4D-ND	4.67	1.41	1.35
28	hB	203	PUB	C4D-ND	4.67	1.41	1.35
28	D3	203	PUB	C4D-ND	4.67	1.41	1.35
28	Y5	1005	PUB	C4D-ND	4.67	1.41	1.35
28	T6	203	PUB	C4D-ND	4.67	1.41	1.35
28	Z6	203	PUB	C4D-ND	4.67	1.41	1.35
28	bn	202	PUB	C4D-ND	4.67	1.41	1.35
28	dP	203	PUB	C4D-ND	4.67	1.41	1.35
28	ep	203	PUB	C4D-ND	4.67	1.41	1.35
28	dR	203	PUB	C4D-ND	4.67	1.41	1.35
28	hY	405	PUB	C4D-ND	4.67	1.41	1.35
28	jO	1003	PUB	C4D-ND	4.67	1.41	1.35
28	T8	305	PUB	C4D-ND	4.67	1.41	1.35
28	dr	203	PUB	C4D-ND	4.67	1.41	1.35
28	gy	305	PUB	C4D-ND	4.67	1.41	1.35
28	P2	203	PUB	C4D-ND	4.67	1.41	1.35
28	bB	203	PUB	C4D-ND	4.67	1.41	1.35
28	gg	203	PUB	C4D-ND	4.67	1.41	1.35
28	iE	1003	PUB	C4D-ND	4.67	1.41	1.35
28	V2	203	PUB	C4D-ND	4.67	1.41	1.35
28	c9	304	PUB	C4D-ND	4.67	1.41	1.35
29	gy	304	PVN	C11-C12	-4.67	1.38	1.45
28	d6	203	PUB	C4D-ND	4.67	1.41	1.35
28	n4	203	PUB	C4D-ND	4.67	1.41	1.35
28	p7	202	PUB	C4D-ND	4.67	1.41	1.35
28	t3	203	PUB	C4D-ND	4.67	1.41	1.35
28	cQ	202	PUB	C4D-ND	4.67	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dv	202	PUB	C4D-ND	4.67	1.41	1.35
28	kS	1003	PUB	C4D-ND	4.67	1.41	1.35
28	n6	203	PUB	C4D-ND	4.66	1.41	1.35
28	H4	203	PUB	C4D-ND	4.66	1.41	1.35
28	R5	203	PUB	C4D-ND	4.66	1.41	1.35
28	R9	203	PUB	C4D-ND	4.66	1.41	1.35
28	p2	203	PUB	C4D-ND	4.66	1.41	1.35
28	P3	203	PUB	C4D-ND	4.66	1.41	1.35
28	cn	202	PUB	C4D-ND	4.66	1.41	1.35
28	eb	202	PUB	C4D-ND	4.66	1.41	1.35
28	lh	203	PUB	C4D-ND	4.66	1.41	1.35
28	at	203	PUB	C4D-ND	4.66	1.41	1.35
28	T4	202	PUB	C4D-ND	4.66	1.41	1.35
28	D5	203	PUB	C4D-ND	4.66	1.41	1.35
28	b8	1005	PUB	C4D-ND	4.66	1.41	1.35
28	eY	405	PUB	C4D-ND	4.66	1.41	1.35
28	fi	203	PUB	C4D-ND	4.66	1.41	1.35
28	K8	203	PUB	C4D-ND	4.66	1.41	1.35
28	dK	203	PUB	C4D-ND	4.66	1.41	1.35
28	iG	1002	PUB	C4D-ND	4.66	1.41	1.35
28	f8	203	PUB	C4D-ND	4.66	1.41	1.35
28	hZ	404	PUB	C4D-ND	4.66	1.41	1.35
28	j3	202	PUB	C4D-ND	4.66	1.41	1.35
28	dw	405	PUB	C4D-ND	4.66	1.41	1.35
28	v3	203	PUB	C4D-ND	4.66	1.41	1.35
28	Z5	306	PUB	C4D-ND	4.66	1.41	1.35
28	H6	203	PUB	C4D-ND	4.66	1.41	1.35
28	dT	203	PUB	C4D-ND	4.66	1.41	1.35
28	C2	305	PUB	C4D-ND	4.65	1.41	1.35
28	Q8	203	PUB	C4D-ND	4.65	1.41	1.35
28	bY	1006	PUB	C4D-ND	4.65	1.41	1.35
28	eF	203	PUB	C4D-ND	4.65	1.41	1.35
28	gk	203	PUB	C4D-ND	4.65	1.41	1.35
28	gx	203	PUB	C4D-ND	4.65	1.41	1.35
28	a6	203	PUB	C4D-ND	4.65	1.41	1.35
28	bD	203	PUB	C4D-ND	4.65	1.41	1.35
28	dH	203	PUB	C4D-ND	4.65	1.41	1.35
28	L7	202	PUB	C4D-ND	4.65	1.41	1.35
28	cM	203	PUB	C4D-ND	4.65	1.41	1.35
28	ll	203	PUB	C4D-ND	4.65	1.41	1.35
28	fj	203	PUB	C4D-ND	4.65	1.41	1.35
28	X6	203	PUB	C4D-ND	4.65	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	fq	203	PUB	C4D-ND	4.65	1.41	1.35
28	kV	1003	PUB	C4D-ND	4.65	1.41	1.35
28	ge	203	PUB	C4D-ND	4.65	1.41	1.35
28	gr	202	PUB	C4D-ND	4.65	1.41	1.35
28	Z7	203	PUB	C4D-ND	4.65	1.41	1.35
28	c8	305	PUB	C4D-ND	4.65	1.41	1.35
28	cz	203	PUB	C4D-ND	4.65	1.41	1.35
28	v7	203	PUB	C4D-ND	4.65	1.41	1.35
28	eT	203	PUB	C4D-ND	4.65	1.41	1.35
28	kW	1003	PUB	C4D-ND	4.65	1.41	1.35
28	L5	203	PUB	C4D-ND	4.65	1.41	1.35
28	V7	203	PUB	C4D-ND	4.65	1.41	1.35
28	hJ	203	PUB	C4D-ND	4.65	1.41	1.35
28	jN	1003	PUB	C4D-ND	4.65	1.41	1.35
28	T8	304	PUB	C4D-ND	4.65	1.41	1.35
28	di	203	PUB	C4D-ND	4.65	1.41	1.35
28	Z5	305	PUB	C4D-ND	4.65	1.41	1.35
28	bP	203	PUB	C4D-ND	4.65	1.41	1.35
28	eL	203	PUB	C4D-ND	4.65	1.41	1.35
28	b8	1006	PUB	C4D-ND	4.65	1.41	1.35
28	z3	203	PUB	C4D-ND	4.64	1.41	1.35
28	d9	305	PUB	C4D-ND	4.64	1.41	1.35
28	fm	203	PUB	C4D-ND	4.64	1.41	1.35
28	gd	202	PUB	C4D-ND	4.64	1.41	1.35
28	en	203	PUB	C4D-ND	4.64	1.41	1.35
29	dw	404	PVN	C4-N1	-4.64	1.38	1.45
28	J5	203	PUB	C4D-ND	4.64	1.41	1.35
28	n5	203	PUB	C4D-ND	4.64	1.41	1.35
28	A2	1006	PUB	C4D-ND	4.64	1.41	1.35
28	H2	202	PUB	C4D-ND	4.64	1.41	1.35
28	y7	203	PUB	C4D-ND	4.64	1.41	1.35
28	y8	203	PUB	C4D-ND	4.64	1.41	1.35
28	aH	203	PUB	C4D-ND	4.64	1.41	1.35
28	gt	203	PUB	C4D-ND	4.63	1.41	1.35
28	hT	203	PUB	C4D-ND	4.63	1.41	1.35
28	N2	203	PUB	C4D-ND	4.63	1.41	1.35
28	R7	203	PUB	C4D-ND	4.63	1.41	1.35
28	cN	202	PUB	C4D-ND	4.63	1.41	1.35
28	N7	203	PUB	C4D-ND	4.62	1.41	1.35
28	T7	203	PUB	C4D-ND	4.62	1.41	1.35
29	T8	303	PVN	C4-N1	-4.62	1.38	1.45
29	Y9	303	PVN	C4-N1	-4.62	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	ly	404	PVN	C4-N1	-4.61	1.38	1.45
29	lz	403	PVN	C4-N1	-4.55	1.38	1.45
28	eX	202	PUB	C4D-ND	4.50	1.41	1.35
27	S1	202	CYC	C1C-NC	-4.46	1.31	1.37
27	a2	901	CYC	C1C-NC	-4.44	1.31	1.37
28	eR	203	PUB	C1C-C2C	-4.42	1.38	1.45
28	bZ	305	PUB	C1C-C2C	-4.42	1.38	1.45
27	M1	1001	CYC	C1C-NC	-4.41	1.31	1.37
28	ax	202	PUB	C1C-C2C	-4.41	1.38	1.45
28	n3	203	PUB	C1C-C2C	-4.41	1.38	1.45
29	eY	403	PVN	C19-C18	-4.41	1.39	1.48
28	lb	203	PUB	C1C-C2C	-4.41	1.38	1.45
28	dX	203	PUB	C1C-C2C	-4.40	1.38	1.45
28	T7	203	PUB	C1C-C2C	-4.40	1.38	1.45
28	bF	203	PUB	C1C-C2C	-4.40	1.38	1.45
28	lh	203	PUB	C1C-C2C	-4.40	1.38	1.45
28	H7	203	PUB	C1C-C2C	-4.40	1.38	1.45
28	X6	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	aJ	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	dF	203	PUB	C1C-C2C	-4.39	1.38	1.45
27	z1	201	CYC	C1C-NC	-4.39	1.31	1.37
28	en	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	Z6	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	D7	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	B9	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	cz	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	et	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	aP	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	v2	203	PUB	C1C-C2C	-4.39	1.38	1.45
28	V3	203	PUB	C1C-C2C	-4.39	1.38	1.45
27	c1	201	CYC	C1C-NC	-4.38	1.31	1.37
28	dR	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	eX	202	PUB	C1C-C2C	-4.38	1.38	1.45
27	J1	201	CYC	C1C-NC	-4.38	1.31	1.37
27	Y1	201	CYC	C1C-NC	-4.38	1.31	1.37
27	v1	201	CYC	C1C-NC	-4.38	1.31	1.37
28	jI	1003	PUB	C1C-C2C	-4.38	1.38	1.45
28	B3	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	R7	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	H5	202	PUB	C1C-C2C	-4.38	1.38	1.45
28	t7	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	hG	202	PUB	C1C-C2C	-4.38	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	hJ	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	F5	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	X7	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	aF	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	ev	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	ap	203	PUB	C1C-C2C	-4.38	1.38	1.45
27	a2	902	CYC	C1C-NC	-4.38	1.31	1.37
27	b2	1001	CYC	C1C-NC	-4.38	1.31	1.37
28	T2	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	J7	202	PUB	C1C-C2C	-4.38	1.38	1.45
28	bD	203	PUB	C1C-C2C	-4.38	1.38	1.45
28	T8	304	PUB	C1C-C2C	-4.37	1.38	1.45
28	gd	202	PUB	C1C-C2C	-4.37	1.38	1.45
28	iE	1003	PUB	C1C-C2C	-4.37	1.38	1.45
28	c7	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	ey	1005	PUB	C1C-C2C	-4.37	1.38	1.45
28	s7	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	w8	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	fw	203	PUB	C1C-C2C	-4.37	1.38	1.45
27	S1	201	CYC	C1C-NC	-4.37	1.31	1.37
27	j1	201	CYC	C1C-NC	-4.37	1.31	1.37
28	U8	1005	PUB	C1C-C2C	-4.37	1.38	1.45
28	ep	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	e9	306	PUB	C1C-C2C	-4.37	1.38	1.45
28	cM	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	t2	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	T3	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	B7	202	PUB	C1C-C2C	-4.37	1.38	1.45
28	y7	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	bL	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	bT	202	PUB	C1C-C2C	-4.37	1.38	1.45
27	h1	201	CYC	C1C-NC	-4.37	1.31	1.37
28	f8	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	jJ	1003	PUB	C1C-C2C	-4.37	1.38	1.45
28	kU	1003	PUB	C1C-C2C	-4.37	1.38	1.45
28	h3	202	PUB	C1C-C2C	-4.37	1.38	1.45
28	D9	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	bZ	306	PUB	C1C-C2C	-4.37	1.38	1.45
28	eF	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	C2	305	PUB	C1C-C2C	-4.37	1.38	1.45
28	c3	305	PUB	C1C-C2C	-4.37	1.38	1.45
28	ey	1006	PUB	C1C-C2C	-4.37	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	lp	203	PUB	C1C-C2C	-4.37	1.38	1.45
29	aY	403	PVN	C31-C3	4.37	1.60	1.51
28	r2	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	Z4	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	p7	202	PUB	C1C-C2C	-4.37	1.38	1.45
28	dv	202	PUB	C1C-C2C	-4.37	1.38	1.45
28	cB	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	dB	202	PUB	C1C-C2C	-4.37	1.38	1.45
28	bJ	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	aH	203	PUB	C1C-C2C	-4.37	1.38	1.45
28	t5	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	N5	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	M8	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	F4	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	p4	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	L9	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	hZ	404	PUB	C1C-C2C	-4.36	1.38	1.45
28	jM	1003	PUB	C1C-C2C	-4.36	1.38	1.45
28	R4	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	eb	202	PUB	C1C-C2C	-4.36	1.38	1.45
28	fo	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	V9	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	kR	1003	PUB	C1C-C2C	-4.36	1.38	1.45
29	eZ	402	PVN	C19-C18	-4.36	1.39	1.48
28	Y9	305	PUB	C1C-C2C	-4.36	1.38	1.45
28	N3	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	eT	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	o8	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	dw	406	PUB	C1C-C2C	-4.36	1.38	1.45
28	eL	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	eY	404	PUB	C1C-C2C	-4.36	1.38	1.45
28	hR	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	y8	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	a7	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	aT	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	hV	203	PUB	C1C-C2C	-4.36	1.38	1.45
27	r1	201	CYC	C1C-NC	-4.36	1.32	1.37
28	ec	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	z5	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	V7	203	PUB	C1C-C2C	-4.36	1.38	1.45
28	X4	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	T5	202	PUB	C1C-C2C	-4.35	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y9	304	PUB	C1C-C2C	-4.35	1.38	1.45
28	A2	1005	PUB	C1C-C2C	-4.35	1.38	1.45
28	A2	1006	PUB	C1C-C2C	-4.35	1.38	1.45
28	44	304	PUB	C1C-C2C	-4.35	1.38	1.45
28	v6	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	eY	405	PUB	C1C-C2C	-4.35	1.38	1.45
28	eZ	404	PUB	C1C-C2C	-4.35	1.38	1.45
27	H1	201	CYC	C1C-NC	-4.35	1.32	1.37
28	F7	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	ly	405	PUB	C1C-C2C	-4.35	1.38	1.45
28	lz	404	PUB	C1C-C2C	-4.35	1.38	1.45
28	fq	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	kW	1003	PUB	C1C-C2C	-4.35	1.38	1.45
28	R5	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	hY	405	PUB	C1C-C2C	-4.35	1.38	1.45
28	x9	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	aR	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	H6	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	d6	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	eD	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	kQ	1003	PUB	C1C-C2C	-4.35	1.38	1.45
28	H3	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	34	1005	PUB	C1C-C2C	-4.35	1.38	1.45
28	n6	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	I8	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	N9	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	cN	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	eV	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	gz	305	PUB	C1C-C2C	-4.35	1.38	1.45
28	jN	1003	PUB	C1C-C2C	-4.35	1.38	1.45
28	v3	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	L4	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	cs	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	x4	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	z4	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	x5	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	cJ	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	cL	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	cQ	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	dH	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	dK	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	iC	1003	PUB	C1C-C2C	-4.35	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	44	305	PUB	C1C-C2C	-4.35	1.38	1.45
28	K8	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	P9	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	b9	407	PUB	C1C-C2C	-4.35	1.38	1.45
28	aL	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	h2	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	y6	204	PUB	C1C-C2C	-4.35	1.38	1.45
28	di	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	lf	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	gi	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	hN	203	PUB	C1C-C2C	-4.35	1.38	1.45
29	bY	1004	PVN	C31-C3	4.35	1.60	1.51
27	t1	201	CYC	C1C-NC	-4.35	1.32	1.37
28	j2	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	C2	304	PUB	C1C-C2C	-4.35	1.38	1.45
28	D6	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	P6	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	R9	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	aN	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	dl	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	lj	202	PUB	C1C-C2C	-4.35	1.38	1.45
28	lx	201	PUB	C1C-C2C	-4.35	1.38	1.45
28	ga	203	PUB	C1C-C2C	-4.35	1.38	1.45
28	P7	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	gt	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	p9	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	V6	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	dY	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	t3	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	R6	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	bB	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	N4	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	J5	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	T6	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	cE	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	ee	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	x3	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	n9	202	PUB	C1C-C2C	-4.34	1.38	1.45
28	an	202	PUB	C1C-C2C	-4.34	1.38	1.45
28	br	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	gp	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	fc	203	PUB	C1C-C2C	-4.34	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	fu	202	PUB	C1C-C2C	-4.34	1.38	1.45
28	gr	202	PUB	C1C-C2C	-4.34	1.38	1.45
28	d8	304	PUB	C1C-C2C	-4.34	1.38	1.45
28	bY	1006	PUB	C1C-C2C	-4.34	1.38	1.45
28	df	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	jP	1003	PUB	C1C-C2C	-4.34	1.38	1.45
28	Z5	305	PUB	C1C-C2C	-4.34	1.38	1.45
28	aV	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	aY	405	PUB	C1C-C2C	-4.34	1.38	1.45
28	bp	202	PUB	C1C-C2C	-4.34	1.38	1.45
28	r5	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	cO	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	dn	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	gk	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	gx	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	jO	1003	PUB	C1C-C2C	-4.34	1.38	1.45
28	z3	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	ei	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	d3	304	PUB	C1C-C2C	-4.34	1.38	1.45
28	c9	305	PUB	C1C-C2C	-4.34	1.38	1.45
28	aD	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	34	1006	PUB	C1C-C2C	-4.34	1.38	1.45
28	gy	305	PUB	C1C-C2C	-4.34	1.38	1.45
28	kS	1003	PUB	C1C-C2C	-4.34	1.38	1.45
28	D4	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	v9	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	T9	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	hY	406	PUB	C1C-C2C	-4.34	1.38	1.45
28	J4	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	E8	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	J9	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	dp	203	PUB	C1C-C2C	-4.34	1.38	1.45
28	hX	203	PUB	C1C-C2C	-4.34	1.38	1.45
27	p1	201	CYC	C1C-NC	-4.33	1.32	1.37
28	gn	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	iF	1003	PUB	C1C-C2C	-4.33	1.38	1.45
28	jK	1003	PUB	C1C-C2C	-4.33	1.38	1.45
28	F6	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	bq	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	dP	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	hT	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	b6	203	PUB	C1C-C2C	-4.33	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	u6	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	cn	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	eP	204	PUB	C1C-C2C	-4.33	1.38	1.45
28	D2	305	PUB	C1C-C2C	-4.33	1.38	1.45
28	c3	304	PUB	C1C-C2C	-4.33	1.38	1.45
28	P5	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	e9	305	PUB	C1C-C2C	-4.33	1.38	1.45
28	bY	1005	PUB	C1C-C2C	-4.33	1.38	1.45
28	ld	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	ln	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	fj	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	v7	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	t9	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	dw	405	PUB	C1C-C2C	-4.33	1.38	1.45
28	er	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	hB	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	hD	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	hL	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	x6	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	z9	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	cH	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	dj	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	dt	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	gv	203	PUB	C1C-C2C	-4.33	1.38	1.45
29	c8	303	PVN	C4-N1	-4.33	1.39	1.45
28	R2	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	d7	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	dh	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	R3	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	t6	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	Z3	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	ez	1005	PUB	C1C-C2C	-4.33	1.38	1.45
28	hP	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	J2	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	j3	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	G8	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	Z9	1006	PUB	C1C-C2C	-4.33	1.38	1.45
28	dT	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	L2	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	l3	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	h8	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	B6	203	PUB	C1C-C2C	-4.33	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	p8	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	bz	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	bP	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	bR	202	PUB	C1C-C2C	-4.33	1.38	1.45
28	x7	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	z7	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	at	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	ll	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	lt	203	PUB	C1C-C2C	-4.33	1.38	1.45
28	hZ	405	PUB	C1C-C2C	-4.33	1.38	1.45
28	Z5	306	PUB	C1C-C2C	-4.32	1.38	1.45
28	e8	304	PUB	C1C-C2C	-4.32	1.38	1.45
28	dr	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	L6	202	PUB	C1C-C2C	-4.32	1.38	1.45
28	n7	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	H9	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	eH	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	N2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	P4	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	L5	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	L7	202	PUB	C1C-C2C	-4.32	1.38	1.45
28	V2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	a3	1006	PUB	C1C-C2C	-4.32	1.38	1.45
28	D5	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	B4	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	t4	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	T8	305	PUB	C1C-C2C	-4.32	1.38	1.45
28	p2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	P3	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	r6	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	eB	204	PUB	C1C-C2C	-4.32	1.38	1.45
28	iD	1003	PUB	C1C-C2C	-4.32	1.38	1.45
28	iG	1002	PUB	C1C-C2C	-4.32	1.38	1.45
28	l6	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	e7	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	lv	202	PUB	C1C-C2C	-4.32	1.38	1.45
28	f2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	F3	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	V4	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	bn	202	PUB	C1C-C2C	-4.32	1.38	1.45
28	dx	407	PUB	C1C-C2C	-4.32	1.38	1.45
28	D2	304	PUB	C1C-C2C	-4.32	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d3	303	PUB	C1C-C2C	-4.32	1.38	1.45
28	r9	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	az	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	l2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	L3	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	l7	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	aY	404	PUB	C1C-C2C	-4.32	1.38	1.45
28	kT	1003	PUB	C1C-C2C	-4.32	1.38	1.45
28	F2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	n4	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	c8	304	PUB	C1C-C2C	-4.32	1.38	1.45
28	X2	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	f3	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	c8	305	PUB	C1C-C2C	-4.32	1.38	1.45
28	c9	304	PUB	C1C-C2C	-4.32	1.38	1.45
28	eZ	403	PUB	C1C-C2C	-4.32	1.38	1.45
28	lr	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	N6	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	z6	203	PUB	C1C-C2C	-4.32	1.38	1.45
28	b8	1005	PUB	C1C-C2C	-4.32	1.38	1.45
28	b9	406	PUB	C1C-C2C	-4.32	1.38	1.45
28	U8	1006	PUB	C1C-C2C	-4.32	1.38	1.45
28	P2	203	PUB	C1C-C2C	-4.32	1.38	1.45
29	ey	1004	PVN	C31-C3	4.32	1.60	1.51
28	Z9	1005	PUB	C1C-C2C	-4.32	1.38	1.45
28	b7	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	C8	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	gz	306	PUB	C1C-C2C	-4.31	1.38	1.45
28	cp	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	ff	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	kX	1003	PUB	C1C-C2C	-4.31	1.38	1.45
28	A8	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	F9	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	ez	1006	PUB	C1C-C2C	-4.31	1.38	1.45
28	ly	406	PUB	C1C-C2C	-4.31	1.38	1.45
28	lz	405	PUB	C1C-C2C	-4.31	1.38	1.45
28	D3	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	Y5	1006	PUB	C1C-C2C	-4.31	1.38	1.45
28	el	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	T4	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	Z7	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	J6	203	PUB	C1C-C2C	-4.31	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a6	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	aZ	304	PUB	C1C-C2C	-4.31	1.38	1.45
28	co	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	cF	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	bN	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	eg	203	PUB	C1C-C2C	-4.31	1.38	1.45
29	D2	303	PVN	C3-C2	4.31	1.39	1.34
29	d3	302	PVN	C3-C2	4.31	1.39	1.34
28	x2	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	X3	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	a3	1005	PUB	C1C-C2C	-4.31	1.38	1.45
28	V5	203	PUB	C1C-C2C	-4.31	1.38	1.45
28	p5	202	PUB	C1C-C2C	-4.31	1.38	1.45
28	d9	305	PUB	C1C-C2C	-4.31	1.38	1.45
28	dx	406	PUB	C1C-C2C	-4.31	1.38	1.45
28	c6	1004	PUB	C1C-C2C	-4.31	1.38	1.45
28	b8	1006	PUB	C1C-C2C	-4.30	1.38	1.45
28	H4	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	gy	306	PUB	C1C-C2C	-4.30	1.38	1.45
28	H2	202	PUB	C1C-C2C	-4.30	1.38	1.45
28	g8	202	PUB	C1C-C2C	-4.30	1.38	1.45
28	bs	1004	PUB	C1C-C2C	-4.30	1.38	1.45
28	ge	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	iH	1002	PUB	C1C-C2C	-4.30	1.38	1.45
28	O8	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	cR	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	eJ	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	gg	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	jL	1003	PUB	C1C-C2C	-4.30	1.38	1.45
28	fs	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	e6	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	N7	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	cq	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	kV	1003	PUB	C1C-C2C	-4.30	1.38	1.45
28	aZ	305	PUB	C1C-C2C	-4.30	1.38	1.45
28	cr	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	n5	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	av	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	eN	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	bo	202	PUB	C1C-C2C	-4.30	1.38	1.45
28	fa	202	PUB	C1C-C2C	-4.30	1.38	1.45
28	fy	202	PUB	C1C-C2C	-4.30	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n2	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	fi	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	p3	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	p6	203	PUB	C1C-C2C	-4.30	1.38	1.45
28	e8	305	PUB	C1C-C2C	-4.29	1.38	1.45
28	bV	203	PUB	C1C-C2C	-4.29	1.38	1.45
27	M1	1001	CYC	C3B-C2B	4.29	1.45	1.36
28	bH	203	PUB	C1C-C2C	-4.29	1.38	1.45
28	r3	203	PUB	C1C-C2C	-4.29	1.38	1.45
28	J3	203	PUB	C1C-C2C	-4.29	1.38	1.45
28	aB	203	PUB	C1C-C2C	-4.29	1.38	1.45
28	dd	203	PUB	C1C-C2C	-4.29	1.38	1.45
27	h1	201	CYC	C3B-C2B	4.29	1.45	1.36
28	cY	203	PUB	C1C-C2C	-4.29	1.38	1.45
28	B5	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	r4	202	PUB	C1C-C2C	-4.28	1.38	1.45
28	v4	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	v5	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	dD	203	PUB	C1C-C2C	-4.28	1.38	1.45
27	J1	201	CYC	C3B-C2B	4.28	1.45	1.36
27	Y1	201	CYC	C3B-C2B	4.28	1.45	1.36
28	Z2	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	cP	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	Q8	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	z2	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	n8	202	PUB	C1C-C2C	-4.28	1.38	1.45
27	S1	202	CYC	C3B-C2B	4.28	1.45	1.36
28	dL	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	hH	203	PUB	C1C-C2C	-4.28	1.38	1.45
28	ar	203	PUB	C1C-C2C	-4.28	1.38	1.45
27	a2	902	CYC	C3B-C2B	4.28	1.45	1.36
27	b2	1001	CYC	C3B-C2B	4.28	1.45	1.36
28	r7	203	PUB	C1C-C2C	-4.28	1.38	1.45
29	c9	303	PVN	C4-N1	-4.27	1.39	1.45
28	fm	203	PUB	C1C-C2C	-4.27	1.38	1.45
27	z1	201	CYC	C3B-C2B	4.27	1.45	1.36
27	c1	201	CYC	C3B-C2B	4.27	1.45	1.36
28	Y5	1005	PUB	C1C-C2C	-4.27	1.38	1.45
27	a2	901	CYC	C3B-C2B	4.26	1.45	1.36
27	H1	201	CYC	C3B-C2B	4.26	1.45	1.36
27	v1	201	CYC	C3B-C2B	4.26	1.45	1.36
27	p1	201	CYC	C3B-C2B	4.25	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	S1	201	CYC	C3B-C2B	4.25	1.45	1.36
27	j1	201	CYC	C3B-C2B	4.25	1.45	1.36
27	r1	201	CYC	C3B-C2B	4.25	1.45	1.36
27	t1	201	CYC	C3B-C2B	4.25	1.45	1.36
28	dN	203	PUB	C1C-C2C	-4.24	1.39	1.45
28	dV	203	PUB	C1C-C2C	-4.23	1.39	1.45
29	Z9	1004	PVN	C4-N1	-4.21	1.39	1.45
29	U8	1004	PVN	C4-N1	-4.20	1.39	1.45
29	ez	1004	PVN	C31-C3	4.18	1.60	1.51
29	b9	405	PVN	C4-N1	-4.16	1.39	1.45
29	eZ	402	PVN	C3-C2	4.14	1.38	1.34
29	b8	1004	PVN	C4-N1	-4.12	1.39	1.45
29	eY	403	PVN	C3-C2	4.08	1.38	1.34
27	y1	201	CYC	C1A-NA	-4.05	1.29	1.38
27	W1	201	CYC	C2C-C1C	-4.04	1.48	1.52
29	d8	303	PVN	C4-N1	-4.04	1.39	1.45
27	U1	201	CYC	C2C-C1C	-4.04	1.48	1.52
27	d2	101	CYC	C2C-C1C	-4.04	1.48	1.52
27	g1	201	CYC	C2C-C1C	-4.04	1.48	1.52
27	q1	201	CYC	C2C-C1C	-4.04	1.48	1.52
27	N1	201	CYC	C2C-C1C	-4.03	1.48	1.52
27	R1	1001	CYC	C1A-NA	-4.03	1.30	1.38
27	i1	1001	CYC	C1A-NA	-4.03	1.30	1.38
27	y1	201	CYC	C2C-C1C	-4.03	1.48	1.52
27	N1	201	CYC	C1A-NA	-4.02	1.30	1.38
27	V1	201	CYC	C1A-NA	-4.02	1.30	1.38
27	w1	201	CYC	C1A-NA	-4.02	1.30	1.38
27	R1	1001	CYC	C2C-C1C	-4.02	1.48	1.52
27	i1	1001	CYC	C2C-C1C	-4.02	1.48	1.52
27	e1	201	CYC	C2C-C1C	-4.02	1.48	1.52
27	q1	201	CYC	C1A-NA	-4.02	1.30	1.38
29	eZ	402	PVN	C4-N1	-4.01	1.39	1.45
27	I1	201	CYC	C1A-NA	-4.01	1.30	1.38
27	o1	1001	CYC	C1A-NA	-4.01	1.30	1.38
29	d9	304	PVN	C4-N1	-4.01	1.39	1.45
27	V1	201	CYC	C2C-C1C	-4.01	1.48	1.52
27	U1	201	CYC	C1A-NA	-4.00	1.30	1.38
27	d1	1001	CYC	C1A-NA	-4.00	1.30	1.38
27	d2	101	CYC	C1A-NA	-4.00	1.30	1.38
27	Q1	201	CYC	C2C-C1C	-4.00	1.48	1.52
27	X1	201	CYC	C1A-NA	-4.00	1.30	1.38
27	L1	201	CYC	C1A-NA	-4.00	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a1	201	CYC	C1A-NA	-4.00	1.30	1.38
27	k1	201	CYC	C1A-NA	-4.00	1.30	1.38
27	G1	1001	CYC	C1A-NA	-4.00	1.30	1.38
27	b1	1001	CYC	C1A-NA	-4.00	1.30	1.38
27	n1	201	CYC	C1A-NA	-4.00	1.30	1.38
27	s1	201	CYC	C1A-NA	-4.00	1.30	1.38
27	u1	1001	CYC	C1A-NA	-4.00	1.30	1.38
27	L1	201	CYC	C2C-C1C	-3.99	1.48	1.52
27	a1	201	CYC	C2C-C1C	-3.99	1.48	1.52
27	f1	201	CYC	C1A-NA	-3.99	1.30	1.38
27	Q1	201	CYC	C1A-NA	-3.99	1.30	1.38
27	W1	201	CYC	C1A-NA	-3.99	1.30	1.38
27	g1	201	CYC	C1A-NA	-3.99	1.30	1.38
29	eY	403	PVN	C4-N1	-3.99	1.39	1.45
27	Z1	201	CYC	C1A-NA	-3.99	1.30	1.38
27	Z1	201	CYC	C2C-C1C	-3.99	1.48	1.52
27	m1	201	CYC	C1A-NA	-3.99	1.30	1.38
27	e1	201	CYC	C1A-NA	-3.98	1.30	1.38
27	n1	201	CYC	C2C-C1C	-3.98	1.48	1.52
27	u1	1001	CYC	C2C-C1C	-3.98	1.48	1.52
27	b1	1001	CYC	C2C-C1C	-3.98	1.48	1.52
27	O1	201	CYC	C1A-NA	-3.98	1.30	1.38
27	s1	201	CYC	C2C-C1C	-3.98	1.48	1.52
27	O1	201	CYC	C2C-C1C	-3.97	1.48	1.52
27	P1	201	CYC	C1A-NA	-3.97	1.30	1.38
27	K1	201	CYC	C1A-NA	-3.97	1.30	1.38
27	P1	201	CYC	C2C-C1C	-3.96	1.48	1.52
26	bP	202	PEB	C2A-C1A	-3.95	1.48	1.52
27	G1	1001	CYC	C2C-C1C	-3.95	1.48	1.52
27	I1	201	CYC	C2C-C1C	-3.95	1.48	1.52
29	e9	304	PVN	C4-N1	-3.95	1.39	1.45
29	bY	1004	PVN	C4-N1	-3.94	1.39	1.45
27	X1	201	CYC	C2C-C1C	-3.94	1.48	1.52
29	e8	303	PVN	C4-N1	-3.93	1.39	1.45
27	k1	201	CYC	C2C-C1C	-3.93	1.48	1.52
26	cr	202	PEB	C2A-C1A	-3.93	1.48	1.52
27	m1	201	CYC	C2C-C1C	-3.91	1.48	1.52
26	N7	202	PEB	C2A-C1A	-3.90	1.48	1.52
27	f1	201	CYC	C2C-C1C	-3.90	1.48	1.52
27	w1	201	CYC	C2C-C1C	-3.90	1.48	1.52
26	h3	201	PEB	C2A-C1A	-3.89	1.48	1.52
26	n7	202	PEB	C2A-C1A	-3.89	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r7	202	PEB	C2A-C1A	-3.88	1.48	1.52
29	c8	303	PVN	C31-C3	3.88	1.59	1.51
29	c9	303	PVN	C31-C3	3.88	1.59	1.51
26	r5	202	PEB	C2A-C1A	-3.88	1.48	1.52
26	cz	202	PEB	C2A-C1A	-3.88	1.48	1.52
29	aY	403	PVN	C4-N1	-3.88	1.39	1.45
27	K1	201	CYC	C2C-C1C	-3.88	1.48	1.52
26	e7	202	PEB	C2A-C1A	-3.87	1.48	1.52
26	cd	202	PEB	C2A-C1A	-3.87	1.48	1.52
27	d1	1001	CYC	C2C-C1C	-3.87	1.48	1.52
26	R6	202	PEB	C2A-C1A	-3.87	1.48	1.52
26	P7	202	PEB	C2A-C1A	-3.87	1.48	1.52
29	gz	304	PVN	C7-C6	-3.87	1.35	1.42
26	B4	202	PEB	C2A-C1A	-3.87	1.48	1.52
26	a7	202	PEB	C2A-C1A	-3.87	1.48	1.52
29	Z5	304	PVN	C3-C2	3.87	1.38	1.34
26	lh	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	ep	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	cl	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	bJ	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	kV	1002	PEB	C2A-C1A	-3.86	1.48	1.52
26	at	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	t5	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	gk	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	bF	202	PEB	C2A-C1A	-3.86	1.48	1.52
26	l7	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	cj	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	cY	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	iE	1002	PEB	C2A-C1A	-3.85	1.48	1.52
26	L9	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	jK	1002	PEB	C2A-C1A	-3.85	1.48	1.52
27	o1	1001	CYC	C2C-C1C	-3.85	1.48	1.52
26	v4	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	ev	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	J3	202	PEB	C2A-C1A	-3.85	1.48	1.52
26	p4	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	B5	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	hL	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	an	201	PEB	C2A-C1A	-3.84	1.48	1.52
26	eX	201	PEB	C2A-C1A	-3.84	1.48	1.52
26	Z3	202	PEB	C2A-C1A	-3.84	1.48	1.52
29	eZ	402	PVN	C16-C17	3.84	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F5	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	y8	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	gp	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	az	202	PEB	C2A-C1A	-3.84	1.48	1.52
26	gv	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	kT	1002	PEB	C2A-C1A	-3.83	1.48	1.52
26	T3	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	jM	1002	PEB	C2A-C1A	-3.83	1.48	1.52
26	F9	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	kS	1002	PEB	C2A-C1A	-3.83	1.48	1.52
26	hH	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	hT	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	Z2	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	fw	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	C8	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	ar	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	ec	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	gn	202	PEB	C2A-C1A	-3.83	1.48	1.52
26	Z7	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	cF	201	PEB	C2A-C1A	-3.82	1.48	1.52
26	dj	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	ei	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	B9	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	eL	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	n6	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	ap	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	hG	201	PEB	C2A-C1A	-3.82	1.48	1.52
26	p5	201	PEB	C2A-C1A	-3.82	1.48	1.52
26	V7	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	bH	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	j3	201	PEB	C2A-C1A	-3.82	1.48	1.52
29	44	303	PVN	C3-C2	3.82	1.38	1.34
26	p8	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	iC	1002	PEB	C2A-C1A	-3.82	1.48	1.52
26	cB	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	ee	202	PEB	C2A-C1A	-3.82	1.48	1.52
26	kX	1002	PEB	C2A-C1A	-3.82	1.48	1.52
26	F7	201	PEB	C2A-C1A	-3.81	1.48	1.52
29	eY	403	PVN	C16-C17	3.81	1.52	1.45
26	gd	201	PEB	C2A-C1A	-3.81	1.48	1.52
26	g5	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	T9	202	PEB	C2A-C1A	-3.81	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hP	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	l2	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	N3	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	v9	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	av	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	f2	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	F3	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	R7	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	v7	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	L2	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	V3	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	J7	201	PEB	C2A-C1A	-3.81	1.48	1.52
26	lw	203	PEB	C2A-C1A	-3.81	1.48	1.52
26	ge	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	V2	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	R3	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	fi	202	PEB	C2A-C1A	-3.81	1.48	1.52
26	kU	1002	PEB	C2A-C1A	-3.81	1.48	1.52
26	T7	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	al	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	N5	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	H7	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	bN	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	fg	201	PEB	C2A-C1A	-3.80	1.48	1.52
26	D7	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	P9	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	h8	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	bB	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	dY	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	et	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	D5	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	Y7	1003	PEB	C2A-C1A	-3.80	1.48	1.52
26	n2	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	P5	201	PEB	C2A-C1A	-3.80	1.48	1.52
26	dL	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	gg	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	dd	202	PEB	C2A-C1A	-3.80	1.48	1.52
26	V9	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	ch	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	cs	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	fj	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	p3	202	PEB	C2A-C1A	-3.79	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	J9	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	er	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	p7	201	PEB	C2A-C1A	-3.79	1.48	1.52
26	bT	201	PEB	C2A-C1A	-3.79	1.48	1.52
26	fc	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	L7	201	PEB	C2A-C1A	-3.79	1.48	1.52
26	aD	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	h2	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	X6	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	gr	201	PEB	C2A-C1A	-3.79	1.48	1.52
26	A5	203	PEB	C2A-C1A	-3.79	1.48	1.52
26	ad	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	ah	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	cE	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	dh	202	PEB	C2A-C1A	-3.79	1.48	1.52
26	li	203	PEB	C2A-C1A	-3.79	1.48	1.52
26	B6	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	cH	201	PEB	C2A-C1A	-3.78	1.48	1.52
26	hR	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	L3	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	fy	201	PEB	C2A-C1A	-3.78	1.48	1.52
26	hJ	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	fs	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	ga	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	34	1002	PEB	C2A-C1A	-3.78	1.48	1.52
26	J5	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	J6	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	jI	1002	PEB	C2A-C1A	-3.78	1.48	1.52
26	df	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	jO	1002	PEB	C2A-C1A	-3.78	1.48	1.52
26	A2	1003	PEB	C2A-C1A	-3.78	1.48	1.52
26	di	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	D4	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	bQ	203	PEB	C2A-C1A	-3.78	1.48	1.52
26	gi	202	PEB	C2A-C1A	-3.78	1.48	1.52
26	j4	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	R5	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	jJ	1002	PEB	C2A-C1A	-3.77	1.48	1.52
26	en	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	T2	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	lr	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	L5	202	PEB	C2A-C1A	-3.77	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B3	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	D9	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	f3	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	ld	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	ln	202	PEB	C2A-C1A	-3.77	1.48	1.52
26	ab	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	cq	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	dl	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	kQ	1002	PEB	C2A-C1A	-3.76	1.48	1.52
26	r4	201	PEB	C2A-C1A	-3.76	1.48	1.52
26	d7	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	g4	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	c7	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	eJ	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	fq	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	cb	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	V5	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	eV	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	aj	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	bV	202	PEB	C2A-C1A	-3.76	1.48	1.52
26	iD	1002	PEB	C2A-C1A	-3.76	1.48	1.52
26	jN	1002	PEB	C2A-C1A	-3.76	1.48	1.52
26	34	1001	PEB	C2A-C1A	-3.75	1.48	1.52
26	jL	1002	PEB	C2A-C1A	-3.75	1.48	1.52
26	e4	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	hV	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	y7	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	hN	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	B7	201	PEB	C2A-C1A	-3.75	1.48	1.52
26	af	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	bD	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	ea	203	PEB	C2A-C1A	-3.75	1.48	1.52
26	fu	201	PEB	C2A-C1A	-3.75	1.48	1.52
26	lf	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	H9	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	gt	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	hD	202	PEB	C2A-C1A	-3.75	1.48	1.52
26	eN	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	z3	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	R9	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	fm	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	j2	202	PEB	C2A-C1A	-3.74	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l4	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	m5	1003	PEB	C2A-C1A	-3.74	1.48	1.52
26	X7	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	v3	202	PEB	C2A-C1A	-3.74	1.48	1.52
26	ax	201	PEB	C2A-C1A	-3.73	1.48	1.52
26	lp	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	W3	203	PEB	C2A-C1A	-3.73	1.48	1.52
26	kW	1002	PEB	C2A-C1A	-3.73	1.48	1.52
26	eB	203	PEB	C2A-C1A	-3.73	1.48	1.52
26	gx	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	n4	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	n5	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	D3	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	N9	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	n8	201	PEB	C2A-C1A	-3.73	1.48	1.52
26	cL	202	PEB	C2A-C1A	-3.73	1.48	1.52
26	cJ	202	PEB	C2A-C1A	-3.72	1.48	1.52
26	eg	202	PEB	C2A-C1A	-3.72	1.48	1.52
29	Y9	303	PVN	C31-C3	3.72	1.59	1.51
26	X2	202	PEB	C2A-C1A	-3.72	1.48	1.52
26	hB	202	PEB	C2A-C1A	-3.72	1.48	1.52
26	p2	202	PEB	C2A-C1A	-3.72	1.48	1.52
26	lo	203	PEB	C2A-C1A	-3.72	1.48	1.52
26	jP	1002	PEB	C2A-C1A	-3.72	1.48	1.52
26	n3	202	PEB	C2A-C1A	-3.72	1.48	1.52
29	D2	303	PVN	C31-C3	3.72	1.59	1.51
29	d3	302	PVN	C31-C3	3.72	1.59	1.51
26	i3	203	PEB	C2A-C1A	-3.72	1.48	1.52
26	hX	202	PEB	C2A-C1A	-3.72	1.48	1.52
26	H3	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	t3	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	x7	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	cn	201	PEB	C2A-C1A	-3.71	1.48	1.52
26	fo	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	P3	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	z7	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	kR	1002	PEB	C2A-C1A	-3.71	1.48	1.52
26	x3	202	PEB	C2A-C1A	-3.71	1.48	1.52
26	cf	201	PEB	C2A-C1A	-3.71	1.48	1.52
26	cp	202	PEB	C2A-C1A	-3.71	1.48	1.52
29	T8	303	PVN	C31-C3	3.71	1.59	1.51
26	aF	202	PEB	C2A-C1A	-3.71	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H2	201	PEB	C2A-C1A	-3.70	1.48	1.52
26	S5	203	PEB	C2A-C1A	-3.70	1.48	1.52
26	A1	301	PEB	C2A-C1A	-3.70	1.48	1.52
26	B1	301	PEB	C2A-C1A	-3.70	1.48	1.52
29	bY	1004	PVN	C14-C13	-3.70	1.37	1.45
26	co	201	PEB	C2A-C1A	-3.69	1.48	1.52
26	v5	202	PEB	C2A-C1A	-3.69	1.48	1.52
26	ff	202	PEB	C2A-C1A	-3.69	1.48	1.52
26	t7	202	PEB	C2A-C1A	-3.69	1.48	1.52
26	el	202	PEB	C2A-C1A	-3.68	1.48	1.52
26	z5	202	PEB	C2A-C1A	-3.68	1.48	1.52
26	dV	202	PEB	C2A-C1A	-3.68	1.48	1.52
29	aY	403	PVN	C14-C13	-3.67	1.37	1.45
26	bL	202	PEB	C2A-C1A	-3.67	1.48	1.52
26	ll	202	PEB	C2A-C1A	-3.67	1.48	1.52
26	r3	202	PEB	C2A-C1A	-3.65	1.48	1.52
29	lz	403	PVN	C31-C3	3.64	1.59	1.51
29	ly	404	PVN	C31-C3	3.63	1.59	1.51
29	C2	303	PVN	C31-C3	3.58	1.59	1.51
29	c3	303	PVN	C31-C3	3.58	1.59	1.51
29	e8	303	PVN	C31-C3	3.57	1.59	1.51
29	e9	304	PVN	C31-C3	3.57	1.59	1.51
29	dx	405	PVN	C31-C3	3.57	1.59	1.51
29	bZ	304	PVN	C3-C2	3.55	1.38	1.34
27	t1	201	CYC	C4A-C3A	3.54	1.53	1.45
29	eY	403	PVN	C31-C3	3.53	1.58	1.51
27	H1	201	CYC	C4A-C3A	3.53	1.53	1.45
29	Y9	303	PVN	C3-C2	3.53	1.38	1.34
26	dO	201	PEB	C4D-ND	3.52	1.39	1.35
29	gy	304	PVN	C9-C10	3.52	1.54	1.41
27	h1	201	CYC	C4A-C3A	3.51	1.53	1.45
29	eZ	402	PVN	C31-C3	3.51	1.58	1.51
27	M1	1001	CYC	C4A-C3A	3.51	1.53	1.45
26	cj	201	PEB	C4D-ND	3.50	1.39	1.35
27	S1	202	CYC	C4A-C3A	3.50	1.53	1.45
29	gy	304	PVN	C16-C17	-3.50	1.38	1.45
27	v1	201	CYC	C4A-C3A	3.50	1.53	1.45
27	a2	901	CYC	C1B-NB	-3.50	1.31	1.37
26	Q3	201	PEB	C4D-ND	3.50	1.39	1.35
27	v1	201	CYC	C1B-NB	-3.50	1.32	1.37
26	H7	201	PEB	C4D-ND	3.50	1.39	1.35
27	J1	201	CYC	C4A-C3A	3.50	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y1	201	CYC	C4A-C3A	3.50	1.53	1.45
26	V7	201	PEB	C4D-ND	3.50	1.39	1.35
27	S1	201	CYC	C4A-C3A	3.49	1.53	1.45
27	j1	201	CYC	C4A-C3A	3.49	1.53	1.45
27	p1	201	CYC	C1B-NB	-3.49	1.32	1.37
27	H1	201	CYC	C1B-NB	-3.49	1.32	1.37
27	a2	901	CYC	C4A-C3A	3.49	1.53	1.45
27	c1	201	CYC	C4A-C3A	3.49	1.53	1.45
26	R9	201	PEB	C4D-ND	3.49	1.39	1.35
29	aZ	303	PVN	C3-C2	3.49	1.38	1.34
26	G4	201	PEB	C4D-ND	3.48	1.39	1.35
27	c1	201	CYC	C1B-NB	-3.48	1.32	1.37
27	M1	1001	CYC	C1B-NB	-3.48	1.32	1.37
27	z1	201	CYC	C4A-C3A	3.48	1.53	1.45
26	eV	201	PEB	C4D-ND	3.48	1.39	1.35
26	l7	201	PEB	C4D-ND	3.48	1.39	1.35
26	X9	401	PEB	C4D-ND	3.48	1.39	1.35
26	dU	201	PEB	C4D-ND	3.48	1.39	1.35
29	34	1004	PVN	C7-C6	-3.48	1.36	1.42
26	G3	201	PEB	C4D-ND	3.48	1.39	1.35
27	a2	902	CYC	C1B-NB	-3.48	1.32	1.37
27	b2	1001	CYC	C1B-NB	-3.48	1.32	1.37
26	n4	201	PEB	C4D-ND	3.48	1.39	1.35
26	cK	201	PEB	C4D-ND	3.48	1.39	1.35
26	x8	202	PEB	C4D-ND	3.47	1.39	1.35
26	ar	201	PEB	C4D-ND	3.47	1.39	1.35
27	r1	201	CYC	C1B-NB	-3.47	1.32	1.37
26	ap	201	PEB	C4D-ND	3.47	1.39	1.35
26	kQ	1001	PEB	C4D-ND	3.47	1.39	1.35
27	a2	902	CYC	C4A-C3A	3.47	1.53	1.45
27	b2	1001	CYC	C4A-C3A	3.47	1.53	1.45
26	l8	201	PEB	C4D-ND	3.47	1.39	1.35
26	ab	201	PEB	C4D-ND	3.47	1.39	1.35
26	eu	201	PEB	C4D-ND	3.47	1.39	1.35
29	c3	303	PVN	C19-C18	-3.47	1.41	1.48
26	a9	602	PEB	C4D-ND	3.47	1.39	1.35
26	eq	202	PEB	C4D-ND	3.47	1.39	1.35
26	iB	1001	PEB	C4D-ND	3.47	1.39	1.35
27	J1	201	CYC	C1B-NB	-3.47	1.32	1.37
27	Y1	201	CYC	C1B-NB	-3.47	1.32	1.37
27	r1	201	CYC	C4A-C3A	3.47	1.53	1.45
29	T8	303	PVN	C3-C2	3.47	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	am	1001	PEB	C4D-ND	3.47	1.39	1.35
26	Z3	201	PEB	C4D-ND	3.46	1.39	1.35
26	w5	201	PEB	C4D-ND	3.46	1.39	1.35
26	K7	201	PEB	C4D-ND	3.46	1.39	1.35
26	i7	201	PEB	C4D-ND	3.46	1.39	1.35
26	dR	202	PEB	C4D-ND	3.46	1.39	1.35
29	U8	1004	PVN	C14-C13	-3.46	1.38	1.45
26	u7	201	PEB	C4D-ND	3.46	1.39	1.35
26	aW	301	PEB	C4D-ND	3.46	1.39	1.35
26	eU	201	PEB	C4D-ND	3.46	1.39	1.35
27	t1	201	CYC	C1B-NB	-3.46	1.32	1.37
26	x8	201	PEB	C4D-ND	3.46	1.39	1.35
26	ll	201	PEB	C4D-ND	3.46	1.39	1.35
26	cR	201	PEB	C4D-ND	3.46	1.39	1.35
26	y3	201	PEB	C4D-ND	3.46	1.39	1.35
26	b9	401	PEB	C4D-ND	3.46	1.39	1.35
26	x9	202	PEB	C4D-ND	3.46	1.39	1.35
26	R7	201	PEB	C4D-ND	3.46	1.39	1.35
26	o4	202	PEB	C4D-ND	3.46	1.39	1.35
26	Z9	1003	PEB	C4D-ND	3.46	1.39	1.35
27	p1	201	CYC	C4A-C3A	3.46	1.53	1.45
26	ey	1002	PEB	C4D-ND	3.46	1.39	1.35
26	ff	204	PEB	C4D-ND	3.46	1.39	1.35
26	W7	201	PEB	C4D-ND	3.45	1.39	1.35
26	dO	202	PEB	C4D-ND	3.45	1.39	1.35
26	lb	202	PEB	C4D-ND	3.45	1.39	1.35
29	U8	1004	PVN	C31-C3	3.45	1.58	1.51
26	l3	201	PEB	C4D-ND	3.45	1.39	1.35
26	cW	202	PEB	C4D-ND	3.45	1.39	1.35
26	j5	202	PEB	C4D-ND	3.45	1.39	1.35
26	jN	1001	PEB	C4D-ND	3.45	1.39	1.35
29	Z9	1004	PVN	C14-C13	-3.45	1.38	1.45
26	I2	202	PEB	C4D-ND	3.45	1.39	1.35
26	N4	201	PEB	C4D-ND	3.45	1.39	1.35
26	P4	202	PEB	C4D-ND	3.45	1.39	1.35
26	Q8	201	PEB	C4D-ND	3.45	1.39	1.35
26	B9	201	PEB	C4D-ND	3.45	1.39	1.35
26	a7	201	PEB	C4D-ND	3.45	1.39	1.35
26	bx	201	PEB	C4D-ND	3.45	1.39	1.35
26	hL	201	PEB	C4D-ND	3.45	1.39	1.35
26	U4	201	PEB	C4D-ND	3.45	1.39	1.35
26	n5	201	PEB	C4D-ND	3.45	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	V6	201	PEB	C4D-ND	3.45	1.39	1.35
26	ey	1003	PEB	C4D-ND	3.45	1.39	1.35
26	S4	201	PEB	C4D-ND	3.45	1.39	1.35
26	f7	201	PEB	C4D-ND	3.45	1.39	1.35
26	b9	404	PEB	C4D-ND	3.45	1.39	1.35
26	ai	201	PEB	C4D-ND	3.45	1.39	1.35
26	bA	201	PEB	C4D-ND	3.45	1.39	1.35
26	bZ	301	PEB	C4D-ND	3.45	1.39	1.35
26	M4	201	PEB	C4D-ND	3.45	1.39	1.35
26	aI	202	PEB	C4D-ND	3.45	1.39	1.35
26	g2	201	PEB	C4D-ND	3.45	1.39	1.35
26	av	201	PEB	C4D-ND	3.45	1.39	1.35
26	eP	202	PEB	C4D-ND	3.45	1.39	1.35
26	G2	202	PEB	C4D-ND	3.45	1.39	1.35
26	s6	202	PEB	C4D-ND	3.45	1.39	1.35
26	aN	204	PEB	C4D-ND	3.45	1.39	1.35
26	bw	201	PEB	C4D-ND	3.45	1.39	1.35
26	dl	201	PEB	C4D-ND	3.45	1.39	1.35
26	eM	1002	PEB	C4D-ND	3.45	1.39	1.35
26	gc	201	PEB	C4D-ND	3.45	1.39	1.35
26	D3	201	PEB	C4D-ND	3.44	1.39	1.35
26	H6	202	PEB	C4D-ND	3.44	1.39	1.35
26	v8	202	PEB	C4D-ND	3.44	1.39	1.35
26	B8	201	PEB	C4D-ND	3.44	1.39	1.35
26	G9	201	PEB	C4D-ND	3.44	1.39	1.35
26	I5	201	PEB	C4D-ND	3.44	1.39	1.35
26	eO	202	PEB	C4D-ND	3.44	1.39	1.35
26	lu	201	PEB	C4D-ND	3.44	1.39	1.35
27	S1	201	CYC	C1B-NB	-3.44	1.32	1.37
27	j1	201	CYC	C1B-NB	-3.44	1.32	1.37
26	v4	201	PEB	C4D-ND	3.44	1.39	1.35
26	k6	1002	PEB	C4D-ND	3.44	1.39	1.35
26	u6	201	PEB	C4D-ND	3.44	1.39	1.35
26	F8	1002	PEB	C4D-ND	3.44	1.39	1.35
26	aC	202	PEB	C4D-ND	3.44	1.39	1.35
26	h2	201	PEB	C4D-ND	3.44	1.39	1.35
26	y2	201	PEB	C4D-ND	3.44	1.39	1.35
26	E6	202	PEB	C4D-ND	3.44	1.39	1.35
26	D2	301	PEB	C4D-ND	3.44	1.39	1.35
26	o7	201	PEB	C4D-ND	3.44	1.39	1.35
26	G8	202	PEB	C4D-ND	3.44	1.39	1.35
26	gk	201	PEB	C4D-ND	3.44	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b9	405	PVN	C31-C3	3.44	1.58	1.51
26	R3	201	PEB	C4D-ND	3.44	1.39	1.35
26	f4	201	PEB	C4D-ND	3.44	1.39	1.35
26	da	1001	PEB	C4D-ND	3.44	1.39	1.35
26	u9	201	PEB	C4D-ND	3.44	1.39	1.35
26	aB	202	PEB	C4D-ND	3.44	1.39	1.35
26	e3	1001	PEB	C4D-ND	3.44	1.39	1.35
26	U5	201	PEB	C4D-ND	3.44	1.39	1.35
26	x7	201	PEB	C4D-ND	3.44	1.39	1.35
26	w9	201	PEB	C4D-ND	3.44	1.39	1.35
26	cU	201	PEB	C4D-ND	3.44	1.39	1.35
26	J3	201	PEB	C4D-ND	3.44	1.39	1.35
26	c6	1003	PEB	C4D-ND	3.44	1.39	1.35
26	d6	201	PEB	C4D-ND	3.44	1.39	1.35
26	gn	201	PEB	C4D-ND	3.44	1.39	1.35
26	gx	201	PEB	C4D-ND	3.44	1.39	1.35
26	iD	1001	PEB	C4D-ND	3.44	1.39	1.35
26	iE	1001	PEB	C4D-ND	3.44	1.39	1.35
26	iF	1001	PEB	C4D-ND	3.44	1.39	1.35
26	t5	201	PEB	C4D-ND	3.44	1.39	1.35
26	c9	301	PEB	C4D-ND	3.44	1.39	1.35
26	h9	202	PEB	C4D-ND	3.44	1.39	1.35
26	hT	201	PEB	C4D-ND	3.44	1.39	1.35
26	k5	201	PEB	C4D-ND	3.44	1.39	1.35
26	dp	201	PEB	C4D-ND	3.44	1.39	1.35
26	dC	202	PEB	C4D-ND	3.44	1.39	1.35
26	dI	1001	PEB	C4D-ND	3.44	1.39	1.35
26	ej	202	PEB	C4D-ND	3.44	1.39	1.35
26	E2	1001	PEB	C4D-ND	3.44	1.39	1.35
26	S4	202	PEB	C4D-ND	3.44	1.39	1.35
26	cD	201	PEB	C4D-ND	3.44	1.39	1.35
26	S3	203	PEB	C4D-ND	3.44	1.39	1.35
26	V4	201	PEB	C4D-ND	3.44	1.39	1.35
26	q4	201	PEB	C4D-ND	3.44	1.39	1.35
26	es	201	PEB	C4D-ND	3.44	1.39	1.35
26	lz	401	PEB	C4D-ND	3.44	1.39	1.35
26	gg	201	PEB	C4D-ND	3.44	1.39	1.35
26	P3	201	PEB	C4D-ND	3.43	1.39	1.35
26	dJ	201	PEB	C4D-ND	3.43	1.39	1.35
26	eh	201	PEB	C4D-ND	3.43	1.39	1.35
26	hY	401	PEB	C4D-ND	3.43	1.39	1.35
26	t4	201	PEB	C4D-ND	3.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D5	201	PEB	C4D-ND	3.43	1.39	1.35
26	E8	201	PEB	C4D-ND	3.43	1.39	1.35
26	bI	201	PEB	C4D-ND	3.43	1.39	1.35
26	gf	201	PEB	C4D-ND	3.43	1.39	1.35
29	Z9	1004	PVN	C31-C3	3.43	1.58	1.51
26	n3	201	PEB	C4D-ND	3.43	1.39	1.35
26	L4	201	PEB	C4D-ND	3.43	1.39	1.35
26	gm	1001	PEB	C4D-ND	3.43	1.39	1.35
27	h1	201	CYC	C1B-NB	-3.43	1.32	1.37
26	bq	201	PEB	C4D-ND	3.43	1.39	1.35
26	bK	1001	PEB	C4D-ND	3.43	1.39	1.35
26	dS	201	PEB	C4D-ND	3.43	1.39	1.35
26	ly	402	PEB	C4D-ND	3.43	1.39	1.35
26	ge	201	PEB	C4D-ND	3.43	1.39	1.35
26	gz	301	PEB	C4D-ND	3.43	1.39	1.35
26	F8	1001	PEB	C4D-ND	3.43	1.39	1.35
26	jP	1001	PEB	C4D-ND	3.43	1.39	1.35
26	m8	202	PEB	C4D-ND	3.43	1.39	1.35
26	L8	201	PEB	C4D-ND	3.43	1.39	1.35
26	aZ	302	PEB	C4D-ND	3.43	1.39	1.35
26	bZ	303	PEB	C4D-ND	3.43	1.39	1.35
26	Y4	202	PEB	C4D-ND	3.43	1.39	1.35
26	a6	201	PEB	C4D-ND	3.43	1.39	1.35
26	b6	202	PEB	C4D-ND	3.43	1.39	1.35
26	E7	201	PEB	C4D-ND	3.43	1.39	1.35
26	hD	201	PEB	C4D-ND	3.43	1.39	1.35
27	z1	201	CYC	C1B-NB	-3.43	1.32	1.37
26	O3	1001	PEB	C4D-ND	3.43	1.39	1.35
26	a3	1001	PEB	C4D-ND	3.43	1.39	1.35
26	u4	202	PEB	C4D-ND	3.43	1.39	1.35
26	s5	201	PEB	C4D-ND	3.43	1.39	1.35
26	d8	302	PEB	C4D-ND	3.43	1.39	1.35
26	de	201	PEB	C4D-ND	3.43	1.39	1.35
26	ef	201	PEB	C4D-ND	3.43	1.39	1.35
26	fc	201	PEB	C4D-ND	3.43	1.39	1.35
26	T5	201	PEB	C4D-ND	3.43	1.39	1.35
26	H8	202	PEB	C4D-ND	3.43	1.39	1.35
26	br	201	PEB	C4D-ND	3.43	1.39	1.35
26	cr	201	PEB	C4D-ND	3.43	1.39	1.35
26	m2	201	PEB	C4D-ND	3.43	1.39	1.35
26	C7	201	PEB	C4D-ND	3.43	1.39	1.35
26	K9	1001	PEB	C4D-ND	3.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cy	1001	PEB	C4D-ND	3.43	1.39	1.35
26	eC	201	PEB	C4D-ND	3.43	1.39	1.35
26	hJ	201	PEB	C4D-ND	3.43	1.39	1.35
29	C2	303	PVN	C19-C18	-3.43	1.41	1.48
26	z2	202	PEB	C4D-ND	3.43	1.39	1.35
26	J2	201	PEB	C4D-ND	3.43	1.39	1.35
26	H3	201	PEB	C4D-ND	3.43	1.39	1.35
26	P7	201	PEB	C4D-ND	3.43	1.39	1.35
26	J8	202	PEB	C4D-ND	3.43	1.39	1.35
26	bm	1002	PEB	C4D-ND	3.43	1.39	1.35
26	bM	201	PEB	C4D-ND	3.43	1.39	1.35
26	eQ	202	PEB	C4D-ND	3.43	1.39	1.35
26	R4	202	PEB	C4D-ND	3.43	1.39	1.35
26	W8	201	PEB	C4D-ND	3.43	1.39	1.35
26	k9	201	PEB	C4D-ND	3.43	1.39	1.35
26	ci	201	PEB	C4D-ND	3.43	1.39	1.35
26	ed	201	PEB	C4D-ND	3.43	1.39	1.35
26	lq	201	PEB	C4D-ND	3.43	1.39	1.35
26	ft	201	PEB	C4D-ND	3.43	1.39	1.35
26	m3	201	PEB	C4D-ND	3.43	1.39	1.35
26	jJ	1001	PEB	C4D-ND	3.43	1.39	1.35
26	s2	202	PEB	C4D-ND	3.43	1.39	1.35
26	B4	201	PEB	C4D-ND	3.43	1.39	1.35
26	L4	202	PEB	C4D-ND	3.43	1.39	1.35
26	k8	202	PEB	C4D-ND	3.43	1.39	1.35
26	R6	201	PEB	C4D-ND	3.43	1.39	1.35
26	z9	202	PEB	C4D-ND	3.43	1.39	1.35
26	bv	202	PEB	C4D-ND	3.43	1.39	1.35
26	cp	201	PEB	C4D-ND	3.43	1.39	1.35
26	cw	201	PEB	C4D-ND	3.43	1.39	1.35
26	gv	201	PEB	C4D-ND	3.43	1.39	1.35
26	kV	1001	PEB	C4D-ND	3.43	1.39	1.35
26	o2	1001	PEB	C4D-ND	3.42	1.39	1.35
26	s3	201	PEB	C4D-ND	3.42	1.39	1.35
26	x4	201	PEB	C4D-ND	3.42	1.39	1.35
26	b5	1001	PEB	C4D-ND	3.42	1.39	1.35
26	m8	201	PEB	C4D-ND	3.42	1.39	1.35
26	K6	201	PEB	C4D-ND	3.42	1.39	1.35
26	U9	201	PEB	C4D-ND	3.42	1.39	1.35
26	bd	201	PEB	C4D-ND	3.42	1.39	1.35
26	bx	202	PEB	C4D-ND	3.42	1.39	1.35
26	by	1001	PEB	C4D-ND	3.42	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bS	201	PEB	C4D-ND	3.42	1.39	1.35
26	dG	201	PEB	C4D-ND	3.42	1.39	1.35
26	ea	201	PEB	C4D-ND	3.42	1.39	1.35
26	lt	201	PEB	C4D-ND	3.42	1.39	1.35
26	fp	201	PEB	C4D-ND	3.42	1.39	1.35
29	hY	404	PVN	C7-C6	-3.42	1.36	1.42
26	v2	201	PEB	C4D-ND	3.42	1.39	1.35
26	Q9	201	PEB	C4D-ND	3.42	1.39	1.35
26	fq	201	PEB	C4D-ND	3.42	1.39	1.35
26	gy	303	PEB	C4D-ND	3.42	1.39	1.35
26	Q4	203	PEB	C4D-ND	3.42	1.39	1.35
26	T4	201	PEB	C4D-ND	3.42	1.39	1.35
26	p4	201	PEB	C4D-ND	3.42	1.39	1.35
26	e6	201	PEB	C4D-ND	3.42	1.39	1.35
26	M7	1002	PEB	C4D-ND	3.42	1.39	1.35
26	L9	201	PEB	C4D-ND	3.42	1.39	1.35
26	cN	201	PEB	C4D-ND	3.42	1.39	1.35
26	K5	1001	PEB	C4D-ND	3.42	1.39	1.35
26	b8	1002	PEB	C4D-ND	3.42	1.39	1.35
26	i9	201	PEB	C4D-ND	3.42	1.39	1.35
26	aT	202	PEB	C4D-ND	3.42	1.39	1.35
26	cV	203	PEB	C4D-ND	3.42	1.39	1.35
26	df	201	PEB	C4D-ND	3.42	1.39	1.35
26	q2	201	PEB	C4D-ND	3.42	1.39	1.35
26	j8	201	PEB	C4D-ND	3.42	1.39	1.35
26	T6	201	PEB	C4D-ND	3.42	1.39	1.35
26	r6	202	PEB	C4D-ND	3.42	1.39	1.35
26	O7	201	PEB	C4D-ND	3.42	1.39	1.35
26	d9	303	PEB	C4D-ND	3.42	1.39	1.35
26	U8	1001	PEB	C4D-ND	3.42	1.39	1.35
26	cV	202	PEB	C4D-ND	3.42	1.39	1.35
26	dj	201	PEB	C4D-ND	3.42	1.39	1.35
26	dA	201	PEB	C4D-ND	3.42	1.39	1.35
26	Q5	201	PEB	C4D-ND	3.42	1.39	1.35
26	y8	201	PEB	C4D-ND	3.42	1.39	1.35
26	N8	201	PEB	C4D-ND	3.42	1.39	1.35
26	cS	202	PEB	C4D-ND	3.42	1.39	1.35
26	dk	1002	PEB	C4D-ND	3.42	1.39	1.35
26	eF	202	PEB	C4D-ND	3.42	1.39	1.35
26	eK	202	PEB	C4D-ND	3.42	1.39	1.35
26	eP	203	PEB	C4D-ND	3.42	1.39	1.35
26	lq	202	PEB	C4D-ND	3.42	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	hZ	403	PVN	C7-C6	-3.42	1.36	1.42
26	m6	201	PEB	C4D-ND	3.42	1.39	1.35
26	x6	202	PEB	C4D-ND	3.42	1.39	1.35
26	U7	201	PEB	C4D-ND	3.42	1.39	1.35
26	Q8	202	PEB	C4D-ND	3.42	1.39	1.35
26	U8	1002	PEB	C4D-ND	3.42	1.39	1.35
26	aV	201	PEB	C4D-ND	3.42	1.39	1.35
26	cE	201	PEB	C4D-ND	3.42	1.39	1.35
26	cP	201	PEB	C4D-ND	3.42	1.39	1.35
26	gq	201	PEB	C4D-ND	3.42	1.39	1.35
26	jI	1001	PEB	C4D-ND	3.42	1.39	1.35
27	S1	202	CYC	C1B-NB	-3.42	1.32	1.37
26	g2	202	PEB	C4D-ND	3.42	1.39	1.35
26	F4	202	PEB	C4D-ND	3.42	1.39	1.35
26	P6	202	PEB	C4D-ND	3.42	1.39	1.35
26	c8	302	PEB	C4D-ND	3.42	1.39	1.35
26	cR	202	PEB	C4D-ND	3.42	1.39	1.35
26	eU	202	PEB	C4D-ND	3.42	1.39	1.35
26	gs	201	PEB	C4D-ND	3.42	1.39	1.35
26	o8	202	PEB	C4D-ND	3.42	1.39	1.35
26	M7	1001	PEB	C4D-ND	3.42	1.39	1.35
26	cM	202	PEB	C4D-ND	3.42	1.39	1.35
26	du	202	PEB	C4D-ND	3.42	1.39	1.35
26	ff	201	PEB	C4D-ND	3.42	1.39	1.35
26	fo	201	PEB	C4D-ND	3.42	1.39	1.35
26	hI	201	PEB	C4D-ND	3.42	1.39	1.35
26	G2	201	PEB	C4D-ND	3.42	1.39	1.35
26	D4	201	PEB	C4D-ND	3.42	1.39	1.35
26	G5	201	PEB	C4D-ND	3.42	1.39	1.35
26	a5	201	PEB	C4D-ND	3.42	1.39	1.35
26	f8	201	PEB	C4D-ND	3.42	1.39	1.35
26	y6	202	PEB	C4D-ND	3.42	1.39	1.35
26	bt	201	PEB	C4D-ND	3.42	1.39	1.35
26	bU	201	PEB	C4D-ND	3.42	1.39	1.35
26	eD	201	PEB	C4D-ND	3.42	1.39	1.35
26	eE	202	PEB	C4D-ND	3.42	1.39	1.35
26	t4	202	PEB	C4D-ND	3.42	1.39	1.35
26	z4	202	PEB	C4D-ND	3.42	1.39	1.35
26	k8	203	PEB	C4D-ND	3.42	1.39	1.35
26	U8	1003	PEB	C4D-ND	3.42	1.39	1.35
26	f9	202	PEB	C4D-ND	3.42	1.39	1.35
26	p9	202	PEB	C4D-ND	3.42	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aC	201	PEB	C4D-ND	3.42	1.39	1.35
26	aO	201	PEB	C4D-ND	3.42	1.39	1.35
26	cW	201	PEB	C4D-ND	3.42	1.39	1.35
26	du	201	PEB	C4D-ND	3.42	1.39	1.35
26	b6	201	PEB	C4D-ND	3.42	1.39	1.35
26	r7	201	PEB	C4D-ND	3.42	1.39	1.35
26	C8	201	PEB	C4D-ND	3.42	1.39	1.35
26	I8	201	PEB	C4D-ND	3.42	1.39	1.35
26	N8	202	PEB	C4D-ND	3.42	1.39	1.35
26	q9	201	PEB	C4D-ND	3.42	1.39	1.35
26	cQ	201	PEB	C4D-ND	3.42	1.39	1.35
26	O2	201	PEB	C4D-ND	3.42	1.39	1.35
26	S6	202	PEB	C4D-ND	3.42	1.39	1.35
26	m9	1001	PEB	C4D-ND	3.42	1.39	1.35
26	aS	201	PEB	C4D-ND	3.42	1.39	1.35
29	Y5	1004	PVN	C7-C6	-3.42	1.36	1.42
26	x2	201	PEB	C4D-ND	3.42	1.39	1.35
26	P2	201	PEB	C4D-ND	3.42	1.39	1.35
26	X3	201	PEB	C4D-ND	3.42	1.39	1.35
26	Y6	201	PEB	C4D-ND	3.42	1.39	1.35
26	I8	202	PEB	C4D-ND	3.42	1.39	1.35
26	J8	201	PEB	C4D-ND	3.42	1.39	1.35
26	I9	201	PEB	C4D-ND	3.42	1.39	1.35
26	bD	201	PEB	C4D-ND	3.42	1.39	1.35
26	cT	1002	PEB	C4D-ND	3.42	1.39	1.35
26	do	202	PEB	C4D-ND	3.42	1.39	1.35
26	fd	303	PEB	C4D-ND	3.42	1.39	1.35
26	fv	201	PEB	C4D-ND	3.42	1.39	1.35
26	kW	1001	PEB	C4D-ND	3.42	1.39	1.35
26	f2	201	PEB	C4D-ND	3.41	1.39	1.35
26	e5	201	PEB	C4D-ND	3.41	1.39	1.35
26	Z6	202	PEB	C4D-ND	3.41	1.39	1.35
26	h6	201	PEB	C4D-ND	3.41	1.39	1.35
26	c7	201	PEB	C4D-ND	3.41	1.39	1.35
26	aI	201	PEB	C4D-ND	3.41	1.39	1.35
26	li	202	PEB	C4D-ND	3.41	1.39	1.35
26	kX	1001	PEB	C4D-ND	3.41	1.39	1.35
29	ly	404	PVN	C3-C2	3.41	1.38	1.34
26	I2	201	PEB	C4D-ND	3.41	1.39	1.35
26	V3	201	PEB	C4D-ND	3.41	1.39	1.35
26	N6	201	PEB	C4D-ND	3.41	1.39	1.35
26	i6	201	PEB	C4D-ND	3.41	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	q8	201	PEB	C4D-ND	3.41	1.39	1.35
26	h9	201	PEB	C4D-ND	3.41	1.39	1.35
26	r9	202	PEB	C4D-ND	3.41	1.39	1.35
26	eF	201	PEB	C4D-ND	3.41	1.39	1.35
26	eN	201	PEB	C4D-ND	3.41	1.39	1.35
26	z2	201	PEB	C4D-ND	3.41	1.39	1.35
26	w3	201	PEB	C4D-ND	3.41	1.39	1.35
26	E4	201	PEB	C4D-ND	3.41	1.39	1.35
26	K4	201	PEB	C4D-ND	3.41	1.39	1.35
26	44	301	PEB	C4D-ND	3.41	1.39	1.35
26	l4	201	PEB	C4D-ND	3.41	1.39	1.35
26	i5	201	PEB	C4D-ND	3.41	1.39	1.35
26	A8	202	PEB	C4D-ND	3.41	1.39	1.35
26	O8	201	PEB	C4D-ND	3.41	1.39	1.35
26	aE	202	PEB	C4D-ND	3.41	1.39	1.35
26	bX	401	PEB	C4D-ND	3.41	1.39	1.35
26	dY	201	PEB	C4D-ND	3.41	1.39	1.35
26	hE	1001	PEB	C4D-ND	3.41	1.39	1.35
26	I6	201	PEB	C4D-ND	3.41	1.39	1.35
26	j6	201	PEB	C4D-ND	3.41	1.39	1.35
26	l6	201	PEB	C4D-ND	3.41	1.39	1.35
26	p9	201	PEB	C4D-ND	3.41	1.39	1.35
26	x9	201	PEB	C4D-ND	3.41	1.39	1.35
26	aL	202	PEB	C4D-ND	3.41	1.39	1.35
26	aM	202	PEB	C4D-ND	3.41	1.39	1.35
26	dt	202	PEB	C4D-ND	3.41	1.39	1.35
26	dQ	201	PEB	C4D-ND	3.41	1.39	1.35
26	lf	201	PEB	C4D-ND	3.41	1.39	1.35
26	fh	1001	PEB	C4D-ND	3.41	1.39	1.35
26	jK	1001	PEB	C4D-ND	3.41	1.39	1.35
26	i2	202	PEB	C4D-ND	3.41	1.39	1.35
26	q2	202	PEB	C4D-ND	3.41	1.39	1.35
26	k3	201	PEB	C4D-ND	3.41	1.39	1.35
26	P4	201	PEB	C4D-ND	3.41	1.39	1.35
26	L5	201	PEB	C4D-ND	3.41	1.39	1.35
26	l8	202	PEB	C4D-ND	3.41	1.39	1.35
26	l9	201	PEB	C4D-ND	3.41	1.39	1.35
26	t9	201	PEB	C4D-ND	3.41	1.39	1.35
26	bd	202	PEB	C4D-ND	3.41	1.39	1.35
26	fi	201	PEB	C4D-ND	3.41	1.39	1.35
26	m4	1001	PEB	C4D-ND	3.41	1.39	1.35
26	m5	1001	PEB	C4D-ND	3.41	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h6	202	PEB	C4D-ND	3.41	1.39	1.35
26	bu	202	PEB	C4D-ND	3.41	1.39	1.35
26	dm	201	PEB	C4D-ND	3.41	1.39	1.35
26	ly	401	PEB	C4D-ND	3.41	1.39	1.35
26	fk	201	PEB	C4D-ND	3.41	1.39	1.35
26	fl	201	PEB	C4D-ND	3.41	1.39	1.35
26	v2	202	PEB	C4D-ND	3.41	1.39	1.35
26	W2	201	PEB	C4D-ND	3.41	1.39	1.35
26	b3	502	PEB	C4D-ND	3.41	1.39	1.35
26	E4	202	PEB	C4D-ND	3.41	1.39	1.35
26	h5	201	PEB	C4D-ND	3.41	1.39	1.35
26	K6	202	PEB	C4D-ND	3.41	1.39	1.35
26	D7	201	PEB	C4D-ND	3.41	1.39	1.35
26	B8	202	PEB	C4D-ND	3.41	1.39	1.35
26	T8	302	PEB	C4D-ND	3.41	1.39	1.35
26	j9	201	PEB	C4D-ND	3.41	1.39	1.35
26	Y9	302	PEB	C4D-ND	3.41	1.39	1.35
26	aj	201	PEB	C4D-ND	3.41	1.39	1.35
26	cB	201	PEB	C4D-ND	3.41	1.39	1.35
26	cU	202	PEB	C4D-ND	3.41	1.39	1.35
26	dq	201	PEB	C4D-ND	3.41	1.39	1.35
26	dw	401	PEB	C4D-ND	3.41	1.39	1.35
26	eg	201	PEB	C4D-ND	3.41	1.39	1.35
26	eS	201	PEB	C4D-ND	3.41	1.39	1.35
26	gi	201	PEB	C4D-ND	3.41	1.39	1.35
26	B2	501	PEB	C4D-ND	3.41	1.39	1.35
26	I3	201	PEB	C4D-ND	3.41	1.39	1.35
26	b3	501	PEB	C4D-ND	3.41	1.39	1.35
26	u5	201	PEB	C4D-ND	3.41	1.39	1.35
26	ag	201	PEB	C4D-ND	3.41	1.39	1.35
26	cT	1001	PEB	C4D-ND	3.41	1.39	1.35
26	ed	202	PEB	C4D-ND	3.41	1.39	1.35
26	eE	201	PEB	C4D-ND	3.41	1.39	1.35
26	lv	201	PEB	C4D-ND	3.41	1.39	1.35
26	fx	201	PEB	C4D-ND	3.41	1.39	1.35
26	hQ	201	PEB	C4D-ND	3.41	1.39	1.35
26	ak	201	PEB	C4D-ND	3.41	1.39	1.35
26	fr	201	PEB	C4D-ND	3.41	1.39	1.35
26	r2	201	PEB	C4D-ND	3.41	1.39	1.35
26	q3	1001	PEB	C4D-ND	3.41	1.39	1.35
26	u4	201	PEB	C4D-ND	3.41	1.39	1.35
26	bh	201	PEB	C4D-ND	3.41	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ch	201	PEB	C4D-ND	3.41	1.39	1.35
26	g3	201	PEB	C4D-ND	3.41	1.39	1.35
26	Q4	202	PEB	C4D-ND	3.41	1.39	1.35
26	x5	201	PEB	C4D-ND	3.41	1.39	1.35
26	U6	201	PEB	C4D-ND	3.41	1.39	1.35
26	z9	201	PEB	C4D-ND	3.41	1.39	1.35
26	az	201	PEB	C4D-ND	3.41	1.39	1.35
26	aR	202	PEB	C4D-ND	3.41	1.39	1.35
26	cv	201	PEB	C4D-ND	3.41	1.39	1.35
26	dq	202	PEB	C4D-ND	3.41	1.39	1.35
26	lm	1001	PEB	C4D-ND	3.41	1.39	1.35
26	gj	201	PEB	C4D-ND	3.41	1.39	1.35
26	C3	1001	PEB	C4D-ND	3.41	1.39	1.35
26	c4	202	PEB	C4D-ND	3.41	1.39	1.35
26	k8	201	PEB	C4D-ND	3.41	1.39	1.35
26	A6	1001	PEB	C4D-ND	3.41	1.39	1.35
26	I6	202	PEB	C4D-ND	3.41	1.39	1.35
26	p8	201	PEB	C4D-ND	3.41	1.39	1.35
26	s8	201	PEB	C4D-ND	3.41	1.39	1.35
26	H9	201	PEB	C4D-ND	3.41	1.39	1.35
26	dM	1002	PEB	C4D-ND	3.41	1.39	1.35
26	eD	202	PEB	C4D-ND	3.41	1.39	1.35
26	i3	201	PEB	C4D-ND	3.41	1.39	1.35
26	O6	201	PEB	C4D-ND	3.41	1.39	1.35
26	t7	201	PEB	C4D-ND	3.41	1.39	1.35
26	z8	201	PEB	C4D-ND	3.41	1.39	1.35
26	cO	202	PEB	C4D-ND	3.41	1.39	1.35
26	ds	201	PEB	C4D-ND	3.41	1.39	1.35
26	eC	202	PEB	C4D-ND	3.41	1.39	1.35
26	o2	1002	PEB	C4D-ND	3.40	1.39	1.35
26	M2	202	PEB	C4D-ND	3.40	1.39	1.35
26	v5	201	PEB	C4D-ND	3.40	1.39	1.35
26	t2	201	PEB	C4D-ND	3.40	1.39	1.35
26	I4	201	PEB	C4D-ND	3.40	1.39	1.35
26	d4	201	PEB	C4D-ND	3.40	1.39	1.35
26	b8	1001	PEB	C4D-ND	3.40	1.39	1.35
26	b9	402	PEB	C4D-ND	3.40	1.39	1.35
26	Y8	201	PEB	C4D-ND	3.40	1.39	1.35
26	n9	201	PEB	C4D-ND	3.40	1.39	1.35
26	ad	201	PEB	C4D-ND	3.40	1.39	1.35
26	aV	202	PEB	C4D-ND	3.40	1.39	1.35
26	dn	202	PEB	C4D-ND	3.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dK	201	PEB	C4D-ND	3.40	1.39	1.35
26	hT	204	PEB	C4D-ND	3.40	1.39	1.35
26	U3	201	PEB	C4D-ND	3.40	1.39	1.35
26	e4	201	PEB	C4D-ND	3.40	1.39	1.35
26	W5	301	PEB	C4D-ND	3.40	1.39	1.35
26	l5	202	PEB	C4D-ND	3.40	1.39	1.35
26	f8	202	PEB	C4D-ND	3.40	1.39	1.35
26	E6	201	PEB	C4D-ND	3.40	1.39	1.35
26	bH	201	PEB	C4D-ND	3.40	1.39	1.35
26	cX	202	PEB	C4D-ND	3.40	1.39	1.35
26	w2	202	PEB	C4D-ND	3.40	1.39	1.35
26	o6	202	PEB	C4D-ND	3.40	1.39	1.35
26	y6	203	PEB	C4D-ND	3.40	1.39	1.35
26	n7	201	PEB	C4D-ND	3.40	1.39	1.35
26	dr	202	PEB	C4D-ND	3.40	1.39	1.35
26	iG	1001	PEB	C4D-ND	3.40	1.39	1.35
26	kR	1001	PEB	C4D-ND	3.40	1.39	1.35
26	C4	1001	PEB	C4D-ND	3.40	1.39	1.35
26	e9	302	PEB	C4D-ND	3.40	1.39	1.35
26	z8	202	PEB	C4D-ND	3.40	1.39	1.35
26	t9	202	PEB	C4D-ND	3.40	1.39	1.35
26	aE	201	PEB	C4D-ND	3.40	1.39	1.35
26	aF	201	PEB	C4D-ND	3.40	1.39	1.35
26	aX	401	PEB	C4D-ND	3.40	1.39	1.35
26	cO	201	PEB	C4D-ND	3.40	1.39	1.35
26	dF	202	PEB	C4D-ND	3.40	1.39	1.35
26	er	201	PEB	C4D-ND	3.40	1.39	1.35
26	T8	301	PEB	C4D-ND	3.40	1.39	1.35
26	aZ	301	PEB	C4D-ND	3.40	1.39	1.35
26	dx	403	PEB	C4D-ND	3.40	1.39	1.35
26	fb	201	PEB	C4D-ND	3.40	1.39	1.35
26	ga	201	PEB	C4D-ND	3.40	1.39	1.35
26	hC	201	PEB	C4D-ND	3.40	1.39	1.35
26	hR	201	PEB	C4D-ND	3.40	1.39	1.35
26	y2	202	PEB	C4D-ND	3.40	1.39	1.35
26	C2	302	PEB	C4D-ND	3.40	1.39	1.35
26	S3	201	PEB	C4D-ND	3.40	1.39	1.35
26	c3	302	PEB	C4D-ND	3.40	1.39	1.35
26	w6	1002	PEB	C4D-ND	3.40	1.39	1.35
26	x6	201	PEB	C4D-ND	3.40	1.39	1.35
26	at	201	PEB	C4D-ND	3.40	1.39	1.35
26	cJ	201	PEB	C4D-ND	3.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dG	202	PEB	C4D-ND	3.40	1.39	1.35
26	M3	201	PEB	C4D-ND	3.40	1.39	1.35
26	A6	1002	PEB	C4D-ND	3.40	1.39	1.35
26	B6	201	PEB	C4D-ND	3.40	1.39	1.35
26	M8	202	PEB	C4D-ND	3.40	1.39	1.35
26	bY	1003	PEB	C4D-ND	3.40	1.39	1.35
26	dW	201	PEB	C4D-ND	3.40	1.39	1.35
26	fw	201	PEB	C4D-ND	3.40	1.39	1.35
26	u2	201	PEB	C4D-ND	3.40	1.39	1.35
26	aD	201	PEB	C4D-ND	3.40	1.39	1.35
26	aJ	202	PEB	C4D-ND	3.40	1.39	1.35
26	aU	202	PEB	C4D-ND	3.40	1.39	1.35
26	eJ	201	PEB	C4D-ND	3.40	1.39	1.35
26	r3	201	PEB	C4D-ND	3.40	1.39	1.35
26	i4	201	PEB	C4D-ND	3.40	1.39	1.35
26	aH	201	PEB	C4D-ND	3.40	1.39	1.35
26	aR	201	PEB	C4D-ND	3.40	1.39	1.35
26	bh	202	PEB	C4D-ND	3.40	1.39	1.35
26	bj	201	PEB	C4D-ND	3.40	1.39	1.35
26	bk	201	PEB	C4D-ND	3.40	1.39	1.35
26	bl	201	PEB	C4D-ND	3.40	1.39	1.35
26	bR	201	PEB	C4D-ND	3.40	1.39	1.35
26	cl	201	PEB	C4D-ND	3.40	1.39	1.35
26	cA	201	PEB	C4D-ND	3.40	1.39	1.35
26	dx	404	PEB	C4D-ND	3.40	1.39	1.35
29	b8	1004	PVN	C31-C3	3.40	1.58	1.51
26	F6	202	PEB	C4D-ND	3.40	1.39	1.35
26	j9	202	PEB	C4D-ND	3.40	1.39	1.35
26	o9	201	PEB	C4D-ND	3.40	1.39	1.35
26	bu	201	PEB	C4D-ND	3.40	1.39	1.35
26	ds	202	PEB	C4D-ND	3.40	1.39	1.35
26	dK	202	PEB	C4D-ND	3.40	1.39	1.35
26	lr	201	PEB	C4D-ND	3.40	1.39	1.35
26	fd	301	PEB	C4D-ND	3.40	1.39	1.35
26	J6	201	PEB	C4D-ND	3.40	1.39	1.35
26	Z8	201	PEB	C4D-ND	3.40	1.39	1.35
26	ae	201	PEB	C4D-ND	3.40	1.39	1.35
26	aw	201	PEB	C4D-ND	3.40	1.39	1.35
26	dp	202	PEB	C4D-ND	3.40	1.39	1.35
26	dt	201	PEB	C4D-ND	3.40	1.39	1.35
26	ln	201	PEB	C4D-ND	3.40	1.39	1.35
26	fj	201	PEB	C4D-ND	3.40	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z2	201	PEB	C4D-ND	3.40	1.39	1.35
26	au	201	PEB	C4D-ND	3.40	1.39	1.35
26	aS	202	PEB	C4D-ND	3.40	1.39	1.35
26	bc	201	PEB	C4D-ND	3.40	1.39	1.35
26	bs	1002	PEB	C4D-ND	3.40	1.39	1.35
26	X2	201	PEB	C4D-ND	3.40	1.39	1.35
26	A3	201	PEB	C4D-ND	3.40	1.39	1.35
26	v3	201	PEB	C4D-ND	3.40	1.39	1.35
26	W6	202	PEB	C4D-ND	3.40	1.39	1.35
26	s6	201	PEB	C4D-ND	3.40	1.39	1.35
26	q7	201	PEB	C4D-ND	3.40	1.39	1.35
26	H8	201	PEB	C4D-ND	3.40	1.39	1.35
26	N9	201	PEB	C4D-ND	3.40	1.39	1.35
26	eI	201	PEB	C4D-ND	3.40	1.39	1.35
26	L2	201	PEB	C4D-ND	3.39	1.39	1.35
26	M2	201	PEB	C4D-ND	3.39	1.39	1.35
26	W2	202	PEB	C4D-ND	3.39	1.39	1.35
26	B3	201	PEB	C4D-ND	3.39	1.39	1.35
26	W3	201	PEB	C4D-ND	3.39	1.39	1.35
26	34	1003	PEB	C4D-ND	3.39	1.39	1.35
26	j4	201	PEB	C4D-ND	3.39	1.39	1.35
26	V5	201	PEB	C4D-ND	3.39	1.39	1.35
26	j5	201	PEB	C4D-ND	3.39	1.39	1.35
26	k6	1001	PEB	C4D-ND	3.39	1.39	1.35
26	v6	201	PEB	C4D-ND	3.39	1.39	1.35
26	s7	201	PEB	C4D-ND	3.39	1.39	1.35
26	L8	202	PEB	C4D-ND	3.39	1.39	1.35
26	J9	201	PEB	C4D-ND	3.39	1.39	1.35
26	aP	202	PEB	C4D-ND	3.39	1.39	1.35
26	bP	201	PEB	C4D-ND	3.39	1.39	1.35
26	du	203	PEB	C4D-ND	3.39	1.39	1.35
26	hB	201	PEB	C4D-ND	3.39	1.39	1.35
26	hK	201	PEB	C4D-ND	3.39	1.39	1.35
26	hY	403	PEB	C4D-ND	3.39	1.39	1.35
29	lz	403	PVN	C3-C2	3.39	1.38	1.34
26	u2	202	PEB	C4D-ND	3.39	1.39	1.35
26	o3	201	PEB	C4D-ND	3.39	1.39	1.35
26	u8	201	PEB	C4D-ND	3.39	1.39	1.35
26	K8	201	PEB	C4D-ND	3.39	1.39	1.35
26	aM	201	PEB	C4D-ND	3.39	1.39	1.35
26	dz	402	PEB	C4D-ND	3.39	1.39	1.35
26	dD	202	PEB	C4D-ND	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hV	201	PEB	C4D-ND	3.39	1.39	1.35
26	C2	301	PEB	C4D-ND	3.39	1.39	1.35
26	N2	202	PEB	C4D-ND	3.39	1.39	1.35
26	Q2	1001	PEB	C4D-ND	3.39	1.39	1.35
26	Z5	301	PEB	C4D-ND	3.39	1.39	1.35
26	O9	201	PEB	C4D-ND	3.39	1.39	1.35
26	cS	201	PEB	C4D-ND	3.39	1.39	1.35
26	ly	403	PEB	C4D-ND	3.39	1.39	1.35
26	lz	402	PEB	C4D-ND	3.39	1.39	1.35
26	K2	202	PEB	C4D-ND	3.39	1.39	1.35
26	G8	201	PEB	C4D-ND	3.39	1.39	1.35
26	E9	201	PEB	C4D-ND	3.39	1.39	1.35
26	aa	1001	PEB	C4D-ND	3.39	1.39	1.35
26	aN	201	PEB	C4D-ND	3.39	1.39	1.35
26	dR	201	PEB	C4D-ND	3.39	1.39	1.35
26	eR	202	PEB	C4D-ND	3.39	1.39	1.35
26	fd	302	PEB	C4D-ND	3.39	1.39	1.35
26	R2	202	PEB	C4D-ND	3.39	1.39	1.35
26	T2	201	PEB	C4D-ND	3.39	1.39	1.35
26	p3	201	PEB	C4D-ND	3.39	1.39	1.35
26	q4	202	PEB	C4D-ND	3.39	1.39	1.35
26	c5	202	PEB	C4D-ND	3.39	1.39	1.35
26	Z9	1007	PEB	C4D-ND	3.39	1.39	1.35
26	bL	201	PEB	C4D-ND	3.39	1.39	1.35
26	bN	201	PEB	C4D-ND	3.39	1.39	1.35
26	dB	201	PEB	C4D-ND	3.39	1.39	1.35
26	dN	202	PEB	C4D-ND	3.39	1.39	1.35
26	n2	201	PEB	C4D-ND	3.39	1.39	1.35
26	t2	202	PEB	C4D-ND	3.39	1.39	1.35
26	Q4	201	PEB	C4D-ND	3.39	1.39	1.35
26	g6	202	PEB	C4D-ND	3.39	1.39	1.35
26	t8	201	PEB	C4D-ND	3.39	1.39	1.35
26	C9	201	PEB	C4D-ND	3.39	1.39	1.35
26	aK	1001	PEB	C4D-ND	3.39	1.39	1.35
26	br	202	PEB	C4D-ND	3.39	1.39	1.35
26	ct	201	PEB	C4D-ND	3.39	1.39	1.35
26	dI	1002	PEB	C4D-ND	3.39	1.39	1.35
26	ek	1001	PEB	C4D-ND	3.39	1.39	1.35
26	fs	201	PEB	C4D-ND	3.39	1.39	1.35
26	P8	201	PEB	C4D-ND	3.39	1.39	1.35
26	l9	202	PEB	C4D-ND	3.39	1.39	1.35
26	aN	202	PEB	C4D-ND	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bj	202	PEB	C4D-ND	3.39	1.39	1.35
26	bt	202	PEB	C4D-ND	3.39	1.39	1.35
26	dE	201	PEB	C4D-ND	3.39	1.39	1.35
26	gy	301	PEB	C4D-ND	3.39	1.39	1.35
26	N3	201	PEB	C4D-ND	3.39	1.39	1.35
26	A5	201	PEB	C4D-ND	3.39	1.39	1.35
26	h8	201	PEB	C4D-ND	3.39	1.39	1.35
26	v6	202	PEB	C4D-ND	3.39	1.39	1.35
26	T7	201	PEB	C4D-ND	3.39	1.39	1.35
26	w8	202	PEB	C4D-ND	3.39	1.39	1.35
26	F9	201	PEB	C4D-ND	3.39	1.39	1.35
26	bi	201	PEB	C4D-ND	3.39	1.39	1.35
26	bF	201	PEB	C4D-ND	3.39	1.39	1.35
26	bY	1001	PEB	C4D-ND	3.39	1.39	1.35
26	gw	201	PEB	C4D-ND	3.39	1.39	1.35
26	K4	202	PEB	C4D-ND	3.39	1.39	1.35
26	Z4	202	PEB	C4D-ND	3.39	1.39	1.35
26	44	302	PEB	C4D-ND	3.39	1.39	1.35
26	a4	201	PEB	C4D-ND	3.39	1.39	1.35
26	S6	201	PEB	C4D-ND	3.39	1.39	1.35
26	c6	1002	PEB	C4D-ND	3.39	1.39	1.35
26	u9	202	PEB	C4D-ND	3.39	1.39	1.35
26	aY	402	PEB	C4D-ND	3.39	1.39	1.35
26	bl	202	PEB	C4D-ND	3.39	1.39	1.35
26	bw	202	PEB	C4D-ND	3.39	1.39	1.35
26	bz	202	PEB	C4D-ND	3.39	1.39	1.35
26	hP	201	PEB	C4D-ND	3.39	1.39	1.35
26	r8	201	PEB	C4D-ND	3.39	1.39	1.35
26	b8	1003	PEB	C4D-ND	3.39	1.39	1.35
26	bf	201	PEB	C4D-ND	3.39	1.39	1.35
26	bQ	201	PEB	C4D-ND	3.39	1.39	1.35
26	dD	201	PEB	C4D-ND	3.39	1.39	1.35
26	e2	201	PEB	C4D-ND	3.39	1.39	1.35
26	A2	1002	PEB	C4D-ND	3.39	1.39	1.35
26	K2	201	PEB	C4D-ND	3.39	1.39	1.35
26	r9	201	PEB	C4D-ND	3.39	1.39	1.35
26	M9	201	PEB	C4D-ND	3.39	1.39	1.35
26	bz	201	PEB	C4D-ND	3.39	1.39	1.35
26	ej	201	PEB	C4D-ND	3.39	1.39	1.35
26	hM	1001	PEB	C4D-ND	3.39	1.39	1.35
26	hX	201	PEB	C4D-ND	3.39	1.39	1.35
26	A4	201	PEB	C4D-ND	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H4	201	PEB	C4D-ND	3.39	1.39	1.35
26	F6	201	PEB	C4D-ND	3.39	1.39	1.35
26	P6	201	PEB	C4D-ND	3.39	1.39	1.35
26	i6	202	PEB	C4D-ND	3.39	1.39	1.35
26	m7	201	PEB	C4D-ND	3.39	1.39	1.35
26	cb	201	PEB	C4D-ND	3.39	1.39	1.35
26	dw	402	PEB	C4D-ND	3.39	1.39	1.35
26	dA	202	PEB	C4D-ND	3.39	1.39	1.35
26	dL	201	PEB	C4D-ND	3.39	1.39	1.35
26	eG	201	PEB	C4D-ND	3.39	1.39	1.35
26	gl	201	PEB	C4D-ND	3.39	1.39	1.35
26	hF	201	PEB	C4D-ND	3.39	1.39	1.35
26	y4	1002	PEB	C4D-ND	3.39	1.39	1.35
26	d5	201	PEB	C4D-ND	3.39	1.39	1.35
26	i8	201	PEB	C4D-ND	3.39	1.39	1.35
26	g7	201	PEB	C4D-ND	3.39	1.39	1.35
26	X8	201	PEB	C4D-ND	3.39	1.39	1.35
26	T9	201	PEB	C4D-ND	3.39	1.39	1.35
26	ay	1001	PEB	C4D-ND	3.39	1.39	1.35
26	aU	201	PEB	C4D-ND	3.39	1.39	1.35
26	bs	1003	PEB	C4D-ND	3.39	1.39	1.35
26	dz	401	PEB	C4D-ND	3.39	1.39	1.35
26	e9	301	PEB	C4D-ND	3.39	1.39	1.35
26	hZ	402	PEB	C4D-ND	3.39	1.39	1.35
26	jM	1001	PEB	C4D-ND	3.39	1.39	1.35
26	kT	1001	PEB	C4D-ND	3.39	1.39	1.35
26	k2	201	PEB	C4D-ND	3.38	1.39	1.35
26	m2	202	PEB	C4D-ND	3.38	1.39	1.35
26	K3	201	PEB	C4D-ND	3.38	1.39	1.35
26	Y3	201	PEB	C4D-ND	3.38	1.39	1.35
26	O4	1002	PEB	C4D-ND	3.38	1.39	1.35
26	o4	201	PEB	C4D-ND	3.38	1.39	1.35
26	o5	201	PEB	C4D-ND	3.38	1.39	1.35
26	k7	1001	PEB	C4D-ND	3.38	1.39	1.35
26	q9	202	PEB	C4D-ND	3.38	1.39	1.35
26	bX	402	PEB	C4D-ND	3.38	1.39	1.35
26	la	1002	PEB	C4D-ND	3.38	1.39	1.35
26	hH	201	PEB	C4D-ND	3.38	1.39	1.35
26	jL	1001	PEB	C4D-ND	3.38	1.39	1.35
26	g5	201	PEB	C4D-ND	3.38	1.39	1.35
26	Q6	202	PEB	C4D-ND	3.38	1.39	1.35
26	z6	202	PEB	C4D-ND	3.38	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h7	201	PEB	C4D-ND	3.38	1.39	1.35
26	A8	201	PEB	C4D-ND	3.38	1.39	1.35
26	bB	201	PEB	C4D-ND	3.38	1.39	1.35
26	dm	202	PEB	C4D-ND	3.38	1.39	1.35
26	dx	402	PEB	C4D-ND	3.38	1.39	1.35
26	k2	202	PEB	C4D-ND	3.38	1.39	1.35
26	h4	202	PEB	C4D-ND	3.38	1.39	1.35
26	b7	201	PEB	C4D-ND	3.38	1.39	1.35
26	a9	601	PEB	C4D-ND	3.38	1.39	1.35
26	b9	403	PEB	C4D-ND	3.38	1.39	1.35
26	bg	201	PEB	C4D-ND	3.38	1.39	1.35
26	ls	201	PEB	C4D-ND	3.38	1.39	1.35
26	F2	201	PEB	C4D-ND	3.38	1.39	1.35
26	Z7	201	PEB	C4D-ND	3.38	1.39	1.35
26	cq	201	PEB	C4D-ND	3.38	1.39	1.35
26	i2	201	PEB	C4D-ND	3.38	1.39	1.35
26	C6	202	PEB	C4D-ND	3.38	1.39	1.35
26	l6	202	PEB	C4D-ND	3.38	1.39	1.35
26	q6	201	PEB	C4D-ND	3.38	1.39	1.35
26	bL	202	PEB	CAD-C3D	-3.38	1.38	1.47
26	g8	201	PEB	C4D-ND	3.38	1.39	1.35
26	V8	1001	PEB	C4D-ND	3.38	1.39	1.35
26	cL	201	PEB	C4D-ND	3.38	1.39	1.35
26	ea	202	PEB	C4D-ND	3.38	1.39	1.35
26	gz	303	PEB	C4D-ND	3.38	1.39	1.35
26	g4	201	PEB	C4D-ND	3.38	1.39	1.35
26	z7	201	PEB	C4D-ND	3.38	1.39	1.35
26	bb	201	PEB	C4D-ND	3.38	1.39	1.35
26	dk	1001	PEB	C4D-ND	3.38	1.39	1.35
26	dC	201	PEB	C4D-ND	3.38	1.39	1.35
26	fa	201	PEB	C4D-ND	3.38	1.39	1.35
26	hN	201	PEB	C4D-ND	3.38	1.39	1.35
26	v9	201	PEB	C4D-ND	3.38	1.39	1.35
26	aG	201	PEB	C4D-ND	3.38	1.39	1.35
26	eB	202	PEB	C4D-ND	3.38	1.39	1.35
26	B5	201	PEB	C4D-ND	3.38	1.39	1.35
26	S8	401	PEB	C4D-ND	3.38	1.39	1.35
26	Y8	202	PEB	C4D-ND	3.38	1.39	1.35
26	cP	202	PEB	C4D-ND	3.38	1.39	1.35
26	dZ	1001	PEB	C4D-ND	3.38	1.39	1.35
26	O2	202	PEB	C4D-ND	3.38	1.39	1.35
26	w4	201	PEB	C4D-ND	3.38	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E8	202	PEB	C4D-ND	3.38	1.39	1.35
26	en	201	PEB	C4D-ND	3.38	1.39	1.35
26	eW	201	PEB	C4D-ND	3.38	1.39	1.35
26	W4	202	PEB	C4D-ND	3.38	1.39	1.35
26	w6	1001	PEB	C4D-ND	3.38	1.39	1.35
26	a9	603	PEB	C4D-ND	3.38	1.39	1.35
26	s9	202	PEB	C4D-ND	3.38	1.39	1.35
26	bo	201	PEB	C4D-ND	3.38	1.39	1.35
26	le	201	PEB	C4D-ND	3.38	1.39	1.35
26	R5	201	PEB	C4D-ND	3.38	1.39	1.35
26	e8	301	PEB	C4D-ND	3.38	1.39	1.35
26	aA	201	PEB	C4D-ND	3.38	1.39	1.35
26	be	201	PEB	C4D-ND	3.38	1.39	1.35
26	dr	201	PEB	C4D-ND	3.38	1.39	1.35
26	dv	201	PEB	C4D-ND	3.38	1.39	1.35
26	dw	403	PEB	C4D-ND	3.38	1.39	1.35
26	go	201	PEB	C4D-ND	3.38	1.39	1.35
26	jO	1001	PEB	C4D-ND	3.38	1.39	1.35
26	O4	1001	PEB	C4D-ND	3.38	1.39	1.35
26	I7	201	PEB	C4D-ND	3.38	1.39	1.35
26	g9	201	PEB	C4D-ND	3.38	1.39	1.35
26	s9	201	PEB	C4D-ND	3.38	1.39	1.35
26	as	201	PEB	C4D-ND	3.38	1.39	1.35
26	t3	201	PEB	C4D-ND	3.38	1.39	1.35
26	H4	202	PEB	C4D-ND	3.38	1.39	1.35
26	z6	201	PEB	C4D-ND	3.38	1.39	1.35
26	bp	201	PEB	C4D-ND	3.38	1.39	1.35
26	hW	201	PEB	C4D-ND	3.38	1.39	1.35
26	a3	1003	PEB	C4D-ND	3.37	1.39	1.35
26	bO	201	PEB	C4D-ND	3.37	1.39	1.35
26	eo	201	PEB	C4D-ND	3.37	1.39	1.35
26	gh	201	PEB	C4D-ND	3.37	1.39	1.35
26	e2	202	PEB	C4D-ND	3.37	1.39	1.35
26	F2	202	PEB	C4D-ND	3.37	1.39	1.35
26	J4	202	PEB	C4D-ND	3.37	1.39	1.35
26	V4	202	PEB	C4D-ND	3.37	1.39	1.35
26	b4	1001	PEB	C4D-ND	3.37	1.39	1.35
26	aA	202	PEB	C4D-ND	3.37	1.39	1.35
26	ce	201	PEB	C4D-ND	3.37	1.39	1.35
26	Y2	201	PEB	C4D-ND	3.37	1.39	1.35
26	Y5	1001	PEB	C4D-ND	3.37	1.39	1.35
26	W6	201	PEB	C4D-ND	3.37	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K8	202	PEB	C4D-ND	3.37	1.39	1.35
26	aW	302	PEB	C4D-ND	3.37	1.39	1.35
26	bV	201	PEB	C4D-ND	3.37	1.39	1.35
26	cC	1001	PEB	C4D-ND	3.37	1.39	1.35
26	dQ	202	PEB	C4D-ND	3.37	1.39	1.35
26	iC	1001	PEB	C4D-ND	3.37	1.39	1.35
26	s2	201	PEB	C4D-ND	3.37	1.39	1.35
26	X7	201	PEB	C4D-ND	3.37	1.39	1.35
26	u3	201	PEB	C4D-ND	3.37	1.39	1.35
26	Y4	201	PEB	C4D-ND	3.37	1.39	1.35
26	M5	201	PEB	C4D-ND	3.37	1.39	1.35
26	S5	201	PEB	C4D-ND	3.37	1.39	1.35
26	C6	201	PEB	C4D-ND	3.37	1.39	1.35
26	f6	201	PEB	C4D-ND	3.37	1.39	1.35
26	t6	202	PEB	C4D-ND	3.37	1.39	1.35
26	S7	201	PEB	C4D-ND	3.37	1.39	1.35
26	a8	601	PEB	C4D-ND	3.37	1.39	1.35
26	f9	201	PEB	C4D-ND	3.37	1.39	1.35
26	A9	201	PEB	C4D-ND	3.37	1.39	1.35
26	S9	201	PEB	C4D-ND	3.37	1.39	1.35
26	eb	201	PEB	C4D-ND	3.37	1.39	1.35
26	el	201	PEB	C4D-ND	3.37	1.39	1.35
26	w2	201	PEB	C4D-ND	3.37	1.39	1.35
26	G6	201	PEB	C4D-ND	3.37	1.39	1.35
26	O8	202	PEB	C4D-ND	3.37	1.39	1.35
26	dd	201	PEB	C4D-ND	3.37	1.39	1.35
26	dH	202	PEB	C4D-ND	3.37	1.39	1.35
26	eH	201	PEB	C4D-ND	3.37	1.39	1.35
26	F3	201	PEB	C4D-ND	3.37	1.39	1.35
26	L6	201	PEB	C4D-ND	3.37	1.39	1.35
26	y7	201	PEB	C4D-ND	3.37	1.39	1.35
26	dT	202	PEB	C4D-ND	3.37	1.39	1.35
26	eA	1001	PEB	C4D-ND	3.37	1.39	1.35
26	X4	202	PEB	C4D-ND	3.37	1.39	1.35
26	T6	202	PEB	C4D-ND	3.37	1.39	1.35
26	c6	1001	PEB	C4D-ND	3.37	1.39	1.35
26	dx	401	PEB	C4D-ND	3.37	1.39	1.35
26	dy	401	PEB	C4D-ND	3.37	1.39	1.35
26	dM	1001	PEB	C4D-ND	3.37	1.39	1.35
26	dN	201	PEB	C4D-ND	3.37	1.39	1.35
26	fe	201	PEB	C4D-ND	3.37	1.39	1.35
26	eV	202	PEB	CAD-C3D	-3.37	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S2	201	PEB	C4D-ND	3.37	1.39	1.35
26	I4	202	PEB	C4D-ND	3.37	1.39	1.35
26	j7	201	PEB	C4D-ND	3.37	1.39	1.35
26	v8	201	PEB	C4D-ND	3.37	1.39	1.35
26	W4	201	PEB	C4D-ND	3.37	1.39	1.35
26	q6	202	PEB	C4D-ND	3.37	1.39	1.35
26	P8	202	PEB	C4D-ND	3.37	1.39	1.35
26	y9	1002	PEB	C4D-ND	3.37	1.39	1.35
26	di	201	PEB	C4D-ND	3.37	1.39	1.35
26	eq	201	PEB	C4D-ND	3.37	1.39	1.35
26	gt	201	PEB	C4D-ND	3.37	1.39	1.35
26	kU	1001	PEB	C4D-ND	3.37	1.39	1.35
26	y4	1001	PEB	C4D-ND	3.37	1.39	1.35
26	D8	201	PEB	C4D-ND	3.37	1.39	1.35
26	V9	201	PEB	C4D-ND	3.37	1.39	1.35
26	aB	201	PEB	C4D-ND	3.37	1.39	1.35
26	do	201	PEB	C4D-ND	3.37	1.39	1.35
26	dF	201	PEB	C4D-ND	3.37	1.39	1.35
26	ee	201	PEB	C4D-ND	3.37	1.39	1.35
26	eH	202	PEB	C4D-ND	3.37	1.39	1.35
26	eK	201	PEB	C4D-ND	3.37	1.39	1.35
26	lc	201	PEB	C4D-ND	3.37	1.39	1.35
26	r2	202	PEB	C4D-ND	3.37	1.39	1.35
26	M4	202	PEB	C4D-ND	3.37	1.39	1.35
26	N5	201	PEB	C4D-ND	3.37	1.39	1.35
26	af	201	PEB	C4D-ND	3.37	1.39	1.35
26	aY	406	PEB	C4D-ND	3.37	1.39	1.35
26	x7	202	PEB	CAD-C3D	-3.37	1.38	1.47
26	l5	201	PEB	C4D-ND	3.37	1.39	1.35
26	cg	201	PEB	C4D-ND	3.37	1.39	1.35
26	cC	1003	PEB	C4D-ND	3.37	1.39	1.35
26	z4	201	PEB	C4D-ND	3.37	1.39	1.35
26	g6	201	PEB	C4D-ND	3.37	1.39	1.35
26	r6	201	PEB	C4D-ND	3.37	1.39	1.35
26	Y7	1001	PEB	C4D-ND	3.37	1.39	1.35
26	w8	201	PEB	C4D-ND	3.37	1.39	1.35
26	aF	204	PEB	C4D-ND	3.37	1.39	1.35
26	eo	202	PEB	C4D-ND	3.37	1.39	1.35
26	ez	1003	PEB	C4D-ND	3.37	1.39	1.35
26	lp	201	PEB	C4D-ND	3.37	1.39	1.35
26	hA	201	PEB	C4D-ND	3.37	1.39	1.35
26	dV	202	PEB	CAD-C3D	-3.37	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F9	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	O6	202	PEB	C4D-ND	3.36	1.39	1.35
26	Q6	201	PEB	C4D-ND	3.36	1.39	1.35
26	w7	1001	PEB	C4D-ND	3.36	1.39	1.35
26	D9	201	PEB	C4D-ND	3.36	1.39	1.35
26	by	1002	PEB	C4D-ND	3.36	1.39	1.35
26	ew	301	PEB	C4D-ND	3.36	1.39	1.35
26	D2	302	PEB	C4D-ND	3.36	1.39	1.35
26	34	1007	PEB	C4D-ND	3.36	1.39	1.35
26	y9	1001	PEB	C4D-ND	3.36	1.39	1.35
26	aK	1002	PEB	C4D-ND	3.36	1.39	1.35
26	cG	201	PEB	C4D-ND	3.36	1.39	1.35
26	dH	201	PEB	C4D-ND	3.36	1.39	1.35
26	eT	202	PEB	C4D-ND	3.36	1.39	1.35
26	p6	201	PEB	C4D-ND	3.36	1.39	1.35
26	iH	1001	PEB	C4D-ND	3.36	1.39	1.35
26	Z5	303	PEB	C4D-ND	3.36	1.39	1.35
26	ao	201	PEB	C4D-ND	3.36	1.39	1.35
26	aH	202	PEB	C4D-ND	3.36	1.39	1.35
26	bq	202	PEB	C4D-ND	3.36	1.39	1.35
26	cu	201	PEB	C4D-ND	3.36	1.39	1.35
26	eQ	201	PEB	C4D-ND	3.36	1.39	1.35
26	hO	201	PEB	C4D-ND	3.36	1.39	1.35
26	cE	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	dc	201	PEB	C4D-ND	3.36	1.39	1.35
26	f3	201	PEB	C4D-ND	3.36	1.39	1.35
26	d9	301	PEB	C4D-ND	3.36	1.39	1.35
26	ah	201	PEB	C4D-ND	3.36	1.39	1.35
26	aJ	201	PEB	C4D-ND	3.36	1.39	1.35
26	eR	201	PEB	C4D-ND	3.36	1.39	1.35
26	la	1001	PEB	C4D-ND	3.36	1.39	1.35
26	hS	201	PEB	C4D-ND	3.36	1.39	1.35
26	p7	201	PEB	CAD-C3D	-3.36	1.38	1.47
26	J5	201	PEB	C4D-ND	3.36	1.39	1.35
26	aX	402	PEB	C4D-ND	3.36	1.39	1.35
26	cm	1001	PEB	C4D-ND	3.36	1.39	1.35
26	cY	201	PEB	C4D-ND	3.36	1.39	1.35
26	dh	201	PEB	C4D-ND	3.36	1.39	1.35
26	av	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	cb	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	bJ	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	kS	1001	PEB	C4D-ND	3.36	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j8	202	PEB	C4D-ND	3.36	1.39	1.35
26	bJ	201	PEB	C4D-ND	3.36	1.39	1.35
26	cx	201	PEB	C4D-ND	3.36	1.39	1.35
26	gb	1001	PEB	C4D-ND	3.36	1.39	1.35
26	p2	201	PEB	C4D-ND	3.36	1.39	1.35
26	D6	201	PEB	C4D-ND	3.36	1.39	1.35
26	lk	201	PEB	C4D-ND	3.36	1.39	1.35
26	t7	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	bC	201	PEB	C4D-ND	3.36	1.39	1.35
26	cX	201	PEB	C4D-ND	3.36	1.39	1.35
26	N3	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	n7	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	T3	201	PEB	C4D-ND	3.36	1.39	1.35
26	X4	201	PEB	C4D-ND	3.36	1.39	1.35
26	F5	201	PEB	C4D-ND	3.36	1.39	1.35
26	N7	201	PEB	C4D-ND	3.36	1.39	1.35
26	dP	202	PEB	C4D-ND	3.36	1.39	1.35
26	fn	1001	PEB	C4D-ND	3.36	1.39	1.35
26	H3	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	cp	202	PEB	CAD-C3D	-3.36	1.38	1.47
26	z3	201	PEB	C4D-ND	3.36	1.39	1.35
26	li	201	PEB	C4D-ND	3.36	1.39	1.35
26	R4	201	PEB	C4D-ND	3.35	1.39	1.35
26	s4	201	PEB	C4D-ND	3.35	1.39	1.35
26	Y5	1003	PEB	C4D-ND	3.35	1.39	1.35
26	y5	1001	PEB	C4D-ND	3.35	1.39	1.35
26	e8	302	PEB	C4D-ND	3.35	1.39	1.35
26	e9	303	PEB	C4D-ND	3.35	1.39	1.35
26	Z9	1001	PEB	C4D-ND	3.35	1.39	1.35
26	aY	401	PEB	C4D-ND	3.35	1.39	1.35
26	bm	1001	PEB	C4D-ND	3.35	1.39	1.35
26	J5	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	aD	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	J4	201	PEB	C4D-ND	3.35	1.39	1.35
26	P9	201	PEB	C4D-ND	3.35	1.39	1.35
26	bn	201	PEB	C4D-ND	3.35	1.39	1.35
26	ca	1001	PEB	C4D-ND	3.35	1.39	1.35
26	cs	201	PEB	C4D-ND	3.35	1.39	1.35
26	cZ	201	PEB	C4D-ND	3.35	1.39	1.35
26	d9	302	PEB	C4D-ND	3.35	1.39	1.35
26	aQ	202	PEB	C4D-ND	3.35	1.39	1.35
26	ez	1002	PEB	C4D-ND	3.35	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eM	1001	PEB	C4D-ND	3.35	1.39	1.35
26	lb	201	PEB	C4D-ND	3.35	1.39	1.35
26	gu	201	PEB	C4D-ND	3.35	1.39	1.35
26	gv	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	p8	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	j2	201	PEB	C4D-ND	3.35	1.39	1.35
26	z5	201	PEB	C4D-ND	3.35	1.39	1.35
26	y6	201	PEB	C4D-ND	3.35	1.39	1.35
26	ep	201	PEB	C4D-ND	3.35	1.39	1.35
26	aF	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	aP	201	PEB	C4D-ND	3.35	1.39	1.35
26	gp	201	PEB	C4D-ND	3.35	1.39	1.35
26	a8	602	PEB	C4D-ND	3.35	1.39	1.35
26	bP	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	B2	502	PEB	C4D-ND	3.35	1.39	1.35
26	c9	302	PEB	C4D-ND	3.35	1.39	1.35
26	cd	201	PEB	C4D-ND	3.35	1.39	1.35
26	cV	201	PEB	C4D-ND	3.35	1.39	1.35
26	dn	201	PEB	C4D-ND	3.35	1.39	1.35
26	ez	1001	PEB	C4D-ND	3.35	1.39	1.35
26	eZ	401	PEB	C4D-ND	3.35	1.39	1.35
26	iA	1001	PEB	C4D-ND	3.35	1.39	1.35
26	Z6	201	PEB	C4D-ND	3.35	1.39	1.35
26	u6	202	PEB	C4D-ND	3.35	1.39	1.35
26	r4	201	PEB	CAD-C3D	-3.35	1.38	1.47
26	r5	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	lr	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	fw	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	fm	201	PEB	C4D-ND	3.35	1.39	1.35
26	P3	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	hX	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	h3	201	PEB	CAD-C3D	-3.35	1.38	1.47
26	V5	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	o6	201	PEB	C4D-ND	3.35	1.39	1.35
26	v7	201	PEB	C4D-ND	3.35	1.39	1.35
26	eG	202	PEB	C4D-ND	3.35	1.39	1.35
26	eY	402	PEB	C4D-ND	3.35	1.39	1.35
26	hN	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	l2	201	PEB	C4D-ND	3.35	1.39	1.35
26	x3	201	PEB	C4D-ND	3.35	1.39	1.35
26	ac	201	PEB	C4D-ND	3.35	1.39	1.35
26	aq	201	PEB	C4D-ND	3.35	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ba	1001	PEB	C4D-ND	3.35	1.39	1.35
26	H9	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	dh	202	PEB	CAD-C3D	-3.35	1.38	1.47
26	34	1001	PEB	CAD-C3D	-3.35	1.38	1.47
26	U2	201	PEB	C4D-ND	3.35	1.39	1.35
26	cz	201	PEB	C4D-ND	3.35	1.39	1.35
26	fo	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	kU	1002	PEB	CAD-C3D	-3.34	1.38	1.47
26	L9	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	S5	203	PEB	CAD-C3D	-3.34	1.38	1.47
26	dd	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	dg	201	PEB	C4D-ND	3.34	1.39	1.35
26	ax	201	PEB	CAD-C3D	-3.34	1.38	1.47
26	E3	201	PEB	C4D-ND	3.34	1.39	1.35
26	m6	202	PEB	C4D-ND	3.34	1.39	1.35
26	cc	201	PEB	C4D-ND	3.34	1.39	1.35
26	H2	201	PEB	CAD-C3D	-3.34	1.38	1.47
26	ei	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	D8	202	PEB	C4D-ND	3.34	1.39	1.35
26	dc	203	PEB	C4D-ND	3.34	1.39	1.35
26	eO	201	PEB	C4D-ND	3.34	1.39	1.35
26	n6	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	df	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	eg	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	eW	202	PEB	C4D-ND	3.34	1.39	1.35
26	ch	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	X5	401	PEB	C4D-ND	3.34	1.39	1.35
26	M6	1002	PEB	C4D-ND	3.34	1.39	1.35
26	dT	201	PEB	C4D-ND	3.34	1.39	1.35
26	D5	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	cl	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	lp	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	N9	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	cq	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	V2	201	PEB	C4D-ND	3.34	1.39	1.35
26	F4	201	PEB	C4D-ND	3.34	1.39	1.35
26	X6	201	PEB	C4D-ND	3.34	1.39	1.35
26	Q7	201	PEB	C4D-ND	3.34	1.39	1.35
26	bD	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	Z2	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	z3	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	k4	201	PEB	C4D-ND	3.34	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aT	201	PEB	C4D-ND	3.34	1.39	1.35
26	eJ	202	PEB	CAD-C3D	-3.34	1.38	1.47
27	Q1	201	CYC	C1D-CHD	3.34	1.54	1.41
26	O5	201	PEB	C4D-ND	3.34	1.39	1.35
26	M8	201	PEB	C4D-ND	3.34	1.39	1.35
26	X7	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	d7	201	PEB	C4D-ND	3.34	1.39	1.35
26	T2	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	cj	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	Y2	202	PEB	C4D-ND	3.34	1.39	1.35
26	w9	202	PEB	C4D-ND	3.34	1.39	1.35
26	cM	201	PEB	C4D-ND	3.34	1.39	1.35
26	db	201	PEB	C4D-ND	3.34	1.39	1.35
26	dX	202	PEB	C4D-ND	3.34	1.39	1.35
26	af	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	ap	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	w2	203	PEB	C4D-ND	3.34	1.39	1.35
26	D4	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	fs	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	gt	202	PEB	CAD-C3D	-3.34	1.38	1.47
27	w1	201	CYC	C1D-CHD	3.34	1.54	1.41
26	A2	1003	PEB	CAD-C3D	-3.34	1.38	1.47
26	24	401	PEB	C4D-ND	3.34	1.39	1.35
26	C5	201	PEB	C4D-ND	3.34	1.39	1.35
26	r5	201	PEB	C4D-ND	3.34	1.39	1.35
26	eT	201	PEB	C4D-ND	3.34	1.39	1.35
26	lf	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	ep	202	PEB	CAD-C3D	-3.34	1.38	1.47
26	bE	201	PEB	C4D-ND	3.33	1.39	1.35
26	em	201	PEB	C4D-ND	3.33	1.39	1.35
26	j4	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	C8	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	lh	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	hH	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	U4	202	PEB	C4D-ND	3.33	1.39	1.35
26	cn	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	bs	1001	PEB	C4D-ND	3.33	1.39	1.35
26	al	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	ee	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	el	202	PEB	CAD-C3D	-3.33	1.38	1.47
27	b1	1001	CYC	C1D-CHD	3.33	1.54	1.41
26	eI	202	PEB	C4D-ND	3.33	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n2	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	P5	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	P9	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	kV	1002	PEB	CAD-C3D	-3.33	1.38	1.47
26	D3	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	bN	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	hP	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	j6	202	PEB	C4D-ND	3.33	1.39	1.35
26	bG	201	PEB	C4D-ND	3.33	1.39	1.35
26	cY	202	PEB	CAD-C3D	-3.33	1.38	1.47
27	W1	201	CYC	C1D-CHD	3.33	1.54	1.41
26	X2	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	x3	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	v4	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	v5	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	ea	203	PEB	CAD-C3D	-3.33	1.38	1.47
26	eL	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	ev	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	fu	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	gk	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	aQ	201	PEB	C4D-ND	3.33	1.39	1.35
26	iC	1002	PEB	CAD-C3D	-3.33	1.38	1.47
26	dY	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	hR	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	hT	202	PEB	CAD-C3D	-3.33	1.38	1.47
27	U1	201	CYC	C1D-CHD	3.33	1.54	1.41
27	d2	101	CYC	C1D-CHD	3.33	1.54	1.41
26	p2	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	B6	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	bH	202	PEB	CAD-C3D	-3.33	1.38	1.47
29	gy	304	PVN	C7-C6	-3.33	1.36	1.42
26	cz	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	cL	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	bQ	203	PEB	CAD-C3D	-3.33	1.38	1.47
26	gg	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	z5	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	ad	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	co	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	hG	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	G4	202	PEB	C4D-ND	3.33	1.39	1.35
26	W8	202	PEB	C4D-ND	3.33	1.39	1.35
26	e4	202	PEB	CAD-C3D	-3.33	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n4	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	v9	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	h2	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	p4	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	p5	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	e7	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	gd	201	PEB	CAD-C3D	-3.33	1.38	1.47
26	hV	202	PEB	CAD-C3D	-3.33	1.38	1.47
27	f1	201	CYC	C1D-CHD	3.33	1.54	1.41
26	N7	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	ab	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	l2	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	A5	203	PEB	CAD-C3D	-3.33	1.38	1.47
26	R5	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	Z7	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	l7	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	v7	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	jI	1002	PEB	CAD-C3D	-3.33	1.38	1.47
26	al	201	PEB	C4D-ND	3.33	1.39	1.35
26	bB	202	PEB	CAD-C3D	-3.33	1.38	1.47
26	r7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	jM	1002	PEB	CAD-C3D	-3.32	1.38	1.47
26	jP	1002	PEB	CAD-C3D	-3.32	1.38	1.47
27	k1	201	CYC	C1D-CHD	3.32	1.54	1.41
27	s1	201	CYC	C1D-CHD	3.32	1.54	1.41
26	m5	1003	PEB	CAD-C3D	-3.32	1.38	1.47
26	t5	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	D7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	fm	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	fq	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	T7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	D9	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	Z4	201	PEB	C4D-ND	3.32	1.39	1.35
26	Y7	1003	PEB	CAD-C3D	-3.32	1.38	1.47
26	B7	201	PEB	CAD-C3D	-3.32	1.38	1.47
26	M6	1001	PEB	C4D-ND	3.32	1.39	1.35
26	aL	201	PEB	C4D-ND	3.32	1.39	1.35
27	d1	1001	CYC	C1D-CHD	3.32	1.54	1.41
26	dL	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	fy	201	PEB	CAD-C3D	-3.32	1.38	1.47
26	gn	202	PEB	CAD-C3D	-3.32	1.38	1.47
27	X1	201	CYC	C1D-CHD	3.32	1.54	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F7	201	PEB	CAD-C3D	-3.32	1.38	1.47
26	ck	201	PEB	C4D-ND	3.32	1.39	1.35
26	cI	201	PEB	C4D-ND	3.32	1.39	1.35
26	dP	201	PEB	C4D-ND	3.32	1.39	1.35
26	gi	202	PEB	CAD-C3D	-3.32	1.38	1.47
27	G1	1001	CYC	C1D-CHD	3.32	1.54	1.41
27	g1	201	CYC	C1D-CHD	3.32	1.54	1.41
26	R9	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	cr	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	lo	203	PEB	CAD-C3D	-3.32	1.38	1.47
26	dl	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	en	202	PEB	CAD-C3D	-3.32	1.38	1.47
27	q1	201	CYC	C1D-CHD	3.32	1.54	1.41
26	cB	202	PEB	CAD-C3D	-3.32	1.38	1.47
27	L1	201	CYC	C1D-CHD	3.32	1.54	1.41
27	a1	201	CYC	C1D-CHD	3.32	1.54	1.41
26	fc	202	PEB	CAD-C3D	-3.32	1.38	1.47
29	A2	1004	PVN	C19-C18	-3.32	1.41	1.48
29	a3	1004	PVN	C19-C18	-3.32	1.41	1.48
26	B5	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	bV	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	es	202	PEB	C4D-ND	3.32	1.39	1.35
26	34	1002	PEB	CAD-C3D	-3.32	1.38	1.47
26	iD	1002	PEB	CAD-C3D	-3.32	1.38	1.47
26	cJ	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	lw	203	PEB	CAD-C3D	-3.32	1.38	1.47
26	E5	201	PEB	C4D-ND	3.32	1.39	1.35
26	R7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	y7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	an	201	PEB	CAD-C3D	-3.32	1.38	1.47
29	dw	404	PVN	C31-C3	3.32	1.58	1.51
27	R1	1001	CYC	C1D-CHD	3.32	1.54	1.41
27	i1	1001	CYC	C1D-CHD	3.32	1.54	1.41
26	c7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	aj	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	kX	1002	PEB	CAD-C3D	-3.32	1.38	1.47
27	u1	1001	CYC	C1D-CHD	3.32	1.54	1.41
26	ge	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	di	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	fi	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	V3	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	cs	202	PEB	CAD-C3D	-3.32	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B9	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	ll	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	fj	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	bW	301	PEB	C4D-ND	3.32	1.39	1.35
26	dV	201	PEB	C4D-ND	3.32	1.39	1.35
26	P7	202	PEB	CAD-C3D	-3.32	1.38	1.47
26	jJ	1002	PEB	CAD-C3D	-3.32	1.38	1.47
27	Z1	201	CYC	C1D-CHD	3.32	1.54	1.41
27	o1	1001	CYC	C1D-CHD	3.32	1.54	1.41
26	N5	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	f3	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	r3	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	L5	202	PEB	CAD-C3D	-3.31	1.38	1.47
27	P1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	a7	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	d7	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	iE	1002	PEB	CAD-C3D	-3.31	1.38	1.47
26	V2	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	v3	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	jO	1002	PEB	CAD-C3D	-3.31	1.38	1.47
26	dj	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	bv	201	PEB	C4D-ND	3.31	1.39	1.35
27	n1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	ga	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	kT	1002	PEB	CAD-C3D	-3.31	1.38	1.47
26	g5	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	eB	203	PEB	CAD-C3D	-3.31	1.38	1.47
27	V1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	L3	201	PEB	C4D-ND	3.31	1.39	1.35
26	bT	201	PEB	CAD-C3D	-3.31	1.38	1.47
26	li	203	PEB	CAD-C3D	-3.31	1.38	1.47
26	A1	301	PEB	CAD-C3D	-3.31	1.38	1.47
26	B1	301	PEB	CAD-C3D	-3.31	1.38	1.47
26	X6	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	V7	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	er	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	ff	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	H5	201	PEB	C4D-ND	3.31	1.39	1.35
26	j2	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	R3	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	R6	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	jL	1002	PEB	CAD-C3D	-3.31	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	kW	1002	PEB	CAD-C3D	-3.31	1.38	1.47
27	N1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	hD	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	kS	1002	PEB	CAD-C3D	-3.31	1.38	1.47
26	L3	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	h8	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	W3	203	PEB	CAD-C3D	-3.31	1.38	1.47
27	e1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	F5	202	PEB	CAD-C3D	-3.31	1.38	1.47
27	K1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	n8	201	PEB	CAD-C3D	-3.31	1.38	1.47
26	fg	201	PEB	CAD-C3D	-3.31	1.38	1.47
26	t3	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	eX	201	PEB	CAD-C3D	-3.31	1.38	1.47
27	m1	201	CYC	C1D-CHD	3.31	1.54	1.41
26	ah	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	hB	202	PEB	CAD-C3D	-3.31	1.38	1.47
26	g4	202	PEB	CAD-C3D	-3.30	1.38	1.47
27	y1	201	CYC	C1D-CHD	3.30	1.54	1.41
26	J6	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	H7	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	F3	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	at	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	B3	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	B4	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	L2	202	PEB	CAD-C3D	-3.30	1.38	1.47
27	O1	201	CYC	C1D-CHD	3.30	1.53	1.41
26	kR	1002	PEB	CAD-C3D	-3.30	1.38	1.47
26	Z3	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	n3	202	PEB	CAD-C3D	-3.30	1.38	1.47
27	I1	201	CYC	C1D-CHD	3.30	1.53	1.41
26	gx	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	f2	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	jK	1002	PEB	CAD-C3D	-3.30	1.38	1.47
26	z7	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	dX	201	PEB	C4D-ND	3.30	1.39	1.35
26	kQ	1002	PEB	CAD-C3D	-3.30	1.38	1.47
26	eS	202	PEB	C4D-ND	3.30	1.39	1.35
26	J9	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	T3	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	hJ	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	J3	202	PEB	CAD-C3D	-3.30	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cH	201	PEB	CAD-C3D	-3.30	1.38	1.47
26	G7	201	PEB	C4D-ND	3.30	1.39	1.35
26	n5	202	PEB	CAD-C3D	-3.30	1.38	1.47
26	ar	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	az	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	V9	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	jN	1002	PEB	CAD-C3D	-3.29	1.38	1.47
26	y8	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	hL	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	ld	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	ln	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	ec	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	i3	203	PEB	CAD-C3D	-3.29	1.38	1.47
26	l4	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	T9	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	cd	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	cf	201	PEB	CAD-C3D	-3.29	1.38	1.47
26	cF	201	PEB	CAD-C3D	-3.29	1.38	1.47
26	L7	201	PEB	CAD-C3D	-3.29	1.38	1.47
26	gp	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	p3	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	eN	202	PEB	CAD-C3D	-3.29	1.38	1.47
26	et	202	PEB	CAD-C3D	-3.28	1.38	1.47
26	j3	201	PEB	CAD-C3D	-3.28	1.38	1.47
29	ey	1004	PVN	C3-C2	3.28	1.37	1.34
29	A2	1004	PVN	C14-C13	-3.28	1.38	1.45
26	gr	201	PEB	CAD-C3D	-3.28	1.38	1.47
26	bF	202	PEB	CAD-C3D	-3.28	1.38	1.47
29	c8	303	PVN	C19-C18	-3.28	1.42	1.48
26	e7	201	PEB	C4D-ND	3.28	1.39	1.35
26	dW	202	PEB	C4D-ND	3.27	1.39	1.35
26	q5	201	PEB	C4D-ND	3.27	1.39	1.35
26	J7	201	PEB	CAD-C3D	-3.27	1.38	1.47
29	ez	1004	PVN	C3-C2	3.26	1.37	1.34
29	c9	303	PVN	C19-C18	-3.26	1.42	1.48
26	eM	1001	PEB	CAD-C3D	-3.25	1.38	1.47
27	a2	902	CYC	C4B-NB	-3.24	1.31	1.38
27	b2	1001	CYC	C4B-NB	-3.24	1.31	1.38
27	S1	202	CYC	C4B-NB	-3.24	1.31	1.38
27	c1	201	CYC	C4B-NB	-3.24	1.31	1.38
29	a3	1004	PVN	C14-C13	-3.24	1.38	1.45
26	ck	201	PEB	CAD-C3D	-3.24	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eo	201	PEB	CAD-C3D	-3.23	1.38	1.47
27	p1	201	CYC	C4B-NB	-3.23	1.31	1.38
27	z1	201	CYC	C4B-NB	-3.23	1.31	1.38
26	eO	201	PEB	CAD-C3D	-3.23	1.38	1.47
27	H1	201	CYC	C4B-NB	-3.23	1.31	1.38
26	el	201	PEB	CAD-C3D	-3.23	1.38	1.47
26	dW	201	PEB	CAD-C3D	-3.22	1.38	1.47
27	J1	201	CYC	C4B-NB	-3.22	1.31	1.38
27	Y1	201	CYC	C4B-NB	-3.22	1.31	1.38
27	t1	201	CYC	C4B-NB	-3.22	1.31	1.38
26	cV	203	PEB	CAD-C3D	-3.22	1.38	1.47
26	ai	201	PEB	CAD-C3D	-3.22	1.38	1.47
26	K3	201	PEB	CAD-C3D	-3.22	1.38	1.47
26	eS	201	PEB	CAD-C3D	-3.22	1.38	1.47
26	t5	201	PEB	CAD-C3D	-3.22	1.38	1.47
26	M6	1002	PEB	CAD-C3D	-3.22	1.38	1.47
26	t7	201	PEB	CAD-C3D	-3.22	1.38	1.47
26	ci	201	PEB	CAD-C3D	-3.22	1.38	1.47
27	S1	201	CYC	C4B-NB	-3.22	1.31	1.38
27	j1	201	CYC	C4B-NB	-3.22	1.31	1.38
26	bI	201	PEB	CAD-C3D	-3.22	1.38	1.47
26	P9	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	eo	202	PEB	CAD-C3D	-3.21	1.38	1.47
26	M5	201	PEB	CAD-C3D	-3.21	1.38	1.47
27	a2	901	CYC	C4B-NB	-3.21	1.31	1.38
26	bJ	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	az	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	hY	403	PEB	CAD-C3D	-3.21	1.38	1.47
26	jP	1001	PEB	CAD-C3D	-3.21	1.38	1.47
27	h1	201	CYC	C4B-NB	-3.21	1.31	1.38
27	M1	1001	CYC	OB-C4B	3.21	1.29	1.23
26	a4	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	dT	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	E3	201	PEB	CAD-C3D	-3.21	1.38	1.47
27	v1	201	CYC	C4B-NB	-3.21	1.31	1.38
26	s6	202	PEB	CAD-C3D	-3.21	1.38	1.47
26	M7	1001	PEB	CAD-C3D	-3.21	1.38	1.47
26	gz	301	PEB	CAD-C3D	-3.21	1.38	1.47
26	O7	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	dh	201	PEB	CAD-C3D	-3.21	1.38	1.47
29	d9	304	PVN	C31-C3	3.21	1.58	1.51
26	l8	201	PEB	CAD-C3D	-3.21	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bZ	301	PEB	CAD-C3D	-3.21	1.38	1.47
26	S6	202	PEB	CAD-C3D	-3.21	1.38	1.47
26	dS	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	gc	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	t2	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	j7	201	PEB	CAD-C3D	-3.21	1.38	1.47
29	d9	304	PVN	C19-C18	-3.21	1.42	1.48
26	dw	401	PEB	CAD-C3D	-3.21	1.38	1.47
26	E8	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	dG	202	PEB	CAD-C3D	-3.21	1.38	1.47
27	p1	201	CYC	OB-C4B	3.21	1.29	1.23
26	u9	201	PEB	CAD-C3D	-3.21	1.38	1.47
26	bp	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	dH	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	cz	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	P8	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	aW	301	PEB	CAD-C3D	-3.20	1.38	1.47
26	ly	401	PEB	CAD-C3D	-3.20	1.38	1.47
27	S1	201	CYC	OB-C4B	3.20	1.29	1.23
27	j1	201	CYC	OB-C4B	3.20	1.29	1.23
27	a2	902	CYC	OB-C4B	3.20	1.29	1.23
27	b2	1001	CYC	OB-C4B	3.20	1.29	1.23
27	M1	1001	CYC	C4B-NB	-3.20	1.31	1.38
26	ed	201	PEB	CAD-C3D	-3.20	1.38	1.47
27	t1	201	CYC	OB-C4B	3.20	1.29	1.23
26	ao	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	en	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	j8	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	i9	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	C9	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	eV	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	kV	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	z2	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	C8	201	PEB	CAD-C3D	-3.20	1.38	1.47
27	h1	201	CYC	OB-C4B	3.20	1.29	1.23
26	o8	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	e3	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	dE	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	I3	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	f9	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	ae	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	G7	201	PEB	CAD-C3D	-3.20	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M7	1002	PEB	CAD-C3D	-3.20	1.38	1.47
26	Y8	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	aR	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	cl	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	cO	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	X2	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	cZ	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	t9	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	dq	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	fp	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	iD	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	aR	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	i2	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	eu	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	I6	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	U7	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	z9	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	bj	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	i7	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	B9	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	cd	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	dN	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	eR	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	fr	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	gb	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	b8	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	c8	302	PEB	CAD-C3D	-3.20	1.38	1.47
26	q9	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	fd	301	PEB	CAD-C3D	-3.20	1.38	1.47
26	r3	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	x6	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	a7	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	aJ	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	dv	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	S7	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	p9	202	PEB	CAD-C3D	-3.20	1.38	1.47
26	ab	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	dk	1002	PEB	CAD-C3D	-3.20	1.38	1.47
26	C3	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	S3	203	PEB	CAD-C3D	-3.20	1.38	1.47
26	bD	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	df	201	PEB	CAD-C3D	-3.20	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	M6	1001	PEB	CAD-C3D	-3.20	1.38	1.47
26	g9	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	ag	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	aX	401	PEB	CAD-C3D	-3.20	1.38	1.47
26	bL	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	dn	201	PEB	CAD-C3D	-3.20	1.38	1.47
26	z9	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	u2	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	w6	1002	PEB	CAD-C3D	-3.19	1.38	1.47
26	aX	402	PEB	CAD-C3D	-3.19	1.38	1.47
26	dY	201	PEB	CAD-C3D	-3.19	1.38	1.47
29	d8	303	PVN	C31-C3	3.19	1.58	1.51
26	E6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	a8	602	PEB	CAD-C3D	-3.19	1.38	1.47
26	y8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	dx	403	PEB	CAD-C3D	-3.19	1.38	1.47
26	aF	204	PEB	CAD-C3D	-3.19	1.38	1.47
26	eG	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	lz	401	PEB	CAD-C3D	-3.19	1.38	1.47
26	ft	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	Z4	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	v5	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	f9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bz	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	l2	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	y4	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	H8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	M9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	E4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	A5	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	h8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	g6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	e9	301	PEB	CAD-C3D	-3.19	1.38	1.47
26	D8	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	ct	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	cV	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	O2	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	q4	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	ga	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	S6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	W7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	o9	201	PEB	CAD-C3D	-3.19	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s9	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	by	1002	PEB	CAD-C3D	-3.19	1.38	1.47
26	dD	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	iB	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	T4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	A6	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	cP	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	eW	202	PEB	CAD-C3D	-3.19	1.38	1.47
27	r1	201	CYC	C4B-NB	-3.19	1.31	1.38
27	J1	201	CYC	OB-C4B	3.19	1.29	1.23
27	Y1	201	CYC	OB-C4B	3.19	1.29	1.23
26	N7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	l7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	cR	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	dt	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	gt	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	iF	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	K2	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	b8	1003	PEB	CAD-C3D	-3.19	1.38	1.47
26	aE	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	do	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	li	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	gn	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	kX	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	T3	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	K6	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	bb	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bi	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bl	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	gs	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	e2	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	v3	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	Y5	1003	PEB	CAD-C3D	-3.19	1.38	1.47
26	f8	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	R7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	T7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	w7	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	h9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	aC	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bd	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	eq	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	eA	1001	PEB	CAD-C3D	-3.19	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	x4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	y4	1002	PEB	CAD-C3D	-3.19	1.38	1.47
26	Z6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	y6	203	PEB	CAD-C3D	-3.19	1.38	1.47
26	cX	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	fw	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	z2	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	Y2	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	L4	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	r8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	e9	303	PEB	CAD-C3D	-3.19	1.38	1.47
26	bd	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	cG	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	cT	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	cY	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	dy	401	PEB	CAD-C3D	-3.19	1.38	1.47
26	dz	402	PEB	CAD-C3D	-3.19	1.38	1.47
26	eG	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	hL	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	jM	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	k2	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	h6	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	q8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bg	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bn	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bS	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	cM	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	fc	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	B2	501	PEB	CAD-C3D	-3.19	1.38	1.47
26	b3	501	PEB	CAD-C3D	-3.19	1.38	1.47
26	q4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	G6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	o6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	r9	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	A9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	af	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bz	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	cy	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	dm	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	dK	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	fs	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	hN	201	PEB	CAD-C3D	-3.19	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l5	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	e6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	q2	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	E7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	D9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	aU	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	cX	202	PEB	CAD-C3D	-3.19	1.38	1.47
27	z1	201	CYC	OB-C4B	3.19	1.29	1.23
26	i4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	X7	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	A8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	j9	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	ac	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	ba	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	bW	301	PEB	CAD-C3D	-3.19	1.38	1.47
26	eg	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	eC	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	ly	403	PEB	CAD-C3D	-3.19	1.38	1.47
26	lz	402	PEB	CAD-C3D	-3.19	1.38	1.47
26	I4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	N4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	C6	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	O6	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	j9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	aj	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	am	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	aH	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bB	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	eh	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	eF	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	eS	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	gv	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	h6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	S9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bl	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	bt	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	hO	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	hT	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	k8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	R9	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	bE	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	dD	202	PEB	CAD-C3D	-3.19	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	a6	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	I8	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	cC	1003	PEB	CAD-C3D	-3.19	1.38	1.47
26	r2	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	U2	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	U4	201	PEB	CAD-C3D	-3.19	1.38	1.47
26	b6	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	V8	1001	PEB	CAD-C3D	-3.19	1.38	1.47
26	cU	202	PEB	CAD-C3D	-3.19	1.38	1.47
26	t6	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	u9	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	aC	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	bh	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	di	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ds	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	eF	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	gq	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	gz	303	PEB	CAD-C3D	-3.18	1.38	1.47
26	hB	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	S2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	u3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	aL	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dz	401	PEB	CAD-C3D	-3.18	1.38	1.47
26	hT	204	PEB	CAD-C3D	-3.18	1.38	1.47
26	u5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	f6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	N9	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	fe	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	m3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	X4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	E5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	d9	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	bw	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	dj	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dr	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	ea	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hK	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	w2	203	PEB	CAD-C3D	-3.18	1.38	1.47
26	f4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	w4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	U8	1001	PEB	CAD-C3D	-3.18	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Z9	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	eb	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hZ	402	PEB	CAD-C3D	-3.18	1.38	1.47
26	r2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	D7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	aA	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	eD	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	x3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	P6	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	D8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	M8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	N8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	S8	401	PEB	CAD-C3D	-3.18	1.38	1.47
26	T8	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	Y9	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	aQ	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	cJ	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dX	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	ea	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	lc	201	PEB	CAD-C3D	-3.18	1.38	1.47
27	P1	201	CYC	OB-C4B	3.18	1.29	1.23
26	O4	1002	PEB	CAD-C3D	-3.18	1.38	1.47
26	Q4	203	PEB	CAD-C3D	-3.18	1.38	1.47
26	R4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	t4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	e5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	k8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	l8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	I7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Z9	1007	PEB	CAD-C3D	-3.18	1.38	1.47
26	gk	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	f3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	D6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Y7	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	b9	403	PEB	CAD-C3D	-3.18	1.38	1.47
26	aI	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	cA	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	cV	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	da	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	ef	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ep	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	fl	201	PEB	CAD-C3D	-3.18	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hC	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Z4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	K7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	e9	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	Q8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	ak	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ar	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	aJ	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	eM	1002	PEB	CAD-C3D	-3.18	1.38	1.47
26	gh	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	j8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	aM	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	do	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	i2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	j4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	X5	401	PEB	CAD-C3D	-3.18	1.38	1.47
26	Z5	301	PEB	CAD-C3D	-3.18	1.38	1.47
26	j5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	b8	1002	PEB	CAD-C3D	-3.18	1.38	1.47
26	aI	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	bv	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	dc	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dW	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	eE	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	gj	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	n2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	S4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Z6	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	K8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	bu	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	cb	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	lk	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	gg	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	jN	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	J6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	l6	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	u6	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	H7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	aU	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	bh	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	bq	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	cq	201	PEB	CAD-C3D	-3.18	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dB	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ey	1002	PEB	CAD-C3D	-3.18	1.38	1.47
26	eH	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	go	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	J4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	K4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Q4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	s6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	q7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	b9	404	PEB	CAD-C3D	-3.18	1.38	1.47
26	v8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	O8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	bV	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	le	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hI	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	h2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	s2	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	x2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	M4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	m8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	W8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	h9	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	bv	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	fd	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	fv	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hW	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	N2	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	Q5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	d9	301	PEB	CAD-C3D	-3.18	1.38	1.47
26	C9	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	aB	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	hE	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	D3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	F4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	c4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	B5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	r5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	bo	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	cW	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	kW	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	g2	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	B2	502	PEB	CAD-C3D	-3.18	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a3	1003	PEB	CAD-C3D	-3.18	1.38	1.47
26	44	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	Z5	303	PEB	CAD-C3D	-3.18	1.38	1.47
26	j6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Q7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	cs	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	eI	202	PEB	CAD-C3D	-3.18	1.38	1.47
27	o1	1001	CYC	OB-C4B	3.18	1.29	1.23
26	m2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	G2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	n3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	u4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	t9	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dX	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	lp	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hQ	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	C2	302	PEB	CAD-C3D	-3.18	1.38	1.47
26	Q4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	N5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	w6	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	c9	301	PEB	CAD-C3D	-3.18	1.38	1.47
26	J8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	M2	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	y3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	G4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	34	1003	PEB	CAD-C3D	-3.18	1.38	1.47
26	H5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	V5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	x8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	G8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	bG	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hX	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	H4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	v4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	L5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	c7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	x7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	J8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	y9	1002	PEB	CAD-C3D	-3.18	1.38	1.47
26	aN	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	bY	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	cp	201	PEB	CAD-C3D	-3.18	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	dk	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	dG	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ln	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	hM	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	iH	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	B3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	K4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	h4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	q5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	F6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	c6	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	m7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	K8	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	aT	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	bw	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	cS	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	eB	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	eR	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ll	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	Y4	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	z4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	L6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	U6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	s8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	aT	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dc	203	PEB	CAD-C3D	-3.18	1.38	1.47
26	dn	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	z3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	o4	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	k5	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	ay	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	bP	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	lt	201	PEB	CAD-C3D	-3.18	1.38	1.47
27	Q1	201	CYC	OB-C4B	3.18	1.29	1.23
27	S1	202	CYC	OB-C4B	3.18	1.29	1.23
26	F3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	N6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	V6	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	i6	202	PEB	CAD-C3D	-3.18	1.38	1.47
26	aY	406	PEB	CAD-C3D	-3.18	1.38	1.47
26	bH	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	o2	1001	PEB	CAD-C3D	-3.18	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	E2	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	O3	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	Y3	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	K5	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	P7	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	M8	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	aF	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	dm	201	PEB	CAD-C3D	-3.18	1.38	1.47
26	iG	1001	PEB	CAD-C3D	-3.18	1.38	1.47
26	E4	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	dA	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	fm	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	w2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	A2	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	g3	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	z6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	f7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	z8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	bO	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dp	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eQ	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eU	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	lf	201	PEB	CAD-C3D	-3.17	1.38	1.47
27	W1	201	CYC	OB-C4B	3.17	1.29	1.23
26	o2	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	c6	1003	PEB	CAD-C3D	-3.17	1.38	1.47
26	t8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	k7	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	x8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	aS	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	lu	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	kU	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	v2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	T6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	W6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	w8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	k9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dx	401	PEB	CAD-C3D	-3.17	1.38	1.47
26	es	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eC	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	lr	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ff	201	PEB	CAD-C3D	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fn	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	fo	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	hS	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	Z3	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	Y6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aY	401	PEB	CAD-C3D	-3.17	1.38	1.47
26	dd	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	jL	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	g2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	k2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	Q2	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	V2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	d4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	F6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	v6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	a9	601	PEB	CAD-C3D	-3.17	1.38	1.47
26	c9	302	PEB	CAD-C3D	-3.17	1.38	1.47
26	F8	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	O8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aM	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aP	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	bF	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cc	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dR	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dR	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	J2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	J5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	K6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	x6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	u7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	w8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	B8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	H8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	p9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	E9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ap	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cO	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	eJ	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	gf	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	y2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	L2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	a8	601	PEB	CAD-C3D	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	aK	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	aP	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	gy	303	PEB	CAD-C3D	-3.17	1.38	1.47
26	hJ	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	kQ	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	F2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	W2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	H4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	S4	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	m4	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	Q6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	r7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	B8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	jI	1001	PEB	CAD-C3D	-3.17	1.38	1.47
27	X1	201	CYC	OB-C4B	3.17	1.29	1.23
26	a3	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	T5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	y6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	e7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	L9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aN	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	dQ	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	gi	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	hR	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	s2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	y2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	k4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	O5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	G8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	L8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	bq	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	bs	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	hA	201	PEB	CAD-C3D	-3.17	1.38	1.47
27	a2	901	CYC	OB-C4B	3.17	1.29	1.23
26	b3	502	PEB	CAD-C3D	-3.17	1.38	1.47
26	W6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	z6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	I9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cL	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cR	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ds	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	eK	202	PEB	CAD-C3D	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	j2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	J4	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	x5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	w9	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	bc	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	bu	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dF	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	eq	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eD	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	fj	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	f2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	u2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	p4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	U9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	bU	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dg	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	D2	301	PEB	CAD-C3D	-3.17	1.38	1.47
26	F4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	W5	301	PEB	CAD-C3D	-3.17	1.38	1.47
26	Z7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	h7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	o7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aV	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	bt	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	cw	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cT	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	dr	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ee	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	la	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	kS	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	Z2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	P4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	V4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	24	401	PEB	CAD-C3D	-3.17	1.38	1.47
26	m6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	r6	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	K9	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	lm	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	iA	1001	PEB	CAD-C3D	-3.17	1.38	1.47
27	c1	201	CYC	OB-C4B	3.17	1.29	1.23
27	e1	201	CYC	OB-C4B	3.17	1.29	1.23
26	w3	201	PEB	CAD-C3D	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	m9	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	G9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	at	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aE	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	bM	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cu	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dw	403	PEB	CAD-C3D	-3.17	1.38	1.47
26	k3	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	X6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	V7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	U8	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	P3	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	R5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	a5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	l6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	p6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	s9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	V9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	as	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	aL	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eO	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eQ	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ls	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	fb	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	d5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	g5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	r6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	F8	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	U8	1003	PEB	CAD-C3D	-3.17	1.38	1.47
26	bk	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	bs	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	bR	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cQ	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ed	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	eP	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	gy	301	PEB	CAD-C3D	-3.17	1.38	1.47
26	p2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	v2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	I2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	K2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	i3	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	B4	201	PEB	CAD-C3D	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	S5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	i8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	k6	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	d7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	X8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	jJ	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	q3	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	O6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	E8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	W8	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cm	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	ez	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	T2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	s4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	C5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	C6	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	d8	302	PEB	CAD-C3D	-3.17	1.38	1.47
26	e8	302	PEB	CAD-C3D	-3.17	1.38	1.47
26	aK	1002	PEB	CAD-C3D	-3.17	1.38	1.47
26	cN	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	ek	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	eH	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	R4	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	j5	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	ad	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cD	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dI	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	O2	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	o3	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	l4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	A8	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	r9	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	br	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	lb	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	lt	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	kT	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	t4	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	l9	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	aO	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	de	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	dC	202	PEB	CAD-C3D	-3.17	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	em	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	hF	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	jO	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	I2	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	U5	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	n7	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	y9	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	be	201	PEB	CAD-C3D	-3.17	1.38	1.47
26	cC	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	dF	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	dH	202	PEB	CAD-C3D	-3.17	1.38	1.47
26	fh	1001	PEB	CAD-C3D	-3.17	1.38	1.47
26	q2	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	M2	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	W4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	b4	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	m8	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	I6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	e8	301	PEB	CAD-C3D	-3.16	1.38	1.47
26	hY	401	PEB	CAD-C3D	-3.16	1.38	1.47
26	O9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	aZ	301	PEB	CAD-C3D	-3.16	1.38	1.47
26	cg	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	gb	1002	PEB	CAD-C3D	-3.16	1.38	1.47
26	hP	201	PEB	CAD-C3D	-3.16	1.38	1.47
27	m1	201	CYC	OB-C4B	3.16	1.29	1.23
26	V4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	m5	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	m6	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	L8	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	aB	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	eN	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	G2	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	c5	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	l5	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	s5	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	aD	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	lw	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	I4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	aG	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	aS	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	aZ	302	PEB	CAD-C3D	-3.16	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ca	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	dN	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	ej	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	gu	201	PEB	CAD-C3D	-3.16	1.38	1.47
27	w1	201	CYC	OB-C4B	3.16	1.29	1.23
26	I5	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	y5	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	k6	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	aQ	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	ez	1003	PEB	CAD-C3D	-3.16	1.38	1.47
26	jK	1001	PEB	CAD-C3D	-3.16	1.38	1.47
27	K1	201	CYC	OB-C4B	3.16	1.29	1.23
26	D2	302	PEB	CAD-C3D	-3.16	1.38	1.47
26	bx	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	eY	402	PEB	CAD-C3D	-3.16	1.38	1.47
26	hD	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	c6	1002	PEB	CAD-C3D	-3.16	1.38	1.47
26	J9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	Z9	1003	PEB	CAD-C3D	-3.16	1.38	1.47
26	cW	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	eZ	401	PEB	CAD-C3D	-3.16	1.38	1.47
26	gl	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	ch	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	cM	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dC	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dK	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	dU	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	la	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	kR	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	44	301	PEB	CAD-C3D	-3.16	1.38	1.47
26	b9	401	PEB	CAD-C3D	-3.16	1.38	1.47
26	v9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bm	1002	PEB	CAD-C3D	-3.16	1.38	1.47
26	gw	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	hM	1002	PEB	CAD-C3D	-3.16	1.38	1.47
26	W2	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	N3	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	O4	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	i5	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bZ	303	PEB	CAD-C3D	-3.16	1.38	1.47
26	ff	204	PEB	CAD-C3D	-3.16	1.38	1.47
26	gp	201	PEB	CAD-C3D	-3.16	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a9	603	PEB	CAD-C3D	-3.16	1.38	1.47
26	N8	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	br	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	gc	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	hV	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	w2	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	X3	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	X4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	z4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	i6	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	cx	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dw	402	PEB	CAD-C3D	-3.16	1.38	1.47
26	fq	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	j6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	u8	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bf	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bK	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	dA	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dI	1002	PEB	CAD-C3D	-3.16	1.38	1.47
26	dQ	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dT	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	eK	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	lv	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	C2	301	PEB	CAD-C3D	-3.16	1.38	1.47
26	o4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	b5	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	o5	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	b6	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	d9	303	PEB	CAD-C3D	-3.16	1.38	1.47
26	bQ	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	eT	201	PEB	CAD-C3D	-3.16	1.38	1.47
27	I1	201	CYC	OB-C4B	3.16	1.29	1.23
26	g4	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bN	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	li	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	E6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	P6	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	w9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	du	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dx	404	PEB	CAD-C3D	-3.16	1.38	1.47
26	hH	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	U3	201	PEB	CAD-C3D	-3.16	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A6	1002	PEB	CAD-C3D	-3.16	1.38	1.47
26	b7	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bx	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	cx	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	dp	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	gz	302	PEB	CAD-C3D	-3.16	1.38	1.47
26	l3	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	Y8	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	dL	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dZ	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	e2	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	F2	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	g6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	o6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	T8	301	PEB	CAD-C3D	-3.16	1.38	1.47
26	bm	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	ly	402	PEB	CAD-C3D	-3.16	1.38	1.47
26	G4	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	q6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	u6	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	w3	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	34	1007	PEB	CAD-C3D	-3.16	1.38	1.47
26	Y5	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	aV	201	PEB	CAD-C3D	-3.16	1.38	1.47
27	b1	1001	CYC	OB-C4B	3.16	1.29	1.23
26	V3	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	C4	1001	PEB	CAD-C3D	-3.16	1.38	1.47
26	M4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	u4	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	Q6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	q9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dl	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dq	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	ej	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	es	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	lq	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	P4	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	T6	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	bA	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bC	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	dO	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	hC	202	PEB	CAD-C3D	-3.16	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Q5	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	g8	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	v8	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	x9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	Q9	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	db	201	PEB	CAD-C3D	-3.16	1.38	1.47
27	L1	201	CYC	OB-C4B	3.16	1.29	1.23
27	a1	201	CYC	OB-C4B	3.16	1.29	1.23
26	f8	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	aW	302	PEB	CAD-C3D	-3.16	1.38	1.47
26	fa	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	h5	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	bY	1003	PEB	CAD-C3D	-3.16	1.38	1.47
26	eE	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	eU	202	PEB	CAD-C3D	-3.16	1.38	1.47
26	eW	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	fx	201	PEB	CAD-C3D	-3.16	1.38	1.47
26	t3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	er	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	R2	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	W3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	K7	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	bj	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	m2	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	d3	301	PEB	CAD-C3D	-3.15	1.38	1.47
26	D4	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	I5	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	w5	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	dJ	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	em	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	eT	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	E2	1002	PEB	CAD-C3D	-3.15	1.38	1.47
26	w5	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	C7	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	aN	204	PEB	CAD-C3D	-3.15	1.38	1.47
26	lq	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	R3	201	PEB	CAD-C3D	-3.15	1.38	1.47
27	U1	201	CYC	OB-C4B	3.15	1.29	1.23
27	d2	101	CYC	OB-C4B	3.15	1.29	1.23
26	s3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	l9	201	PEB	CAD-C3D	-3.15	1.38	1.47
27	k1	201	CYC	OB-C4B	3.15	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v6	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	aa	1001	PEB	CAD-C3D	-3.15	1.38	1.47
26	cv	201	PEB	CAD-C3D	-3.15	1.38	1.47
29	d8	303	PVN	C19-C18	-3.15	1.42	1.48
26	C3	1002	PEB	CAD-C3D	-3.15	1.38	1.47
26	y6	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	P8	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	fd	303	PEB	CAD-C3D	-3.15	1.38	1.47
26	gm	1001	PEB	CAD-C3D	-3.15	1.38	1.47
26	A3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	J3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	B6	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	au	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	cU	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	dM	1001	PEB	CAD-C3D	-3.15	1.38	1.47
27	f1	201	CYC	OB-C4B	3.15	1.29	1.23
26	Y2	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	Z8	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	H9	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	M3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	Z5	302	PEB	CAD-C3D	-3.15	1.38	1.47
26	y7	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	by	1001	PEB	CAD-C3D	-3.15	1.38	1.47
26	ce	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	T9	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	lj	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	ge	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	iE	1001	PEB	CAD-C3D	-3.15	1.38	1.47
26	K3	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	s7	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	dt	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	A4	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	w4	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	ev	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	gx	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	A3	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	L4	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	z5	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	H6	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	O7	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	cj	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	eI	201	PEB	CAD-C3D	-3.15	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c3	302	PEB	CAD-C3D	-3.15	1.38	1.47
26	d6	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	Q8	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	aH	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	cP	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	ez	1002	PEB	CAD-C3D	-3.15	1.38	1.47
27	R1	1001	CYC	OB-C4B	3.15	1.29	1.23
27	i1	1001	CYC	OB-C4B	3.15	1.29	1.23
26	aY	402	PEB	CAD-C3D	-3.15	1.38	1.47
26	de	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	q6	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	x9	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	ei	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	fi	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	i3	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	v7	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	I8	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	bs	1003	PEB	CAD-C3D	-3.15	1.38	1.47
27	v1	201	CYC	OB-C4B	3.15	1.29	1.23
26	L3	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	e4	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	cB	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	du	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	F5	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	G5	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	f7	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	b9	402	PEB	CAD-C3D	-3.15	1.38	1.47
26	t2	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	dx	402	PEB	CAD-C3D	-3.15	1.38	1.47
26	dP	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	ew	301	PEB	CAD-C3D	-3.15	1.38	1.47
26	lo	202	PEB	CAD-C3D	-3.15	1.38	1.47
27	d1	1001	CYC	OB-C4B	3.15	1.29	1.23
27	n1	201	CYC	OB-C4B	3.15	1.29	1.23
26	a9	602	PEB	CAD-C3D	-3.15	1.38	1.47
26	n9	201	PEB	CAD-C3D	-3.15	1.38	1.47
26	bO	202	PEB	CAD-C3D	-3.15	1.38	1.47
27	r1	201	CYC	OB-C4B	3.15	1.29	1.23
26	U4	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	bG	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	ey	1003	PEB	CAD-C3D	-3.15	1.38	1.47
26	cK	201	PEB	CAD-C3D	-3.15	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	le	202	PEB	CAD-C3D	-3.15	1.38	1.47
26	S2	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	S3	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	s3	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	P2	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	G3	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	o3	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	G6	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	cS	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	lc	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	n5	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	C7	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	aq	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	iC	1001	PEB	CAD-C3D	-3.14	1.38	1.47
27	H1	201	CYC	OB-C4B	3.14	1.29	1.23
26	du	203	PEB	CAD-C3D	-3.14	1.38	1.47
27	y1	201	CYC	OB-C4B	3.14	1.29	1.23
26	bX	402	PEB	CAD-C3D	-3.14	1.38	1.47
26	Q3	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	c5	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	k8	203	PEB	CAD-C3D	-3.14	1.38	1.47
26	U7	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	eP	203	PEB	CAD-C3D	-3.14	1.38	1.47
26	dZ	1002	PEB	CAD-C3D	-3.14	1.38	1.47
26	R6	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	I7	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	cr	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	cI	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	dM	1002	PEB	CAD-C3D	-3.14	1.38	1.47
26	p6	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	U9	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	cy	1002	PEB	CAD-C3D	-3.14	1.38	1.47
26	hI	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	N6	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	S7	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	k7	1002	PEB	CAD-C3D	-3.14	1.38	1.47
26	z8	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	cE	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	lq	203	PEB	CAD-C3D	-3.14	1.38	1.47
26	hQ	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	F9	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	lb	202	PEB	CAD-C3D	-3.14	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fe	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	fn	1002	PEB	CAD-C3D	-3.14	1.38	1.47
26	X9	401	PEB	CAD-C3D	-3.14	1.38	1.47
27	G1	1001	CYC	OB-C4B	3.14	1.29	1.23
26	U3	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	fk	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	gj	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	hS	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	D5	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	lo	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	lw	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	s8	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	bU	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	A5	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	aA	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	U5	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	aq	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	o5	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	gq	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	O5	202	PEB	CAD-C3D	-3.14	1.38	1.47
27	q1	201	CYC	OB-C4B	3.14	1.29	1.23
26	W4	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	as	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	gu	202	PEB	CAD-C3D	-3.14	1.38	1.47
27	N1	201	CYC	OB-C4B	3.14	1.29	1.23
26	H3	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	d6	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	bA	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	fr	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	fz	301	PEB	CAD-C3D	-3.14	1.38	1.47
26	hZ	401	PEB	CAD-C3D	-3.14	1.38	1.47
26	z7	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	bM	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	lg	201	PEB	CAD-C3D	-3.14	1.38	1.47
26	q7	202	PEB	CAD-C3D	-3.14	1.38	1.47
26	ef	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	cA	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	av	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	I3	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	C5	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	s7	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	gf	202	PEB	CAD-C3D	-3.13	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	iF	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	G9	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	bX	401	PEB	CAD-C3D	-3.13	1.38	1.47
26	ct	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	N2	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	Q9	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	hK	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	ek	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	lm	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	hW	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	iA	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	dU	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	P2	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	W3	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	O9	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	et	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	ey	1001	PEB	CAD-C3D	-3.13	1.38	1.47
26	ls	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	u3	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	cD	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	cI	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	m3	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	bI	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	cw	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	dg	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	hA	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	hF	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	hU	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	h4	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	ah	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	aw	201	PEB	CAD-C3D	-3.13	1.38	1.47
27	s1	201	CYC	OB-C4B	3.13	1.29	1.23
26	m7	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	h7	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	fh	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	hY	402	PEB	CAD-C3D	-3.13	1.38	1.47
27	g1	201	CYC	OB-C4B	3.13	1.29	1.23
26	K5	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	gl	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	e3	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	eP	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	ld	201	PEB	CAD-C3D	-3.13	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H6	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	Y7	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	al	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	u7	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	I9	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	eL	201	PEB	CAD-C3D	-3.13	1.38	1.47
26	fk	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	S5	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	a6	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	w7	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	ft	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	Y9	301	PEB	CAD-C3D	-3.13	1.38	1.47
26	bK	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	eA	1002	PEB	CAD-C3D	-3.13	1.38	1.47
26	fg	202	PEB	CAD-C3D	-3.13	1.38	1.47
26	dO	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	dP	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	eB	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	fp	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	G3	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	S3	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	lk	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	f5	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	t6	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	bS	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	s4	202	PEB	CAD-C3D	-3.12	1.38	1.47
27	z1	201	CYC	C2A-C3A	3.12	1.43	1.36
26	Q3	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	c8	301	PEB	CAD-C3D	-3.12	1.38	1.47
26	lu	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	E3	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	i7	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	fv	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	Y5	1002	PEB	CAD-C3D	-3.12	1.38	1.47
26	o8	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	q5	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	cG	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	g7	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	u5	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	y3	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	dV	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	p3	201	PEB	CAD-C3D	-3.12	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c4	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	ay	1002	PEB	CAD-C3D	-3.12	1.38	1.47
26	hO	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	V6	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	M7	1003	PEB	CAD-C3D	-3.12	1.38	1.47
26	g7	201	PEB	CAD-C3D	-3.12	1.38	1.47
26	K9	1002	PEB	CAD-C3D	-3.12	1.38	1.47
26	cZ	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	U2	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	M9	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	S9	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	gy	302	PEB	CAD-C3D	-3.12	1.38	1.47
26	E9	202	PEB	CAD-C3D	-3.12	1.38	1.47
29	dx	405	PVN	C3-C2	3.12	1.37	1.34
27	O1	201	CYC	OB-C4B	3.12	1.29	1.23
26	Z9	1002	PEB	CAD-C3D	-3.12	1.38	1.47
26	hE	1002	PEB	CAD-C3D	-3.12	1.38	1.47
26	fl	202	PEB	CAD-C3D	-3.12	1.38	1.47
26	G5	202	PEB	CAD-C3D	-3.11	1.38	1.47
26	au	202	PEB	CAD-C3D	-3.11	1.38	1.47
26	gs	202	PEB	CAD-C3D	-3.11	1.38	1.47
26	n6	201	PEB	CAD-C3D	-3.11	1.39	1.47
26	fx	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	G7	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	ao	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	lg	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	gm	1002	PEB	CAD-C3D	-3.11	1.39	1.47
26	g3	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	k3	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	y5	1002	PEB	CAD-C3D	-3.11	1.39	1.47
26	q8	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	p8	201	PEB	CAD-C3D	-3.11	1.39	1.47
26	bQ	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	r8	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	lh	201	PEB	CAD-C3D	-3.11	1.39	1.47
26	gw	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	N4	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	e6	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	da	1002	PEB	CAD-C3D	-3.11	1.39	1.47
26	s5	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	A9	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	W7	202	PEB	CAD-C3D	-3.11	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	gh	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	eh	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	A7	201	PEB	CAD-C3D	-3.11	1.39	1.47
26	eu	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	M3	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	dJ	202	PEB	CAD-C3D	-3.11	1.39	1.47
27	Z1	201	CYC	OB-C4B	3.11	1.29	1.23
26	a3	1002	PEB	CAD-C3D	-3.11	1.39	1.47
26	c3	301	PEB	CAD-C3D	-3.11	1.39	1.47
26	U6	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	t8	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	d8	301	PEB	CAD-C3D	-3.11	1.39	1.47
26	bZ	302	PEB	CAD-C3D	-3.11	1.39	1.47
26	u8	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	cC	1002	PEB	CAD-C3D	-3.11	1.39	1.47
27	u1	1001	CYC	OB-C4B	3.11	1.29	1.23
26	cv	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	Y3	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	aw	202	PEB	CAD-C3D	-3.11	1.39	1.47
26	bC	202	PEB	CAD-C3D	-3.11	1.39	1.47
27	V1	201	CYC	OB-C4B	3.11	1.29	1.23
26	E7	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	ec	201	PEB	CAD-C3D	-3.10	1.39	1.47
26	fb	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	iB	1002	PEB	CAD-C3D	-3.10	1.39	1.47
27	g1	201	CYC	C3D-C2D	3.10	1.46	1.37
27	a2	901	CYC	C2A-C3A	3.10	1.43	1.36
26	db	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	dc	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	A4	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	M5	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	m5	1002	PEB	CAD-C3D	-3.10	1.39	1.47
26	f6	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	A2	1001	PEB	CAD-C3D	-3.10	1.39	1.47
26	cK	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	R2	201	PEB	CAD-C3D	-3.10	1.39	1.47
27	K1	201	CYC	C4A-C3A	3.10	1.52	1.45
26	j7	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	Q7	202	PEB	CAD-C3D	-3.10	1.39	1.47
29	gz	304	PVN	C9-C10	3.10	1.53	1.41
27	m1	201	CYC	C4A-C3A	3.10	1.52	1.45
26	h5	202	PEB	CAD-C3D	-3.10	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	o7	202	PEB	CAD-C3D	-3.10	1.39	1.47
26	O3	1002	PEB	CAD-C3D	-3.10	1.39	1.47
27	I1	201	CYC	C4A-C3A	3.10	1.52	1.45
29	dx	405	PVN	C14-C13	-3.10	1.39	1.45
26	E5	202	PEB	CAD-C3D	-3.09	1.39	1.47
27	g1	201	CYC	C4A-C3A	3.09	1.52	1.45
26	cm	1002	PEB	CAD-C3D	-3.09	1.39	1.47
27	M1	1001	CYC	C2A-C3A	3.09	1.43	1.36
26	C4	1002	PEB	CAD-C3D	-3.09	1.39	1.47
27	S1	201	CYC	C1D-CHD	3.09	1.53	1.41
27	j1	201	CYC	C1D-CHD	3.09	1.53	1.41
26	bY	1002	PEB	CAD-C3D	-3.09	1.39	1.47
26	go	202	PEB	CAD-C3D	-3.09	1.39	1.47
27	t1	201	CYC	C1D-CHD	3.09	1.53	1.41
27	Q1	201	CYC	C4A-C3A	3.09	1.52	1.45
27	S1	201	CYC	C2A-C3A	3.09	1.43	1.36
27	j1	201	CYC	C2A-C3A	3.09	1.43	1.36
26	bE	202	PEB	CAD-C3D	-3.09	1.39	1.47
26	eY	401	PEB	CAD-C3D	-3.09	1.39	1.47
27	H1	201	CYC	C1D-CHD	3.09	1.53	1.41
27	k1	201	CYC	C4A-C3A	3.09	1.52	1.45
27	v1	201	CYC	C1D-CHD	3.09	1.53	1.41
26	cu	202	PEB	CAD-C3D	-3.09	1.39	1.47
27	z1	201	CYC	C1D-CHD	3.09	1.53	1.41
27	J1	201	CYC	C2A-C3A	3.09	1.43	1.36
27	Y1	201	CYC	C2A-C3A	3.09	1.43	1.36
27	e1	201	CYC	C4A-C3A	3.09	1.52	1.45
27	s1	201	CYC	C4A-C3A	3.08	1.52	1.45
27	f1	201	CYC	C4A-C3A	3.08	1.52	1.45
27	r1	201	CYC	C2A-C3A	3.08	1.43	1.36
27	M1	1001	CYC	C1D-CHD	3.08	1.53	1.41
27	c1	201	CYC	C2A-C3A	3.08	1.43	1.36
27	k1	201	CYC	C3D-C2D	3.08	1.46	1.37
27	I1	201	CYC	C3D-C2D	3.08	1.46	1.37
27	w1	201	CYC	C3D-C2D	3.08	1.46	1.37
27	y1	201	CYC	C4A-C3A	3.08	1.52	1.45
27	W1	201	CYC	C3D-C2D	3.08	1.46	1.37
27	p1	201	CYC	C2A-C3A	3.08	1.43	1.36
27	N1	201	CYC	C3D-C2D	3.08	1.46	1.37
27	r1	201	CYC	C1D-CHD	3.08	1.53	1.41
27	t1	201	CYC	C2A-C3A	3.08	1.43	1.36
27	c1	201	CYC	C1D-CHD	3.07	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	J1	201	CYC	C1D-CHD	3.07	1.53	1.41
27	Y1	201	CYC	C1D-CHD	3.07	1.53	1.41
27	a2	902	CYC	C2A-C3A	3.07	1.43	1.36
27	b2	1001	CYC	C2A-C3A	3.07	1.43	1.36
27	a2	901	CYC	C1D-CHD	3.07	1.53	1.41
27	N1	201	CYC	C4A-C3A	3.07	1.52	1.45
27	d1	1001	CYC	C4A-C3A	3.07	1.52	1.45
27	n1	201	CYC	C3D-C2D	3.07	1.46	1.37
27	G1	1001	CYC	C4A-C3A	3.07	1.52	1.45
27	S1	202	CYC	C1D-CHD	3.07	1.53	1.41
27	s1	201	CYC	C3D-C2D	3.07	1.46	1.37
27	U1	201	CYC	C4A-C3A	3.07	1.52	1.45
27	d2	101	CYC	C4A-C3A	3.07	1.52	1.45
27	m1	201	CYC	C3D-C2D	3.07	1.46	1.37
27	L1	201	CYC	C4A-C3A	3.07	1.52	1.45
27	a1	201	CYC	C4A-C3A	3.07	1.52	1.45
27	O1	201	CYC	C4A-C3A	3.07	1.52	1.45
27	h1	201	CYC	C1D-CHD	3.07	1.53	1.41
27	f1	201	CYC	C3D-C2D	3.07	1.46	1.37
27	O1	201	CYC	C3D-C2D	3.07	1.46	1.37
27	p1	201	CYC	C1D-CHD	3.07	1.53	1.41
27	R1	1001	CYC	C4A-C3A	3.06	1.52	1.45
27	i1	1001	CYC	C4A-C3A	3.06	1.52	1.45
27	U1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	d2	101	CYC	C3D-C2D	3.06	1.46	1.37
27	d1	1001	CYC	C3D-C2D	3.06	1.46	1.37
27	L1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	a1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	R1	1001	CYC	C3D-C2D	3.06	1.46	1.37
27	i1	1001	CYC	C3D-C2D	3.06	1.46	1.37
27	K1	201	CYC	C3D-C2D	3.06	1.46	1.37
29	hZ	403	PVN	C14-C13	-3.06	1.39	1.45
27	h1	201	CYC	C2A-C3A	3.06	1.43	1.36
27	n1	201	CYC	C4A-C3A	3.06	1.52	1.45
27	W1	201	CYC	C4A-C3A	3.06	1.52	1.45
27	H1	201	CYC	C2A-C3A	3.06	1.43	1.36
27	X1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	e1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	V1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	y1	201	CYC	C3D-C2D	3.06	1.46	1.37
27	a2	902	CYC	C1D-CHD	3.06	1.53	1.41
27	b2	1001	CYC	C1D-CHD	3.06	1.53	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b1	1001	CYC	C4A-C3A	3.06	1.52	1.45
26	bL	202	PEB	C3C-C4C	3.06	1.46	1.42
29	b9	405	PVN	C14-C13	-3.06	1.39	1.45
27	b1	1001	CYC	C3D-C2D	3.05	1.46	1.37
27	q1	201	CYC	C4A-C3A	3.05	1.52	1.45
29	ly	404	PVN	C19-C18	-3.05	1.42	1.48
27	X1	201	CYC	C4A-C3A	3.05	1.52	1.45
27	q1	201	CYC	C3D-C2D	3.05	1.46	1.37
29	b8	1004	PVN	C14-C13	-3.05	1.39	1.45
27	v1	201	CYC	C2A-C3A	3.05	1.43	1.36
27	Z1	201	CYC	C3D-C2D	3.05	1.46	1.37
27	V1	201	CYC	C4A-C3A	3.05	1.52	1.45
27	Z1	201	CYC	C4A-C3A	3.05	1.52	1.45
27	o1	1001	CYC	C3D-C2D	3.05	1.46	1.37
27	u1	1001	CYC	C3D-C2D	3.04	1.46	1.37
27	G1	1001	CYC	C3D-C2D	3.04	1.46	1.37
27	o1	1001	CYC	C4A-C3A	3.04	1.52	1.45
27	u1	1001	CYC	C4A-C3A	3.04	1.52	1.45
29	hY	404	PVN	C14-C13	-3.04	1.39	1.45
29	U8	1004	PVN	C19-C18	-3.04	1.42	1.48
29	34	1004	PVN	C14-C13	-3.04	1.39	1.45
29	Y5	1004	PVN	C14-C13	-3.04	1.39	1.45
27	Q1	201	CYC	C3D-C2D	3.04	1.46	1.37
27	w1	201	CYC	C4A-C3A	3.04	1.52	1.45
27	P1	201	CYC	C3D-C2D	3.04	1.46	1.37
27	S1	202	CYC	C2A-C3A	3.04	1.43	1.36
29	Z9	1004	PVN	C19-C18	-3.03	1.42	1.48
26	v3	202	PEB	C3C-C4C	3.03	1.46	1.42
27	P1	201	CYC	C4A-C3A	3.03	1.52	1.45
26	n3	202	PEB	C3C-C4C	3.03	1.46	1.42
29	hY	404	PVN	C19-C18	-3.03	1.42	1.48
26	R3	202	PEB	C3C-C4C	3.02	1.46	1.42
26	i3	203	PEB	C3C-C4C	3.02	1.46	1.42
26	j4	202	PEB	C3C-C4C	3.02	1.46	1.42
26	cn	201	PEB	C3C-C4C	3.02	1.46	1.42
26	t5	202	PEB	C3C-C4C	3.01	1.46	1.42
26	en	202	PEB	C3C-C4C	3.01	1.46	1.42
26	cb	202	PEB	C3C-C4C	3.00	1.46	1.42
26	L9	202	PEB	C3C-C4C	3.00	1.46	1.42
26	az	202	PEB	C3C-C4C	3.00	1.46	1.42
26	lo	203	PEB	C3C-C4C	3.00	1.46	1.42
26	n4	202	PEB	C3C-C4C	3.00	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B9	202	PEB	C3C-C4C	3.00	1.46	1.42
26	y8	202	PEB	C3C-C4C	3.00	1.46	1.42
26	eX	201	PEB	C3C-C4C	3.00	1.46	1.42
26	ga	202	PEB	C3C-C4C	3.00	1.46	1.42
27	f1	201	CYC	O2A-CGA	-3.00	1.20	1.30
27	g1	201	CYC	O2A-CGA	-3.00	1.20	1.30
26	hG	201	PEB	C3C-C4C	3.00	1.46	1.42
27	L1	201	CYC	O2A-CGA	-3.00	1.20	1.30
26	eJ	202	PEB	C3C-C4C	3.00	1.46	1.42
26	Z2	202	PEB	C3C-C4C	3.00	1.46	1.42
27	b1	1001	CYC	O2A-CGA	-3.00	1.20	1.30
26	m5	1003	PEB	C3C-C4C	3.00	1.46	1.42
26	e7	202	PEB	C3C-C4C	2.99	1.46	1.42
26	ah	202	PEB	C3C-C4C	2.99	1.46	1.42
29	eY	403	PVN	C15-C16	2.99	1.45	1.38
26	H7	202	PEB	C3C-C4C	2.99	1.46	1.42
26	hV	202	PEB	C3C-C4C	2.99	1.46	1.42
26	B4	202	PEB	C3C-C4C	2.99	1.46	1.42
26	F3	202	PEB	C3C-C4C	2.99	1.46	1.42
26	cB	202	PEB	C3C-C4C	2.99	1.46	1.42
26	kS	1002	PEB	C3C-C4C	2.99	1.46	1.42
26	N3	202	PEB	C3C-C4C	2.99	1.46	1.42
26	34	1002	PEB	C3C-C4C	2.99	1.46	1.42
27	q1	201	CYC	O2A-CGA	-2.99	1.20	1.30
29	34	1004	PVN	C19-C18	-2.99	1.42	1.48
29	Y5	1004	PVN	C19-C18	-2.99	1.42	1.48
27	y1	201	CYC	O2A-CGA	-2.99	1.20	1.30
26	ld	202	PEB	C3C-C4C	2.99	1.46	1.42
26	ln	202	PEB	C3C-C4C	2.99	1.46	1.42
27	K1	201	CYC	O2A-CGA	-2.99	1.20	1.30
26	L3	202	PEB	C3C-C4C	2.99	1.46	1.42
26	gk	202	PEB	C3C-C4C	2.99	1.46	1.42
27	e1	201	CYC	O2A-CGA	-2.99	1.20	1.30
26	a7	202	PEB	C3C-C4C	2.99	1.46	1.42
27	w1	201	CYC	O2A-CGA	-2.99	1.20	1.30
26	bN	202	PEB	C3C-C4C	2.99	1.46	1.42
26	lf	202	PEB	C3C-C4C	2.99	1.46	1.42
27	u1	1001	CYC	O2A-CGA	-2.98	1.20	1.30
26	F5	202	PEB	C3C-C4C	2.98	1.46	1.42
27	G1	1001	CYC	O2A-CGA	-2.98	1.20	1.30
26	cY	202	PEB	C3C-C4C	2.98	1.46	1.42
29	gz	304	PVN	C1-C2	2.98	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ea	203	PEB	C3C-C4C	2.98	1.46	1.42
26	cs	202	PEB	C3C-C4C	2.98	1.46	1.42
26	z3	202	PEB	C3C-C4C	2.98	1.46	1.42
26	co	201	PEB	C3C-C4C	2.98	1.46	1.42
29	lz	403	PVN	C19-C18	-2.98	1.42	1.48
26	ei	202	PEB	C3C-C4C	2.98	1.46	1.42
26	ev	202	PEB	C3C-C4C	2.98	1.46	1.42
26	hH	202	PEB	C3C-C4C	2.98	1.46	1.42
29	A2	1004	PVN	C31-C3	2.98	1.57	1.51
29	a3	1004	PVN	C31-C3	2.98	1.57	1.51
29	hZ	403	PVN	C19-C18	-2.98	1.42	1.48
26	y7	202	PEB	C3C-C4C	2.98	1.46	1.42
26	dd	202	PEB	C3C-C4C	2.98	1.46	1.42
26	kX	1002	PEB	C3C-C4C	2.98	1.46	1.42
27	Q1	201	CYC	O2A-CGA	-2.98	1.20	1.30
26	D9	202	PEB	C3C-C4C	2.98	1.46	1.42
26	cr	202	PEB	C3C-C4C	2.98	1.46	1.42
26	T2	202	PEB	C3C-C4C	2.98	1.46	1.42
26	n6	202	PEB	C3C-C4C	2.98	1.46	1.42
26	gi	202	PEB	C3C-C4C	2.98	1.46	1.42
26	gp	202	PEB	C3C-C4C	2.98	1.46	1.42
27	k1	201	CYC	O2A-CGA	-2.98	1.20	1.30
27	s1	201	CYC	O2A-CGA	-2.98	1.20	1.30
27	N1	201	CYC	O2A-CGA	-2.98	1.20	1.30
26	cL	202	PEB	C3C-C4C	2.98	1.46	1.42
26	jI	1002	PEB	C3C-C4C	2.98	1.46	1.42
27	X1	201	CYC	O2A-CGA	-2.98	1.20	1.30
27	Z1	201	CYC	O2A-CGA	-2.98	1.20	1.30
26	n8	201	PEB	C3C-C4C	2.97	1.46	1.42
26	Y7	1003	PEB	C3C-C4C	2.97	1.46	1.42
26	B6	202	PEB	C3C-C4C	2.97	1.46	1.42
26	L7	201	PEB	C3C-C4C	2.97	1.46	1.42
27	o1	1001	CYC	O2A-CGA	-2.97	1.20	1.30
27	a1	201	CYC	O2A-CGA	-2.97	1.20	1.30
26	aF	202	PEB	C3C-C4C	2.97	1.46	1.42
26	dL	202	PEB	C3C-C4C	2.97	1.46	1.42
26	kQ	1002	PEB	C3C-C4C	2.97	1.46	1.42
27	V1	201	CYC	O2A-CGA	-2.97	1.20	1.30
26	cF	201	PEB	C3C-C4C	2.97	1.46	1.42
27	O1	201	CYC	O2A-CGA	-2.97	1.20	1.30
26	hX	202	PEB	C3C-C4C	2.97	1.46	1.42
29	eZ	402	PVN	C15-C16	2.97	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F7	201	PEB	C3C-C4C	2.97	1.46	1.42
26	ap	202	PEB	C3C-C4C	2.97	1.46	1.42
26	bB	202	PEB	C3C-C4C	2.97	1.46	1.42
26	hD	202	PEB	C3C-C4C	2.97	1.46	1.42
26	f3	202	PEB	C3C-C4C	2.97	1.46	1.42
27	d1	1001	CYC	O2A-CGA	-2.97	1.20	1.30
27	n1	201	CYC	O2A-CGA	-2.97	1.20	1.30
26	af	202	PEB	C3C-C4C	2.97	1.46	1.42
26	an	201	PEB	C3C-C4C	2.97	1.46	1.42
26	fg	201	PEB	C3C-C4C	2.97	1.46	1.42
26	fj	202	PEB	C3C-C4C	2.97	1.46	1.42
27	W1	201	CYC	O2A-CGA	-2.97	1.20	1.30
26	p5	201	PEB	C3C-C4C	2.97	1.46	1.42
26	al	202	PEB	C3C-C4C	2.97	1.46	1.42
26	eg	202	PEB	C3C-C4C	2.97	1.46	1.42
26	gg	202	PEB	C3C-C4C	2.97	1.46	1.42
27	U1	201	CYC	O2A-CGA	-2.97	1.20	1.30
27	d2	101	CYC	O2A-CGA	-2.97	1.20	1.30
26	jN	1002	PEB	C3C-C4C	2.97	1.46	1.42
26	dY	202	PEB	C3C-C4C	2.97	1.46	1.42
26	cH	201	PEB	C3C-C4C	2.97	1.46	1.42
26	dV	202	PEB	C3C-C4C	2.97	1.46	1.42
26	jO	1002	PEB	C3C-C4C	2.97	1.46	1.42
26	x3	202	PEB	C3C-C4C	2.97	1.46	1.42
26	R5	202	PEB	C3C-C4C	2.97	1.46	1.42
26	d7	202	PEB	C3C-C4C	2.97	1.46	1.42
26	fw	202	PEB	C3C-C4C	2.96	1.46	1.42
26	C8	202	PEB	C3C-C4C	2.96	1.46	1.42
26	T3	202	PEB	C3C-C4C	2.96	1.46	1.42
26	D5	202	PEB	C3C-C4C	2.96	1.46	1.42
26	eV	202	PEB	C3C-C4C	2.96	1.46	1.42
27	I1	201	CYC	O2A-CGA	-2.96	1.20	1.30
26	r7	202	PEB	C3C-C4C	2.96	1.46	1.42
26	P9	202	PEB	C3C-C4C	2.96	1.46	1.42
26	gx	202	PEB	C3C-C4C	2.96	1.46	1.42
27	R1	1001	CYC	O2A-CGA	-2.96	1.20	1.30
27	i1	1001	CYC	O2A-CGA	-2.96	1.20	1.30
26	cj	202	PEB	C3C-C4C	2.96	1.46	1.42
26	kU	1002	PEB	C3C-C4C	2.96	1.46	1.42
26	bQ	203	PEB	C3C-C4C	2.96	1.46	1.42
27	P1	201	CYC	O2A-CGA	-2.96	1.20	1.30
26	D3	202	PEB	C3C-C4C	2.96	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	gn	202	PEB	C3C-C4C	2.96	1.46	1.42
27	m1	201	CYC	O2A-CGA	-2.96	1.20	1.30
26	z7	202	PEB	C3C-C4C	2.96	1.46	1.42
26	r4	201	PEB	C3C-C4C	2.96	1.46	1.42
26	F9	202	PEB	C3C-C4C	2.96	1.46	1.42
26	lr	202	PEB	C3C-C4C	2.96	1.46	1.42
26	gr	201	PEB	C3C-C4C	2.96	1.46	1.42
26	iD	1002	PEB	C3C-C4C	2.96	1.46	1.42
26	B7	201	PEB	C3C-C4C	2.96	1.46	1.42
26	T9	202	PEB	C3C-C4C	2.96	1.46	1.42
26	B5	202	PEB	C3C-C4C	2.96	1.46	1.42
26	bV	202	PEB	C3C-C4C	2.96	1.46	1.42
26	H9	202	PEB	C3C-C4C	2.96	1.46	1.42
26	di	202	PEB	C3C-C4C	2.96	1.46	1.42
26	ab	202	PEB	C3C-C4C	2.96	1.46	1.42
26	dh	202	PEB	C3C-C4C	2.96	1.46	1.42
26	dl	202	PEB	C3C-C4C	2.96	1.46	1.42
26	hR	202	PEB	C3C-C4C	2.96	1.46	1.42
26	h2	202	PEB	C3C-C4C	2.95	1.46	1.42
26	N5	202	PEB	C3C-C4C	2.95	1.46	1.42
26	V9	202	PEB	C3C-C4C	2.95	1.46	1.42
26	fi	202	PEB	C3C-C4C	2.95	1.46	1.42
26	t7	202	PEB	C3C-C4C	2.95	1.46	1.42
26	jL	1002	PEB	C3C-C4C	2.95	1.46	1.42
26	p2	202	PEB	C3C-C4C	2.95	1.46	1.42
26	X6	202	PEB	C3C-C4C	2.95	1.46	1.42
26	cJ	202	PEB	C3C-C4C	2.95	1.46	1.42
26	kW	1002	PEB	C3C-C4C	2.95	1.46	1.42
26	v4	202	PEB	C3C-C4C	2.95	1.46	1.42
26	v5	202	PEB	C3C-C4C	2.95	1.46	1.42
26	av	202	PEB	C3C-C4C	2.95	1.46	1.42
26	cq	202	PEB	C3C-C4C	2.95	1.46	1.42
26	fm	202	PEB	C3C-C4C	2.95	1.46	1.42
26	H2	201	PEB	C3C-C4C	2.95	1.46	1.42
26	g4	202	PEB	C3C-C4C	2.95	1.46	1.42
26	cd	202	PEB	C3C-C4C	2.95	1.46	1.42
26	B1	301	PEB	C3C-C4C	2.95	1.46	1.42
26	V5	202	PEB	C3C-C4C	2.95	1.46	1.42
26	R9	202	PEB	C3C-C4C	2.95	1.46	1.42
26	at	202	PEB	C3C-C4C	2.95	1.46	1.42
26	lh	202	PEB	C3C-C4C	2.95	1.46	1.42
26	ff	202	PEB	C3C-C4C	2.95	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fo	202	PEB	C3C-C4C	2.95	1.46	1.42
26	A2	1003	PEB	C3C-C4C	2.95	1.46	1.42
26	B3	202	PEB	C3C-C4C	2.95	1.46	1.42
26	P5	201	PEB	C3C-C4C	2.95	1.46	1.42
26	p8	202	PEB	C3C-C4C	2.95	1.46	1.42
29	C2	303	PVN	C18-C17	2.95	1.43	1.36
26	D7	202	PEB	C3C-C4C	2.95	1.46	1.42
26	ar	202	PEB	C3C-C4C	2.95	1.46	1.42
26	cE	202	PEB	C3C-C4C	2.95	1.46	1.42
26	hP	202	PEB	C3C-C4C	2.95	1.46	1.42
26	jM	1002	PEB	C3C-C4C	2.95	1.46	1.42
26	eL	202	PEB	C3C-C4C	2.95	1.46	1.42
26	fu	201	PEB	C3C-C4C	2.95	1.46	1.42
26	hN	202	PEB	C3C-C4C	2.95	1.46	1.42
29	ey	1004	PVN	C14-C13	-2.95	1.39	1.45
26	V3	202	PEB	C3C-C4C	2.94	1.46	1.42
26	hB	202	PEB	C3C-C4C	2.94	1.46	1.42
26	l2	202	PEB	C3C-C4C	2.94	1.46	1.42
26	P7	202	PEB	C3C-C4C	2.94	1.46	1.42
26	bP	202	PEB	C3C-C4C	2.94	1.46	1.42
26	H3	202	PEB	C3C-C4C	2.94	1.46	1.42
28	eR	203	PUB	CHC-C1D	2.94	1.60	1.53
29	c3	303	PVN	C18-C17	2.94	1.43	1.36
26	X2	202	PEB	C3C-C4C	2.94	1.46	1.42
26	kR	1002	PEB	C3C-C4C	2.94	1.46	1.42
26	kT	1002	PEB	C3C-C4C	2.94	1.46	1.42
26	j2	202	PEB	C3C-C4C	2.94	1.46	1.42
26	J3	202	PEB	C3C-C4C	2.94	1.46	1.42
26	h3	201	PEB	C3C-C4C	2.94	1.46	1.42
26	r3	202	PEB	C3C-C4C	2.94	1.46	1.42
27	d1	1001	CYC	C1B-C2B	2.94	1.50	1.45
26	p3	202	PEB	C3C-C4C	2.94	1.46	1.42
26	R6	202	PEB	C3C-C4C	2.94	1.46	1.42
26	N7	202	PEB	C3C-C4C	2.94	1.46	1.42
27	H1	201	CYC	C3D-C2D	2.94	1.46	1.37
26	jJ	1002	PEB	C3C-C4C	2.94	1.46	1.42
26	T7	202	PEB	C3C-C4C	2.94	1.46	1.42
26	bD	202	PEB	C3C-C4C	2.94	1.46	1.42
26	eB	203	PEB	C3C-C4C	2.94	1.46	1.42
26	lp	202	PEB	C3C-C4C	2.94	1.46	1.42
26	N9	202	PEB	C3C-C4C	2.94	1.46	1.42
26	gd	201	PEB	C3C-C4C	2.94	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f2	202	PEB	C3C-C4C	2.94	1.46	1.42
26	l4	202	PEB	C3C-C4C	2.94	1.46	1.42
26	J9	202	PEB	C3C-C4C	2.94	1.46	1.42
26	h8	202	PEB	C3C-C4C	2.94	1.46	1.42
26	R7	202	PEB	C3C-C4C	2.94	1.46	1.42
26	fy	201	PEB	C3C-C4C	2.94	1.46	1.42
26	iC	1002	PEB	C3C-C4C	2.94	1.46	1.42
26	n2	202	PEB	C3C-C4C	2.94	1.46	1.42
26	L2	202	PEB	C3C-C4C	2.94	1.46	1.42
26	p7	201	PEB	C3C-C4C	2.94	1.46	1.42
27	b1	1001	CYC	C1B-C2B	2.94	1.50	1.45
26	J6	202	PEB	C3C-C4C	2.94	1.46	1.42
26	v9	202	PEB	C3C-C4C	2.94	1.46	1.42
26	ge	202	PEB	C3C-C4C	2.94	1.46	1.42
27	a2	902	CYC	C3D-C2D	2.94	1.46	1.37
27	b2	1001	CYC	C3D-C2D	2.94	1.46	1.37
26	v7	202	PEB	C3C-C4C	2.93	1.46	1.42
26	fc	202	PEB	C3C-C4C	2.93	1.46	1.42
26	r5	202	PEB	C3C-C4C	2.93	1.46	1.42
26	z5	202	PEB	C3C-C4C	2.93	1.46	1.42
27	Q1	201	CYC	C1B-C2B	2.93	1.50	1.45
27	K1	201	CYC	C1B-C2B	2.93	1.50	1.45
27	p1	201	CYC	C3D-C2D	2.93	1.46	1.37
26	er	202	PEB	C3C-C4C	2.93	1.46	1.42
28	eF	203	PUB	CHC-C1D	2.93	1.60	1.53
27	J1	201	CYC	C3D-C2D	2.93	1.46	1.37
27	Y1	201	CYC	C3D-C2D	2.93	1.46	1.37
26	S5	203	PEB	C3C-C4C	2.93	1.46	1.42
26	V7	202	PEB	C3C-C4C	2.93	1.46	1.42
26	W3	203	PEB	C3C-C4C	2.93	1.46	1.42
26	L5	202	PEB	C3C-C4C	2.93	1.46	1.42
26	ee	202	PEB	C3C-C4C	2.93	1.46	1.42
27	t1	201	CYC	C3D-C2D	2.93	1.46	1.37
26	J5	202	PEB	C3C-C4C	2.93	1.46	1.42
26	n7	202	PEB	C3C-C4C	2.93	1.46	1.42
26	df	202	PEB	C3C-C4C	2.93	1.46	1.42
26	gv	202	PEB	C3C-C4C	2.93	1.46	1.42
28	ez	1006	PUB	CHC-C1D	2.93	1.60	1.53
26	ep	202	PEB	C3C-C4C	2.93	1.46	1.42
26	hL	202	PEB	C3C-C4C	2.93	1.46	1.42
26	jP	1002	PEB	C3C-C4C	2.93	1.46	1.42
27	f1	201	CYC	C1B-C2B	2.93	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ad	202	PEB	C3C-C4C	2.93	1.46	1.42
26	p4	202	PEB	C3C-C4C	2.93	1.46	1.42
28	hY	405	PUB	CHC-C1D	2.92	1.60	1.53
26	V2	202	PEB	C3C-C4C	2.92	1.46	1.42
26	ll	202	PEB	C3C-C4C	2.92	1.46	1.42
26	gt	202	PEB	C3C-C4C	2.92	1.46	1.42
27	U1	201	CYC	C1B-C2B	2.92	1.50	1.45
27	d2	101	CYC	C1B-C2B	2.92	1.50	1.45
27	a2	901	CYC	C3D-C2D	2.92	1.46	1.37
27	O1	201	CYC	C1B-C2B	2.92	1.50	1.45
26	j3	201	PEB	C3C-C4C	2.92	1.46	1.42
26	l7	202	PEB	C3C-C4C	2.92	1.46	1.42
26	bT	201	PEB	C3C-C4C	2.92	1.46	1.42
26	P3	202	PEB	C3C-C4C	2.92	1.46	1.42
26	aD	202	PEB	C3C-C4C	2.92	1.46	1.42
26	iE	1002	PEB	C3C-C4C	2.92	1.46	1.42
27	h1	201	CYC	C3D-C2D	2.92	1.46	1.37
26	cp	202	PEB	C3C-C4C	2.92	1.46	1.42
28	f3	203	PUB	CHC-C1D	2.92	1.60	1.53
26	34	1001	PEB	C3C-C4C	2.92	1.46	1.42
28	L7	202	PUB	CHC-C1D	2.92	1.60	1.53
27	n1	201	CYC	C1B-C2B	2.92	1.50	1.45
27	c1	201	CYC	C3D-C2D	2.92	1.46	1.37
28	n5	203	PUB	CHC-C1D	2.92	1.60	1.53
28	F9	203	PUB	CHC-C1D	2.92	1.60	1.53
27	S1	201	CYC	C3D-C2D	2.92	1.46	1.37
27	j1	201	CYC	C3D-C2D	2.92	1.46	1.37
28	ly	406	PUB	CHC-C1D	2.92	1.60	1.53
28	lz	405	PUB	CHC-C1D	2.92	1.60	1.53
26	fs	202	PEB	C3C-C4C	2.92	1.46	1.42
27	I1	201	CYC	C1B-C2B	2.92	1.50	1.45
28	fq	203	PUB	CHC-C1D	2.92	1.60	1.53
28	z6	203	PUB	CHC-C1D	2.92	1.60	1.53
26	bF	202	PEB	C3C-C4C	2.92	1.46	1.42
28	er	203	PUB	CHC-C1D	2.92	1.60	1.53
27	N1	201	CYC	C1B-C2B	2.92	1.50	1.45
28	e8	304	PUB	CHC-C1D	2.92	1.60	1.53
28	bB	203	PUB	CHC-C1D	2.91	1.60	1.53
27	u1	1001	CYC	C1B-C2B	2.91	1.50	1.45
27	w1	201	CYC	C1B-C2B	2.91	1.50	1.45
27	W1	201	CYC	C1B-C2B	2.91	1.50	1.45
28	d3	304	PUB	CHC-C1D	2.91	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	cJ	203	PUB	CHC-C1D	2.91	1.60	1.53
26	Z7	202	PEB	C3C-C4C	2.91	1.46	1.42
26	lw	203	PEB	C3C-C4C	2.91	1.46	1.42
28	R6	203	PUB	CHC-C1D	2.91	1.60	1.53
26	hT	202	PEB	C3C-C4C	2.91	1.46	1.42
27	r1	201	CYC	C3D-C2D	2.91	1.46	1.37
27	o1	1001	CYC	C1B-C2B	2.91	1.50	1.45
26	cf	201	PEB	C3C-C4C	2.91	1.46	1.42
26	dj	202	PEB	C3C-C4C	2.91	1.46	1.42
28	H6	203	PUB	CHC-C1D	2.91	1.60	1.53
28	di	203	PUB	CHC-C1D	2.91	1.60	1.53
26	cl	202	PEB	C3C-C4C	2.91	1.46	1.42
28	cQ	202	PUB	CHC-C1D	2.91	1.60	1.53
26	el	202	PEB	C3C-C4C	2.91	1.46	1.42
26	hJ	202	PEB	C3C-C4C	2.91	1.46	1.42
26	bJ	202	PEB	C3C-C4C	2.91	1.46	1.42
26	ch	202	PEB	C3C-C4C	2.91	1.46	1.42
28	ep	203	PUB	CHC-C1D	2.91	1.60	1.53
28	fm	203	PUB	CHC-C1D	2.91	1.60	1.53
26	J7	201	PEB	C3C-C4C	2.91	1.46	1.42
28	V5	203	PUB	CHC-C1D	2.91	1.60	1.53
28	bJ	203	PUB	CHC-C1D	2.91	1.60	1.53
26	jK	1002	PEB	C3C-C4C	2.91	1.46	1.42
27	H1	201	CYC	C4C-NC	-2.91	1.31	1.37
28	eP	204	PUB	CHC-C1D	2.91	1.60	1.53
27	S1	202	CYC	C3D-C2D	2.91	1.46	1.37
28	t4	203	PUB	CHC-C1D	2.91	1.60	1.53
28	bn	202	PUB	CHC-C1D	2.91	1.60	1.53
28	dT	203	PUB	CHC-C1D	2.91	1.60	1.53
28	b7	202	PUB	CHC-C1D	2.91	1.60	1.53
28	Y9	304	PUB	CHC-C1D	2.91	1.60	1.53
28	gy	305	PUB	CHC-C1D	2.91	1.60	1.53
28	t9	203	PUB	CHC-C1D	2.91	1.60	1.53
28	R2	203	PUB	CHC-C1D	2.91	1.60	1.53
28	cN	202	PUB	CHC-C1D	2.91	1.60	1.53
28	gp	203	PUB	CHC-C1D	2.91	1.60	1.53
26	Z3	202	PEB	C3C-C4C	2.90	1.46	1.42
26	e4	202	PEB	C3C-C4C	2.90	1.46	1.42
28	en	203	PUB	CHC-C1D	2.90	1.60	1.53
26	ec	202	PEB	C3C-C4C	2.90	1.46	1.42
28	hZ	405	PUB	CHC-C1D	2.90	1.60	1.53
26	n5	202	PEB	C3C-C4C	2.90	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dd	203	PUB	CHC-C1D	2.90	1.60	1.53
28	dL	203	PUB	CHC-C1D	2.90	1.60	1.53
28	D5	203	PUB	CHC-C1D	2.90	1.60	1.53
28	X6	203	PUB	CHC-C1D	2.90	1.60	1.53
28	c8	305	PUB	CHC-C1D	2.90	1.60	1.53
28	dx	407	PUB	CHC-C1D	2.90	1.60	1.53
26	eN	202	PEB	C3C-C4C	2.90	1.46	1.42
28	r9	203	PUB	CHC-C1D	2.90	1.60	1.53
26	bH	202	PEB	C3C-C4C	2.90	1.46	1.42
26	kV	1002	PEB	C3C-C4C	2.90	1.46	1.42
27	m1	201	CYC	C1B-C2B	2.90	1.50	1.45
28	z5	203	PUB	CHC-C1D	2.90	1.60	1.53
28	lb	203	PUB	CHC-C1D	2.90	1.60	1.53
27	z1	201	CYC	C3D-C2D	2.90	1.46	1.37
26	A1	301	PEB	C3C-C4C	2.90	1.46	1.42
28	v3	203	PUB	CHC-C1D	2.90	1.60	1.53
28	H9	203	PUB	CHC-C1D	2.90	1.60	1.53
28	hZ	404	PUB	CHC-C1D	2.90	1.60	1.53
28	Z7	203	PUB	CHC-C1D	2.90	1.60	1.53
26	X7	202	PEB	C3C-C4C	2.90	1.46	1.42
28	N7	203	PUB	CHC-C1D	2.90	1.60	1.53
27	M1	1001	CYC	C3D-C2D	2.90	1.46	1.37
26	t3	202	PEB	C3C-C4C	2.90	1.46	1.42
27	e1	201	CYC	C1B-C2B	2.90	1.50	1.45
28	a3	1005	PUB	CHC-C1D	2.90	1.60	1.53
28	bT	202	PUB	CHC-C1D	2.90	1.60	1.53
28	ld	203	PUB	CHC-C1D	2.90	1.60	1.53
28	ln	203	PUB	CHC-C1D	2.90	1.60	1.53
28	iC	1003	PUB	CHC-C1D	2.90	1.60	1.53
28	gd	202	PUB	CHC-C1D	2.90	1.59	1.53
26	fq	202	PEB	C3C-C4C	2.90	1.46	1.42
28	aP	203	PUB	CHC-C1D	2.90	1.59	1.53
28	bs	1004	PUB	CHC-C1D	2.90	1.59	1.53
28	ec	203	PUB	CHC-C1D	2.90	1.59	1.53
27	L1	201	CYC	C1B-C2B	2.90	1.50	1.45
27	a1	201	CYC	C1B-C2B	2.90	1.50	1.45
28	F3	203	PUB	CHC-C1D	2.90	1.59	1.53
27	G1	1001	CYC	C1B-C2B	2.90	1.50	1.45
27	v1	201	CYC	C3D-C2D	2.90	1.46	1.37
28	L2	203	PUB	CHC-C1D	2.90	1.59	1.53
28	z7	203	PUB	CHC-C1D	2.90	1.59	1.53
28	d8	304	PUB	CHC-C1D	2.90	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R4	203	PUB	CHC-C1D	2.89	1.59	1.53
28	N5	203	PUB	CHC-C1D	2.89	1.59	1.53
27	J1	201	CYC	C4C-NC	-2.89	1.31	1.37
27	Y1	201	CYC	C4C-NC	-2.89	1.31	1.37
28	aZ	304	PUB	CHC-C1D	2.89	1.59	1.53
28	hV	203	PUB	CHC-C1D	2.89	1.59	1.53
26	c7	202	PEB	C3C-C4C	2.89	1.46	1.42
28	gz	306	PUB	CHC-C1D	2.89	1.59	1.53
28	a3	1006	PUB	CHC-C1D	2.89	1.59	1.53
28	j3	202	PUB	CHC-C1D	2.89	1.59	1.53
28	eJ	203	PUB	CHC-C1D	2.89	1.59	1.53
28	jN	1003	PUB	CHC-C1D	2.89	1.59	1.53
28	Z2	203	PUB	CHC-C1D	2.89	1.59	1.53
28	ax	202	PUB	CHC-C1D	2.89	1.59	1.53
27	S1	201	CYC	C4C-NC	-2.89	1.31	1.37
27	j1	201	CYC	C4C-NC	-2.89	1.31	1.37
28	Z9	1006	PUB	CHC-C1D	2.89	1.59	1.53
28	cL	203	PUB	CHC-C1D	2.89	1.59	1.53
27	V1	201	CYC	C1B-C2B	2.89	1.50	1.45
28	ee	203	PUB	CHC-C1D	2.89	1.59	1.53
27	s1	201	CYC	C1B-C2B	2.89	1.50	1.45
28	n2	203	PUB	CHC-C1D	2.89	1.59	1.53
28	V3	203	PUB	CHC-C1D	2.89	1.59	1.53
28	a6	203	PUB	CHC-C1D	2.89	1.59	1.53
26	D4	202	PEB	C3C-C4C	2.89	1.46	1.42
26	li	203	PEB	C3C-C4C	2.89	1.46	1.42
27	P1	201	CYC	C1B-C2B	2.89	1.50	1.45
27	Z1	201	CYC	C1B-C2B	2.89	1.50	1.45
28	p4	203	PUB	CHC-C1D	2.89	1.59	1.53
28	dj	203	PUB	CHC-C1D	2.89	1.59	1.53
28	dt	203	PUB	CHC-C1D	2.89	1.59	1.53
28	kQ	1003	PUB	CHC-C1D	2.89	1.59	1.53
26	A5	203	PEB	C3C-C4C	2.89	1.46	1.42
28	n6	203	PUB	CHC-C1D	2.89	1.59	1.53
28	v6	203	PUB	CHC-C1D	2.89	1.59	1.53
28	dl	203	PUB	CHC-C1D	2.89	1.59	1.53
28	hH	203	PUB	CHC-C1D	2.89	1.59	1.53
27	v1	201	CYC	C4C-NC	-2.89	1.31	1.37
28	aD	203	PUB	CHC-C1D	2.89	1.59	1.53
28	hP	203	PUB	CHC-C1D	2.89	1.59	1.53
28	J9	203	PUB	CHC-C1D	2.89	1.59	1.53
26	x7	202	PEB	C3C-C4C	2.89	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	l6	203	PUB	CHC-C1D	2.89	1.59	1.53
28	r7	203	PUB	CHC-C1D	2.89	1.59	1.53
28	c9	305	PUB	CHC-C1D	2.89	1.59	1.53
28	hJ	203	PUB	CHC-C1D	2.89	1.59	1.53
29	e9	304	PVN	C19-C18	-2.89	1.42	1.48
27	c1	201	CYC	C4C-NC	-2.89	1.31	1.37
26	et	202	PEB	C3C-C4C	2.89	1.46	1.42
28	R9	203	PUB	CHC-C1D	2.89	1.59	1.53
28	br	203	PUB	CHC-C1D	2.89	1.59	1.53
28	dv	202	PUB	CHC-C1D	2.89	1.59	1.53
28	iH	1002	PUB	CHC-C1D	2.89	1.59	1.53
28	D2	305	PUB	CHC-C1D	2.89	1.59	1.53
28	aY	404	PUB	CHC-C1D	2.89	1.59	1.53
28	bD	203	PUB	CHC-C1D	2.89	1.59	1.53
28	cO	203	PUB	CHC-C1D	2.89	1.59	1.53
28	hT	203	PUB	CHC-C1D	2.89	1.59	1.53
28	c6	1004	PUB	CHC-C1D	2.89	1.59	1.53
28	bY	1005	PUB	CHC-C1D	2.89	1.59	1.53
28	eY	404	PUB	CHC-C1D	2.89	1.59	1.53
28	fw	203	PUB	CHC-C1D	2.89	1.59	1.53
28	hR	203	PUB	CHC-C1D	2.89	1.59	1.53
28	f2	203	PUB	CHC-C1D	2.89	1.59	1.53
28	34	1006	PUB	CHC-C1D	2.89	1.59	1.53
28	c7	203	PUB	CHC-C1D	2.89	1.59	1.53
28	s7	203	PUB	CHC-C1D	2.89	1.59	1.53
28	b9	407	PUB	CHC-C1D	2.89	1.59	1.53
28	bN	203	PUB	CHC-C1D	2.89	1.59	1.53
28	gg	203	PUB	CHC-C1D	2.89	1.59	1.53
28	aJ	203	PUB	CHC-C1D	2.89	1.59	1.53
28	eZ	403	PUB	CHC-C1D	2.89	1.59	1.53
28	ga	203	PUB	CHC-C1D	2.89	1.59	1.53
28	gt	203	PUB	CHC-C1D	2.89	1.59	1.53
26	aj	202	PEB	C3C-C4C	2.89	1.46	1.42
28	Z6	203	PUB	CHC-C1D	2.89	1.59	1.53
28	dV	203	PUB	CHC-C1D	2.89	1.59	1.53
28	fc	203	PUB	CHC-C1D	2.89	1.59	1.53
28	iE	1003	PUB	CHC-C1D	2.89	1.59	1.53
28	H5	202	PUB	CHC-C1D	2.89	1.59	1.53
28	aN	203	PUB	CHC-C1D	2.89	1.59	1.53
28	lx	201	PUB	CHC-C1D	2.89	1.59	1.53
28	X2	203	PUB	CHC-C1D	2.88	1.59	1.53
28	p5	202	PUB	CHC-C1D	2.88	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	ll	203	PUB	CHC-C1D	2.88	1.59	1.53
28	t6	203	PUB	CHC-C1D	2.88	1.59	1.53
28	B7	202	PUB	CHC-C1D	2.88	1.59	1.53
28	c9	304	PUB	CHC-C1D	2.88	1.59	1.53
28	v9	203	PUB	CHC-C1D	2.88	1.59	1.53
28	eT	203	PUB	CHC-C1D	2.88	1.59	1.53
28	e8	305	PUB	CHC-C1D	2.88	1.59	1.53
28	e9	306	PUB	CHC-C1D	2.88	1.59	1.53
28	cr	203	PUB	CHC-C1D	2.88	1.59	1.53
28	cs	203	PUB	CHC-C1D	2.88	1.59	1.53
28	lh	203	PUB	CHC-C1D	2.88	1.59	1.53
28	V4	203	PUB	CHC-C1D	2.88	1.59	1.53
28	d9	305	PUB	CHC-C1D	2.88	1.59	1.53
28	cB	203	PUB	CHC-C1D	2.88	1.59	1.53
26	F9	202	PEB	C4D-ND	2.88	1.39	1.35
27	X1	201	CYC	C1B-C2B	2.88	1.50	1.45
28	h8	203	PUB	CHC-C1D	2.88	1.59	1.53
28	r6	203	PUB	CHC-C1D	2.88	1.59	1.53
28	az	203	PUB	CHC-C1D	2.88	1.59	1.53
28	hL	203	PUB	CHC-C1D	2.88	1.59	1.53
28	hN	203	PUB	CHC-C1D	2.88	1.59	1.53
27	g1	201	CYC	C1B-C2B	2.88	1.50	1.45
28	V7	203	PUB	CHC-C1D	2.88	1.59	1.53
28	aH	203	PUB	CHC-C1D	2.88	1.59	1.53
28	dN	203	PUB	CHC-C1D	2.88	1.59	1.53
28	F5	203	PUB	CHC-C1D	2.88	1.59	1.53
28	b8	1005	PUB	CHC-C1D	2.88	1.59	1.53
28	B5	203	PUB	CHC-C1D	2.88	1.59	1.53
28	cp	203	PUB	CHC-C1D	2.88	1.59	1.53
28	Y9	305	PUB	CHC-C1D	2.88	1.59	1.53
28	dD	203	PUB	CHC-C1D	2.88	1.59	1.53
28	gv	203	PUB	CHC-C1D	2.88	1.59	1.53
26	cB	202	PEB	C4D-ND	2.88	1.39	1.35
26	dV	202	PEB	C4D-ND	2.88	1.39	1.35
28	z2	203	PUB	CHC-C1D	2.88	1.59	1.53
28	l3	202	PUB	CHC-C1D	2.88	1.59	1.53
28	T4	202	PUB	CHC-C1D	2.88	1.59	1.53
28	x4	202	PUB	CHC-C1D	2.88	1.59	1.53
28	x5	202	PUB	CHC-C1D	2.88	1.59	1.53
28	aV	203	PUB	CHC-C1D	2.88	1.59	1.53
28	bq	203	PUB	CHC-C1D	2.88	1.59	1.53
28	jK	1003	PUB	CHC-C1D	2.88	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	j2	203	PUB	CHC-C1D	2.88	1.59	1.53
28	F6	203	PUB	CHC-C1D	2.88	1.59	1.53
28	c8	304	PUB	CHC-C1D	2.88	1.59	1.53
28	bp	202	PUB	CHC-C1D	2.88	1.59	1.53
28	bz	203	PUB	CHC-C1D	2.88	1.59	1.53
28	bY	1006	PUB	CHC-C1D	2.88	1.59	1.53
28	dH	203	PUB	CHC-C1D	2.88	1.59	1.53
28	eY	405	PUB	CHC-C1D	2.88	1.59	1.53
28	eZ	404	PUB	CHC-C1D	2.88	1.59	1.53
28	gr	202	PUB	CHC-C1D	2.88	1.59	1.53
28	c3	304	PUB	CHC-C1D	2.88	1.59	1.53
28	cP	203	PUB	CHC-C1D	2.88	1.59	1.53
27	y1	201	CYC	C1B-C2B	2.88	1.50	1.45
27	t1	201	CYC	C4C-NC	-2.88	1.31	1.37
28	A2	1005	PUB	CHC-C1D	2.88	1.59	1.53
28	e7	203	PUB	CHC-C1D	2.88	1.59	1.53
29	aZ	303	PVN	C31-C3	2.88	1.57	1.51
28	ey	1005	PUB	CHC-C1D	2.88	1.59	1.53
26	cz	202	PEB	C3C-C4C	2.88	1.46	1.42
28	C2	304	PUB	CHC-C1D	2.88	1.59	1.53
28	b6	203	PUB	CHC-C1D	2.88	1.59	1.53
28	D7	203	PUB	CHC-C1D	2.88	1.59	1.53
28	y8	203	PUB	CHC-C1D	2.88	1.59	1.53
28	aB	203	PUB	CHC-C1D	2.88	1.59	1.53
28	kW	1003	PUB	CHC-C1D	2.88	1.59	1.53
29	gz	304	PVN	C10-C11	-2.88	1.32	1.35
28	c3	305	PUB	CHC-C1D	2.88	1.59	1.53
28	h3	202	PUB	CHC-C1D	2.88	1.59	1.53
28	X4	203	PUB	CHC-C1D	2.88	1.59	1.53
28	t5	203	PUB	CHC-C1D	2.88	1.59	1.53
28	cY	203	PUB	CHC-C1D	2.88	1.59	1.53
28	df	203	PUB	CHC-C1D	2.88	1.59	1.53
28	dY	203	PUB	CHC-C1D	2.88	1.59	1.53
28	lj	202	PUB	CHC-C1D	2.88	1.59	1.53
28	gx	203	PUB	CHC-C1D	2.88	1.59	1.53
27	z1	201	CYC	C4C-NC	-2.88	1.31	1.37
28	44	304	PUB	CHC-C1D	2.88	1.59	1.53
28	U8	1005	PUB	CHC-C1D	2.88	1.59	1.53
28	bZ	305	PUB	CHC-C1D	2.88	1.59	1.53
28	hG	202	PUB	CHC-C1D	2.88	1.59	1.53
28	hY	406	PUB	CHC-C1D	2.88	1.59	1.53
26	ap	202	PEB	C4D-ND	2.88	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D6	202	PUB	CHC-C1D	2.88	1.59	1.53
28	A8	203	PUB	CHC-C1D	2.88	1.59	1.53
28	bL	203	PUB	CHC-C1D	2.88	1.59	1.53
28	dw	406	PUB	CHC-C1D	2.88	1.59	1.53
28	fy	202	PUB	CHC-C1D	2.88	1.59	1.53
28	p3	203	PUB	CHC-C1D	2.87	1.59	1.53
28	t7	203	PUB	CHC-C1D	2.87	1.59	1.53
28	C8	203	PUB	CHC-C1D	2.87	1.59	1.53
28	T8	304	PUB	CHC-C1D	2.87	1.59	1.53
28	eb	202	PUB	CHC-C1D	2.87	1.59	1.53
26	ax	201	PEB	C3C-C4C	2.87	1.46	1.42
28	cE	203	PUB	CHC-C1D	2.87	1.59	1.53
28	gk	203	PUB	CHC-C1D	2.87	1.59	1.53
28	T8	305	PUB	CHC-C1D	2.87	1.59	1.53
28	U8	1006	PUB	CHC-C1D	2.87	1.59	1.53
28	aF	203	PUB	CHC-C1D	2.87	1.59	1.53
28	bF	203	PUB	CHC-C1D	2.87	1.59	1.53
28	dp	203	PUB	CHC-C1D	2.87	1.59	1.53
27	q1	201	CYC	C1B-C2B	2.87	1.50	1.45
28	l2	203	PUB	CHC-C1D	2.87	1.59	1.53
28	L3	203	PUB	CHC-C1D	2.87	1.59	1.53
28	r4	202	PUB	CHC-C1D	2.87	1.59	1.53
28	r5	203	PUB	CHC-C1D	2.87	1.59	1.53
28	L6	202	PUB	CHC-C1D	2.87	1.59	1.53
28	dX	203	PUB	CHC-C1D	2.87	1.59	1.53
28	cq	203	PUB	CHC-C1D	2.87	1.59	1.53
28	dr	203	PUB	CHC-C1D	2.87	1.59	1.53
28	fs	203	PUB	CHC-C1D	2.87	1.59	1.53
26	g5	202	PEB	C3C-C4C	2.87	1.46	1.42
28	D2	304	PUB	CHC-C1D	2.87	1.59	1.53
28	eg	203	PUB	CHC-C1D	2.87	1.59	1.53
28	H3	203	PUB	CHC-C1D	2.87	1.59	1.53
28	p6	203	PUB	CHC-C1D	2.87	1.59	1.53
28	D3	203	PUB	CHC-C1D	2.87	1.59	1.53
28	r3	203	PUB	CHC-C1D	2.87	1.59	1.53
28	44	305	PUB	CHC-C1D	2.87	1.59	1.53
28	Z5	306	PUB	CHC-C1D	2.87	1.59	1.53
28	P9	203	PUB	CHC-C1D	2.87	1.59	1.53
27	a2	901	CYC	C4C-NC	-2.87	1.31	1.37
28	J6	203	PUB	CHC-C1D	2.87	1.59	1.53
28	y7	203	PUB	CHC-C1D	2.87	1.59	1.53
28	eH	203	PUB	CHC-C1D	2.87	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P2	203	PUB	CHC-C1D	2.87	1.59	1.53
28	o8	203	PUB	CHC-C1D	2.87	1.59	1.53
28	Q8	203	PUB	CHC-C1D	2.87	1.59	1.53
28	p9	203	PUB	CHC-C1D	2.87	1.59	1.53
28	V9	203	PUB	CHC-C1D	2.87	1.59	1.53
28	aZ	305	PUB	CHC-C1D	2.87	1.59	1.53
28	co	202	PUB	CHC-C1D	2.87	1.59	1.53
28	eN	203	PUB	CHC-C1D	2.87	1.59	1.53
28	b8	1006	PUB	CHC-C1D	2.87	1.59	1.53
28	I8	203	PUB	CHC-C1D	2.87	1.59	1.53
28	N9	203	PUB	CHC-C1D	2.87	1.59	1.53
28	ap	203	PUB	CHC-C1D	2.87	1.59	1.53
28	ey	1006	PUB	CHC-C1D	2.87	1.59	1.53
27	h1	201	CYC	C4C-NC	-2.87	1.31	1.37
29	bZ	304	PVN	C31-C3	2.87	1.57	1.51
28	p2	203	PUB	CHC-C1D	2.87	1.59	1.53
28	e6	203	PUB	CHC-C1D	2.87	1.59	1.53
28	K8	203	PUB	CHC-C1D	2.87	1.59	1.53
28	lp	203	PUB	CHC-C1D	2.87	1.59	1.53
28	hX	203	PUB	CHC-C1D	2.87	1.59	1.53
28	jI	1003	PUB	CHC-C1D	2.87	1.59	1.53
28	N4	203	PUB	CHC-C1D	2.87	1.59	1.53
28	J5	203	PUB	CHC-C1D	2.87	1.59	1.53
28	eB	204	PUB	CHC-C1D	2.87	1.59	1.53
28	iD	1003	PUB	CHC-C1D	2.87	1.59	1.53
28	bZ	306	PUB	CHC-C1D	2.87	1.59	1.53
28	fa	202	PUB	CHC-C1D	2.87	1.59	1.53
28	iG	1002	PUB	CHC-C1D	2.87	1.59	1.53
28	J4	203	PUB	CHC-C1D	2.87	1.59	1.53
28	34	1005	PUB	CHC-C1D	2.87	1.59	1.53
27	p1	201	CYC	C4C-NC	-2.87	1.31	1.37
28	L5	203	PUB	CHC-C1D	2.87	1.59	1.53
28	G8	203	PUB	CHC-C1D	2.87	1.59	1.53
28	x9	203	PUB	CHC-C1D	2.87	1.59	1.53
28	L9	203	PUB	CHC-C1D	2.87	1.59	1.53
28	an	202	PUB	CHC-C1D	2.87	1.59	1.53
28	dh	203	PUB	CHC-C1D	2.87	1.59	1.53
28	ly	405	PUB	CHC-C1D	2.87	1.59	1.53
28	lz	404	PUB	CHC-C1D	2.87	1.59	1.53
28	hD	203	PUB	CHC-C1D	2.87	1.59	1.53
28	V2	203	PUB	CHC-C1D	2.87	1.59	1.53
28	n4	203	PUB	CHC-C1D	2.87	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C2	303	PVN	C14-C13	-2.87	1.39	1.45
29	c3	303	PVN	C14-C13	-2.87	1.39	1.45
28	H2	202	PUB	CHC-C1D	2.87	1.59	1.53
28	n7	203	PUB	CHC-C1D	2.87	1.59	1.53
28	el	203	PUB	CHC-C1D	2.87	1.59	1.53
28	lf	203	PUB	CHC-C1D	2.87	1.59	1.53
28	dx	406	PUB	CHC-C1D	2.87	1.59	1.53
28	Z3	203	PUB	CHC-C1D	2.87	1.59	1.53
28	B4	203	PUB	CHC-C1D	2.87	1.59	1.53
28	d7	203	PUB	CHC-C1D	2.87	1.59	1.53
28	x7	203	PUB	CHC-C1D	2.87	1.59	1.53
28	dw	405	PUB	CHC-C1D	2.87	1.59	1.53
28	H4	203	PUB	CHC-C1D	2.87	1.59	1.53
28	Y5	1005	PUB	CHC-C1D	2.87	1.59	1.53
28	fj	203	PUB	CHC-C1D	2.87	1.59	1.53
28	t3	203	PUB	CHC-C1D	2.86	1.59	1.53
28	z3	203	PUB	CHC-C1D	2.86	1.59	1.53
28	n9	202	PUB	CHC-C1D	2.86	1.59	1.53
28	gi	203	PUB	CHC-C1D	2.86	1.59	1.53
28	eR	203	PUB	C1A-NA	2.86	1.39	1.35
28	f8	203	PUB	CHC-C1D	2.86	1.59	1.53
28	u6	203	PUB	CHC-C1D	2.86	1.59	1.53
28	aY	405	PUB	CHC-C1D	2.86	1.59	1.53
28	cz	203	PUB	CHC-C1D	2.86	1.59	1.53
28	eV	203	PUB	CHC-C1D	2.86	1.59	1.53
28	ff	203	PUB	CHC-C1D	2.86	1.59	1.53
28	fo	203	PUB	CHC-C1D	2.86	1.59	1.53
28	gy	306	PUB	CHC-C1D	2.86	1.59	1.53
28	gz	305	PUB	CHC-C1D	2.86	1.59	1.53
27	r1	201	CYC	C4C-NC	-2.86	1.31	1.37
27	k1	201	CYC	C1B-C2B	2.86	1.50	1.45
28	Z4	203	PUB	CHC-C1D	2.86	1.59	1.53
28	v4	203	PUB	CHC-C1D	2.86	1.59	1.53
28	v5	203	PUB	CHC-C1D	2.86	1.59	1.53
28	bo	202	PUB	CHC-C1D	2.86	1.59	1.53
28	eD	203	PUB	CHC-C1D	2.86	1.59	1.53
28	iF	1003	PUB	CHC-C1D	2.86	1.59	1.53
28	kX	1003	PUB	CHC-C1D	2.86	1.59	1.53
28	d6	203	PUB	CHC-C1D	2.86	1.59	1.53
28	v7	203	PUB	CHC-C1D	2.86	1.59	1.53
27	M1	1001	CYC	C4C-NC	-2.86	1.31	1.37
28	l7	203	PUB	CHC-C1D	2.86	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	eL	203	PUB	CHC-C1D	2.86	1.59	1.53
28	ge	203	PUB	CHC-C1D	2.86	1.59	1.53
28	r2	203	PUB	CHC-C1D	2.86	1.59	1.53
28	T2	203	PUB	CHC-C1D	2.86	1.59	1.53
28	R3	203	PUB	CHC-C1D	2.86	1.59	1.53
28	p8	203	PUB	CHC-C1D	2.86	1.59	1.53
28	P7	203	PUB	CHC-C1D	2.86	1.59	1.53
28	gn	203	PUB	CHC-C1D	2.86	1.59	1.53
28	jL	1003	PUB	CHC-C1D	2.86	1.59	1.53
27	a2	902	CYC	C4C-NC	-2.86	1.31	1.37
27	b2	1001	CYC	C4C-NC	-2.86	1.31	1.37
28	L4	203	PUB	CHC-C1D	2.86	1.59	1.53
28	P4	203	PUB	CHC-C1D	2.86	1.59	1.53
28	e9	305	PUB	CHC-C1D	2.86	1.59	1.53
28	w8	203	PUB	CHC-C1D	2.86	1.59	1.53
28	kU	1003	PUB	CHC-C1D	2.86	1.59	1.53
28	B3	203	PUB	CHC-C1D	2.86	1.59	1.53
28	R5	203	PUB	CHC-C1D	2.86	1.59	1.53
28	cR	203	PUB	CHC-C1D	2.86	1.59	1.53
26	B5	202	PEB	C4D-ND	2.86	1.39	1.35
28	T5	202	PUB	CHC-C1D	2.86	1.59	1.53
28	p7	202	PUB	CHC-C1D	2.86	1.59	1.53
28	Z9	1005	PUB	CHC-C1D	2.86	1.59	1.53
28	dF	203	PUB	CHC-C1D	2.86	1.59	1.53
27	R1	1001	CYC	C1B-C2B	2.86	1.50	1.45
27	i1	1001	CYC	C1B-C2B	2.86	1.50	1.45
28	z4	203	PUB	CHC-C1D	2.86	1.59	1.53
28	Y5	1006	PUB	CHC-C1D	2.86	1.59	1.53
28	ei	203	PUB	CHC-C1D	2.86	1.59	1.53
29	gy	304	PVN	C4-N1	-2.86	1.41	1.45
28	x3	203	PUB	CHC-C1D	2.86	1.59	1.53
28	cH	202	PUB	CHC-C1D	2.86	1.59	1.53
27	S1	202	CYC	C4C-NC	-2.86	1.31	1.37
28	C2	305	PUB	CHC-C1D	2.86	1.59	1.53
28	cM	203	PUB	CHC-C1D	2.86	1.59	1.53
28	F2	203	PUB	CHC-C1D	2.86	1.59	1.53
28	bP	203	PUB	CHC-C1D	2.86	1.59	1.53
28	cF	202	PUB	CHC-C1D	2.86	1.59	1.53
28	Z5	305	PUB	CHC-C1D	2.86	1.59	1.53
28	P6	203	PUB	CHC-C1D	2.86	1.59	1.53
28	a7	203	PUB	CHC-C1D	2.86	1.59	1.53
26	ev	202	PEB	C4D-ND	2.86	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	h2	203	PUB	CHC-C1D	2.86	1.59	1.53
28	g8	202	PUB	CHC-C1D	2.86	1.59	1.53
28	lv	202	PUB	CHC-C1D	2.86	1.59	1.53
28	kS	1003	PUB	CHC-C1D	2.86	1.59	1.53
29	gy	304	PVN	O1-C1	-2.86	1.18	1.23
28	P5	202	PUB	CHC-C1D	2.85	1.59	1.53
28	hB	203	PUB	CHC-C1D	2.85	1.59	1.53
28	V6	203	PUB	CHC-C1D	2.85	1.59	1.53
28	T7	203	PUB	CHC-C1D	2.85	1.59	1.53
28	dB	202	PUB	CHC-C1D	2.85	1.59	1.53
28	ez	1005	PUB	CHC-C1D	2.85	1.59	1.53
28	kV	1003	PUB	CHC-C1D	2.85	1.59	1.53
29	c8	303	PVN	C3-C2	2.85	1.37	1.34
28	J7	202	PUB	CHC-C1D	2.85	1.59	1.53
28	kR	1003	PUB	CHC-C1D	2.85	1.59	1.53
28	J2	202	PUB	CHC-C1D	2.85	1.59	1.53
28	et	203	PUB	CHC-C1D	2.85	1.59	1.53
28	lt	203	PUB	CHC-C1D	2.85	1.59	1.53
28	dK	203	PUB	CHC-C1D	2.85	1.59	1.53
28	fi	203	PUB	CHC-C1D	2.85	1.59	1.53
28	aR	203	PUB	CHC-C1D	2.85	1.59	1.53
28	at	203	PUB	CHC-C1D	2.85	1.59	1.53
26	d7	202	PEB	C4D-ND	2.85	1.38	1.35
28	B6	203	PUB	CHC-C1D	2.85	1.59	1.53
28	x6	203	PUB	CHC-C1D	2.85	1.59	1.53
28	fu	202	PUB	CHC-C1D	2.85	1.59	1.53
28	jJ	1003	PUB	CHC-C1D	2.85	1.59	1.53
28	kT	1003	PUB	CHC-C1D	2.85	1.59	1.53
29	e8	303	PVN	C19-C18	-2.85	1.42	1.48
29	44	303	PVN	O1-C1	-2.85	1.18	1.23
29	Z5	304	PVN	O1-C1	-2.85	1.18	1.23
28	D4	203	PUB	CHC-C1D	2.85	1.59	1.53
28	bV	203	PUB	CHC-C1D	2.85	1.59	1.53
28	n8	202	PUB	CHC-C1D	2.85	1.59	1.53
28	z9	203	PUB	CHC-C1D	2.85	1.59	1.53
28	J3	203	PUB	CHC-C1D	2.85	1.59	1.53
28	y6	204	PUB	CHC-C1D	2.85	1.59	1.53
28	aT	203	PUB	CHC-C1D	2.85	1.59	1.53
28	N2	203	PUB	CHC-C1D	2.85	1.59	1.53
28	n3	203	PUB	CHC-C1D	2.85	1.59	1.53
28	x2	202	PUB	CHC-C1D	2.85	1.59	1.53
28	X3	202	PUB	CHC-C1D	2.85	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	gy	304	PVN	C10-C11	-2.85	1.32	1.35
28	N6	203	PUB	CHC-C1D	2.85	1.59	1.53
28	av	203	PUB	CHC-C1D	2.85	1.59	1.53
28	R7	203	PUB	CHC-C1D	2.85	1.59	1.53
28	t2	203	PUB	CHC-C1D	2.84	1.59	1.53
28	T3	203	PUB	CHC-C1D	2.84	1.59	1.53
28	cn	202	PUB	CHC-C1D	2.84	1.59	1.53
26	T3	202	PEB	C4D-ND	2.84	1.38	1.35
28	O8	203	PUB	CHC-C1D	2.84	1.59	1.53
28	ev	203	PUB	CHC-C1D	2.84	1.59	1.53
28	b9	406	PUB	CHC-C1D	2.84	1.59	1.53
28	M8	203	PUB	CHC-C1D	2.84	1.59	1.53
28	dR	203	PUB	CHC-C1D	2.84	1.59	1.53
26	aj	202	PEB	C4D-ND	2.84	1.38	1.35
28	v2	203	PUB	CHC-C1D	2.84	1.59	1.53
28	jO	1003	PUB	CHC-C1D	2.84	1.59	1.53
26	f3	202	PEB	C4D-ND	2.84	1.38	1.35
28	bH	203	PUB	CHC-C1D	2.84	1.59	1.53
28	bR	202	PUB	CHC-C1D	2.84	1.59	1.53
28	dn	203	PUB	CHC-C1D	2.84	1.59	1.53
28	F7	202	PUB	CHC-C1D	2.84	1.59	1.53
28	aL	203	PUB	CHC-C1D	2.84	1.59	1.53
28	A2	1006	PUB	CHC-C1D	2.84	1.59	1.53
28	d3	303	PUB	CHC-C1D	2.84	1.59	1.53
28	B9	203	PUB	CHC-C1D	2.84	1.59	1.53
28	lr	203	PUB	CHC-C1D	2.84	1.59	1.53
28	H7	203	PUB	CHC-C1D	2.84	1.59	1.53
28	eX	202	PUB	CHC-C1D	2.84	1.59	1.53
28	N3	203	PUB	CHC-C1D	2.84	1.59	1.53
26	H3	202	PEB	C4D-ND	2.83	1.38	1.35
26	n8	201	PEB	C4D-ND	2.83	1.38	1.35
28	P3	203	PUB	CHC-C1D	2.83	1.59	1.53
28	E8	203	PUB	CHC-C1D	2.83	1.59	1.53
26	cs	202	PEB	C4D-ND	2.83	1.38	1.35
28	T6	203	PUB	CHC-C1D	2.83	1.59	1.53
28	X7	203	PUB	CHC-C1D	2.83	1.59	1.53
28	F4	203	PUB	CHC-C1D	2.83	1.59	1.53
28	jM	1003	PUB	CHC-C1D	2.83	1.59	1.53
29	gz	304	PVN	O19-C19	-2.83	1.18	1.23
26	L9	202	PEB	C4D-ND	2.83	1.38	1.35
26	eL	202	PEB	C4D-ND	2.83	1.38	1.35
26	cY	202	PEB	C4D-ND	2.83	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ll	202	PEB	C4D-ND	2.83	1.38	1.35
28	jP	1003	PUB	CHC-C1D	2.83	1.59	1.53
29	Z9	1004	PVN	C3-C2	2.83	1.37	1.34
29	ez	1004	PVN	C14-C13	-2.83	1.39	1.45
29	dw	404	PVN	C14-C13	-2.83	1.39	1.45
26	bH	202	PEB	C4D-ND	2.83	1.38	1.35
29	dx	405	PVN	C19-C18	-2.83	1.42	1.48
26	ax	201	PEB	C4D-ND	2.83	1.38	1.35
26	et	202	PEB	C4D-ND	2.83	1.38	1.35
28	D9	203	PUB	CHC-C1D	2.83	1.59	1.53
26	j4	202	PEB	C4D-ND	2.83	1.38	1.35
28	eT	203	PUB	C1A-NA	2.83	1.38	1.35
26	bV	202	PEB	C4D-ND	2.83	1.38	1.35
29	c9	303	PVN	C3-C2	2.83	1.37	1.34
26	lh	202	PEB	C4D-ND	2.82	1.38	1.35
26	dL	202	PEB	C4D-ND	2.82	1.38	1.35
26	er	202	PEB	C4D-ND	2.82	1.38	1.35
26	ge	202	PEB	C4D-ND	2.82	1.38	1.35
26	t3	202	PEB	C4D-ND	2.82	1.38	1.35
28	dP	203	PUB	CHC-C1D	2.82	1.59	1.53
26	co	201	PEB	C4D-ND	2.82	1.38	1.35
26	el	202	PEB	C4D-ND	2.82	1.38	1.35
28	ar	203	PUB	CHC-C1D	2.82	1.59	1.53
26	bJ	202	PEB	C4D-ND	2.82	1.38	1.35
26	hN	202	PEB	C4D-ND	2.82	1.38	1.35
26	z3	202	PEB	C4D-ND	2.82	1.38	1.35
28	T9	203	PUB	CHC-C1D	2.82	1.59	1.53
26	jK	1002	PEB	C4D-ND	2.82	1.38	1.35
26	ei	202	PEB	C4D-ND	2.82	1.38	1.35
26	ff	202	PEB	C4D-ND	2.82	1.38	1.35
26	fo	202	PEB	C4D-ND	2.82	1.38	1.35
26	jN	1002	PEB	C4D-ND	2.82	1.38	1.35
26	v4	202	PEB	C4D-ND	2.82	1.38	1.35
26	cH	201	PEB	C4D-ND	2.82	1.38	1.35
26	kS	1002	PEB	C4D-ND	2.82	1.38	1.35
26	at	202	PEB	C4D-ND	2.82	1.38	1.35
26	di	202	PEB	C4D-ND	2.82	1.38	1.35
26	D3	202	PEB	C4D-ND	2.81	1.38	1.35
26	D4	202	PEB	C4D-ND	2.81	1.38	1.35
26	af	202	PEB	C4D-ND	2.81	1.38	1.35
26	fy	201	PEB	C4D-ND	2.81	1.38	1.35
26	jI	1002	PEB	C4D-ND	2.81	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N5	202	PEB	C4D-ND	2.81	1.38	1.35
26	P3	202	PEB	C4D-ND	2.81	1.38	1.35
26	F7	201	PEB	C4D-ND	2.81	1.38	1.35
26	al	202	PEB	C4D-ND	2.81	1.38	1.35
26	ec	202	PEB	C4D-ND	2.81	1.38	1.35
26	ld	202	PEB	C4D-ND	2.81	1.38	1.35
26	ln	202	PEB	C4D-ND	2.81	1.38	1.35
26	A2	1003	PEB	C4D-ND	2.81	1.38	1.35
26	X2	202	PEB	C4D-ND	2.81	1.38	1.35
26	34	1002	PEB	C4D-ND	2.81	1.38	1.35
26	N7	202	PEB	C4D-ND	2.81	1.38	1.35
26	cq	202	PEB	C4D-ND	2.81	1.38	1.35
26	B3	202	PEB	C4D-ND	2.81	1.38	1.35
26	dl	202	PEB	C4D-ND	2.81	1.38	1.35
29	gz	304	PVN	C16-C17	-2.81	1.40	1.45
26	n4	202	PEB	C4D-ND	2.81	1.38	1.35
26	n5	202	PEB	C4D-ND	2.81	1.38	1.35
26	cL	202	PEB	C4D-ND	2.81	1.38	1.35
26	hB	202	PEB	C4D-ND	2.81	1.38	1.35
26	F3	202	PEB	C4D-ND	2.80	1.38	1.35
26	L3	202	PEB	C4D-ND	2.80	1.38	1.35
26	n6	202	PEB	C4D-ND	2.80	1.38	1.35
26	V7	202	PEB	C4D-ND	2.80	1.38	1.35
26	cr	202	PEB	C4D-ND	2.80	1.38	1.35
26	dj	202	PEB	C4D-ND	2.80	1.38	1.35
26	L2	202	PEB	C4D-ND	2.80	1.38	1.35
26	a7	202	PEB	C4D-ND	2.80	1.38	1.35
26	gi	202	PEB	C4D-ND	2.80	1.38	1.35
26	gr	201	PEB	C4D-ND	2.80	1.38	1.35
26	v3	202	PEB	C4D-ND	2.80	1.38	1.35
26	lp	202	PEB	C4D-ND	2.80	1.38	1.35
26	n7	202	PEB	C4D-ND	2.80	1.38	1.35
26	lr	202	PEB	C4D-ND	2.80	1.38	1.35
26	j2	202	PEB	C4D-ND	2.80	1.38	1.35
26	eX	201	PEB	C4D-ND	2.80	1.38	1.35
26	i3	203	PEB	C4D-ND	2.80	1.38	1.35
26	T7	202	PEB	C4D-ND	2.80	1.38	1.35
26	J9	202	PEB	C4D-ND	2.80	1.38	1.35
26	l7	202	PEB	C4D-ND	2.80	1.38	1.35
26	an	201	PEB	C4D-ND	2.80	1.38	1.35
26	V2	202	PEB	C4D-ND	2.80	1.38	1.35
26	D5	202	PEB	C4D-ND	2.80	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	iC	1002	PEB	C4D-ND	2.80	1.38	1.35
26	kW	1002	PEB	C4D-ND	2.80	1.38	1.35
29	U8	1004	PVN	C3-C2	2.80	1.37	1.34
26	N3	202	PEB	C4D-ND	2.80	1.38	1.35
26	r4	201	PEB	C4D-ND	2.80	1.38	1.35
26	D7	202	PEB	C4D-ND	2.80	1.38	1.35
26	gx	202	PEB	C4D-ND	2.80	1.38	1.35
28	D7	203	PUB	C1A-NA	2.80	1.38	1.35
26	gk	202	PEB	C4D-ND	2.79	1.38	1.35
26	kX	1002	PEB	C4D-ND	2.79	1.38	1.35
28	bD	203	PUB	C1A-NA	2.79	1.38	1.35
26	kU	1002	PEB	C4D-ND	2.79	1.38	1.35
26	A5	203	PEB	C4D-ND	2.79	1.38	1.35
26	P5	201	PEB	C4D-ND	2.79	1.38	1.35
26	B6	202	PEB	C4D-ND	2.79	1.38	1.35
26	dh	202	PEB	C4D-ND	2.79	1.38	1.35
26	jL	1002	PEB	C4D-ND	2.79	1.38	1.35
26	jP	1002	PEB	C4D-ND	2.79	1.38	1.35
26	fu	201	PEB	C4D-ND	2.79	1.38	1.35
26	p2	202	PEB	C4D-ND	2.79	1.38	1.35
26	R3	202	PEB	C4D-ND	2.79	1.38	1.35
26	t5	202	PEB	C4D-ND	2.79	1.38	1.35
26	z5	202	PEB	C4D-ND	2.79	1.38	1.35
26	J6	202	PEB	C4D-ND	2.79	1.38	1.35
26	H7	202	PEB	C4D-ND	2.79	1.38	1.35
28	T5	202	PUB	C1A-NA	2.79	1.38	1.35
26	cl	202	PEB	C4D-ND	2.79	1.38	1.35
26	p8	202	PEB	C4D-ND	2.79	1.38	1.35
26	X7	202	PEB	C4D-ND	2.79	1.38	1.35
26	t7	202	PEB	C4D-ND	2.79	1.38	1.35
26	P9	202	PEB	C4D-ND	2.79	1.38	1.35
26	cf	201	PEB	C4D-ND	2.79	1.38	1.35
26	fj	202	PEB	C4D-ND	2.79	1.38	1.35
26	jO	1002	PEB	C4D-ND	2.79	1.38	1.35
26	B7	201	PEB	C4D-ND	2.79	1.38	1.35
26	aD	202	PEB	C4D-ND	2.79	1.38	1.35
26	bD	202	PEB	C4D-ND	2.79	1.38	1.35
26	bQ	203	PEB	C4D-ND	2.79	1.38	1.35
26	c7	202	PEB	C4D-ND	2.79	1.38	1.35
28	g8	202	PUB	C1A-NA	2.79	1.38	1.35
26	eV	202	PEB	C4D-ND	2.79	1.38	1.35
26	gg	202	PEB	C4D-ND	2.79	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ch	202	PEB	C4D-ND	2.79	1.38	1.35
26	l2	202	PEB	C4D-ND	2.78	1.38	1.35
28	ar	203	PUB	C1A-NA	2.78	1.38	1.35
26	Z7	202	PEB	C4D-ND	2.78	1.38	1.35
26	ga	202	PEB	C4D-ND	2.78	1.38	1.35
26	dY	202	PEB	C4D-ND	2.78	1.38	1.35
26	bT	201	PEB	C4D-ND	2.78	1.38	1.35
26	eB	203	PEB	C4D-ND	2.78	1.38	1.35
26	fs	202	PEB	C4D-ND	2.78	1.38	1.35
26	kQ	1002	PEB	C4D-ND	2.78	1.38	1.35
26	J5	202	PEB	C4D-ND	2.78	1.38	1.35
26	cj	202	PEB	C4D-ND	2.78	1.38	1.35
28	N9	203	PUB	C1A-NA	2.78	1.38	1.35
26	F5	202	PEB	C4D-ND	2.78	1.38	1.35
26	fq	202	PEB	C4D-ND	2.78	1.38	1.35
26	bN	202	PEB	C4D-ND	2.78	1.38	1.35
26	iE	1002	PEB	C4D-ND	2.78	1.38	1.35
28	dV	203	PUB	C1A-NA	2.78	1.38	1.35
26	V5	202	PEB	C4D-ND	2.78	1.38	1.35
26	hJ	202	PEB	C4D-ND	2.78	1.38	1.35
28	gy	306	PUB	C1A-NA	2.78	1.38	1.35
26	gd	201	PEB	C4D-ND	2.78	1.38	1.35
26	gt	202	PEB	C4D-ND	2.78	1.38	1.35
26	H2	201	PEB	C4D-ND	2.78	1.38	1.35
26	gv	202	PEB	C4D-ND	2.78	1.38	1.35
26	v9	202	PEB	C4D-ND	2.77	1.38	1.35
26	dd	202	PEB	C4D-ND	2.77	1.38	1.35
26	hH	202	PEB	C4D-ND	2.77	1.38	1.35
26	ea	203	PEB	C4D-ND	2.77	1.38	1.35
28	ep	203	PUB	C1A-NA	2.77	1.38	1.35
26	h3	201	PEB	C4D-ND	2.77	1.38	1.35
26	R6	202	PEB	C4D-ND	2.77	1.38	1.35
28	V6	203	PUB	C1A-NA	2.77	1.38	1.35
28	o8	203	PUB	C1A-NA	2.77	1.38	1.35
28	H7	203	PUB	C1A-NA	2.77	1.38	1.35
26	y8	202	PEB	C4D-ND	2.77	1.38	1.35
26	D9	202	PEB	C4D-ND	2.77	1.38	1.35
26	lw	203	PEB	C4D-ND	2.77	1.38	1.35
29	dw	404	PVN	C19-C18	-2.77	1.43	1.48
26	n2	202	PEB	C4D-ND	2.77	1.38	1.35
28	bH	203	PUB	C1A-NA	2.77	1.38	1.35
26	cn	201	PEB	C4D-ND	2.77	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	fc	202	PEB	C4D-ND	2.77	1.38	1.35
28	n5	203	PUB	C1A-NA	2.77	1.38	1.35
28	bP	203	PUB	C1A-NA	2.77	1.38	1.35
28	cn	202	PUB	C1A-NA	2.77	1.38	1.35
28	di	203	PUB	C1A-NA	2.77	1.38	1.35
26	cz	202	PEB	C4D-ND	2.77	1.38	1.35
28	t5	203	PUB	C1A-NA	2.77	1.38	1.35
26	R9	202	PEB	C4D-ND	2.77	1.38	1.35
26	eJ	202	PEB	C4D-ND	2.77	1.38	1.35
26	jJ	1002	PEB	C4D-ND	2.77	1.38	1.35
28	b6	203	PUB	C1A-NA	2.77	1.38	1.35
28	dL	203	PUB	C1A-NA	2.77	1.38	1.35
26	T2	202	PEB	C4D-ND	2.77	1.38	1.35
26	T9	202	PEB	C4D-ND	2.77	1.38	1.35
26	fm	202	PEB	C4D-ND	2.77	1.38	1.35
26	gn	202	PEB	C4D-ND	2.77	1.38	1.35
26	kV	1002	PEB	C4D-ND	2.77	1.38	1.35
28	lr	203	PUB	C1A-NA	2.77	1.38	1.35
26	kT	1002	PEB	C4D-ND	2.77	1.38	1.35
28	bz	203	PUB	C1A-NA	2.77	1.38	1.35
29	A2	1004	PVN	C3-C2	2.77	1.37	1.34
29	a3	1004	PVN	C3-C2	2.77	1.37	1.34
26	R7	202	PEB	C4D-ND	2.77	1.38	1.35
26	y7	202	PEB	C4D-ND	2.77	1.38	1.35
26	lf	202	PEB	C4D-ND	2.77	1.38	1.35
26	fg	201	PEB	C4D-ND	2.77	1.38	1.35
28	cR	203	PUB	C1A-NA	2.77	1.38	1.35
26	B9	202	PEB	C4D-ND	2.77	1.38	1.35
26	cd	202	PEB	C4D-ND	2.77	1.38	1.35
28	T7	203	PUB	C1A-NA	2.77	1.38	1.35
26	H9	202	PEB	C4D-ND	2.77	1.38	1.35
26	eN	202	PEB	C4D-ND	2.77	1.38	1.35
28	X3	202	PUB	C1A-NA	2.76	1.38	1.35
26	z7	202	PEB	C4D-ND	2.76	1.38	1.35
26	lo	203	PEB	C4D-ND	2.76	1.38	1.35
28	r2	203	PUB	C1A-NA	2.76	1.38	1.35
28	R3	203	PUB	C1A-NA	2.76	1.38	1.35
28	hG	202	PUB	C1A-NA	2.76	1.38	1.35
26	S5	203	PEB	C4D-ND	2.76	1.38	1.35
26	ep	202	PEB	C4D-ND	2.76	1.38	1.35
28	y8	203	PUB	C1A-NA	2.76	1.38	1.35
28	df	203	PUB	C1A-NA	2.76	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L7	201	PEB	C4D-ND	2.76	1.38	1.35
26	hP	202	PEB	C4D-ND	2.76	1.38	1.35
28	l7	203	PUB	C1A-NA	2.76	1.38	1.35
26	Y7	1003	PEB	C4D-ND	2.76	1.38	1.35
28	bY	1005	PUB	C1A-NA	2.76	1.38	1.35
28	dX	203	PUB	C1A-NA	2.76	1.38	1.35
26	V9	202	PEB	C4D-ND	2.76	1.38	1.35
26	bB	202	PEB	C4D-ND	2.76	1.38	1.35
26	bP	202	PEB	C4D-ND	2.76	1.38	1.35
26	hL	202	PEB	C4D-ND	2.76	1.38	1.35
26	hX	202	PEB	C4D-ND	2.76	1.38	1.35
28	p4	203	PUB	C1A-NA	2.76	1.38	1.35
26	r3	202	PEB	C4D-ND	2.76	1.38	1.35
28	gi	203	PUB	C1A-NA	2.76	1.38	1.35
28	v5	203	PUB	C1A-NA	2.76	1.38	1.35
28	J6	203	PUB	C1A-NA	2.76	1.38	1.35
28	K8	203	PUB	C1A-NA	2.76	1.38	1.35
26	x3	202	PEB	C4D-ND	2.76	1.38	1.35
26	p5	201	PEB	C4D-ND	2.76	1.38	1.35
26	N9	202	PEB	C4D-ND	2.76	1.38	1.35
28	G8	203	PUB	C1A-NA	2.76	1.38	1.35
28	L9	203	PUB	C1A-NA	2.76	1.38	1.35
28	an	202	PUB	C1A-NA	2.76	1.38	1.35
28	bY	1006	PUB	C1A-NA	2.76	1.38	1.35
28	hD	203	PUB	C1A-NA	2.76	1.38	1.35
28	hY	405	PUB	C1A-NA	2.76	1.38	1.35
26	J3	202	PEB	C4D-ND	2.76	1.38	1.35
28	aV	203	PUB	C1A-NA	2.76	1.38	1.35
28	bL	203	PUB	C1A-NA	2.76	1.38	1.35
28	gz	306	PUB	C1A-NA	2.76	1.38	1.35
26	x7	202	PEB	C4D-ND	2.76	1.38	1.35
28	cB	203	PUB	C1A-NA	2.76	1.38	1.35
26	Z3	202	PEB	C4D-ND	2.76	1.38	1.35
26	r7	202	PEB	C4D-ND	2.76	1.38	1.35
26	eg	202	PEB	C4D-ND	2.76	1.38	1.35
26	hD	202	PEB	C4D-ND	2.76	1.38	1.35
28	aP	203	PUB	C1A-NA	2.76	1.38	1.35
26	li	203	PEB	C4D-ND	2.76	1.38	1.35
28	L4	203	PUB	C1A-NA	2.76	1.38	1.35
28	eZ	404	PUB	C1A-NA	2.76	1.38	1.35
29	e8	303	PVN	C3-C2	2.76	1.37	1.34
29	e9	304	PVN	C3-C2	2.76	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A1	301	PEB	C4D-ND	2.76	1.38	1.35
26	B1	301	PEB	C4D-ND	2.76	1.38	1.35
26	34	1001	PEB	C4D-ND	2.76	1.38	1.35
26	C8	202	PEB	C4D-ND	2.76	1.38	1.35
26	av	202	PEB	C4D-ND	2.76	1.38	1.35
26	cp	202	PEB	C4D-ND	2.76	1.38	1.35
28	a3	1006	PUB	C1A-NA	2.76	1.38	1.35
26	jM	1002	PEB	C4D-ND	2.75	1.38	1.35
28	c3	304	PUB	C1A-NA	2.75	1.38	1.35
28	Z4	203	PUB	C1A-NA	2.75	1.38	1.35
28	l6	203	PUB	C1A-NA	2.75	1.38	1.35
28	ld	203	PUB	C1A-NA	2.75	1.38	1.35
28	hZ	404	PUB	C1A-NA	2.75	1.38	1.35
26	l4	202	PEB	C4D-ND	2.75	1.38	1.35
26	e7	202	PEB	C4D-ND	2.75	1.38	1.35
28	ax	202	PUB	C1A-NA	2.75	1.38	1.35
28	eX	202	PUB	C1A-NA	2.75	1.38	1.35
28	gp	203	PUB	C1A-NA	2.75	1.38	1.35
26	B4	202	PEB	C4D-ND	2.75	1.38	1.35
26	e4	202	PEB	C4D-ND	2.75	1.38	1.35
28	fj	203	PUB	C1A-NA	2.75	1.38	1.35
28	gn	203	PUB	C1A-NA	2.75	1.38	1.35
26	ab	202	PEB	C4D-ND	2.75	1.38	1.35
28	bq	203	PUB	C1A-NA	2.75	1.38	1.35
28	F4	203	PUB	C1A-NA	2.75	1.38	1.35
28	Q8	203	PUB	C1A-NA	2.75	1.38	1.35
28	aZ	305	PUB	C1A-NA	2.75	1.38	1.35
28	dY	203	PUB	C1A-NA	2.75	1.38	1.35
28	gz	305	PUB	C1A-NA	2.75	1.38	1.35
26	aF	202	PEB	C4D-ND	2.75	1.38	1.35
26	bF	202	PEB	C4D-ND	2.75	1.38	1.35
26	m5	1003	PEB	C4D-ND	2.75	1.38	1.35
26	v5	202	PEB	C4D-ND	2.75	1.38	1.35
28	r7	203	PUB	C1A-NA	2.75	1.38	1.35
28	t9	203	PUB	C1A-NA	2.75	1.38	1.35
28	Y9	304	PUB	C1A-NA	2.75	1.38	1.35
28	lj	202	PUB	C1A-NA	2.75	1.38	1.35
28	lx	201	PUB	C1A-NA	2.75	1.38	1.35
26	p3	202	PEB	C4D-ND	2.75	1.38	1.35
26	bL	202	PEB	C4D-ND	2.75	1.38	1.35
28	H3	203	PUB	C1A-NA	2.75	1.38	1.35
26	h8	202	PEB	C4D-ND	2.75	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p7	201	PEB	C4D-ND	2.75	1.38	1.35
26	hG	201	PEB	C4D-ND	2.75	1.38	1.35
28	dD	203	PUB	C1A-NA	2.75	1.38	1.35
28	fc	203	PUB	C1A-NA	2.75	1.38	1.35
28	gx	203	PUB	C1A-NA	2.75	1.38	1.35
26	fw	202	PEB	C4D-ND	2.75	1.38	1.35
28	y6	204	PUB	C1A-NA	2.75	1.38	1.35
28	dl	203	PUB	C1A-NA	2.75	1.38	1.35
28	aB	203	PUB	C1A-NA	2.75	1.38	1.35
28	lp	203	PUB	C1A-NA	2.75	1.38	1.35
26	h2	202	PEB	C4D-ND	2.74	1.38	1.35
26	az	202	PEB	C4D-ND	2.74	1.38	1.35
26	hV	202	PEB	C4D-ND	2.74	1.38	1.35
28	x2	202	PUB	C1A-NA	2.74	1.38	1.35
28	ga	203	PUB	C1A-NA	2.74	1.38	1.35
28	gy	305	PUB	C1A-NA	2.74	1.38	1.35
28	Y5	1005	PUB	C1A-NA	2.74	1.38	1.35
28	bp	202	PUB	C1A-NA	2.74	1.38	1.35
28	co	202	PUB	C1A-NA	2.74	1.38	1.35
28	cQ	202	PUB	C1A-NA	2.74	1.38	1.35
28	hV	203	PUB	C1A-NA	2.74	1.38	1.35
29	ly	404	PVN	C14-C13	-2.74	1.39	1.45
26	W3	203	PEB	C4D-ND	2.74	1.38	1.35
28	N7	203	PUB	C1A-NA	2.74	1.38	1.35
28	eP	204	PUB	C1A-NA	2.74	1.38	1.35
28	lt	203	PUB	C1A-NA	2.74	1.38	1.35
28	ly	405	PUB	C1A-NA	2.74	1.38	1.35
28	lz	404	PUB	C1A-NA	2.74	1.38	1.35
26	gp	202	PEB	C4D-ND	2.74	1.38	1.35
26	kR	1002	PEB	C4D-ND	2.74	1.38	1.35
28	aZ	304	PUB	C1A-NA	2.74	1.38	1.35
28	lf	203	PUB	C1A-NA	2.74	1.38	1.35
28	V3	203	PUB	C1A-NA	2.74	1.38	1.35
28	z4	203	PUB	C1A-NA	2.74	1.38	1.35
28	F6	203	PUB	C1A-NA	2.74	1.38	1.35
26	j3	201	PEB	C4D-ND	2.74	1.38	1.35
26	ad	202	PEB	C4D-ND	2.74	1.38	1.35
28	T2	203	PUB	C1A-NA	2.74	1.38	1.35
28	t3	203	PUB	C1A-NA	2.74	1.38	1.35
28	d9	305	PUB	C1A-NA	2.74	1.38	1.35
28	dB	202	PUB	C1A-NA	2.74	1.38	1.35
28	ey	1005	PUB	C1A-NA	2.74	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	eV	203	PUB	C1A-NA	2.74	1.38	1.35
28	c8	304	PUB	C1A-NA	2.74	1.38	1.35
26	cb	202	PEB	C4D-ND	2.74	1.38	1.35
28	J4	203	PUB	C1A-NA	2.74	1.38	1.35
28	R7	203	PUB	C1A-NA	2.74	1.38	1.35
28	cp	203	PUB	C1A-NA	2.74	1.38	1.35
28	H2	202	PUB	C1A-NA	2.74	1.38	1.35
28	e9	305	PUB	C1A-NA	2.74	1.38	1.35
28	bJ	203	PUB	C1A-NA	2.74	1.38	1.35
28	jJ	1003	PUB	C1A-NA	2.74	1.38	1.35
26	fi	202	PEB	C4D-ND	2.74	1.38	1.35
26	hT	202	PEB	C4D-ND	2.74	1.38	1.35
28	F5	203	PUB	C1A-NA	2.74	1.38	1.35
28	eD	203	PUB	C1A-NA	2.74	1.38	1.35
26	R5	202	PEB	C4D-ND	2.74	1.38	1.35
28	T6	203	PUB	C1A-NA	2.74	1.38	1.35
28	X7	203	PUB	C1A-NA	2.74	1.38	1.35
28	en	203	PUB	C1A-NA	2.74	1.38	1.35
28	eF	203	PUB	C1A-NA	2.74	1.38	1.35
26	g5	202	PEB	C4D-ND	2.74	1.38	1.35
26	X6	202	PEB	C4D-ND	2.74	1.38	1.35
28	x3	203	PUB	C1A-NA	2.74	1.38	1.35
28	L5	203	PUB	C1A-NA	2.74	1.38	1.35
28	cO	203	PUB	C1A-NA	2.74	1.38	1.35
26	v7	202	PEB	C4D-ND	2.74	1.38	1.35
26	cF	201	PEB	C4D-ND	2.74	1.38	1.35
28	ff	203	PUB	C1A-NA	2.74	1.38	1.35
28	jK	1003	PUB	C1A-NA	2.74	1.38	1.35
26	V3	202	PEB	C4D-ND	2.73	1.38	1.35
26	ee	202	PEB	C4D-ND	2.73	1.38	1.35
26	en	202	PEB	C4D-ND	2.73	1.38	1.35
28	dj	203	PUB	C1A-NA	2.73	1.38	1.35
28	dn	203	PUB	C1A-NA	2.73	1.38	1.35
28	dt	203	PUB	C1A-NA	2.73	1.38	1.35
28	l2	203	PUB	C1A-NA	2.73	1.38	1.35
28	L3	203	PUB	C1A-NA	2.73	1.38	1.35
28	el	203	PUB	C1A-NA	2.73	1.38	1.35
26	f2	202	PEB	C4D-ND	2.73	1.38	1.35
26	cE	202	PEB	C4D-ND	2.73	1.38	1.35
28	C2	305	PUB	C1A-NA	2.73	1.38	1.35
28	B9	203	PUB	C1A-NA	2.73	1.38	1.35
28	dv	202	PUB	C1A-NA	2.73	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dK	203	PUB	C1A-NA	2.73	1.38	1.35
28	x4	202	PUB	C1A-NA	2.73	1.38	1.35
28	x5	202	PUB	C1A-NA	2.73	1.38	1.35
28	iH	1002	PUB	C1A-NA	2.73	1.38	1.35
28	kU	1003	PUB	C1A-NA	2.73	1.38	1.35
28	p6	203	PUB	C1A-NA	2.73	1.38	1.35
28	z7	203	PUB	C1A-NA	2.73	1.38	1.35
28	J9	203	PUB	C1A-NA	2.73	1.38	1.35
28	fm	203	PUB	C1A-NA	2.73	1.38	1.35
26	p4	202	PEB	C4D-ND	2.73	1.38	1.35
26	cJ	202	PEB	C4D-ND	2.73	1.38	1.35
26	iD	1002	PEB	C4D-ND	2.73	1.38	1.35
28	L2	203	PUB	C1A-NA	2.73	1.38	1.35
28	h3	202	PUB	C1A-NA	2.73	1.38	1.35
28	v7	203	PUB	C1A-NA	2.73	1.38	1.35
28	P9	203	PUB	C1A-NA	2.73	1.38	1.35
28	aN	203	PUB	C1A-NA	2.73	1.38	1.35
26	Z2	202	PEB	C4D-ND	2.73	1.38	1.35
26	L5	202	PEB	C4D-ND	2.73	1.38	1.35
26	P7	202	PEB	C4D-ND	2.73	1.38	1.35
28	J7	202	PUB	C1A-NA	2.73	1.38	1.35
28	Z7	203	PUB	C1A-NA	2.73	1.38	1.35
28	ez	1005	PUB	C1A-NA	2.73	1.38	1.35
28	v6	203	PUB	C1A-NA	2.73	1.38	1.35
28	jM	1003	PUB	C1A-NA	2.73	1.38	1.35
28	c3	305	PUB	C1A-NA	2.73	1.38	1.35
28	X4	203	PUB	C1A-NA	2.73	1.38	1.35
28	b7	202	PUB	C1A-NA	2.73	1.38	1.35
28	eY	405	PUB	C1A-NA	2.73	1.38	1.35
28	gk	203	PUB	C1A-NA	2.73	1.38	1.35
28	34	1006	PUB	C1A-NA	2.73	1.38	1.35
28	d7	203	PUB	C1A-NA	2.73	1.38	1.35
28	b9	406	PUB	C1A-NA	2.73	1.38	1.35
28	N3	203	PUB	C1A-NA	2.73	1.38	1.35
28	N5	203	PUB	C1A-NA	2.73	1.38	1.35
28	p5	202	PUB	C1A-NA	2.73	1.38	1.35
28	Z9	1006	PUB	C1A-NA	2.73	1.38	1.35
28	cF	202	PUB	C1A-NA	2.73	1.38	1.35
28	dp	203	PUB	C1A-NA	2.73	1.38	1.35
28	dF	203	PUB	C1A-NA	2.73	1.38	1.35
29	c9	303	PVN	C14-C13	-2.73	1.39	1.45
28	R2	203	PUB	C1A-NA	2.73	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X2	203	PUB	C1A-NA	2.73	1.38	1.35
28	p3	203	PUB	C1A-NA	2.73	1.38	1.35
28	r3	203	PUB	C1A-NA	2.73	1.38	1.35
28	b8	1006	PUB	C1A-NA	2.73	1.38	1.35
29	D2	303	PVN	C19-C18	-2.73	1.43	1.48
29	d3	302	PVN	C19-C18	-2.73	1.43	1.48
28	h2	203	PUB	C1A-NA	2.73	1.38	1.35
28	hN	203	PUB	C1A-NA	2.73	1.38	1.35
28	jL	1003	PUB	C1A-NA	2.73	1.38	1.35
26	J7	201	PEB	C4D-ND	2.72	1.38	1.35
28	l3	202	PUB	C1A-NA	2.72	1.38	1.35
28	X6	203	PUB	C1A-NA	2.72	1.38	1.35
28	cL	203	PUB	C1A-NA	2.72	1.38	1.35
28	ec	203	PUB	C1A-NA	2.72	1.38	1.35
28	hP	203	PUB	C1A-NA	2.72	1.38	1.35
28	z9	203	PUB	C1A-NA	2.72	1.38	1.35
26	n3	202	PEB	C4D-ND	2.72	1.38	1.35
28	A2	1005	PUB	C1A-NA	2.72	1.38	1.35
28	F2	203	PUB	C1A-NA	2.72	1.38	1.35
28	a3	1005	PUB	C1A-NA	2.72	1.38	1.35
28	H5	202	PUB	C1A-NA	2.72	1.38	1.35
28	Y9	305	PUB	C1A-NA	2.72	1.38	1.35
28	bT	202	PUB	C1A-NA	2.72	1.38	1.35
28	dw	405	PUB	C1A-NA	2.72	1.38	1.35
28	j3	202	PUB	C1A-NA	2.72	1.38	1.35
28	at	203	PUB	C1A-NA	2.72	1.38	1.35
28	cJ	203	PUB	C1A-NA	2.72	1.38	1.35
28	aF	203	PUB	C1A-NA	2.72	1.38	1.35
28	bF	203	PUB	C1A-NA	2.72	1.38	1.35
28	bN	203	PUB	C1A-NA	2.72	1.38	1.35
28	dR	203	PUB	C1A-NA	2.72	1.38	1.35
28	lb	203	PUB	C1A-NA	2.72	1.38	1.35
28	iC	1003	PUB	C1A-NA	2.72	1.38	1.35
28	iD	1003	PUB	C1A-NA	2.72	1.38	1.35
28	J2	202	PUB	C1A-NA	2.72	1.38	1.35
28	er	203	PUB	C1A-NA	2.72	1.38	1.35
28	ll	203	PUB	C1A-NA	2.72	1.38	1.35
26	g4	202	PEB	C4D-ND	2.72	1.38	1.35
28	D3	203	PUB	C1A-NA	2.72	1.38	1.35
28	eb	202	PUB	C1A-NA	2.72	1.38	1.35
28	D2	305	PUB	C1A-NA	2.72	1.38	1.35
28	fa	202	PUB	C1A-NA	2.72	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ah	202	PEB	C4D-ND	2.72	1.38	1.35
28	f8	203	PUB	C1A-NA	2.72	1.38	1.35
28	D6	202	PUB	C1A-NA	2.72	1.38	1.35
28	fy	202	PUB	C1A-NA	2.72	1.38	1.35
28	B7	202	PUB	C1A-NA	2.72	1.38	1.35
28	P7	203	PUB	C1A-NA	2.72	1.38	1.35
28	cs	203	PUB	C1A-NA	2.72	1.38	1.35
28	eJ	203	PUB	C1A-NA	2.72	1.38	1.35
28	fs	203	PUB	C1A-NA	2.72	1.38	1.35
28	kQ	1003	PUB	C1A-NA	2.72	1.38	1.35
28	z2	203	PUB	C1A-NA	2.72	1.38	1.35
28	F3	203	PUB	C1A-NA	2.72	1.38	1.35
28	Z3	203	PUB	C1A-NA	2.72	1.38	1.35
28	A8	203	PUB	C1A-NA	2.72	1.38	1.35
28	F9	203	PUB	C1A-NA	2.72	1.38	1.35
28	Z9	1005	PUB	C1A-NA	2.72	1.38	1.35
28	dP	203	PUB	C1A-NA	2.72	1.38	1.35
28	ee	203	PUB	C1A-NA	2.72	1.38	1.35
28	P6	203	PUB	C1A-NA	2.72	1.38	1.35
28	gg	203	PUB	C1A-NA	2.72	1.38	1.35
26	hR	202	PEB	C4D-ND	2.72	1.38	1.35
28	c9	304	PUB	C1A-NA	2.72	1.38	1.35
28	bZ	305	PUB	C1A-NA	2.72	1.38	1.35
26	ar	202	PEB	C4D-ND	2.72	1.38	1.35
28	bn	202	PUB	C1A-NA	2.72	1.38	1.35
28	h8	203	PUB	C1A-NA	2.71	1.38	1.35
28	a7	203	PUB	C1A-NA	2.71	1.38	1.35
28	j2	203	PUB	C1A-NA	2.71	1.38	1.35
28	B3	203	PUB	C1A-NA	2.71	1.38	1.35
28	u6	203	PUB	C1A-NA	2.71	1.38	1.35
28	cz	203	PUB	C1A-NA	2.71	1.38	1.35
28	gd	202	PUB	C1A-NA	2.71	1.38	1.35
28	44	304	PUB	C1A-NA	2.71	1.38	1.35
28	v4	203	PUB	C1A-NA	2.71	1.38	1.35
28	Z5	305	PUB	C1A-NA	2.71	1.38	1.35
28	d6	203	PUB	C1A-NA	2.71	1.38	1.35
28	aH	203	PUB	C1A-NA	2.71	1.38	1.35
28	bs	1004	PUB	C1A-NA	2.71	1.38	1.35
29	lz	403	PVN	C14-C13	-2.71	1.40	1.45
28	D2	304	PUB	C1A-NA	2.71	1.38	1.35
28	z5	203	PUB	C1A-NA	2.71	1.38	1.35
28	C8	203	PUB	C1A-NA	2.71	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	r9	203	PUB	C1A-NA	2.71	1.38	1.35
28	ez	1006	PUB	C1A-NA	2.71	1.38	1.35
28	r4	202	PUB	C1A-NA	2.71	1.38	1.35
28	Z5	306	PUB	C1A-NA	2.71	1.38	1.35
28	H6	203	PUB	C1A-NA	2.71	1.38	1.35
28	aR	203	PUB	C1A-NA	2.71	1.38	1.35
28	dN	203	PUB	C1A-NA	2.71	1.38	1.35
28	n8	202	PUB	C1A-NA	2.71	1.38	1.35
28	f2	203	PUB	C1A-NA	2.71	1.38	1.35
28	p2	203	PUB	C1A-NA	2.71	1.38	1.35
28	N2	203	PUB	C1A-NA	2.71	1.38	1.35
28	P3	203	PUB	C1A-NA	2.71	1.38	1.35
28	U8	1006	PUB	C1A-NA	2.71	1.38	1.35
28	ge	203	PUB	C1A-NA	2.71	1.38	1.35
28	hL	203	PUB	C1A-NA	2.71	1.38	1.35
28	hR	203	PUB	C1A-NA	2.71	1.38	1.35
28	jP	1003	PUB	C1A-NA	2.71	1.38	1.35
26	r5	202	PEB	C4D-ND	2.71	1.38	1.35
26	df	202	PEB	C4D-ND	2.71	1.38	1.35
28	w8	203	PUB	C1A-NA	2.71	1.38	1.35
28	hT	203	PUB	C1A-NA	2.71	1.38	1.35
28	d3	303	PUB	C1A-NA	2.71	1.38	1.35
28	I8	203	PUB	C1A-NA	2.71	1.38	1.35
28	T4	202	PUB	C1A-NA	2.71	1.38	1.35
28	dw	406	PUB	C1A-NA	2.71	1.38	1.35
28	eB	204	PUB	C1A-NA	2.71	1.38	1.35
28	eH	203	PUB	C1A-NA	2.71	1.38	1.35
28	J3	203	PUB	C1A-NA	2.71	1.38	1.35
28	v3	203	PUB	C1A-NA	2.71	1.38	1.35
28	D4	203	PUB	C1A-NA	2.71	1.38	1.35
28	v9	203	PUB	C1A-NA	2.71	1.38	1.35
28	av	203	PUB	C1A-NA	2.71	1.38	1.35
28	eg	203	PUB	C1A-NA	2.71	1.38	1.35
28	P5	202	PUB	C1A-NA	2.70	1.38	1.35
28	b8	1005	PUB	C1A-NA	2.70	1.38	1.35
28	N6	203	PUB	C1A-NA	2.70	1.38	1.35
28	bR	202	PUB	C1A-NA	2.70	1.38	1.35
28	et	203	PUB	C1A-NA	2.70	1.38	1.35
28	gr	202	PUB	C1A-NA	2.70	1.38	1.35
28	t2	203	PUB	C1A-NA	2.70	1.38	1.35
28	c6	1004	PUB	C1A-NA	2.70	1.38	1.35
28	ap	203	PUB	C1A-NA	2.70	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dx	407	PUB	C1A-NA	2.70	1.38	1.35
28	T3	203	PUB	C1A-NA	2.70	1.38	1.35
28	x6	203	PUB	C1A-NA	2.70	1.38	1.35
28	V7	203	PUB	C1A-NA	2.70	1.38	1.35
28	az	203	PUB	C1A-NA	2.70	1.38	1.35
28	fq	203	PUB	C1A-NA	2.70	1.38	1.35
28	44	305	PUB	C1A-NA	2.70	1.38	1.35
28	e6	203	PUB	C1A-NA	2.70	1.38	1.35
28	n9	202	PUB	C1A-NA	2.70	1.38	1.35
28	cE	203	PUB	C1A-NA	2.70	1.38	1.35
28	kX	1003	PUB	C1A-NA	2.70	1.38	1.35
28	kR	1003	PUB	C1A-NA	2.70	1.38	1.35
28	kS	1003	PUB	C1A-NA	2.70	1.38	1.35
28	C2	304	PUB	C1A-NA	2.70	1.38	1.35
28	dH	203	PUB	C1A-NA	2.70	1.38	1.35
28	n6	203	PUB	C1A-NA	2.70	1.38	1.35
28	z6	203	PUB	C1A-NA	2.70	1.38	1.35
28	dN	203	PUB	C4D-C3D	-2.70	1.43	1.48
28	Z2	203	PUB	C1A-NA	2.70	1.38	1.35
28	D5	203	PUB	C1A-NA	2.70	1.38	1.35
28	Y5	1006	PUB	C1A-NA	2.70	1.38	1.35
28	D9	203	PUB	C1A-NA	2.70	1.38	1.35
28	dh	203	PUB	C1A-NA	2.70	1.38	1.35
28	iF	1003	PUB	C1A-NA	2.70	1.38	1.35
28	F7	202	PUB	C1A-NA	2.70	1.38	1.35
28	H9	203	PUB	C1A-NA	2.70	1.38	1.35
28	V9	203	PUB	C1A-NA	2.70	1.38	1.35
28	cH	202	PUB	C1A-NA	2.70	1.38	1.35
28	fw	203	PUB	C1A-NA	2.70	1.38	1.35
28	hX	203	PUB	C1A-NA	2.70	1.38	1.35
28	aY	405	PUB	C1A-NA	2.70	1.38	1.35
28	er	203	PUB	C4D-C3D	-2.70	1.43	1.48
28	R6	203	PUB	C1A-NA	2.70	1.38	1.35
28	U8	1005	PUB	C1A-NA	2.70	1.38	1.35
28	hJ	203	PUB	C1A-NA	2.70	1.38	1.35
28	t4	203	PUB	C1A-NA	2.70	1.38	1.35
28	c7	203	PUB	C1A-NA	2.70	1.38	1.35
28	p7	202	PUB	C1A-NA	2.70	1.38	1.35
28	d8	304	PUB	C1A-NA	2.70	1.38	1.35
28	e8	305	PUB	C1A-NA	2.70	1.38	1.35
28	bZ	306	PUB	C1A-NA	2.70	1.38	1.35
28	cq	203	PUB	C1A-NA	2.70	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	cr	203	PUB	C1A-NA	2.70	1.38	1.35
28	r6	203	PUB	C1A-NA	2.69	1.38	1.35
28	iG	1002	PUB	C1A-NA	2.69	1.38	1.35
28	aZ	304	PUB	C4D-C3D	-2.69	1.43	1.48
28	R4	203	PUB	C1A-NA	2.69	1.38	1.35
28	hB	203	PUB	C1A-NA	2.69	1.38	1.35
28	v2	203	PUB	C1A-NA	2.69	1.38	1.35
28	jI	1003	PUB	C1A-NA	2.69	1.38	1.35
28	T8	304	PUB	C1A-NA	2.69	1.38	1.35
28	F9	203	PUB	C4D-C3D	-2.69	1.43	1.48
28	dr	203	PUB	C1A-NA	2.69	1.38	1.35
28	eY	404	PUB	C1A-NA	2.69	1.38	1.35
28	eZ	403	PUB	C1A-NA	2.69	1.38	1.35
28	P3	203	PUB	C4D-C3D	-2.69	1.43	1.48
28	fi	203	PUB	C1A-NA	2.69	1.38	1.35
28	D7	203	PUB	C4D-C3D	-2.69	1.43	1.48
28	34	1005	PUB	C1A-NA	2.69	1.38	1.35
28	aD	203	PUB	C1A-NA	2.69	1.38	1.35
28	lv	202	PUB	C1A-NA	2.69	1.38	1.35
28	D9	203	PUB	C4D-C3D	-2.69	1.43	1.48
28	V2	203	PUB	C1A-NA	2.69	1.38	1.35
28	L6	202	PUB	C1A-NA	2.69	1.38	1.35
28	Z6	203	PUB	C1A-NA	2.69	1.38	1.35
28	x7	203	PUB	C1A-NA	2.69	1.38	1.35
28	c9	305	PUB	C1A-NA	2.69	1.38	1.35
28	M8	203	PUB	C1A-NA	2.69	1.38	1.35
28	R9	203	PUB	C1A-NA	2.69	1.38	1.35
28	lh	203	PUB	C1A-NA	2.69	1.38	1.35
29	44	303	PVN	C15-C16	2.69	1.44	1.38
29	Z5	304	PVN	C15-C16	2.69	1.44	1.38
28	y7	203	PUB	C1A-NA	2.69	1.38	1.35
28	hY	406	PUB	C1A-NA	2.69	1.38	1.35
26	ao	202	PEB	C2A-C1A	-2.69	1.49	1.52
28	el	203	PUB	C4D-C3D	-2.69	1.43	1.48
28	b9	407	PUB	C1A-NA	2.69	1.38	1.35
28	bV	203	PUB	C1A-NA	2.69	1.38	1.35
28	N4	203	PUB	C1A-NA	2.69	1.38	1.35
28	P4	203	PUB	C1A-NA	2.69	1.38	1.35
28	J5	203	PUB	C1A-NA	2.69	1.38	1.35
28	E8	203	PUB	C1A-NA	2.69	1.38	1.35
28	cY	203	PUB	C1A-NA	2.69	1.38	1.35
28	H4	203	PUB	C1A-NA	2.69	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	s7	203	PUB	C1A-NA	2.69	1.38	1.35
28	cN	202	PUB	C1A-NA	2.69	1.38	1.35
28	fu	202	PUB	C1A-NA	2.69	1.38	1.35
28	L7	202	PUB	C1A-NA	2.69	1.38	1.35
28	cL	203	PUB	C4D-C3D	-2.69	1.43	1.48
28	eP	204	PUB	C4D-C3D	-2.68	1.43	1.48
28	P2	203	PUB	C1A-NA	2.68	1.38	1.35
28	aL	203	PUB	C1A-NA	2.68	1.38	1.35
28	jO	1003	PUB	C1A-NA	2.68	1.38	1.35
28	kV	1003	PUB	C1A-NA	2.68	1.38	1.35
29	c8	303	PVN	C14-C13	-2.68	1.40	1.45
28	V4	203	PUB	C1A-NA	2.68	1.38	1.35
28	R5	203	PUB	C1A-NA	2.68	1.38	1.35
28	p8	203	PUB	C1A-NA	2.68	1.38	1.35
28	x9	203	PUB	C1A-NA	2.68	1.38	1.35
28	p9	203	PUB	C1A-NA	2.68	1.38	1.35
28	aY	404	PUB	C1A-NA	2.68	1.38	1.35
28	eN	203	PUB	C1A-NA	2.68	1.38	1.35
28	gt	203	PUB	C1A-NA	2.68	1.38	1.35
28	kW	1003	PUB	C1A-NA	2.68	1.38	1.35
28	eT	203	PUB	C4D-C3D	-2.68	1.43	1.48
28	bq	203	PUB	C4D-C3D	-2.68	1.43	1.48
28	bo	202	PUB	C1A-NA	2.68	1.38	1.35
28	cP	203	PUB	C1A-NA	2.68	1.38	1.35
28	fo	203	PUB	C1A-NA	2.68	1.38	1.35
28	e9	306	PUB	C1A-NA	2.68	1.38	1.35
28	f3	203	PUB	C1A-NA	2.68	1.38	1.35
28	z7	203	PUB	C4D-C3D	-2.68	1.43	1.48
28	bF	203	PUB	C4D-C3D	-2.68	1.43	1.48
28	eY	404	PUB	C4D-C3D	-2.68	1.43	1.48
28	eZ	403	PUB	C4D-C3D	-2.68	1.43	1.48
28	ln	203	PUB	C1A-NA	2.68	1.38	1.35
28	dR	203	PUB	C4D-C3D	-2.68	1.43	1.48
28	d3	304	PUB	C4D-C3D	-2.68	1.43	1.48
28	z3	203	PUB	C1A-NA	2.68	1.38	1.35
28	t7	203	PUB	C1A-NA	2.68	1.38	1.35
28	jN	1003	PUB	C1A-NA	2.68	1.38	1.35
28	n2	203	PUB	C1A-NA	2.68	1.38	1.35
28	T8	305	PUB	C1A-NA	2.68	1.38	1.35
28	gv	203	PUB	C1A-NA	2.68	1.38	1.35
28	R5	203	PUB	C4D-C3D	-2.68	1.43	1.48
28	t5	203	PUB	C4D-C3D	-2.68	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n3	203	PUB	C1A-NA	2.67	1.38	1.35
28	dx	406	PUB	C1A-NA	2.67	1.38	1.35
28	Z9	1005	PUB	C4D-C3D	-2.67	1.43	1.48
28	c8	305	PUB	C1A-NA	2.67	1.38	1.35
28	bB	203	PUB	C1A-NA	2.67	1.38	1.35
28	c7	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	kX	1003	PUB	C4D-C3D	-2.67	1.43	1.48
28	V5	203	PUB	C1A-NA	2.67	1.38	1.35
28	ei	203	PUB	C1A-NA	2.67	1.38	1.35
28	hH	203	PUB	C1A-NA	2.67	1.38	1.35
28	cY	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	iF	1003	PUB	C4D-C3D	-2.67	1.43	1.48
28	B5	203	PUB	C1A-NA	2.67	1.38	1.35
28	eg	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	dT	203	PUB	C1A-NA	2.67	1.38	1.35
28	bZ	305	PUB	C4D-C3D	-2.67	1.43	1.48
28	e9	306	PUB	C4D-C3D	-2.67	1.43	1.48
28	O8	203	PUB	C1A-NA	2.67	1.38	1.35
28	T9	203	PUB	C1A-NA	2.67	1.38	1.35
28	A2	1006	PUB	C1A-NA	2.67	1.38	1.35
28	br	203	PUB	C1A-NA	2.67	1.38	1.35
28	ey	1006	PUB	C1A-NA	2.67	1.38	1.35
28	eL	203	PUB	C1A-NA	2.67	1.38	1.35
28	dY	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	Z2	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	B4	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	N4	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	at	203	PUB	C4D-C3D	-2.67	1.43	1.48
28	aJ	203	PUB	C1A-NA	2.67	1.38	1.35
28	ev	203	PUB	C1A-NA	2.67	1.38	1.35
28	eJ	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	a6	203	PUB	C1A-NA	2.66	1.38	1.35
28	P5	202	PUB	C4D-C3D	-2.66	1.43	1.48
28	Z5	306	PUB	C4D-C3D	-2.66	1.43	1.48
28	bs	1004	PUB	C4D-C3D	-2.66	1.43	1.48
28	x7	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	n9	202	PUB	C4D-C3D	-2.66	1.43	1.48
28	d3	304	PUB	C1A-NA	2.66	1.38	1.35
28	B9	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	o8	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	cr	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	kT	1003	PUB	C1A-NA	2.66	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	R7	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	c8	304	PUB	C4D-C3D	-2.66	1.43	1.48
28	hV	203	PUB	C4D-C3D	-2.66	1.43	1.48
26	et	201	PEB	C2A-C1A	-2.66	1.49	1.52
28	r5	203	PUB	C1A-NA	2.66	1.38	1.35
28	hZ	405	PUB	C1A-NA	2.66	1.38	1.35
28	v6	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	r9	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	Y9	305	PUB	C4D-C3D	-2.66	1.43	1.48
28	Z4	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	aD	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	ei	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	N5	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	z5	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	hP	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	n4	203	PUB	C1A-NA	2.66	1.38	1.35
28	cM	203	PUB	C1A-NA	2.66	1.38	1.35
28	ly	406	PUB	C1A-NA	2.66	1.38	1.35
28	lz	405	PUB	C1A-NA	2.66	1.38	1.35
28	F6	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	gy	305	PUB	C4D-C3D	-2.66	1.43	1.48
28	dp	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	B4	203	PUB	C1A-NA	2.66	1.38	1.35
28	x6	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	aP	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	dj	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	dt	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	dx	407	PUB	C4D-C3D	-2.66	1.43	1.48
28	dF	203	PUB	C4D-C3D	-2.66	1.43	1.48
28	U8	1005	PUB	C4D-C3D	-2.65	1.43	1.48
28	ec	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	B6	203	PUB	C1A-NA	2.65	1.38	1.35
28	t6	203	PUB	C1A-NA	2.65	1.38	1.35
28	dd	203	PUB	C1A-NA	2.65	1.38	1.35
28	y6	204	PUB	C4D-C3D	-2.65	1.43	1.48
28	ez	1006	PUB	C4D-C3D	-2.65	1.43	1.48
28	iE	1003	PUB	C1A-NA	2.65	1.38	1.35
28	n7	203	PUB	C1A-NA	2.65	1.38	1.35
28	F4	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	B5	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	fw	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	B3	203	PUB	C4D-C3D	-2.65	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	gv	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	hY	405	PUB	C4D-C3D	-2.65	1.43	1.48
28	kU	1003	PUB	C4D-C3D	-2.65	1.43	1.48
28	b6	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	dn	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	kS	1003	PUB	C4D-C3D	-2.65	1.43	1.48
28	e7	203	PUB	C1A-NA	2.65	1.38	1.35
28	p2	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	e7	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	fu	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	jI	1003	PUB	C4D-C3D	-2.65	1.43	1.48
28	t7	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	J9	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	aF	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	bp	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	fa	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	d6	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	d8	304	PUB	C4D-C3D	-2.65	1.43	1.48
28	U8	1006	PUB	C4D-C3D	-2.65	1.43	1.48
28	bH	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	bY	1006	PUB	C4D-C3D	-2.65	1.43	1.48
28	co	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	lt	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	R3	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	cJ	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	z4	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	n6	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	eR	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	cp	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	kT	1003	PUB	C4D-C3D	-2.65	1.43	1.48
28	A2	1006	PUB	C4D-C3D	-2.65	1.43	1.48
28	a3	1006	PUB	C4D-C3D	-2.65	1.43	1.48
28	n3	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	R4	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	e9	305	PUB	C4D-C3D	-2.65	1.43	1.48
28	aR	203	PUB	C4D-C3D	-2.65	1.43	1.48
29	dw	404	PVN	C3-C2	2.65	1.37	1.34
28	e8	304	PUB	C1A-NA	2.65	1.38	1.35
28	F2	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	x4	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	T5	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	x5	202	PUB	C4D-C3D	-2.65	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H4	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	D5	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	F7	202	PUB	C4D-C3D	-2.65	1.43	1.48
28	cE	203	PUB	C4D-C3D	-2.65	1.43	1.48
28	dx	406	PUB	C4D-C3D	-2.64	1.43	1.48
28	iG	1002	PUB	C4D-C3D	-2.64	1.43	1.48
28	D2	304	PUB	C4D-C3D	-2.64	1.43	1.48
28	d3	303	PUB	C4D-C3D	-2.64	1.43	1.48
28	gr	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	dX	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	v9	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	lr	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	hB	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	aT	203	PUB	C1A-NA	2.64	1.38	1.35
28	r3	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	x9	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	Z9	1006	PUB	C4D-C3D	-2.64	1.43	1.48
28	aV	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	cO	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	C2	305	PUB	C4D-C3D	-2.64	1.43	1.48
28	F3	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	cz	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	dd	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	dV	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	l7	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	z9	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	cF	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	lj	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	lx	201	PUB	C4D-C3D	-2.64	1.43	1.48
28	gn	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	p8	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	b8	1005	PUB	C4D-C3D	-2.64	1.43	1.48
28	b9	406	PUB	C4D-C3D	-2.64	1.43	1.48
28	C8	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	K8	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	t2	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	t6	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	n7	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	dh	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	gg	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	T3	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	V4	203	PUB	C4D-C3D	-2.64	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	p4	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	c6	1004	PUB	C4D-C3D	-2.64	1.43	1.48
28	v7	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	bV	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	hR	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	F5	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	R6	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	b7	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	T9	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	dr	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	jP	1003	PUB	C4D-C3D	-2.64	1.43	1.48
28	n5	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	aT	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	gi	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	A8	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	cB	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	iH	1002	PUB	C4D-C3D	-2.64	1.43	1.48
28	f2	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	V2	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	Y5	1005	PUB	C4D-C3D	-2.64	1.43	1.48
28	c9	304	PUB	C4D-C3D	-2.64	1.43	1.48
28	hN	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	c9	305	PUB	C4D-C3D	-2.64	1.43	1.48
28	aJ	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	bY	1005	PUB	C4D-C3D	-2.64	1.43	1.48
28	p6	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	cs	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	dw	406	PUB	C4D-C3D	-2.64	1.43	1.48
28	h2	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	D2	305	PUB	C4D-C3D	-2.64	1.43	1.48
28	T4	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	a6	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	B7	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	bD	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	iE	1003	PUB	C4D-C3D	-2.64	1.43	1.48
28	a3	1005	PUB	C4D-C3D	-2.64	1.43	1.48
28	L5	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	p5	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	Q8	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	V9	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	aN	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	dD	203	PUB	C4D-C3D	-2.64	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	ep	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	ga	203	PUB	C4D-C3D	-2.64	1.43	1.48
28	eB	204	PUB	C4D-C3D	-2.64	1.43	1.48
28	lz	405	PUB	C4D-C3D	-2.64	1.43	1.48
28	gd	202	PUB	C4D-C3D	-2.64	1.43	1.48
28	z3	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	44	305	PUB	C4D-C3D	-2.63	1.43	1.48
28	dB	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	dP	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	ee	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	fo	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	f8	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	H6	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	kV	1003	PUB	C4D-C3D	-2.63	1.43	1.48
28	fc	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	r4	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	r5	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	ly	405	PUB	C4D-C3D	-2.63	1.43	1.48
28	lz	404	PUB	C4D-C3D	-2.63	1.43	1.48
28	fy	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	hH	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	eH	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	ge	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	hD	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	hX	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	jJ	1003	PUB	C4D-C3D	-2.63	1.43	1.48
26	S9	202	PEB	C2A-C1A	-2.63	1.49	1.52
28	J3	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	kR	1003	PUB	C4D-C3D	-2.63	1.43	1.48
28	z6	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	eY	405	PUB	C4D-C3D	-2.63	1.43	1.48
28	eZ	404	PUB	C4D-C3D	-2.63	1.43	1.48
28	J2	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	X6	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	d9	305	PUB	C4D-C3D	-2.63	1.43	1.48
28	E8	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	dT	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	ez	1005	PUB	C4D-C3D	-2.63	1.43	1.48
28	lh	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	X4	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	a7	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	cn	202	PUB	C4D-C3D	-2.63	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	lv	202	PUB	C4D-C3D	-2.63	1.43	1.48
29	d9	304	PVN	C14-C13	-2.63	1.40	1.45
28	h3	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	34	1006	PUB	C4D-C3D	-2.63	1.43	1.48
28	t4	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	Y5	1006	PUB	C4D-C3D	-2.63	1.43	1.48
28	e8	305	PUB	C4D-C3D	-2.63	1.43	1.48
28	t9	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	gy	306	PUB	C4D-C3D	-2.63	1.43	1.48
28	h8	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	V7	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	P9	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	n2	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	t3	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	e6	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	O8	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	aZ	305	PUB	C4D-C3D	-2.63	1.43	1.48
28	J7	202	PUB	C4D-C3D	-2.63	1.43	1.48
26	gf	202	PEB	C2A-C1A	-2.63	1.49	1.52
28	z2	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	Z3	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	v3	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	L6	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	r7	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	bB	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	dL	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	ld	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	ln	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	u6	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	n8	202	PUB	C4D-C3D	-2.63	1.43	1.48
28	s7	203	PUB	C4D-C3D	-2.63	1.43	1.48
28	az	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	R9	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	d7	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	dH	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	ev	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	jL	1003	PUB	C4D-C3D	-2.62	1.43	1.48
28	v4	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	v5	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	bT	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	fj	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	gp	203	PUB	C4D-C3D	-2.62	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	X2	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	dK	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	fs	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	n4	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	r6	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	av	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	dv	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	cN	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	T2	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	J5	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	T8	305	PUB	C4D-C3D	-2.62	1.43	1.48
28	ey	1005	PUB	C4D-C3D	-2.62	1.43	1.48
28	I8	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	N9	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	dw	405	PUB	C4D-C3D	-2.62	1.43	1.48
28	kQ	1003	PUB	C4D-C3D	-2.62	1.43	1.48
28	X3	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	p7	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	cP	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	b9	407	PUB	C4D-C3D	-2.62	1.43	1.48
28	cQ	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	eX	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	hL	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	j3	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	bo	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	bL	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	fi	203	PUB	C4D-C3D	-2.62	1.43	1.48
26	cI	202	PEB	C2A-C1A	-2.62	1.49	1.52
28	y8	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	gk	203	PUB	C4D-C3D	-2.62	1.43	1.48
29	C2	303	PVN	C15-C16	2.62	1.44	1.38
29	c3	303	PVN	C15-C16	2.62	1.44	1.38
28	c8	305	PUB	C4D-C3D	-2.62	1.43	1.48
26	gc	202	PEB	C2A-C1A	-2.62	1.49	1.52
28	C2	304	PUB	C4D-C3D	-2.62	1.43	1.48
28	N6	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	L7	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	lp	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	et	203	PUB	C4D-C3D	-2.62	1.43	1.48
26	de	202	PEB	C2A-C1A	-2.62	1.49	1.52
28	N3	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	br	203	PUB	C4D-C3D	-2.62	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	eZ	402	PVN	C14-C13	-2.62	1.40	1.45
28	g8	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	P7	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	gz	305	PUB	C4D-C3D	-2.62	1.43	1.48
28	cH	202	PUB	C4D-C3D	-2.62	1.43	1.48
28	lf	203	PUB	C4D-C3D	-2.62	1.43	1.48
28	hZ	404	PUB	C4D-C3D	-2.62	1.43	1.48
28	c3	305	PUB	C4D-C3D	-2.61	1.43	1.48
28	M8	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	gt	203	PUB	C4D-C3D	-2.61	1.43	1.48
29	d8	303	PVN	C14-C13	-2.61	1.40	1.45
28	T6	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	X7	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	aY	404	PUB	C4D-C3D	-2.61	1.43	1.48
28	aY	405	PUB	C4D-C3D	-2.61	1.43	1.48
28	gx	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	jM	1003	PUB	C4D-C3D	-2.61	1.43	1.48
26	dU	202	PEB	C2A-C1A	-2.61	1.49	1.52
28	l2	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	Y9	304	PUB	C4D-C3D	-2.61	1.43	1.48
28	bn	202	PUB	C4D-C3D	-2.61	1.43	1.48
28	w8	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	aB	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	bz	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	bJ	203	PUB	C4D-C3D	-2.61	1.43	1.48
26	C9	202	PEB	C2A-C1A	-2.61	1.49	1.52
28	L3	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	y7	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	l3	202	PUB	C4D-C3D	-2.61	1.43	1.48
28	cR	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	ly	406	PUB	C4D-C3D	-2.61	1.43	1.48
28	gz	306	PUB	C4D-C3D	-2.61	1.43	1.48
28	c3	304	PUB	C4D-C3D	-2.61	1.43	1.48
28	D6	202	PUB	C4D-C3D	-2.61	1.43	1.48
28	cM	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	r2	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	34	1005	PUB	C4D-C3D	-2.61	1.43	1.48
28	V5	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	df	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	eF	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	V3	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	44	304	PUB	C4D-C3D	-2.61	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	di	203	PUB	C4D-C3D	-2.61	1.43	1.48
29	gz	304	PVN	C4-N1	-2.61	1.41	1.45
28	L2	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	e8	304	PUB	C4D-C3D	-2.61	1.43	1.48
28	N7	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	G8	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	L9	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	dl	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	ey	1006	PUB	C4D-C3D	-2.61	1.43	1.48
28	P2	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	Z6	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	bZ	306	PUB	C4D-C3D	-2.61	1.43	1.48
26	gz	302	PEB	C2A-C1A	-2.61	1.49	1.52
28	j2	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	D3	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	H2	202	PUB	C4D-C3D	-2.61	1.43	1.48
28	p3	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	T8	304	PUB	C4D-C3D	-2.61	1.43	1.48
29	eY	403	PVN	C14-C13	-2.61	1.40	1.45
28	P6	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	ar	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	eD	203	PUB	C4D-C3D	-2.61	1.43	1.48
28	b8	1006	PUB	C4D-C3D	-2.61	1.43	1.48
28	H3	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	J6	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	H7	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	eV	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	hY	406	PUB	C4D-C3D	-2.60	1.43	1.48
28	l6	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	lb	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	ll	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	iC	1003	PUB	C4D-C3D	-2.60	1.43	1.48
28	iD	1003	PUB	C4D-C3D	-2.60	1.43	1.48
28	fm	203	PUB	C4D-C3D	-2.60	1.43	1.48
26	bI	202	PEB	C2A-C1A	-2.60	1.49	1.52
28	L4	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	cq	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	jO	1003	PUB	C4D-C3D	-2.60	1.43	1.48
28	hJ	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	H5	202	PUB	C4D-C3D	-2.60	1.43	1.48
28	bP	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	hT	203	PUB	C4D-C3D	-2.60	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D4	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	B6	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	eL	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	jK	1003	PUB	C4D-C3D	-2.60	1.43	1.48
28	V6	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	aL	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	ff	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	p9	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	ap	203	PUB	C4D-C3D	-2.60	1.43	1.48
26	f5	201	PEB	C2A-C1A	-2.60	1.49	1.52
28	N2	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	Z7	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	bR	202	PUB	C4D-C3D	-2.60	1.43	1.48
28	A2	1005	PUB	C4D-C3D	-2.60	1.43	1.48
28	P4	203	PUB	C4D-C3D	-2.60	1.43	1.48
26	hS	202	PEB	C2A-C1A	-2.60	1.49	1.52
28	f3	203	PUB	C4D-C3D	-2.60	1.43	1.48
28	Z5	305	PUB	C4D-C3D	-2.60	1.43	1.48
28	R2	203	PUB	C4D-C3D	-2.59	1.43	1.48
28	fq	203	PUB	C4D-C3D	-2.59	1.43	1.48
26	U9	202	PEB	C2A-C1A	-2.59	1.49	1.52
26	hM	1002	PEB	C2A-C1A	-2.59	1.49	1.52
28	ax	202	PUB	C4D-C3D	-2.59	1.43	1.48
26	E3	202	PEB	C2A-C1A	-2.59	1.49	1.52
26	c4	201	PEB	C2A-C1A	-2.59	1.49	1.52
28	eb	202	PUB	C4D-C3D	-2.59	1.43	1.48
28	an	202	PUB	C4D-C3D	-2.59	1.43	1.48
26	C4	1002	PEB	C2A-C1A	-2.59	1.49	1.52
26	g7	202	PEB	C2A-C1A	-2.59	1.49	1.52
28	jN	1003	PUB	C4D-C3D	-2.59	1.43	1.48
28	J4	203	PUB	C4D-C3D	-2.59	1.43	1.48
26	d8	301	PEB	C2A-C1A	-2.59	1.49	1.52
28	aH	203	PUB	C4D-C3D	-2.59	1.43	1.48
28	v2	203	PUB	C4D-C3D	-2.59	1.43	1.48
26	lj	201	PEB	C2A-C1A	-2.59	1.49	1.52
28	hZ	405	PUB	C4D-C3D	-2.59	1.43	1.48
28	kW	1003	PUB	C4D-C3D	-2.58	1.43	1.48
26	Q3	202	PEB	C2A-C1A	-2.58	1.49	1.52
28	en	203	PUB	C4D-C3D	-2.58	1.43	1.48
28	hG	202	PUB	C4D-C3D	-2.58	1.43	1.48
28	bN	203	PUB	C4D-C3D	-2.58	1.43	1.48
26	r8	202	PEB	C2A-C1A	-2.58	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	x2	202	PUB	C4D-C3D	-2.58	1.43	1.48
26	eA	1002	PEB	C2A-C1A	-2.58	1.49	1.52
26	lo	202	PEB	C2A-C1A	-2.58	1.49	1.52
28	x3	203	PUB	C4D-C3D	-2.57	1.43	1.48
26	k7	1002	PEB	C2A-C1A	-2.57	1.49	1.52
26	fb	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	E2	1002	PEB	C2A-C1A	-2.57	1.49	1.52
26	I7	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	G5	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	M7	1003	PEB	C2A-C1A	-2.57	1.49	1.52
26	j7	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	A4	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	h7	202	PEB	C2A-C1A	-2.57	1.49	1.52
26	e3	1002	PEB	C2A-C1A	-2.57	1.49	1.52
28	H9	203	PUB	C4D-C3D	-2.57	1.43	1.48
26	hU	201	PEB	C2A-C1A	-2.57	1.49	1.52
29	b9	405	PVN	C19-C18	-2.57	1.43	1.48
26	bC	202	PEB	C2A-C1A	-2.56	1.49	1.52
29	bZ	304	PVN	C15-C16	2.56	1.44	1.38
26	o8	201	PEB	C3C-C4C	2.56	1.46	1.42
26	e6	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	iF	1002	PEB	C2A-C1A	-2.56	1.49	1.52
26	bS	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	gm	1002	PEB	C2A-C1A	-2.56	1.49	1.52
28	T7	203	PUB	C4D-C3D	-2.56	1.43	1.48
26	i7	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	cI	202	PEB	C3C-C4C	2.56	1.46	1.42
26	u3	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	H6	201	PEB	C2A-C1A	-2.56	1.49	1.52
26	ec	201	PEB	C2A-C1A	-2.56	1.49	1.52
26	ev	201	PEB	C2A-C1A	-2.56	1.49	1.52
26	fz	301	PEB	C2A-C1A	-2.56	1.49	1.52
28	eN	203	PUB	C4D-C3D	-2.56	1.43	1.48
26	O9	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	bQ	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	fe	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	fg	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	hK	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	p6	202	PEB	C2A-C1A	-2.56	1.49	1.52
26	ld	201	PEB	C2A-C1A	-2.56	1.49	1.52
26	Y5	1002	PEB	C2A-C1A	-2.55	1.49	1.52
26	q5	202	PEB	C2A-C1A	-2.55	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cw	202	PEB	C3C-C4C	2.55	1.46	1.42
26	q7	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	bY	1002	PEB	C2A-C1A	-2.55	1.49	1.52
26	dJ	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	fh	1002	PEB	C2A-C1A	-2.55	1.49	1.52
26	gu	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	t6	201	PEB	C2A-C1A	-2.55	1.49	1.52
26	cv	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	eh	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	f7	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	K3	202	PEB	C3C-C4C	2.55	1.46	1.42
26	A5	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	d6	202	PEB	C2A-C1A	-2.55	1.49	1.52
26	lo	201	PEB	C2A-C1A	-2.55	1.49	1.52
26	fp	202	PEB	C2A-C1A	-2.55	1.49	1.52
29	aZ	303	PVN	C15-C16	2.55	1.44	1.38
26	h5	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	t8	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	dZ	1002	PEB	C2A-C1A	-2.54	1.49	1.52
26	gh	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	u7	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	c9	303	PVN	C15-C16	2.54	1.44	1.38
26	N2	201	PEB	C2A-C1A	-2.54	1.49	1.52
26	a3	1002	PEB	C2A-C1A	-2.54	1.49	1.52
26	gw	202	PEB	C3C-C4C	2.54	1.46	1.42
26	m7	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	I5	202	PEB	C3C-C4C	2.54	1.46	1.42
26	ek	1002	PEB	C2A-C1A	-2.54	1.49	1.52
26	lm	1002	PEB	C2A-C1A	-2.54	1.49	1.52
26	C3	1002	PEB	C3C-C4C	2.54	1.46	1.42
26	bY	1002	PEB	C3C-C4C	2.54	1.46	1.42
26	w3	202	PEB	C2A-C1A	-2.54	1.49	1.52
29	D2	303	PVN	C14-C13	-2.54	1.40	1.45
29	d3	302	PVN	C14-C13	-2.54	1.40	1.45
26	Q7	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	eY	401	PEB	C2A-C1A	-2.54	1.49	1.52
26	hF	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	lg	202	PEB	C3C-C4C	2.54	1.46	1.42
26	m5	1002	PEB	C2A-C1A	-2.54	1.49	1.52
26	cG	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	eu	202	PEB	C2A-C1A	-2.54	1.49	1.52
26	hY	402	PEB	C2A-C1A	-2.54	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A9	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	ct	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	fv	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	bG	202	PEB	C3C-C4C	2.53	1.46	1.42
26	I5	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	Q5	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	Y7	1002	PEB	C2A-C1A	-2.53	1.49	1.52
26	gw	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	dc	202	PEB	C3C-C4C	2.53	1.46	1.42
26	au	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	fn	1002	PEB	C2A-C1A	-2.53	1.49	1.52
26	iB	1002	PEB	C2A-C1A	-2.53	1.49	1.52
26	eA	1002	PEB	C3C-C4C	2.53	1.46	1.42
26	A3	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	y3	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	da	1002	PEB	C2A-C1A	-2.53	1.49	1.52
26	ay	1002	PEB	C2A-C1A	-2.53	1.49	1.52
26	dc	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	lg	201	PEB	C2A-C1A	-2.53	1.49	1.52
26	O3	1002	PEB	C2A-C1A	-2.53	1.49	1.52
26	S7	202	PEB	C3C-C4C	2.53	1.46	1.42
26	fk	202	PEB	C3C-C4C	2.53	1.46	1.42
27	H1	201	CYC	O2D-CGD	-2.53	1.22	1.30
26	bG	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	gl	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	ct	202	PEB	C3C-C4C	2.53	1.46	1.42
27	v1	201	CYC	O2D-CGD	-2.53	1.22	1.30
26	C7	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	gq	202	PEB	C2A-C1A	-2.53	1.49	1.52
26	A4	202	PEB	C3C-C4C	2.52	1.46	1.42
26	go	202	PEB	C3C-C4C	2.52	1.46	1.42
27	z1	201	CYC	O2D-CGD	-2.52	1.22	1.30
26	ay	1002	PEB	C3C-C4C	2.52	1.46	1.42
29	ez	1004	PVN	C19-C18	-2.52	1.43	1.48
29	c8	303	PVN	C15-C16	2.52	1.44	1.38
26	cZ	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	go	202	PEB	C2A-C1A	-2.52	1.49	1.52
27	S1	201	CYC	O2D-CGD	-2.52	1.22	1.30
27	j1	201	CYC	O2D-CGD	-2.52	1.22	1.30
26	E3	202	PEB	C3C-C4C	2.52	1.46	1.42
26	d3	301	PEB	C2A-C1A	-2.52	1.49	1.52
26	bM	202	PEB	C2A-C1A	-2.52	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eB	201	PEB	C2A-C1A	-2.52	1.49	1.52
26	eP	201	PEB	C2A-C1A	-2.52	1.49	1.52
27	M1	1001	CYC	O2D-CGD	-2.52	1.22	1.30
26	p6	202	PEB	C3C-C4C	2.52	1.46	1.42
27	a2	901	CYC	O2D-CGD	-2.52	1.22	1.30
26	cw	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	Y5	1002	PEB	C3C-C4C	2.52	1.46	1.42
26	S2	202	PEB	C3C-C4C	2.52	1.46	1.42
26	s3	202	PEB	C3C-C4C	2.52	1.46	1.42
26	f7	202	PEB	C3C-C4C	2.52	1.46	1.42
26	eY	401	PEB	C3C-C4C	2.52	1.46	1.42
26	hY	402	PEB	C3C-C4C	2.52	1.46	1.42
26	w5	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	a6	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	q8	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	e3	1002	PEB	C3C-C4C	2.52	1.46	1.42
27	r1	201	CYC	O2D-CGD	-2.52	1.22	1.30
26	o5	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	H6	201	PEB	C3C-C4C	2.52	1.46	1.42
26	Y7	1002	PEB	C3C-C4C	2.52	1.46	1.42
26	iA	1002	PEB	C3C-C4C	2.52	1.46	1.42
29	gz	304	PVN	O1-C1	-2.52	1.18	1.23
26	Q7	202	PEB	C3C-C4C	2.52	1.46	1.42
26	k3	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	M5	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	fl	202	PEB	C2A-C1A	-2.52	1.49	1.52
26	q5	202	PEB	C3C-C4C	2.52	1.46	1.42
26	o7	202	PEB	C3C-C4C	2.51	1.46	1.42
26	gc	202	PEB	C3C-C4C	2.51	1.46	1.42
26	S3	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	lq	203	PEB	C2A-C1A	-2.51	1.49	1.52
26	ls	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	hO	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	cK	202	PEB	C3C-C4C	2.51	1.46	1.42
27	J1	201	CYC	O2D-CGD	-2.51	1.22	1.30
26	h4	201	PEB	C3C-C4C	2.51	1.46	1.42
26	w7	1002	PEB	C2A-C1A	-2.51	1.49	1.52
26	bM	202	PEB	C3C-C4C	2.51	1.45	1.42
26	lo	201	PEB	C3C-C4C	2.51	1.45	1.42
26	O5	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	G7	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	I9	202	PEB	C2A-C1A	-2.51	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	lt	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	lw	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	hZ	401	PEB	C2A-C1A	-2.51	1.49	1.52
27	a2	902	CYC	O2D-CGD	-2.51	1.22	1.30
27	b2	1001	CYC	O2D-CGD	-2.51	1.22	1.30
26	S2	202	PEB	C2A-C1A	-2.51	1.49	1.52
27	c1	201	CYC	O2D-CGD	-2.51	1.22	1.30
26	Q5	202	PEB	C3C-C4C	2.51	1.45	1.42
26	r8	202	PEB	C3C-C4C	2.51	1.45	1.42
26	cZ	202	PEB	C3C-C4C	2.51	1.45	1.42
26	de	202	PEB	C3C-C4C	2.51	1.45	1.42
26	hK	202	PEB	C3C-C4C	2.51	1.45	1.42
26	R2	201	PEB	C2A-C1A	-2.51	1.49	1.52
26	K5	1002	PEB	C2A-C1A	-2.51	1.49	1.52
26	E9	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	f5	201	PEB	C3C-C4C	2.51	1.45	1.42
26	bA	202	PEB	C3C-C4C	2.51	1.45	1.42
26	bU	202	PEB	C3C-C4C	2.51	1.45	1.42
26	R2	201	PEB	C3C-C4C	2.51	1.45	1.42
26	U6	202	PEB	C3C-C4C	2.51	1.45	1.42
26	ec	201	PEB	C3C-C4C	2.51	1.45	1.42
26	V6	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	lc	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	G3	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	h4	201	PEB	C2A-C1A	-2.51	1.49	1.52
26	C5	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	lk	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	hW	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	lq	203	PEB	C3C-C4C	2.51	1.45	1.42
26	m5	1002	PEB	C3C-C4C	2.51	1.45	1.42
26	n6	201	PEB	C2A-C1A	-2.51	1.49	1.52
26	hI	202	PEB	C2A-C1A	-2.51	1.49	1.52
26	Q3	202	PEB	C3C-C4C	2.50	1.45	1.42
27	p1	201	CYC	O2D-CGD	-2.50	1.22	1.30
27	t1	201	CYC	O2D-CGD	-2.50	1.22	1.30
26	bS	202	PEB	C3C-C4C	2.50	1.45	1.42
26	cv	202	PEB	C3C-C4C	2.50	1.45	1.42
26	O7	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	lg	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	G3	202	PEB	C3C-C4C	2.50	1.45	1.42
26	gb	1002	PEB	C3C-C4C	2.50	1.45	1.42
26	Z5	302	PEB	C3C-C4C	2.50	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a6	202	PEB	C3C-C4C	2.50	1.45	1.42
26	iA	1002	PEB	C2A-C1A	-2.50	1.49	1.52
29	ey	1004	PVN	C19-C18	-2.50	1.43	1.48
26	s8	202	PEB	C3C-C4C	2.50	1.45	1.42
26	cm	1002	PEB	C3C-C4C	2.50	1.45	1.42
27	Y1	201	CYC	O2D-CGD	-2.50	1.22	1.30
26	ef	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	as	202	PEB	C3C-C4C	2.50	1.45	1.42
26	ek	1002	PEB	C3C-C4C	2.50	1.45	1.42
26	U2	202	PEB	C3C-C4C	2.50	1.45	1.42
26	o3	202	PEB	C3C-C4C	2.50	1.45	1.42
26	G7	202	PEB	C3C-C4C	2.50	1.45	1.42
27	S1	202	CYC	O2D-CGD	-2.50	1.22	1.30
26	M9	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	k3	202	PEB	C3C-C4C	2.50	1.45	1.42
26	c5	201	PEB	C3C-C4C	2.50	1.45	1.42
26	fb	202	PEB	C3C-C4C	2.50	1.45	1.42
26	fl	202	PEB	C3C-C4C	2.50	1.45	1.42
26	dg	202	PEB	C3C-C4C	2.50	1.45	1.42
26	U5	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	c5	201	PEB	C2A-C1A	-2.50	1.49	1.52
26	aw	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	fr	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	s5	202	PEB	C3C-C4C	2.50	1.45	1.42
26	ei	201	PEB	C3C-C4C	2.50	1.45	1.42
26	M7	1003	PEB	C3C-C4C	2.50	1.45	1.42
26	bO	202	PEB	C3C-C4C	2.50	1.45	1.42
26	eL	201	PEB	C3C-C4C	2.50	1.45	1.42
26	le	202	PEB	C3C-C4C	2.50	1.45	1.42
26	cK	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	ei	201	PEB	C2A-C1A	-2.50	1.49	1.52
26	N2	201	PEB	C3C-C4C	2.50	1.45	1.42
26	g3	202	PEB	C3C-C4C	2.50	1.45	1.42
26	G5	202	PEB	C3C-C4C	2.50	1.45	1.42
26	d6	202	PEB	C3C-C4C	2.50	1.45	1.42
26	M9	202	PEB	C3C-C4C	2.50	1.45	1.42
26	ao	202	PEB	C3C-C4C	2.50	1.45	1.42
26	au	202	PEB	C3C-C4C	2.50	1.45	1.42
26	Z5	302	PEB	C2A-C1A	-2.50	1.49	1.52
26	hE	1002	PEB	C2A-C1A	-2.50	1.49	1.52
26	bK	1002	PEB	C3C-C4C	2.50	1.45	1.42
26	cu	202	PEB	C3C-C4C	2.50	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	gf	202	PEB	C3C-C4C	2.50	1.45	1.42
26	bQ	202	PEB	C3C-C4C	2.50	1.45	1.42
26	cD	202	PEB	C3C-C4C	2.50	1.45	1.42
26	c3	301	PEB	C2A-C1A	-2.50	1.49	1.52
26	g3	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	o3	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	I3	202	PEB	C3C-C4C	2.50	1.45	1.42
26	m7	202	PEB	C3C-C4C	2.50	1.45	1.42
29	b8	1004	PVN	C19-C18	-2.50	1.43	1.48
26	dg	202	PEB	C2A-C1A	-2.50	1.49	1.52
26	gy	302	PEB	C2A-C1A	-2.50	1.49	1.52
26	E2	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	gy	302	PEB	C3C-C4C	2.49	1.45	1.42
26	M3	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	Z9	1002	PEB	C2A-C1A	-2.49	1.49	1.52
26	bA	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	cu	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	cy	1002	PEB	C2A-C1A	-2.49	1.49	1.52
26	db	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	fx	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	dU	202	PEB	C3C-C4C	2.49	1.45	1.42
27	h1	201	CYC	O2D-CGD	-2.49	1.22	1.30
29	Z9	1004	PVN	C15-C16	2.49	1.43	1.38
26	iB	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	da	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	hW	202	PEB	C3C-C4C	2.49	1.45	1.42
26	I3	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	u5	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	N6	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	cD	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	gs	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	N4	202	PEB	C3C-C4C	2.49	1.45	1.42
26	ef	202	PEB	C3C-C4C	2.49	1.45	1.42
26	et	201	PEB	C3C-C4C	2.49	1.45	1.42
26	P2	202	PEB	C3C-C4C	2.49	1.45	1.42
26	y3	202	PEB	C3C-C4C	2.49	1.45	1.42
26	y5	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	U9	202	PEB	C3C-C4C	2.49	1.45	1.42
26	lj	201	PEB	C3C-C4C	2.49	1.45	1.42
26	gq	202	PEB	C3C-C4C	2.49	1.45	1.42
26	lg	201	PEB	C3C-C4C	2.49	1.45	1.42
26	I7	202	PEB	C3C-C4C	2.49	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y9	301	PEB	C3C-C4C	2.49	1.45	1.42
26	hM	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	gb	1002	PEB	C2A-C1A	-2.49	1.49	1.52
26	O9	202	PEB	C3C-C4C	2.49	1.45	1.42
26	Z9	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	cx	202	PEB	C3C-C4C	2.49	1.45	1.42
26	w3	202	PEB	C3C-C4C	2.49	1.45	1.42
26	E5	202	PEB	C3C-C4C	2.49	1.45	1.42
29	e9	304	PVN	C15-C16	2.49	1.43	1.38
26	Y3	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	K9	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	dJ	202	PEB	C3C-C4C	2.49	1.45	1.42
26	dZ	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	ev	201	PEB	C3C-C4C	2.49	1.45	1.42
26	lm	1002	PEB	C3C-C4C	2.49	1.45	1.42
26	hF	202	PEB	C3C-C4C	2.49	1.45	1.42
26	hU	201	PEB	C3C-C4C	2.49	1.45	1.42
26	K7	202	PEB	C3C-C4C	2.49	1.45	1.42
26	w5	202	PEB	C3C-C4C	2.49	1.45	1.42
26	lt	202	PEB	C3C-C4C	2.49	1.45	1.42
26	lw	201	PEB	C3C-C4C	2.49	1.45	1.42
26	bO	202	PEB	C2A-C1A	-2.49	1.49	1.52
26	fg	202	PEB	C3C-C4C	2.48	1.45	1.42
26	gu	202	PEB	C3C-C4C	2.48	1.45	1.42
29	U8	1004	PVN	C15-C16	2.48	1.43	1.38
29	e8	303	PVN	C15-C16	2.48	1.43	1.38
26	db	202	PEB	C3C-C4C	2.48	1.45	1.42
26	bK	1002	PEB	C2A-C1A	-2.48	1.49	1.52
26	k7	1002	PEB	C3C-C4C	2.48	1.45	1.42
26	G9	202	PEB	C3C-C4C	2.48	1.45	1.42
26	A2	1001	PEB	C2A-C1A	-2.48	1.49	1.52
26	t6	201	PEB	C3C-C4C	2.48	1.45	1.42
26	U7	202	PEB	C3C-C4C	2.48	1.45	1.42
26	bC	202	PEB	C3C-C4C	2.48	1.45	1.42
26	fx	202	PEB	C3C-C4C	2.48	1.45	1.42
26	s4	202	PEB	C2A-C1A	-2.48	1.49	1.52
26	i3	202	PEB	C3C-C4C	2.48	1.45	1.42
26	em	202	PEB	C3C-C4C	2.48	1.45	1.42
26	G6	202	PEB	C3C-C4C	2.48	1.45	1.42
26	w4	202	PEB	C2A-C1A	-2.48	1.49	1.52
26	M3	202	PEB	C3C-C4C	2.48	1.45	1.42
26	i7	202	PEB	C3C-C4C	2.48	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eB	201	PEB	C3C-C4C	2.48	1.45	1.42
26	O5	202	PEB	C3C-C4C	2.48	1.45	1.42
26	A9	202	PEB	C3C-C4C	2.48	1.45	1.42
26	Q9	202	PEB	C3C-C4C	2.48	1.45	1.42
26	V6	202	PEB	C3C-C4C	2.48	1.45	1.42
26	S9	202	PEB	C3C-C4C	2.48	1.45	1.42
26	cy	1002	PEB	C3C-C4C	2.48	1.45	1.42
26	m3	202	PEB	C2A-C1A	-2.48	1.49	1.52
26	c3	301	PEB	C3C-C4C	2.48	1.45	1.42
26	gs	202	PEB	C3C-C4C	2.48	1.45	1.42
26	C4	1002	PEB	C3C-C4C	2.48	1.45	1.42
29	C2	303	PVN	C11-C12	-2.48	1.41	1.45
29	c3	303	PVN	C11-C12	-2.48	1.41	1.45
26	cA	202	PEB	C2A-C1A	-2.48	1.49	1.52
26	cC	1002	PEB	C2A-C1A	-2.48	1.49	1.52
26	lu	202	PEB	C3C-C4C	2.48	1.45	1.42
26	fv	202	PEB	C3C-C4C	2.47	1.45	1.42
26	S7	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	ey	1001	PEB	C2A-C1A	-2.47	1.49	1.52
26	bE	202	PEB	C3C-C4C	2.47	1.45	1.42
26	S3	202	PEB	C3C-C4C	2.47	1.45	1.42
26	s4	202	PEB	C3C-C4C	2.47	1.45	1.42
26	bI	202	PEB	C3C-C4C	2.47	1.45	1.42
26	gj	202	PEB	C3C-C4C	2.47	1.45	1.42
26	O3	1002	PEB	C3C-C4C	2.47	1.45	1.42
26	A5	202	PEB	C3C-C4C	2.47	1.45	1.42
26	K5	1002	PEB	C3C-C4C	2.47	1.45	1.42
26	o5	202	PEB	C3C-C4C	2.47	1.45	1.42
26	lk	202	PEB	C3C-C4C	2.47	1.45	1.42
26	fr	202	PEB	C3C-C4C	2.47	1.45	1.42
26	a3	1002	PEB	C3C-C4C	2.47	1.45	1.42
26	h5	202	PEB	C3C-C4C	2.47	1.45	1.42
26	d8	301	PEB	C3C-C4C	2.47	1.45	1.42
26	h7	202	PEB	C3C-C4C	2.47	1.45	1.42
26	m3	202	PEB	C3C-C4C	2.47	1.45	1.42
26	w7	1002	PEB	C3C-C4C	2.47	1.45	1.42
26	gm	1002	PEB	C3C-C4C	2.47	1.45	1.42
26	hO	202	PEB	C3C-C4C	2.47	1.45	1.42
26	s8	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	A2	1001	PEB	C3C-C4C	2.47	1.45	1.42
26	C7	202	PEB	C3C-C4C	2.47	1.45	1.42
26	cA	202	PEB	C3C-C4C	2.47	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hA	202	PEB	C3C-C4C	2.47	1.45	1.42
26	o7	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	hA	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	d3	301	PEB	C3C-C4C	2.47	1.45	1.42
26	E7	202	PEB	C3C-C4C	2.47	1.45	1.42
26	ls	202	PEB	C3C-C4C	2.47	1.45	1.42
26	w4	202	PEB	C3C-C4C	2.47	1.45	1.42
26	lo	202	PEB	C3C-C4C	2.47	1.45	1.42
26	lw	202	PEB	C3C-C4C	2.47	1.45	1.42
26	fz	301	PEB	C3C-C4C	2.47	1.45	1.42
29	hY	404	PVN	C5-C4	-2.47	1.47	1.54
26	eh	202	PEB	C3C-C4C	2.47	1.45	1.42
26	ft	202	PEB	C3C-C4C	2.47	1.45	1.42
26	o8	201	PEB	C2A-C1A	-2.47	1.49	1.52
26	K7	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	G9	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	as	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	Y3	202	PEB	C3C-C4C	2.47	1.45	1.42
26	bZ	302	PEB	C3C-C4C	2.47	1.45	1.42
26	hC	202	PEB	C3C-C4C	2.47	1.45	1.42
26	ey	1001	PEB	C3C-C4C	2.47	1.45	1.42
26	K3	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	U6	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	f6	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	U7	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	em	202	PEB	C2A-C1A	-2.47	1.49	1.52
26	W3	202	PEB	C3C-C4C	2.47	1.45	1.42
26	C5	202	PEB	C3C-C4C	2.47	1.45	1.42
26	j7	202	PEB	C3C-C4C	2.47	1.45	1.42
26	c8	301	PEB	C3C-C4C	2.47	1.45	1.42
26	hS	202	PEB	C3C-C4C	2.47	1.45	1.42
26	lc	202	PEB	C3C-C4C	2.46	1.45	1.42
26	hI	202	PEB	C3C-C4C	2.46	1.45	1.42
26	W3	202	PEB	C2A-C1A	-2.46	1.49	1.52
26	le	202	PEB	C2A-C1A	-2.46	1.49	1.52
26	lw	201	PEB	C2A-C1A	-2.46	1.49	1.52
29	T8	303	PVN	C14-C13	-2.46	1.40	1.45
29	Y9	303	PVN	C14-C13	-2.46	1.40	1.45
26	eP	201	PEB	C3C-C4C	2.46	1.45	1.42
26	A7	201	PEB	C2A-C1A	-2.46	1.49	1.52
26	bZ	302	PEB	C2A-C1A	-2.46	1.49	1.52
26	U3	202	PEB	C3C-C4C	2.46	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c4	201	PEB	C3C-C4C	2.46	1.45	1.42
26	hE	1002	PEB	C3C-C4C	2.46	1.45	1.42
26	y5	1002	PEB	C2A-C1A	-2.46	1.49	1.52
26	aw	202	PEB	C3C-C4C	2.46	1.45	1.42
26	gj	202	PEB	C2A-C1A	-2.46	1.49	1.52
29	hZ	403	PVN	C5-C4	-2.46	1.47	1.54
26	Y9	301	PEB	C2A-C1A	-2.46	1.49	1.52
26	u5	202	PEB	C3C-C4C	2.46	1.45	1.42
26	gl	202	PEB	C3C-C4C	2.46	1.45	1.42
26	U3	202	PEB	C2A-C1A	-2.46	1.49	1.52
26	A3	202	PEB	C3C-C4C	2.46	1.45	1.42
26	fe	202	PEB	C3C-C4C	2.46	1.45	1.42
26	C3	1002	PEB	C2A-C1A	-2.46	1.49	1.52
26	hC	202	PEB	C2A-C1A	-2.46	1.49	1.52
26	hQ	202	PEB	C2A-C1A	-2.46	1.49	1.52
26	M5	202	PEB	C3C-C4C	2.46	1.45	1.42
26	E9	202	PEB	C3C-C4C	2.46	1.45	1.42
26	S5	202	PEB	C3C-C4C	2.46	1.45	1.42
29	34	1004	PVN	C5-C4	-2.46	1.47	1.54
29	Y5	1004	PVN	C5-C4	-2.46	1.47	1.54
26	fk	202	PEB	C2A-C1A	-2.45	1.49	1.52
26	ft	202	PEB	C2A-C1A	-2.45	1.49	1.52
26	s7	202	PEB	C3C-C4C	2.45	1.45	1.42
26	C9	202	PEB	C3C-C4C	2.45	1.45	1.42
26	cC	1002	PEB	C3C-C4C	2.45	1.45	1.42
26	s5	202	PEB	C2A-C1A	-2.45	1.49	1.52
26	q8	202	PEB	C3C-C4C	2.45	1.45	1.42
26	g7	202	PEB	C3C-C4C	2.45	1.45	1.42
26	I9	202	PEB	C3C-C4C	2.45	1.45	1.42
26	hZ	401	PEB	C3C-C4C	2.45	1.45	1.42
26	eu	202	PEB	C3C-C4C	2.45	1.45	1.42
26	t8	202	PEB	C3C-C4C	2.45	1.45	1.42
26	E7	202	PEB	C2A-C1A	-2.45	1.49	1.52
26	E5	202	PEB	C2A-C1A	-2.45	1.49	1.52
26	ld	201	PEB	C3C-C4C	2.45	1.45	1.42
26	U5	202	PEB	C3C-C4C	2.45	1.45	1.42
26	gh	202	PEB	C3C-C4C	2.45	1.45	1.42
26	gz	302	PEB	C3C-C4C	2.45	1.45	1.42
26	q7	202	PEB	C3C-C4C	2.45	1.45	1.42
26	lh	201	PEB	C3C-C4C	2.45	1.45	1.42
26	A7	201	PEB	C3C-C4C	2.45	1.45	1.42
26	K9	1002	PEB	C2A-C1A	-2.44	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	lu	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	f6	202	PEB	C3C-C4C	2.44	1.45	1.42
26	n6	201	PEB	C3C-C4C	2.44	1.45	1.42
26	O7	202	PEB	C3C-C4C	2.44	1.45	1.42
26	u8	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	P2	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	W7	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	i3	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	S5	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	e6	202	PEB	C3C-C4C	2.44	1.45	1.42
26	W7	202	PEB	C3C-C4C	2.44	1.45	1.42
26	fh	1002	PEB	C3C-C4C	2.44	1.45	1.42
26	cx	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	iF	1002	PEB	C3C-C4C	2.44	1.45	1.42
26	Q9	202	PEB	C2A-C1A	-2.44	1.49	1.52
26	aq	202	PEB	C3C-C4C	2.44	1.45	1.42
26	fp	202	PEB	C3C-C4C	2.44	1.45	1.42
26	eL	201	PEB	C2A-C1A	-2.44	1.49	1.52
26	N6	202	PEB	C3C-C4C	2.44	1.45	1.42
26	cG	202	PEB	C3C-C4C	2.44	1.45	1.42
29	aZ	303	PVN	C14-C13	-2.44	1.40	1.45
29	D2	303	PVN	C15-C16	2.43	1.43	1.38
29	d3	302	PVN	C15-C16	2.43	1.43	1.38
26	u3	202	PEB	C3C-C4C	2.43	1.45	1.42
26	N4	202	PEB	C2A-C1A	-2.43	1.49	1.52
26	hQ	202	PEB	C3C-C4C	2.43	1.45	1.42
26	u8	202	PEB	C3C-C4C	2.43	1.45	1.42
29	ly	404	PVN	C15-C16	2.43	1.43	1.38
26	u7	202	PEB	C3C-C4C	2.43	1.45	1.42
26	G6	202	PEB	C2A-C1A	-2.43	1.49	1.52
26	lh	201	PEB	C2A-C1A	-2.43	1.49	1.52
26	s7	202	PEB	C2A-C1A	-2.43	1.49	1.52
26	c8	301	PEB	C2A-C1A	-2.43	1.49	1.52
26	U2	202	PEB	C2A-C1A	-2.43	1.49	1.52
29	A2	1004	PVN	C1-N1	-2.43	1.31	1.35
29	a3	1004	PVN	C1-N1	-2.43	1.31	1.35
26	fn	1002	PEB	C3C-C4C	2.42	1.45	1.42
29	lz	403	PVN	C15-C16	2.42	1.43	1.38
29	T8	303	PVN	C15-C16	2.42	1.43	1.38
29	Y9	303	PVN	C15-C16	2.42	1.43	1.38
29	bZ	304	PVN	C14-C13	-2.42	1.40	1.45
26	bU	202	PEB	C2A-C1A	-2.41	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cm	1002	PEB	C2A-C1A	-2.41	1.49	1.52
26	bE	202	PEB	C2A-C1A	-2.41	1.49	1.52
27	v1	201	CYC	C1B-C2B	2.41	1.49	1.45
27	J1	201	CYC	C1B-C2B	2.41	1.49	1.45
26	s3	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	hZ	403	PVN	C5-C6	-2.41	1.45	1.50
29	Y5	1004	PVN	C5-C6	-2.41	1.45	1.50
26	aq	202	PEB	C2A-C1A	-2.41	1.49	1.52
29	hY	404	PVN	C5-C6	-2.40	1.45	1.50
29	C2	303	PVN	C3-C2	2.40	1.36	1.34
29	c3	303	PVN	C3-C2	2.40	1.36	1.34
29	gy	304	PVN	C1-C2	2.40	1.54	1.47
27	Y1	201	CYC	C1B-C2B	2.40	1.49	1.45
29	A2	1004	PVN	C15-C16	2.39	1.43	1.38
29	a3	1004	PVN	C15-C16	2.39	1.43	1.38
29	bY	1004	PVN	C3-C2	2.39	1.36	1.34
27	z1	201	CYC	C1B-C2B	2.39	1.49	1.45
29	34	1004	PVN	C5-C6	-2.39	1.45	1.50
29	d8	303	PVN	C15-C16	2.39	1.43	1.38
29	gy	304	PVN	C15-C16	-2.38	1.32	1.38
27	c1	201	CYC	C1B-C2B	2.38	1.49	1.45
27	a2	902	CYC	C1B-C2B	2.38	1.49	1.45
27	b2	1001	CYC	C1B-C2B	2.38	1.49	1.45
29	hZ	403	PVN	C15-C16	2.38	1.43	1.38
29	ey	1004	PVN	C11-C12	-2.38	1.41	1.45
27	h1	201	CYC	C1B-C2B	2.37	1.49	1.45
27	p1	201	CYC	C1B-C2B	2.37	1.49	1.45
27	M1	1001	CYC	C1B-C2B	2.37	1.49	1.45
27	S1	201	CYC	C1B-C2B	2.37	1.49	1.45
27	j1	201	CYC	C1B-C2B	2.37	1.49	1.45
29	hY	404	PVN	C15-C16	2.37	1.43	1.38
28	n3	203	PUB	C2C-C3C	2.37	1.41	1.36
27	r1	201	CYC	C1B-C2B	2.37	1.49	1.45
28	J4	203	PUB	C2C-C3C	2.36	1.41	1.36
29	gy	304	PVN	O19-C19	-2.36	1.19	1.23
28	bq	203	PUB	C2C-C3C	2.36	1.41	1.36
28	Y5	1006	PUB	C2C-C3C	2.36	1.41	1.36
27	H1	201	CYC	C1B-C2B	2.36	1.49	1.45
28	dT	203	PUB	C2C-C3C	2.36	1.41	1.36
29	d9	304	PVN	C15-C16	2.35	1.43	1.38
28	t2	203	PUB	C2C-C3C	2.35	1.41	1.36
28	T3	203	PUB	C2C-C3C	2.35	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	cQ	202	PUB	C2C-C3C	2.35	1.41	1.36
28	P3	203	PUB	C2C-C3C	2.35	1.41	1.36
28	gr	202	PUB	C2C-C3C	2.35	1.41	1.36
28	t4	203	PUB	C2C-C3C	2.35	1.41	1.36
29	aY	403	PVN	C7-C6	-2.35	1.38	1.42
29	bY	1004	PVN	C7-C6	-2.35	1.38	1.42
27	a2	901	CYC	C1B-C2B	2.35	1.49	1.45
28	t6	203	PUB	C2C-C3C	2.35	1.41	1.36
26	g5	202	PEB	C3B-C2B	2.35	1.41	1.36
28	d7	203	PUB	C2C-C3C	2.35	1.41	1.36
28	aL	203	PUB	C2C-C3C	2.35	1.41	1.36
28	x2	202	PUB	C2C-C3C	2.35	1.41	1.36
28	H5	202	PUB	C2C-C3C	2.35	1.41	1.36
27	t1	201	CYC	C1B-C2B	2.35	1.49	1.45
28	eV	203	PUB	C2C-C3C	2.35	1.41	1.36
28	T6	203	PUB	C2C-C3C	2.35	1.41	1.36
28	n5	203	PUB	C2C-C3C	2.35	1.41	1.36
28	l3	202	PUB	C2C-C3C	2.35	1.41	1.36
28	v7	203	PUB	C2C-C3C	2.35	1.41	1.36
28	dw	406	PUB	C2C-C3C	2.35	1.41	1.36
28	lj	202	PUB	C2C-C3C	2.35	1.41	1.36
28	lx	201	PUB	C2C-C3C	2.35	1.41	1.36
28	d6	203	PUB	C2C-C3C	2.35	1.41	1.36
28	bH	203	PUB	C2C-C3C	2.35	1.41	1.36
28	a6	203	PUB	C2C-C3C	2.35	1.41	1.36
28	co	202	PUB	C2C-C3C	2.34	1.41	1.36
28	eP	204	PUB	C2C-C3C	2.34	1.41	1.36
28	V7	203	PUB	C2C-C3C	2.34	1.41	1.36
28	T8	304	PUB	C2C-C3C	2.34	1.41	1.36
28	bZ	305	PUB	C2C-C3C	2.34	1.41	1.36
28	R5	203	PUB	C2C-C3C	2.34	1.41	1.36
28	dH	203	PUB	C2C-C3C	2.34	1.41	1.36
28	R2	203	PUB	C2C-C3C	2.34	1.41	1.36
28	bJ	203	PUB	C2C-C3C	2.34	1.41	1.36
28	fc	203	PUB	C2C-C3C	2.34	1.41	1.36
28	o8	203	PUB	C2C-C3C	2.34	1.41	1.36
28	jL	1003	PUB	C2C-C3C	2.34	1.41	1.36
28	gy	305	PUB	C2C-C3C	2.34	1.41	1.36
28	b9	406	PUB	C2C-C3C	2.34	1.41	1.36
28	az	203	PUB	C2C-C3C	2.34	1.41	1.36
28	cB	203	PUB	C2C-C3C	2.34	1.41	1.36
28	ev	203	PUB	C2C-C3C	2.34	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	L3	203	PUB	C2C-C3C	2.34	1.41	1.36
28	p4	203	PUB	C2C-C3C	2.34	1.41	1.36
28	c8	304	PUB	C2C-C3C	2.34	1.41	1.36
28	kQ	1003	PUB	C2C-C3C	2.34	1.41	1.36
28	gx	203	PUB	C2C-C3C	2.34	1.41	1.36
28	V2	203	PUB	C2C-C3C	2.34	1.41	1.36
28	M8	203	PUB	C2C-C3C	2.34	1.41	1.36
28	R9	203	PUB	C2C-C3C	2.34	1.41	1.36
28	P5	202	PUB	C2C-C3C	2.34	1.41	1.36
28	F6	203	PUB	C2C-C3C	2.34	1.41	1.36
28	cq	203	PUB	C2C-C3C	2.34	1.41	1.36
28	ee	203	PUB	C2C-C3C	2.34	1.41	1.36
28	A2	1005	PUB	C2C-C3C	2.34	1.41	1.36
28	en	203	PUB	C2C-C3C	2.34	1.41	1.36
28	kR	1003	PUB	C2C-C3C	2.34	1.41	1.36
28	F2	203	PUB	C2C-C3C	2.34	1.41	1.36
28	v6	203	PUB	C2C-C3C	2.34	1.41	1.36
29	44	303	PVN	C14-C13	-2.34	1.40	1.45
29	Z5	304	PVN	C14-C13	-2.34	1.40	1.45
28	cs	203	PUB	C2C-C3C	2.34	1.41	1.36
28	T5	202	PUB	C2C-C3C	2.34	1.41	1.36
26	V7	202	PEB	C3B-C2B	2.34	1.41	1.36
28	E8	203	PUB	C2C-C3C	2.33	1.41	1.36
28	aY	404	PUB	C2C-C3C	2.33	1.41	1.36
28	ei	203	PUB	C2C-C3C	2.33	1.41	1.36
26	ar	202	PEB	C3B-C2B	2.33	1.41	1.36
28	H2	202	PUB	C2C-C3C	2.33	1.41	1.36
28	et	203	PUB	C2C-C3C	2.33	1.41	1.36
28	eJ	203	PUB	C2C-C3C	2.33	1.41	1.36
26	ep	202	PEB	C3B-C2B	2.33	1.41	1.36
28	X6	203	PUB	C2C-C3C	2.33	1.41	1.36
28	ec	203	PUB	C2C-C3C	2.33	1.41	1.36
28	p9	203	PUB	C2C-C3C	2.33	1.41	1.36
28	aJ	203	PUB	C2C-C3C	2.33	1.41	1.36
28	h3	202	PUB	C2C-C3C	2.33	1.41	1.36
28	F7	202	PUB	C2C-C3C	2.33	1.41	1.36
28	eH	203	PUB	C2C-C3C	2.33	1.41	1.36
28	fo	203	PUB	C2C-C3C	2.33	1.41	1.36
28	N5	203	PUB	C2C-C3C	2.33	1.41	1.36
28	c7	203	PUB	C2C-C3C	2.33	1.41	1.36
28	iH	1002	PUB	C2C-C3C	2.33	1.41	1.36
28	P4	203	PUB	C2C-C3C	2.33	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	dD	203	PUB	C2C-C3C	2.33	1.41	1.36
28	x9	203	PUB	C2C-C3C	2.33	1.41	1.36
28	hV	203	PUB	C2C-C3C	2.33	1.41	1.36
28	b9	407	PUB	C2C-C3C	2.33	1.41	1.36
28	dX	203	PUB	C2C-C3C	2.33	1.41	1.36
28	J6	203	PUB	C2C-C3C	2.33	1.41	1.36
28	Q8	203	PUB	C2C-C3C	2.33	1.41	1.36
28	P9	203	PUB	C2C-C3C	2.33	1.41	1.36
28	V9	203	PUB	C2C-C3C	2.33	1.41	1.36
28	ep	203	PUB	C2C-C3C	2.33	1.41	1.36
28	bP	203	PUB	C2C-C3C	2.33	1.41	1.36
28	dP	203	PUB	C2C-C3C	2.33	1.41	1.36
28	fj	203	PUB	C2C-C3C	2.33	1.41	1.36
28	hJ	203	PUB	C2C-C3C	2.33	1.41	1.36
27	S1	202	CYC	C1B-C2B	2.33	1.49	1.45
28	bn	202	PUB	C2C-C3C	2.33	1.41	1.36
28	D7	203	PUB	C2C-C3C	2.33	1.41	1.36
28	ln	203	PUB	C2C-C3C	2.33	1.41	1.36
28	lp	203	PUB	C2C-C3C	2.33	1.41	1.36
26	er	202	PEB	C3B-C2B	2.33	1.41	1.36
28	J7	202	PUB	C2C-C3C	2.33	1.41	1.36
28	ey	1006	PUB	C2C-C3C	2.33	1.41	1.36
28	R7	203	PUB	C2C-C3C	2.33	1.41	1.36
28	cz	203	PUB	C2C-C3C	2.33	1.41	1.36
28	kS	1003	PUB	C2C-C3C	2.33	1.41	1.36
28	r2	203	PUB	C2C-C3C	2.33	1.41	1.36
28	R3	203	PUB	C2C-C3C	2.33	1.41	1.36
28	B5	203	PUB	C2C-C3C	2.33	1.41	1.36
28	d8	304	PUB	C2C-C3C	2.33	1.41	1.36
28	34	1005	PUB	C2C-C3C	2.33	1.41	1.36
28	n7	203	PUB	C2C-C3C	2.32	1.41	1.36
28	gg	203	PUB	C2C-C3C	2.32	1.41	1.36
29	ez	1004	PVN	C15-C16	2.32	1.43	1.38
28	D6	202	PUB	C2C-C3C	2.32	1.41	1.36
28	Z9	1006	PUB	C2C-C3C	2.32	1.41	1.36
28	dB	202	PUB	C2C-C3C	2.32	1.41	1.36
28	C2	305	PUB	C2C-C3C	2.32	1.41	1.36
28	U8	1006	PUB	C2C-C3C	2.32	1.41	1.36
28	D9	203	PUB	C2C-C3C	2.32	1.41	1.36
29	34	1004	PVN	C15-C16	2.32	1.43	1.38
29	Y5	1004	PVN	C15-C16	2.32	1.43	1.38
26	v5	202	PEB	C3B-C2B	2.32	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eJ	202	PEB	C3B-C2B	2.32	1.41	1.36
28	r3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	L5	203	PUB	C2C-C3C	2.32	1.41	1.36
28	cr	203	PUB	C2C-C3C	2.32	1.41	1.36
28	gk	203	PUB	C2C-C3C	2.32	1.41	1.36
28	D3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	e9	306	PUB	C2C-C3C	2.32	1.41	1.36
28	dN	203	PUB	C2C-C3C	2.32	1.41	1.36
28	f3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	c9	305	PUB	C2C-C3C	2.32	1.41	1.36
28	w8	203	PUB	C2C-C3C	2.32	1.41	1.36
28	br	203	PUB	C2C-C3C	2.32	1.41	1.36
28	ge	203	PUB	C2C-C3C	2.32	1.41	1.36
28	v4	203	PUB	C2C-C3C	2.32	1.41	1.36
28	x4	202	PUB	C2C-C3C	2.32	1.41	1.36
28	v5	203	PUB	C2C-C3C	2.32	1.41	1.36
28	x5	202	PUB	C2C-C3C	2.32	1.41	1.36
28	hB	203	PUB	C2C-C3C	2.32	1.41	1.36
28	A2	1006	PUB	C2C-C3C	2.32	1.41	1.36
28	cM	203	PUB	C2C-C3C	2.32	1.41	1.36
28	V4	203	PUB	C2C-C3C	2.32	1.41	1.36
28	P6	203	PUB	C2C-C3C	2.32	1.41	1.36
28	y6	204	PUB	C2C-C3C	2.32	1.41	1.36
28	aF	203	PUB	C2C-C3C	2.32	1.41	1.36
28	bF	203	PUB	C2C-C3C	2.32	1.41	1.36
26	D4	202	PEB	C3B-C2B	2.32	1.41	1.36
28	T2	203	PUB	C2C-C3C	2.32	1.41	1.36
28	t3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	Z9	1005	PUB	C2C-C3C	2.32	1.41	1.36
28	eF	203	PUB	C2C-C3C	2.32	1.41	1.36
28	hG	202	PUB	C2C-C3C	2.32	1.41	1.36
28	l7	203	PUB	C2C-C3C	2.32	1.41	1.36
28	lv	202	PUB	C2C-C3C	2.32	1.41	1.36
28	H3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	e6	203	PUB	C2C-C3C	2.32	1.41	1.36
28	aD	203	PUB	C2C-C3C	2.32	1.41	1.36
28	b8	1005	PUB	C2C-C3C	2.32	1.41	1.36
28	aH	203	PUB	C2C-C3C	2.32	1.41	1.36
28	aP	203	PUB	C2C-C3C	2.32	1.41	1.36
28	z4	203	PUB	C2C-C3C	2.32	1.41	1.36
28	z5	203	PUB	C2C-C3C	2.32	1.41	1.36
28	Z7	203	PUB	C2C-C3C	2.32	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B9	203	PUB	C2C-C3C	2.32	1.41	1.36
28	D2	305	PUB	C2C-C3C	2.32	1.41	1.36
28	d3	304	PUB	C2C-C3C	2.32	1.41	1.36
28	y8	203	PUB	C2C-C3C	2.32	1.41	1.36
28	J9	203	PUB	C2C-C3C	2.32	1.41	1.36
28	bT	202	PUB	C2C-C3C	2.32	1.41	1.36
28	z7	203	PUB	C2C-C3C	2.32	1.41	1.36
28	e7	203	PUB	C2C-C3C	2.32	1.41	1.36
28	at	203	PUB	C2C-C3C	2.32	1.41	1.36
28	eY	405	PUB	C2C-C3C	2.32	1.41	1.36
28	eZ	404	PUB	C2C-C3C	2.32	1.41	1.36
28	ld	203	PUB	C2C-C3C	2.32	1.41	1.36
28	N3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	B4	203	PUB	C2C-C3C	2.32	1.41	1.36
28	hR	203	PUB	C2C-C3C	2.32	1.41	1.36
26	cq	202	PEB	C3B-C2B	2.32	1.41	1.36
28	f2	203	PUB	C2C-C3C	2.32	1.41	1.36
28	z2	203	PUB	C2C-C3C	2.32	1.41	1.36
28	Z3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	L7	202	PUB	C2C-C3C	2.32	1.41	1.36
28	P7	203	PUB	C2C-C3C	2.32	1.41	1.36
28	t7	203	PUB	C2C-C3C	2.32	1.41	1.36
28	hD	203	PUB	C2C-C3C	2.32	1.41	1.36
26	p2	202	PEB	C3B-C2B	2.32	1.41	1.36
28	V3	203	PUB	C2C-C3C	2.32	1.41	1.36
28	c8	305	PUB	C2C-C3C	2.32	1.41	1.36
26	cn	201	PEB	C3B-C2B	2.31	1.41	1.36
28	X3	202	PUB	C2C-C3C	2.31	1.41	1.36
28	p7	202	PUB	C2C-C3C	2.31	1.41	1.36
28	cF	202	PUB	C2C-C3C	2.31	1.41	1.36
28	B3	203	PUB	C2C-C3C	2.31	1.41	1.36
28	r4	202	PUB	C2C-C3C	2.31	1.41	1.36
28	r5	203	PUB	C2C-C3C	2.31	1.41	1.36
28	c6	1004	PUB	C2C-C3C	2.31	1.41	1.36
28	cN	202	PUB	C2C-C3C	2.31	1.41	1.36
28	lb	203	PUB	C2C-C3C	2.31	1.41	1.36
26	ap	202	PEB	C3B-C2B	2.31	1.41	1.36
28	J3	203	PUB	C2C-C3C	2.31	1.41	1.36
28	r6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	T9	203	PUB	C2C-C3C	2.31	1.41	1.36
28	ez	1005	PUB	C2C-C3C	2.31	1.41	1.36
28	hH	203	PUB	C2C-C3C	2.31	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	cs	202	PEB	C3B-C2B	2.31	1.41	1.36
28	n4	203	PUB	C2C-C3C	2.31	1.41	1.36
28	F5	203	PUB	C2C-C3C	2.31	1.41	1.36
28	cY	203	PUB	C2C-C3C	2.31	1.41	1.36
28	hY	406	PUB	C2C-C3C	2.31	1.41	1.36
28	a3	1006	PUB	C2C-C3C	2.31	1.41	1.36
28	H4	203	PUB	C2C-C3C	2.31	1.41	1.36
28	Z4	203	PUB	C2C-C3C	2.31	1.41	1.36
28	D5	203	PUB	C2C-C3C	2.31	1.41	1.36
28	V5	203	PUB	C2C-C3C	2.31	1.41	1.36
28	p5	202	PUB	C2C-C3C	2.31	1.41	1.36
28	bo	202	PUB	C2C-C3C	2.31	1.41	1.36
28	cp	203	PUB	C2C-C3C	2.31	1.41	1.36
28	eL	203	PUB	C2C-C3C	2.31	1.41	1.36
26	e7	202	PEB	C3B-C2B	2.31	1.41	1.36
26	bQ	203	PEB	C3B-C2B	2.31	1.41	1.36
28	R6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	z6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	O8	203	PUB	C2C-C3C	2.31	1.41	1.36
28	aN	203	PUB	C2C-C3C	2.31	1.41	1.36
28	aT	203	PUB	C2C-C3C	2.31	1.41	1.36
28	cP	203	PUB	C2C-C3C	2.31	1.41	1.36
28	dx	407	PUB	C2C-C3C	2.31	1.41	1.36
28	dF	203	PUB	C2C-C3C	2.31	1.41	1.36
28	lf	203	PUB	C2C-C3C	2.31	1.41	1.36
28	hZ	405	PUB	C2C-C3C	2.31	1.41	1.36
26	Z7	202	PEB	C3B-C2B	2.31	1.41	1.36
26	cb	202	PEB	C3B-C2B	2.31	1.41	1.36
28	h2	203	PUB	C2C-C3C	2.31	1.41	1.36
28	C2	304	PUB	C2C-C3C	2.31	1.41	1.36
28	cJ	203	PUB	C2C-C3C	2.31	1.41	1.36
26	H3	202	PEB	C3B-C2B	2.31	1.41	1.36
28	X2	203	PUB	C2C-C3C	2.31	1.41	1.36
28	H6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	gn	203	PUB	C2C-C3C	2.31	1.41	1.36
28	Z6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	b6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	df	203	PUB	C2C-C3C	2.31	1.41	1.36
28	gy	306	PUB	C2C-C3C	2.31	1.41	1.36
26	ga	202	PEB	C3B-C2B	2.31	1.41	1.36
28	dh	203	PUB	C2C-C3C	2.31	1.41	1.36
28	fu	202	PUB	C2C-C3C	2.31	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P2	203	PUB	C2C-C3C	2.31	1.41	1.36
28	p3	203	PUB	C2C-C3C	2.31	1.41	1.36
28	y7	203	PUB	C2C-C3C	2.31	1.41	1.36
28	ax	202	PUB	C2C-C3C	2.31	1.41	1.36
28	dx	406	PUB	C2C-C3C	2.31	1.41	1.36
28	dK	203	PUB	C2C-C3C	2.31	1.41	1.36
28	lr	203	PUB	C2C-C3C	2.31	1.41	1.36
26	hB	202	PEB	C3B-C2B	2.31	1.41	1.36
28	34	1006	PUB	C2C-C3C	2.31	1.41	1.36
28	aZ	304	PUB	C2C-C3C	2.31	1.41	1.36
28	ll	203	PUB	C2C-C3C	2.31	1.41	1.36
28	lt	203	PUB	C2C-C3C	2.31	1.41	1.36
28	v2	203	PUB	C2C-C3C	2.31	1.41	1.36
28	N4	203	PUB	C2C-C3C	2.31	1.41	1.36
28	t5	203	PUB	C2C-C3C	2.31	1.41	1.36
28	cE	203	PUB	C2C-C3C	2.31	1.41	1.36
28	fs	203	PUB	C2C-C3C	2.31	1.41	1.36
28	hT	203	PUB	C2C-C3C	2.31	1.41	1.36
28	iD	1003	PUB	C2C-C3C	2.31	1.41	1.36
26	J9	202	PEB	C3B-C2B	2.31	1.41	1.36
28	p8	203	PUB	C2C-C3C	2.31	1.41	1.36
28	bN	203	PUB	C2C-C3C	2.31	1.41	1.36
28	fi	203	PUB	C2C-C3C	2.31	1.41	1.36
26	e4	202	PEB	C3B-C2B	2.31	1.41	1.36
28	r9	203	PUB	C2C-C3C	2.31	1.41	1.36
28	kU	1003	PUB	C2C-C3C	2.31	1.41	1.36
28	j2	203	PUB	C2C-C3C	2.31	1.41	1.36
28	cH	202	PUB	C2C-C3C	2.31	1.41	1.36
28	fy	202	PUB	C2C-C3C	2.31	1.41	1.36
28	gp	203	PUB	C2C-C3C	2.31	1.41	1.36
28	iC	1003	PUB	C2C-C3C	2.31	1.41	1.36
28	b8	1006	PUB	C2C-C3C	2.31	1.41	1.36
28	hL	203	PUB	C2C-C3C	2.31	1.41	1.36
28	eY	404	PUB	C2C-C3C	2.31	1.41	1.36
28	eZ	403	PUB	C2C-C3C	2.31	1.41	1.36
28	hN	203	PUB	C2C-C3C	2.31	1.41	1.36
28	hX	203	PUB	C2C-C3C	2.31	1.41	1.36
28	iF	1003	PUB	C2C-C3C	2.31	1.41	1.36
28	Z5	306	PUB	C2C-C3C	2.31	1.41	1.36
28	e8	304	PUB	C2C-C3C	2.31	1.41	1.36
28	e9	305	PUB	C2C-C3C	2.31	1.41	1.36
28	lh	203	PUB	C2C-C3C	2.31	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	ly	405	PUB	C2C-C3C	2.31	1.41	1.36
28	lz	404	PUB	C2C-C3C	2.31	1.41	1.36
29	dw	404	PVN	C15-C16	2.31	1.43	1.38
26	v9	202	PEB	C3B-C2B	2.31	1.41	1.36
28	N6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	V6	203	PUB	C2C-C3C	2.31	1.41	1.36
28	T7	203	PUB	C2C-C3C	2.31	1.41	1.36
28	H9	203	PUB	C2C-C3C	2.31	1.41	1.36
26	n3	202	PEB	C3B-C2B	2.31	1.41	1.36
26	kR	1002	PEB	C3B-C2B	2.31	1.41	1.36
28	D2	304	PUB	C2C-C3C	2.31	1.41	1.36
28	d3	303	PUB	C2C-C3C	2.31	1.41	1.36
28	X7	203	PUB	C2C-C3C	2.31	1.41	1.36
28	s7	203	PUB	C2C-C3C	2.31	1.41	1.36
28	kX	1003	PUB	C2C-C3C	2.31	1.41	1.36
28	U8	1005	PUB	C2C-C3C	2.30	1.41	1.36
28	gz	306	PUB	C2C-C3C	2.30	1.41	1.36
28	jJ	1003	PUB	C2C-C3C	2.30	1.41	1.36
26	z5	202	PEB	C3B-C2B	2.30	1.41	1.36
26	bN	202	PEB	C3B-C2B	2.30	1.41	1.36
26	eX	201	PEB	C3B-C2B	2.30	1.41	1.36
28	D4	203	PUB	C2C-C3C	2.30	1.41	1.36
28	B7	202	PUB	C2C-C3C	2.30	1.41	1.36
28	H7	203	PUB	C2C-C3C	2.30	1.41	1.36
28	ar	203	PUB	C2C-C3C	2.30	1.41	1.36
28	eN	203	PUB	C2C-C3C	2.30	1.41	1.36
28	h8	203	PUB	C2C-C3C	2.30	1.41	1.36
26	aj	202	PEB	C3B-C2B	2.30	1.41	1.36
26	ff	202	PEB	C3B-C2B	2.30	1.41	1.36
26	fo	202	PEB	C3B-C2B	2.30	1.41	1.36
28	44	305	PUB	C2C-C3C	2.30	1.41	1.36
28	l6	203	PUB	C2C-C3C	2.30	1.41	1.36
28	n9	202	PUB	C2C-C3C	2.30	1.41	1.36
28	an	202	PUB	C2C-C3C	2.30	1.41	1.36
28	gd	202	PUB	C2C-C3C	2.30	1.41	1.36
26	fy	201	PEB	C3B-C2B	2.30	1.41	1.36
28	r7	203	PUB	C2C-C3C	2.30	1.41	1.36
28	T8	305	PUB	C2C-C3C	2.30	1.41	1.36
28	Y9	305	PUB	C2C-C3C	2.30	1.41	1.36
28	bV	203	PUB	C2C-C3C	2.30	1.41	1.36
28	l2	203	PUB	C2C-C3C	2.30	1.41	1.36
28	a7	203	PUB	C2C-C3C	2.30	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b7	202	PUB	C2C-C3C	2.30	1.41	1.36
28	I8	203	PUB	C2C-C3C	2.30	1.41	1.36
28	N9	203	PUB	C2C-C3C	2.30	1.41	1.36
28	Y9	304	PUB	C2C-C3C	2.30	1.41	1.36
28	bL	203	PUB	C2C-C3C	2.30	1.41	1.36
28	eg	203	PUB	C2C-C3C	2.30	1.41	1.36
28	hZ	404	PUB	C2C-C3C	2.30	1.41	1.36
28	j3	202	PUB	C2C-C3C	2.30	1.41	1.36
28	B6	203	PUB	C2C-C3C	2.30	1.41	1.36
28	cR	203	PUB	C2C-C3C	2.30	1.41	1.36
28	jK	1003	PUB	C2C-C3C	2.30	1.41	1.36
26	fj	202	PEB	C3B-C2B	2.30	1.41	1.36
28	eR	203	PUB	C2C-C3C	2.30	1.41	1.36
26	d7	202	PEB	C3B-C2B	2.30	1.41	1.36
26	ah	202	PEB	C3B-C2B	2.30	1.41	1.36
28	G8	203	PUB	C2C-C3C	2.30	1.41	1.36
28	cL	203	PUB	C2C-C3C	2.30	1.41	1.36
28	eB	204	PUB	C2C-C3C	2.30	1.41	1.36
28	e8	305	PUB	C2C-C3C	2.30	1.41	1.36
28	dr	203	PUB	C2C-C3C	2.30	1.41	1.36
28	dv	202	PUB	C2C-C3C	2.30	1.41	1.36
29	aY	403	PVN	C3-C2	2.30	1.36	1.34
28	L4	203	PUB	C2C-C3C	2.30	1.41	1.36
28	L9	203	PUB	C2C-C3C	2.30	1.41	1.36
28	ff	203	PUB	C2C-C3C	2.30	1.41	1.36
28	fw	203	PUB	C2C-C3C	2.30	1.41	1.36
28	ap	203	PUB	C2C-C3C	2.30	1.41	1.36
28	fa	202	PUB	C2C-C3C	2.30	1.41	1.36
28	gz	305	PUB	C2C-C3C	2.30	1.41	1.36
26	cB	202	PEB	C3B-C2B	2.30	1.41	1.36
26	dY	202	PEB	C3B-C2B	2.30	1.41	1.36
26	ee	202	PEB	C3B-C2B	2.30	1.41	1.36
26	hV	202	PEB	C3B-C2B	2.30	1.41	1.36
26	jI	1002	PEB	C3B-C2B	2.30	1.41	1.36
26	kW	1002	PEB	C3B-C2B	2.30	1.41	1.36
28	n2	203	PUB	C2C-C3C	2.30	1.41	1.36
28	dw	405	PUB	C2C-C3C	2.30	1.41	1.36
26	j4	202	PEB	C3B-C2B	2.30	1.41	1.36
26	n8	201	PEB	C3B-C2B	2.30	1.41	1.36
26	kQ	1002	PEB	C3B-C2B	2.30	1.41	1.36
28	z3	203	PUB	C2C-C3C	2.30	1.41	1.36
28	bp	202	PUB	C2C-C3C	2.30	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	bD	203	PUB	C2C-C3C	2.30	1.41	1.36
28	Z2	203	PUB	C2C-C3C	2.30	1.41	1.36
28	t9	203	PUB	C2C-C3C	2.30	1.41	1.36
28	aR	203	PUB	C2C-C3C	2.30	1.41	1.36
28	bR	202	PUB	C2C-C3C	2.30	1.41	1.36
28	gi	203	PUB	C2C-C3C	2.30	1.41	1.36
28	iE	1003	PUB	C2C-C3C	2.30	1.41	1.36
26	bD	202	PEB	C3B-C2B	2.30	1.41	1.36
26	fm	202	PEB	C3B-C2B	2.30	1.41	1.36
28	T4	202	PUB	C2C-C3C	2.30	1.41	1.36
28	x6	203	PUB	C2C-C3C	2.30	1.41	1.36
28	aV	203	PUB	C2C-C3C	2.30	1.41	1.36
28	dn	203	PUB	C2C-C3C	2.30	1.41	1.36
28	jP	1003	PUB	C2C-C3C	2.30	1.41	1.36
26	cY	202	PEB	C3B-C2B	2.30	1.41	1.36
28	f8	203	PUB	C2C-C3C	2.30	1.41	1.36
28	jN	1003	PUB	C2C-C3C	2.30	1.41	1.36
26	A2	1003	PEB	C3B-C2B	2.30	1.41	1.36
26	l4	202	PEB	C3B-C2B	2.30	1.41	1.36
26	cf	201	PEB	C3B-C2B	2.30	1.41	1.36
26	lh	202	PEB	C3B-C2B	2.30	1.41	1.36
28	p6	203	PUB	C2C-C3C	2.30	1.41	1.36
28	bZ	306	PUB	C2C-C3C	2.30	1.41	1.36
28	kW	1003	PUB	C2C-C3C	2.30	1.41	1.36
26	Y7	1003	PEB	C3B-C2B	2.30	1.41	1.36
26	R9	202	PEB	C3B-C2B	2.30	1.41	1.36
26	ec	202	PEB	C3B-C2B	2.30	1.41	1.36
28	N2	203	PUB	C2C-C3C	2.30	1.41	1.36
28	di	203	PUB	C2C-C3C	2.30	1.41	1.36
28	eb	202	PUB	C2C-C3C	2.30	1.41	1.36
28	ez	1006	PUB	C2C-C3C	2.30	1.41	1.36
26	bL	202	PEB	C3B-C2B	2.30	1.41	1.36
28	dj	203	PUB	C2C-C3C	2.30	1.41	1.36
28	dt	203	PUB	C2C-C3C	2.30	1.41	1.36
28	dL	203	PUB	C2C-C3C	2.30	1.41	1.36
26	j2	202	PEB	C3B-C2B	2.30	1.41	1.36
26	J3	202	PEB	C3B-C2B	2.30	1.41	1.36
26	t5	202	PEB	C3B-C2B	2.30	1.41	1.36
28	aB	203	PUB	C2C-C3C	2.30	1.41	1.36
28	hY	405	PUB	C2C-C3C	2.30	1.41	1.36
26	m5	1003	PEB	C3B-C2B	2.30	1.41	1.36
28	n6	203	PUB	C2C-C3C	2.30	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	ch	202	PEB	C3B-C2B	2.29	1.41	1.36
26	gn	202	PEB	C3B-C2B	2.29	1.41	1.36
26	hR	202	PEB	C3B-C2B	2.29	1.41	1.36
28	c9	304	PUB	C2C-C3C	2.29	1.41	1.36
28	v9	203	PUB	C2C-C3C	2.29	1.41	1.36
28	av	203	PUB	C2C-C3C	2.29	1.41	1.36
28	aZ	305	PUB	C2C-C3C	2.29	1.41	1.36
26	R6	202	PEB	C3B-C2B	2.29	1.41	1.36
26	N7	202	PEB	C3B-C2B	2.29	1.41	1.36
26	hH	202	PEB	C3B-C2B	2.29	1.41	1.36
28	a3	1005	PUB	C2C-C3C	2.29	1.41	1.36
28	c3	304	PUB	C2C-C3C	2.29	1.41	1.36
28	44	304	PUB	C2C-C3C	2.29	1.41	1.36
28	Z5	305	PUB	C2C-C3C	2.29	1.41	1.36
26	X6	202	PEB	C3B-C2B	2.29	1.41	1.36
26	dj	202	PEB	C3B-C2B	2.29	1.41	1.36
26	gx	202	PEB	C3B-C2B	2.29	1.41	1.36
28	R4	203	PUB	C2C-C3C	2.29	1.41	1.36
28	kT	1003	PUB	C2C-C3C	2.29	1.41	1.36
26	jM	1002	PEB	C3B-C2B	2.29	1.41	1.36
26	hX	202	PEB	C3B-C2B	2.29	1.41	1.36
28	jO	1003	PUB	C2C-C3C	2.29	1.41	1.36
26	cl	202	PEB	C3B-C2B	2.29	1.41	1.36
26	cH	201	PEB	C3B-C2B	2.29	1.41	1.36
26	ea	203	PEB	C3B-C2B	2.29	1.41	1.36
28	p2	203	PUB	C2C-C3C	2.29	1.41	1.36
28	c3	305	PUB	C2C-C3C	2.29	1.41	1.36
28	n8	202	PUB	C2C-C3C	2.29	1.41	1.36
28	eD	203	PUB	C2C-C3C	2.29	1.41	1.36
26	bH	202	PEB	C3B-C2B	2.29	1.41	1.36
26	ld	202	PEB	C3B-C2B	2.29	1.41	1.36
26	ln	202	PEB	C3B-C2B	2.29	1.41	1.36
28	iG	1002	PUB	C2C-C3C	2.29	1.41	1.36
26	cz	202	PEB	C3B-C2B	2.29	1.41	1.36
28	bs	1004	PUB	C2C-C3C	2.29	1.41	1.36
28	gv	203	PUB	C2C-C3C	2.29	1.41	1.36
28	B9	203	PUB	C4C-NC	2.29	1.39	1.35
26	kX	1002	PEB	C3B-C2B	2.29	1.41	1.36
28	dl	203	PUB	C2C-C3C	2.29	1.41	1.36
26	di	202	PEB	C3B-C2B	2.29	1.41	1.36
28	J5	203	PUB	C2C-C3C	2.29	1.41	1.36
26	J5	202	PEB	C3B-C2B	2.29	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f2	202	PEB	C3B-C2B	2.29	1.41	1.36
26	P3	202	PEB	C3B-C2B	2.29	1.41	1.36
26	x7	202	PEB	C3B-C2B	2.29	1.41	1.36
26	cE	202	PEB	C3B-C2B	2.29	1.41	1.36
26	eN	202	PEB	C3B-C2B	2.29	1.41	1.36
28	cO	203	PUB	C2C-C3C	2.29	1.41	1.36
28	dR	203	PUB	C2C-C3C	2.29	1.41	1.36
28	dY	203	PUB	C2C-C3C	2.29	1.41	1.36
26	bB	202	PEB	C3B-C2B	2.29	1.41	1.36
26	dl	202	PEB	C3B-C2B	2.29	1.41	1.36
28	fq	203	PUB	C2C-C3C	2.29	1.41	1.36
28	hP	203	PUB	C2C-C3C	2.29	1.41	1.36
28	jI	1003	PUB	C2C-C3C	2.29	1.41	1.36
26	p3	202	PEB	C3B-C2B	2.29	1.41	1.36
26	B5	202	PEB	C3B-C2B	2.29	1.41	1.36
26	df	202	PEB	C3B-C2B	2.29	1.41	1.36
26	fq	202	PEB	C3B-C2B	2.29	1.41	1.36
28	dd	203	PUB	C2C-C3C	2.29	1.41	1.36
26	fs	202	PEB	C3B-C2B	2.29	1.41	1.36
26	ge	202	PEB	C3B-C2B	2.29	1.41	1.36
28	gt	203	PUB	C2C-C3C	2.29	1.41	1.36
26	h2	202	PEB	C3B-C2B	2.29	1.41	1.36
26	Z3	202	PEB	C3B-C2B	2.29	1.41	1.36
26	a7	202	PEB	C3B-C2B	2.29	1.41	1.36
26	C8	202	PEB	C3B-C2B	2.29	1.41	1.36
26	ei	202	PEB	C3B-C2B	2.29	1.41	1.36
26	D3	202	PEB	C3B-C2B	2.29	1.41	1.36
26	fg	201	PEB	C3B-C2B	2.29	1.41	1.36
28	J2	202	PUB	C2C-C3C	2.29	1.41	1.36
26	L2	202	PEB	C3B-C2B	2.29	1.41	1.36
26	V2	202	PEB	C3B-C2B	2.29	1.41	1.36
26	R3	202	PEB	C3B-C2B	2.29	1.41	1.36
26	v3	202	PEB	C3B-C2B	2.29	1.41	1.36
26	n7	202	PEB	C3B-C2B	2.29	1.41	1.36
26	v7	202	PEB	C3B-C2B	2.29	1.41	1.36
26	kS	1002	PEB	C3B-C2B	2.29	1.41	1.36
28	X4	203	PUB	C2C-C3C	2.29	1.41	1.36
26	F3	202	PEB	C3B-C2B	2.28	1.41	1.36
26	av	202	PEB	C3B-C2B	2.28	1.41	1.36
28	v3	203	PUB	C2C-C3C	2.28	1.41	1.36
28	bz	203	PUB	C2C-C3C	2.28	1.41	1.36
26	r5	202	PEB	C3B-C2B	2.28	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	bJ	202	PEB	C3B-C2B	2.28	1.41	1.36
26	lw	203	PEB	C3B-C2B	2.28	1.41	1.36
26	hG	201	PEB	C3B-C2B	2.28	1.41	1.36
26	jJ	1002	PEB	C3B-C2B	2.28	1.41	1.36
28	d9	305	PUB	C2C-C3C	2.28	1.41	1.36
26	D5	202	PEB	C3B-C2B	2.28	1.41	1.36
26	V5	202	PEB	C3B-C2B	2.28	1.41	1.36
26	eL	202	PEB	C3B-C2B	2.28	1.41	1.36
26	eV	202	PEB	C3B-C2B	2.28	1.41	1.36
26	jL	1002	PEB	C3B-C2B	2.28	1.41	1.36
28	F4	203	PUB	C2C-C3C	2.28	1.41	1.36
28	kV	1003	PUB	C2C-C3C	2.28	1.41	1.36
26	T3	202	PEB	C3B-C2B	2.28	1.41	1.36
26	F7	201	PEB	C3B-C2B	2.28	1.41	1.36
26	V9	202	PEB	C3B-C2B	2.28	1.41	1.36
28	Y5	1005	PUB	C2C-C3C	2.28	1.41	1.36
26	L3	202	PEB	C3B-C2B	2.28	1.41	1.36
26	n4	202	PEB	C3B-C2B	2.28	1.41	1.36
26	S5	203	PEB	C3B-C2B	2.28	1.41	1.36
26	X7	202	PEB	C3B-C2B	2.28	1.41	1.36
26	cr	202	PEB	C3B-C2B	2.28	1.41	1.36
26	gd	201	PEB	C3B-C2B	2.28	1.41	1.36
26	X2	202	PEB	C3B-C2B	2.28	1.41	1.36
26	v4	202	PEB	C3B-C2B	2.28	1.41	1.36
26	y8	202	PEB	C3B-C2B	2.28	1.41	1.36
26	lr	202	PEB	C3B-C2B	2.28	1.41	1.36
28	A8	203	PUB	C2C-C3C	2.28	1.41	1.36
28	K8	203	PUB	C2C-C3C	2.28	1.41	1.36
28	F9	203	PUB	C2C-C3C	2.28	1.41	1.36
28	ey	1005	PUB	C2C-C3C	2.28	1.41	1.36
26	R7	202	PEB	C3B-C2B	2.28	1.41	1.36
26	cp	202	PEB	C3B-C2B	2.28	1.41	1.36
28	eT	203	PUB	C2C-C3C	2.28	1.41	1.36
28	fm	203	PUB	C2C-C3C	2.28	1.41	1.36
26	eB	203	PEB	C3B-C2B	2.28	1.41	1.36
28	er	203	PUB	C2C-C3C	2.28	1.41	1.36
28	az	203	PUB	C4C-NC	2.28	1.39	1.35
26	34	1001	PEB	C3B-C2B	2.28	1.41	1.36
26	n5	202	PEB	C3B-C2B	2.28	1.41	1.36
26	bV	202	PEB	C3B-C2B	2.28	1.41	1.36
28	g8	202	PUB	C2C-C3C	2.28	1.41	1.36
28	cn	202	PUB	C2C-C3C	2.28	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	eX	202	PUB	C2C-C3C	2.28	1.41	1.36
26	ax	201	PEB	C3B-C2B	2.28	1.41	1.36
28	L6	202	PUB	C2C-C3C	2.28	1.41	1.36
28	aY	405	PUB	C2C-C3C	2.28	1.41	1.36
26	T2	202	PEB	C3B-C2B	2.28	1.41	1.36
26	t3	202	PEB	C3B-C2B	2.28	1.41	1.36
26	fw	202	PEB	C3B-C2B	2.28	1.41	1.36
26	hL	202	PEB	C3B-C2B	2.28	1.41	1.36
26	kU	1002	PEB	C3B-C2B	2.28	1.41	1.36
28	F3	203	PUB	C2C-C3C	2.28	1.41	1.36
29	b8	1004	PVN	C15-C16	2.28	1.43	1.38
26	dh	202	PEB	C3B-C2B	2.28	1.41	1.36
26	gp	202	PEB	C3B-C2B	2.28	1.41	1.36
28	el	203	PUB	C2C-C3C	2.28	1.41	1.36
26	A5	203	PEB	C3B-C2B	2.28	1.41	1.36
26	h8	202	PEB	C3B-C2B	2.28	1.41	1.36
26	r7	202	PEB	C3B-C2B	2.28	1.41	1.36
28	jM	1003	PUB	C2C-C3C	2.28	1.41	1.36
26	H2	201	PEB	C3B-C2B	2.28	1.41	1.36
26	N3	202	PEB	C3B-C2B	2.28	1.41	1.36
26	dd	202	PEB	C3B-C2B	2.28	1.41	1.36
26	ll	202	PEB	C3B-C2B	2.28	1.41	1.36
28	x3	203	PUB	C2C-C3C	2.28	1.41	1.36
28	z9	203	PUB	C2C-C3C	2.27	1.41	1.36
28	bY	1006	PUB	C2C-C3C	2.27	1.41	1.36
28	x4	202	PUB	C4C-NC	2.27	1.39	1.35
26	ad	202	PEB	C3B-C2B	2.27	1.41	1.36
28	dp	203	PUB	C2C-C3C	2.27	1.41	1.36
26	fc	202	PEB	C3B-C2B	2.27	1.41	1.36
26	g4	202	PEB	C3B-C2B	2.27	1.41	1.36
26	kT	1002	PEB	C3B-C2B	2.27	1.41	1.36
28	r3	203	PUB	C4C-NC	2.27	1.39	1.35
28	eX	202	PUB	C4C-NC	2.27	1.39	1.35
26	n2	202	PEB	C3B-C2B	2.27	1.41	1.36
26	V3	202	PEB	C3B-C2B	2.27	1.41	1.36
26	lf	202	PEB	C3B-C2B	2.27	1.41	1.36
28	x7	203	PUB	C2C-C3C	2.27	1.41	1.36
27	w1	201	CYC	C4D-CHA	2.27	1.49	1.41
26	J6	202	PEB	C3B-C2B	2.27	1.41	1.36
26	H7	202	PEB	C3B-C2B	2.27	1.41	1.36
26	jP	1002	PEB	C3B-C2B	2.27	1.41	1.36
28	dV	203	PUB	C2C-C3C	2.27	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	ga	203	PUB	C2C-C3C	2.27	1.41	1.36
26	l2	202	PEB	C3B-C2B	2.27	1.41	1.36
26	N5	202	PEB	C3B-C2B	2.27	1.41	1.36
26	dL	202	PEB	C3B-C2B	2.27	1.41	1.36
28	ap	203	PUB	C4C-NC	2.27	1.39	1.35
26	j3	201	PEB	C3B-C2B	2.27	1.41	1.36
26	az	202	PEB	C3B-C2B	2.27	1.41	1.36
28	et	203	PUB	C4C-NC	2.27	1.39	1.35
26	bP	202	PEB	C3B-C2B	2.27	1.41	1.36
26	hD	202	PEB	C3B-C2B	2.27	1.41	1.36
28	34	1006	PUB	C4C-NC	2.27	1.39	1.35
28	dK	203	PUB	C4C-NC	2.27	1.39	1.35
26	T7	202	PEB	C3B-C2B	2.27	1.41	1.36
26	z7	202	PEB	C3B-C2B	2.27	1.41	1.36
28	br	203	PUB	C4C-NC	2.27	1.39	1.35
26	N9	202	PEB	C3B-C2B	2.27	1.41	1.36
26	ab	202	PEB	C3B-C2B	2.27	1.41	1.36
26	hN	202	PEB	C3B-C2B	2.27	1.41	1.36
28	L2	203	PUB	C2C-C3C	2.27	1.41	1.36
26	Z2	202	PEB	C3B-C2B	2.27	1.41	1.36
26	z3	202	PEB	C3B-C2B	2.27	1.41	1.36
26	gk	202	PEB	C3B-C2B	2.27	1.41	1.36
26	lp	202	PEB	C3B-C2B	2.27	1.41	1.36
28	dw	406	PUB	C4C-NC	2.27	1.39	1.35
26	F9	202	PEB	C3B-C2B	2.27	1.41	1.36
26	an	201	PEB	C3B-C2B	2.27	1.41	1.36
26	aD	202	PEB	C3B-C2B	2.27	1.41	1.36
26	gt	202	PEB	C3B-C2B	2.27	1.41	1.36
28	y6	204	PUB	C4C-NC	2.27	1.39	1.35
28	bL	203	PUB	C4C-NC	2.27	1.39	1.35
26	L9	202	PEB	C3B-C2B	2.27	1.41	1.36
28	C8	203	PUB	C2C-C3C	2.27	1.41	1.36
26	at	202	PEB	C3B-C2B	2.27	1.41	1.36
28	ly	406	PUB	C2C-C3C	2.27	1.41	1.36
28	lz	405	PUB	C2C-C3C	2.27	1.41	1.36
28	P2	203	PUB	C4C-NC	2.27	1.39	1.35
28	p3	203	PUB	C4C-NC	2.27	1.39	1.35
28	iC	1003	PUB	C4C-NC	2.27	1.39	1.35
26	dV	202	PEB	C3B-C2B	2.27	1.41	1.36
26	gv	202	PEB	C3B-C2B	2.27	1.41	1.36
26	cL	202	PEB	C3B-C2B	2.27	1.41	1.36
28	F3	203	PUB	C4C-NC	2.27	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f3	202	PEB	C3B-C2B	2.27	1.41	1.36
26	c7	202	PEB	C3B-C2B	2.27	1.41	1.36
29	bY	1004	PVN	C19-C18	-2.26	1.43	1.48
26	iC	1002	PEB	C3B-C2B	2.26	1.41	1.36
26	l7	202	PEB	C3B-C2B	2.26	1.41	1.36
26	al	202	PEB	C3B-C2B	2.26	1.41	1.36
29	b9	405	PVN	C15-C16	2.26	1.43	1.38
28	bP	203	PUB	C4C-NC	2.26	1.39	1.35
28	dP	203	PUB	C4C-NC	2.26	1.39	1.35
28	n4	203	PUB	C4C-NC	2.26	1.39	1.35
27	e1	201	CYC	C4D-CHA	2.26	1.49	1.41
26	P9	202	PEB	C3B-C2B	2.26	1.41	1.36
26	cF	201	PEB	C3B-C2B	2.26	1.41	1.36
28	u6	203	PUB	C2C-C3C	2.26	1.41	1.36
26	hJ	202	PEB	C3B-C2B	2.26	1.41	1.36
26	J7	201	PEB	C3B-C2B	2.26	1.41	1.36
26	y7	202	PEB	C3B-C2B	2.26	1.41	1.36
26	jO	1002	PEB	C3B-C2B	2.26	1.41	1.36
26	kV	1002	PEB	C3B-C2B	2.26	1.41	1.36
27	O1	201	CYC	C4D-CHA	2.26	1.49	1.41
28	bY	1005	PUB	C4C-NC	2.26	1.39	1.35
26	bT	201	PEB	C3B-C2B	2.26	1.41	1.36
28	c8	304	PUB	C4C-NC	2.26	1.39	1.35
29	gz	304	PVN	C15-C16	-2.26	1.32	1.38
27	Z1	201	CYC	C4D-CHA	2.26	1.49	1.41
28	bB	203	PUB	C2C-C3C	2.26	1.41	1.36
28	N3	203	PUB	C4C-NC	2.26	1.39	1.35
28	aJ	203	PUB	C4C-NC	2.26	1.39	1.35
28	cY	203	PUB	C4C-NC	2.26	1.39	1.35
26	fu	201	PEB	C3B-C2B	2.26	1.41	1.36
27	b1	1001	CYC	C4D-CHA	2.26	1.49	1.41
26	r4	201	PEB	C3B-C2B	2.26	1.41	1.36
26	T9	202	PEB	C3B-C2B	2.26	1.41	1.36
26	lo	203	PEB	C3B-C2B	2.26	1.41	1.36
26	iD	1002	PEB	C3B-C2B	2.26	1.41	1.36
26	jN	1002	PEB	C3B-C2B	2.26	1.41	1.36
27	U1	201	CYC	C4D-CHA	2.26	1.49	1.41
27	d2	101	CYC	C4D-CHA	2.26	1.49	1.41
26	t7	202	PEB	C3B-C2B	2.26	1.41	1.36
26	fi	202	PEB	C3B-C2B	2.26	1.41	1.36
28	bY	1005	PUB	C2C-C3C	2.26	1.41	1.36
26	F5	202	PEB	C3B-C2B	2.26	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	af	202	PEB	C3B-C2B	2.26	1.41	1.36
26	B6	202	PEB	C3B-C2B	2.26	1.41	1.36
26	B7	201	PEB	C3B-C2B	2.26	1.41	1.36
26	L7	201	PEB	C3B-C2B	2.26	1.41	1.36
26	hP	202	PEB	C3B-C2B	2.26	1.41	1.36
28	N7	203	PUB	C4C-NC	2.26	1.39	1.35
26	p4	202	PEB	C3B-C2B	2.26	1.41	1.36
26	H9	202	PEB	C3B-C2B	2.26	1.41	1.36
26	en	202	PEB	C3B-C2B	2.26	1.41	1.36
28	r7	203	PUB	C4C-NC	2.26	1.39	1.35
28	an	202	PUB	C4C-NC	2.26	1.39	1.35
27	k1	201	CYC	C4D-CHA	2.26	1.49	1.41
26	ev	202	PEB	C3B-C2B	2.26	1.41	1.36
28	aT	203	PUB	C4C-NC	2.26	1.39	1.35
29	44	303	PVN	C19-C18	-2.26	1.44	1.48
29	Z5	304	PVN	C19-C18	-2.26	1.44	1.48
26	iE	1002	PEB	C3B-C2B	2.26	1.41	1.36
28	eY	404	PUB	C4C-NC	2.26	1.39	1.35
29	gy	304	PVN	C3-C2	2.25	1.36	1.34
28	Y5	1005	PUB	C4C-NC	2.25	1.39	1.35
28	U8	1005	PUB	C4C-NC	2.25	1.39	1.35
26	gr	201	PEB	C3B-C2B	2.25	1.41	1.36
26	hT	202	PEB	C3B-C2B	2.25	1.41	1.36
27	o1	1001	CYC	C4D-CHA	2.25	1.49	1.41
28	eN	203	PUB	C4C-NC	2.25	1.39	1.35
28	fy	202	PUB	C4C-NC	2.25	1.39	1.35
26	r3	202	PEB	C3B-C2B	2.25	1.41	1.36
28	Z4	203	PUB	C4C-NC	2.25	1.39	1.35
28	bD	203	PUB	C4C-NC	2.25	1.39	1.35
26	B4	202	PEB	C3B-C2B	2.25	1.41	1.36
26	n6	202	PEB	C3B-C2B	2.25	1.41	1.36
26	D7	202	PEB	C3B-C2B	2.25	1.41	1.36
26	cj	202	PEB	C3B-C2B	2.25	1.41	1.36
27	u1	1001	CYC	C4D-CHA	2.25	1.49	1.41
26	34	1002	PEB	C3B-C2B	2.25	1.41	1.36
26	cJ	202	PEB	C3B-C2B	2.25	1.41	1.36
28	aB	203	PUB	C4C-NC	2.25	1.39	1.35
28	aF	203	PUB	C4C-NC	2.25	1.39	1.35
28	bF	203	PUB	C4C-NC	2.25	1.39	1.35
26	jK	1002	PEB	C3B-C2B	2.25	1.41	1.36
28	d9	305	PUB	C4C-NC	2.25	1.39	1.35
28	cP	203	PUB	C4C-NC	2.25	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P5	201	PEB	C3B-C2B	2.25	1.41	1.36
28	ev	203	PUB	C4C-NC	2.25	1.39	1.35
26	L5	202	PEB	C3B-C2B	2.25	1.41	1.36
27	K1	201	CYC	C4D-CHA	2.25	1.49	1.41
26	p7	201	PEB	C3B-C2B	2.25	1.41	1.36
26	p5	201	PEB	C3B-C2B	2.25	1.41	1.36
27	f1	201	CYC	C4D-CHA	2.25	1.49	1.41
28	hT	203	PUB	C4C-NC	2.25	1.39	1.35
26	W3	203	PEB	C3B-C2B	2.25	1.41	1.36
27	y1	201	CYC	C4D-CHA	2.25	1.49	1.41
26	B3	202	PEB	C3B-C2B	2.25	1.41	1.36
28	d6	203	PUB	C4C-NC	2.25	1.39	1.35
29	e9	304	PVN	C14-C13	-2.25	1.41	1.45
28	r2	203	PUB	C4C-NC	2.25	1.39	1.35
28	d8	304	PUB	C4C-NC	2.25	1.39	1.35
26	P7	202	PEB	C3B-C2B	2.25	1.41	1.36
27	V1	201	CYC	C4D-CHA	2.25	1.49	1.41
28	Y5	1006	PUB	C4C-NC	2.25	1.39	1.35
28	x5	202	PUB	C4C-NC	2.25	1.39	1.35
28	t9	203	PUB	C4C-NC	2.25	1.39	1.35
27	I1	201	CYC	C4D-CHA	2.25	1.49	1.41
27	W1	201	CYC	C4D-CHA	2.25	1.49	1.41
27	m1	201	CYC	C4D-CHA	2.25	1.49	1.41
28	D6	202	PUB	C4C-NC	2.25	1.39	1.35
28	z7	203	PUB	C4C-NC	2.25	1.39	1.35
28	hD	203	PUB	C4C-NC	2.25	1.39	1.35
27	d1	1001	CYC	C4D-CHA	2.25	1.49	1.41
27	q1	201	CYC	C4D-CHA	2.25	1.49	1.41
29	aY	403	PVN	C19-C18	-2.25	1.44	1.48
28	gg	203	PUB	C4C-NC	2.25	1.39	1.35
28	hZ	405	PUB	C4C-NC	2.25	1.39	1.35
26	A1	301	PEB	C3B-C2B	2.25	1.41	1.36
26	B1	301	PEB	C3B-C2B	2.25	1.41	1.36
28	cM	203	PUB	C4C-NC	2.25	1.39	1.35
28	dw	405	PUB	C4C-NC	2.25	1.39	1.35
27	n1	201	CYC	C4D-CHA	2.25	1.49	1.41
27	z1	201	CYC	CAD-C3D	-2.25	1.48	1.52
26	aF	202	PEB	C3B-C2B	2.25	1.41	1.36
26	gi	202	PEB	C3B-C2B	2.25	1.41	1.36
28	R2	203	PUB	C4C-NC	2.25	1.39	1.35
28	V6	203	PUB	C4C-NC	2.24	1.39	1.35
28	p5	202	PUB	C4C-NC	2.24	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J6	203	PUB	C4C-NC	2.24	1.39	1.35
28	H7	203	PUB	C4C-NC	2.24	1.39	1.35
28	D9	203	PUB	C4C-NC	2.24	1.39	1.35
27	N1	201	CYC	C4D-CHA	2.24	1.49	1.41
27	Q1	201	CYC	C4D-CHA	2.24	1.49	1.41
26	D9	202	PEB	C3B-C2B	2.24	1.41	1.36
28	J2	202	PUB	C4C-NC	2.24	1.39	1.35
28	dd	203	PUB	C4C-NC	2.24	1.39	1.35
27	P1	201	CYC	C4D-CHA	2.24	1.49	1.41
28	fw	203	PUB	C4C-NC	2.24	1.39	1.35
27	G1	1001	CYC	C4D-CHA	2.24	1.49	1.41
28	iH	1002	PUB	C4C-NC	2.24	1.39	1.35
28	aN	203	PUB	C4C-NC	2.24	1.39	1.35
26	li	203	PEB	C3B-C2B	2.24	1.41	1.36
28	hV	203	PUB	C4C-NC	2.24	1.39	1.35
28	n6	203	PUB	C4C-NC	2.24	1.39	1.35
27	R1	1001	CYC	C4D-CHA	2.24	1.49	1.41
27	i1	1001	CYC	C4D-CHA	2.24	1.49	1.41
28	d3	304	PUB	C4C-NC	2.24	1.39	1.35
28	B4	203	PUB	C4C-NC	2.24	1.39	1.35
26	co	201	PEB	C3B-C2B	2.24	1.41	1.36
27	H1	201	CYC	CAD-C3D	-2.24	1.48	1.52
28	b8	1006	PUB	C4C-NC	2.24	1.39	1.35
28	kS	1003	PUB	C4C-NC	2.24	1.39	1.35
26	p8	202	PEB	C3B-C2B	2.24	1.41	1.36
29	e8	303	PVN	C14-C13	-2.24	1.41	1.45
26	cd	202	PEB	C3B-C2B	2.24	1.41	1.36
28	c3	304	PUB	C4C-NC	2.24	1.39	1.35
28	T9	203	PUB	C4C-NC	2.24	1.39	1.35
28	cL	203	PUB	C4C-NC	2.24	1.39	1.35
28	eP	204	PUB	C4C-NC	2.24	1.39	1.35
28	N7	203	PUB	C2C-C3C	2.24	1.41	1.36
28	ar	203	PUB	C4C-NC	2.24	1.39	1.35
28	gy	306	PUB	C4C-NC	2.24	1.39	1.35
26	h3	201	PEB	C3B-C2B	2.24	1.41	1.36
28	cq	203	PUB	C4C-NC	2.24	1.39	1.35
28	gn	203	PUB	C4C-NC	2.24	1.39	1.35
27	X1	201	CYC	C4D-CHA	2.24	1.49	1.41
26	R5	202	PEB	C3B-C2B	2.24	1.41	1.36
26	bF	202	PEB	C3B-C2B	2.24	1.41	1.36
28	r4	202	PUB	C4C-NC	2.24	1.39	1.35
28	r5	203	PUB	C4C-NC	2.24	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H6	203	PUB	C4C-NC	2.24	1.39	1.35
28	y7	203	PUB	C4C-NC	2.24	1.39	1.35
28	R6	203	PUB	C4C-NC	2.24	1.39	1.35
28	v6	203	PUB	C4C-NC	2.24	1.39	1.35
28	a7	203	PUB	C4C-NC	2.24	1.39	1.35
28	aP	203	PUB	C4C-NC	2.24	1.39	1.35
28	hJ	203	PUB	C4C-NC	2.24	1.39	1.35
28	kW	1003	PUB	C4C-NC	2.24	1.39	1.35
28	C2	305	PUB	C4C-NC	2.24	1.39	1.35
28	P3	203	PUB	C4C-NC	2.24	1.39	1.35
28	c3	305	PUB	C4C-NC	2.24	1.39	1.35
28	f8	203	PUB	C4C-NC	2.24	1.39	1.35
28	T8	304	PUB	C4C-NC	2.24	1.39	1.35
27	L1	201	CYC	C4D-CHA	2.24	1.49	1.41
27	a1	201	CYC	C4D-CHA	2.24	1.49	1.41
28	fo	203	PUB	C4C-NC	2.23	1.39	1.35
28	gz	306	PUB	C4C-NC	2.23	1.39	1.35
28	x3	203	PUB	C4C-NC	2.23	1.39	1.35
28	eL	203	PUB	C4C-NC	2.23	1.39	1.35
28	fq	203	PUB	C4C-NC	2.23	1.39	1.35
28	V5	203	PUB	C4C-NC	2.23	1.39	1.35
28	ld	203	PUB	C4C-NC	2.23	1.39	1.35
28	ln	203	PUB	C4C-NC	2.23	1.39	1.35
28	H5	202	PUB	C4C-NC	2.23	1.39	1.35
28	ez	1006	PUB	C4C-NC	2.23	1.39	1.35
28	fu	202	PUB	C4C-NC	2.23	1.39	1.35
28	hX	203	PUB	C4C-NC	2.23	1.39	1.35
26	gg	202	PEB	C3B-C2B	2.23	1.41	1.36
28	u6	203	PUB	C4C-NC	2.23	1.39	1.35
28	jN	1003	PUB	C4C-NC	2.23	1.39	1.35
26	eg	202	PEB	C3B-C2B	2.23	1.41	1.36
28	gk	203	PUB	C4C-NC	2.23	1.39	1.35
28	R4	203	PUB	C4C-NC	2.23	1.39	1.35
28	N5	203	PUB	C4C-NC	2.23	1.39	1.35
28	U8	1006	PUB	C4C-NC	2.23	1.39	1.35
28	cz	203	PUB	C4C-NC	2.23	1.39	1.35
28	dV	203	PUB	C4C-NC	2.23	1.39	1.35
28	L2	203	PUB	C4C-NC	2.23	1.39	1.35
28	I8	203	PUB	C4C-NC	2.23	1.39	1.35
28	N9	203	PUB	C4C-NC	2.23	1.39	1.35
28	el	203	PUB	C4C-NC	2.23	1.39	1.35
28	bZ	306	PUB	C4C-NC	2.23	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H9	203	PUB	C4C-NC	2.23	1.39	1.35
28	aZ	304	PUB	C4C-NC	2.23	1.39	1.35
28	bY	1006	PUB	C4C-NC	2.23	1.39	1.35
28	bZ	305	PUB	C4C-NC	2.23	1.39	1.35
28	hP	203	PUB	C4C-NC	2.23	1.39	1.35
29	lz	403	PVN	C11-C12	-2.23	1.42	1.45
28	jI	1003	PUB	C4C-NC	2.23	1.39	1.35
26	B9	202	PEB	C3B-C2B	2.23	1.41	1.36
28	dF	203	PUB	C4C-NC	2.23	1.39	1.35
28	eV	203	PUB	C4C-NC	2.23	1.39	1.35
28	gd	202	PUB	C4C-NC	2.23	1.39	1.35
28	C2	304	PUB	C4C-NC	2.23	1.39	1.35
28	cQ	202	PUB	C4C-NC	2.23	1.39	1.35
28	V2	203	PUB	C4C-NC	2.23	1.39	1.35
28	Z2	203	PUB	C4C-NC	2.23	1.39	1.35
28	dh	203	PUB	C4C-NC	2.23	1.39	1.35
28	eB	204	PUB	C4C-NC	2.23	1.39	1.35
28	kT	1003	PUB	C4C-NC	2.23	1.39	1.35
28	L3	203	PUB	C4C-NC	2.23	1.39	1.35
28	F6	203	PUB	C4C-NC	2.23	1.39	1.35
28	K8	203	PUB	C4C-NC	2.23	1.39	1.35
28	p9	203	PUB	C4C-NC	2.23	1.39	1.35
28	D3	203	PUB	C4C-NC	2.23	1.39	1.35
28	R5	203	PUB	C4C-NC	2.23	1.39	1.35
28	c6	1004	PUB	C4C-NC	2.23	1.39	1.35
28	hZ	404	PUB	C4C-NC	2.23	1.39	1.35
28	kU	1003	PUB	C4C-NC	2.23	1.39	1.35
27	g1	201	CYC	C4D-CHA	2.23	1.49	1.41
28	e8	305	PUB	C4C-NC	2.23	1.39	1.35
28	J9	203	PUB	C4C-NC	2.23	1.39	1.35
28	bJ	203	PUB	C4C-NC	2.23	1.39	1.35
28	ge	203	PUB	C4C-NC	2.23	1.39	1.35
28	h3	202	PUB	C4C-NC	2.23	1.39	1.35
28	l6	203	PUB	C4C-NC	2.23	1.39	1.35
28	bN	203	PUB	C4C-NC	2.23	1.39	1.35
28	cO	203	PUB	C4C-NC	2.23	1.39	1.35
28	dl	203	PUB	C4C-NC	2.23	1.39	1.35
28	L9	203	PUB	C4C-NC	2.23	1.39	1.35
28	ec	203	PUB	C4C-NC	2.23	1.39	1.35
28	A2	1005	PUB	C4C-NC	2.22	1.39	1.35
28	a3	1005	PUB	C4C-NC	2.22	1.39	1.35
28	z2	203	PUB	C4C-NC	2.22	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	n3	203	PUB	C4C-NC	2.22	1.39	1.35
28	n9	202	PUB	C4C-NC	2.22	1.39	1.35
28	r9	203	PUB	C4C-NC	2.22	1.39	1.35
28	L6	202	PUB	C4C-NC	2.22	1.39	1.35
28	T8	305	PUB	C4C-NC	2.22	1.39	1.35
28	Y9	305	PUB	C4C-NC	2.22	1.39	1.35
28	fj	203	PUB	C4C-NC	2.22	1.39	1.35
26	et	202	PEB	C3B-C2B	2.22	1.41	1.36
28	aY	404	PUB	C4C-NC	2.22	1.39	1.35
28	cJ	203	PUB	C4C-NC	2.22	1.39	1.35
28	dL	203	PUB	C4C-NC	2.22	1.39	1.35
28	dX	203	PUB	C4C-NC	2.22	1.39	1.35
28	j2	203	PUB	C4C-NC	2.22	1.39	1.35
28	x2	202	PUB	C4C-NC	2.22	1.39	1.35
28	n7	203	PUB	C4C-NC	2.22	1.39	1.35
28	dY	203	PUB	C4C-NC	2.22	1.39	1.35
28	f2	203	PUB	C4C-NC	2.22	1.39	1.35
28	n8	202	PUB	C4C-NC	2.22	1.39	1.35
28	y8	203	PUB	C4C-NC	2.22	1.39	1.35
28	cF	202	PUB	C4C-NC	2.22	1.39	1.35
28	ez	1005	PUB	C4C-NC	2.22	1.39	1.35
28	X7	203	PUB	C4C-NC	2.22	1.39	1.35
28	Z9	1006	PUB	C4C-NC	2.22	1.39	1.35
27	s1	201	CYC	C4D-CHA	2.22	1.49	1.41
28	X3	202	PUB	C4C-NC	2.22	1.39	1.35
28	t7	203	PUB	C4C-NC	2.22	1.39	1.35
28	T5	202	PUB	C4C-NC	2.22	1.39	1.35
28	x7	203	PUB	C4C-NC	2.22	1.39	1.35
28	x6	203	PUB	C4C-NC	2.22	1.39	1.35
28	eg	203	PUB	C4C-NC	2.22	1.39	1.35
28	jM	1003	PUB	C4C-NC	2.22	1.39	1.35
28	kR	1003	PUB	C4C-NC	2.22	1.39	1.35
28	h2	203	PUB	C4C-NC	2.22	1.39	1.35
28	n5	203	PUB	C4C-NC	2.22	1.39	1.35
28	eD	203	PUB	C4C-NC	2.22	1.39	1.35
28	hH	203	PUB	C4C-NC	2.22	1.39	1.35
26	i3	203	PEB	C3B-C2B	2.22	1.41	1.36
28	p6	203	PUB	C4C-NC	2.22	1.39	1.35
28	jO	1003	PUB	C4C-NC	2.22	1.39	1.35
28	dp	203	PUB	C4C-NC	2.22	1.39	1.35
28	dx	407	PUB	C4C-NC	2.22	1.39	1.35
28	D4	203	PUB	C4C-NC	2.22	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P6	203	PUB	C4C-NC	2.22	1.39	1.35
28	Z7	203	PUB	C4C-NC	2.22	1.39	1.35
28	X4	203	PUB	C4C-NC	2.22	1.39	1.35
28	h8	203	PUB	C4C-NC	2.22	1.39	1.35
28	lr	203	PUB	C4C-NC	2.22	1.39	1.35
28	bz	203	PUB	C4C-NC	2.22	1.39	1.35
28	B7	202	PUB	C4C-NC	2.22	1.39	1.35
28	cE	203	PUB	C4C-NC	2.22	1.39	1.35
28	M8	203	PUB	C4C-NC	2.22	1.39	1.35
28	Q8	203	PUB	C4C-NC	2.22	1.39	1.35
28	V9	203	PUB	C4C-NC	2.22	1.39	1.35
28	lt	203	PUB	C4C-NC	2.22	1.39	1.35
28	H3	203	PUB	C4C-NC	2.21	1.39	1.35
28	d7	203	PUB	C4C-NC	2.21	1.39	1.35
28	w8	203	PUB	C4C-NC	2.21	1.39	1.35
28	cs	203	PUB	C4C-NC	2.21	1.39	1.35
28	lj	202	PUB	C4C-NC	2.21	1.39	1.35
28	lx	201	PUB	C4C-NC	2.21	1.39	1.35
28	p4	203	PUB	C4C-NC	2.21	1.39	1.35
28	Z6	203	PUB	C4C-NC	2.21	1.39	1.35
28	cR	203	PUB	C4C-NC	2.21	1.39	1.35
28	b8	1005	PUB	C4C-NC	2.21	1.39	1.35
28	bq	203	PUB	C4C-NC	2.21	1.39	1.35
28	N4	203	PUB	C4C-NC	2.21	1.39	1.35
28	J5	203	PUB	C4C-NC	2.21	1.39	1.35
28	c7	203	PUB	C4C-NC	2.21	1.39	1.35
28	v9	203	PUB	C4C-NC	2.21	1.39	1.35
28	cH	202	PUB	C4C-NC	2.21	1.39	1.35
28	eY	405	PUB	C4C-NC	2.21	1.39	1.35
28	eZ	404	PUB	C4C-NC	2.21	1.39	1.35
27	J1	201	CYC	CAD-C3D	-2.21	1.48	1.52
28	P4	203	PUB	C4C-NC	2.21	1.39	1.35
28	N6	203	PUB	C4C-NC	2.21	1.39	1.35
28	bR	202	PUB	C4C-NC	2.21	1.39	1.35
28	L4	203	PUB	C4C-NC	2.21	1.39	1.35
28	X2	203	PUB	C4C-NC	2.21	1.39	1.35
28	b9	407	PUB	C4C-NC	2.21	1.39	1.35
28	cr	203	PUB	C4C-NC	2.21	1.39	1.35
28	v3	203	PUB	C4C-NC	2.21	1.39	1.35
28	A8	203	PUB	C4C-NC	2.21	1.39	1.35
28	F9	203	PUB	C4C-NC	2.21	1.39	1.35
28	R9	203	PUB	C4C-NC	2.21	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Z9	1005	PUB	C4C-NC	2.21	1.39	1.35
28	lh	203	PUB	C4C-NC	2.21	1.39	1.35
28	hY	406	PUB	C4C-NC	2.21	1.39	1.35
28	iF	1003	PUB	C4C-NC	2.21	1.39	1.35
28	jL	1003	PUB	C4C-NC	2.21	1.39	1.35
28	D2	305	PUB	C4C-NC	2.21	1.39	1.35
28	j3	202	PUB	C4C-NC	2.21	1.39	1.35
28	J4	203	PUB	C4C-NC	2.21	1.39	1.35
28	t4	203	PUB	C4C-NC	2.21	1.39	1.35
28	g8	202	PUB	C4C-NC	2.21	1.39	1.35
28	dR	203	PUB	C4C-NC	2.21	1.39	1.35
28	fc	203	PUB	C4C-NC	2.21	1.39	1.35
28	gt	203	PUB	C4C-NC	2.21	1.39	1.35
28	gv	203	PUB	C4C-NC	2.21	1.39	1.35
28	z3	203	PUB	C4C-NC	2.21	1.39	1.35
28	e8	304	PUB	C4C-NC	2.21	1.39	1.35
28	bn	202	PUB	C4C-NC	2.21	1.39	1.35
28	v2	203	PUB	C4C-NC	2.21	1.39	1.35
28	F2	203	PUB	C4C-NC	2.21	1.39	1.35
28	V3	203	PUB	C4C-NC	2.21	1.39	1.35
28	dn	203	PUB	C4C-NC	2.21	1.39	1.35
28	ei	203	PUB	C4C-NC	2.21	1.39	1.35
28	fi	203	PUB	C4C-NC	2.21	1.39	1.35
28	X6	203	PUB	C4C-NC	2.21	1.39	1.35
28	c8	305	PUB	C4C-NC	2.21	1.39	1.35
28	Y9	304	PUB	C4C-NC	2.21	1.39	1.35
28	df	203	PUB	C4C-NC	2.21	1.39	1.35
29	dx	405	PVN	C15-C16	2.21	1.43	1.38
28	bT	202	PUB	C4C-NC	2.21	1.39	1.35
28	ll	203	PUB	C4C-NC	2.21	1.39	1.35
28	cN	202	PUB	C4C-NC	2.21	1.39	1.35
28	en	203	PUB	C4C-NC	2.21	1.39	1.35
28	hB	203	PUB	C4C-NC	2.21	1.39	1.35
29	ez	1004	PVN	C11-C12	-2.21	1.42	1.45
27	p1	201	CYC	CAD-C3D	-2.21	1.48	1.52
26	x3	202	PEB	C3B-C2B	2.21	1.41	1.36
28	F5	203	PUB	C4C-NC	2.21	1.39	1.35
28	Z5	305	PUB	C4C-NC	2.21	1.39	1.35
28	B6	203	PUB	C4C-NC	2.21	1.39	1.35
28	V7	203	PUB	C4C-NC	2.21	1.39	1.35
28	cB	203	PUB	C4C-NC	2.21	1.39	1.35
28	gy	305	PUB	C4C-NC	2.21	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	iE	1003	PUB	C4C-NC	2.21	1.39	1.35
28	T4	202	PUB	C4C-NC	2.21	1.39	1.35
28	P5	202	PUB	C4C-NC	2.21	1.39	1.35
28	Z5	306	PUB	C4C-NC	2.21	1.39	1.35
28	a6	203	PUB	C4C-NC	2.21	1.39	1.35
28	R7	203	PUB	C4C-NC	2.21	1.39	1.35
28	dr	203	PUB	C4C-NC	2.21	1.39	1.35
28	hN	203	PUB	C4C-NC	2.21	1.39	1.35
28	kQ	1003	PUB	C4C-NC	2.21	1.39	1.35
28	kV	1003	PUB	C4C-NC	2.21	1.39	1.35
28	34	1005	PUB	C4C-NC	2.21	1.39	1.35
28	at	203	PUB	C4C-NC	2.21	1.39	1.35
28	di	203	PUB	C4C-NC	2.21	1.39	1.35
28	ey	1006	PUB	C4C-NC	2.21	1.39	1.35
28	z4	203	PUB	C4C-NC	2.20	1.39	1.35
28	z5	203	PUB	C4C-NC	2.20	1.39	1.35
28	iG	1002	PUB	C4C-NC	2.20	1.39	1.35
28	f3	203	PUB	C4C-NC	2.20	1.39	1.35
28	F4	203	PUB	C4C-NC	2.20	1.39	1.35
28	x9	203	PUB	C4C-NC	2.20	1.39	1.35
28	aZ	305	PUB	C4C-NC	2.20	1.39	1.35
28	eH	203	PUB	C4C-NC	2.20	1.39	1.35
28	T2	203	PUB	C4C-NC	2.20	1.39	1.35
28	t3	203	PUB	C4C-NC	2.20	1.39	1.35
28	v4	203	PUB	C4C-NC	2.20	1.39	1.35
28	v5	203	PUB	C4C-NC	2.20	1.39	1.35
28	t6	203	PUB	C4C-NC	2.20	1.39	1.35
28	jK	1003	PUB	C4C-NC	2.20	1.39	1.35
28	B3	203	PUB	C4C-NC	2.20	1.39	1.35
28	bV	203	PUB	C4C-NC	2.20	1.39	1.35
28	bo	202	PUB	C4C-NC	2.20	1.39	1.35
28	N2	203	PUB	C4C-NC	2.20	1.39	1.35
28	b7	202	PUB	C4C-NC	2.20	1.39	1.35
28	dx	406	PUB	C4C-NC	2.20	1.39	1.35
28	lb	203	PUB	C4C-NC	2.20	1.39	1.35
28	ff	203	PUB	C4C-NC	2.20	1.39	1.35
28	O8	203	PUB	C4C-NC	2.20	1.39	1.35
28	B5	203	PUB	C4C-NC	2.20	1.39	1.35
28	aH	203	PUB	C4C-NC	2.20	1.39	1.35
28	cp	203	PUB	C4C-NC	2.20	1.39	1.35
28	jP	1003	PUB	C4C-NC	2.20	1.39	1.35
28	D2	304	PUB	C4C-NC	2.20	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d3	303	PUB	C4C-NC	2.20	1.39	1.35
28	z6	203	PUB	C4C-NC	2.20	1.39	1.35
28	fm	203	PUB	C4C-NC	2.20	1.39	1.35
28	J3	203	PUB	C4C-NC	2.20	1.39	1.35
28	cn	202	PUB	C4C-NC	2.20	1.39	1.35
28	co	202	PUB	C4C-NC	2.20	1.39	1.35
28	ee	203	PUB	C4C-NC	2.20	1.39	1.35
28	gr	202	PUB	C4C-NC	2.20	1.39	1.35
28	gx	203	PUB	C4C-NC	2.20	1.39	1.35
28	bH	203	PUB	C4C-NC	2.20	1.39	1.35
28	eb	202	PUB	C4C-NC	2.20	1.39	1.35
28	ey	1005	PUB	C4C-NC	2.20	1.39	1.35
28	eZ	403	PUB	C4C-NC	2.20	1.39	1.35
28	H4	203	PUB	C4C-NC	2.20	1.39	1.35
28	44	304	PUB	C4C-NC	2.20	1.39	1.35
28	D5	203	PUB	C4C-NC	2.20	1.39	1.35
28	v7	203	PUB	C4C-NC	2.20	1.39	1.35
28	eT	203	PUB	C4C-NC	2.20	1.39	1.35
28	T3	203	PUB	C4C-NC	2.20	1.39	1.35
28	V4	203	PUB	C4C-NC	2.20	1.39	1.35
28	c9	304	PUB	C4C-NC	2.20	1.39	1.35
28	dH	203	PUB	C4C-NC	2.20	1.39	1.35
28	lv	202	PUB	C4C-NC	2.20	1.39	1.35
29	aZ	303	PVN	C19-C18	-2.20	1.44	1.48
28	bB	203	PUB	C4C-NC	2.20	1.39	1.35
28	t2	203	PUB	C4C-NC	2.20	1.39	1.35
28	R3	203	PUB	C4C-NC	2.20	1.39	1.35
28	44	305	PUB	C4C-NC	2.20	1.39	1.35
28	gp	203	PUB	C4C-NC	2.20	1.39	1.35
28	L5	203	PUB	C4C-NC	2.19	1.39	1.35
28	o8	203	PUB	C4C-NC	2.19	1.39	1.35
28	ly	406	PUB	C4C-NC	2.19	1.39	1.35
28	lz	405	PUB	C4C-NC	2.19	1.39	1.35
28	A2	1006	PUB	C4C-NC	2.19	1.39	1.35
28	a3	1006	PUB	C4C-NC	2.19	1.39	1.35
28	F7	202	PUB	C4C-NC	2.19	1.39	1.35
28	dv	202	PUB	C4C-NC	2.19	1.39	1.35
28	lp	203	PUB	C4C-NC	2.19	1.39	1.35
27	a2	902	CYC	CAD-C3D	-2.19	1.48	1.52
27	b2	1001	CYC	CAD-C3D	-2.19	1.48	1.52
28	H2	202	PUB	C4C-NC	2.19	1.39	1.35
28	aV	203	PUB	C4C-NC	2.19	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	S1	201	CYC	CAD-C3D	-2.19	1.48	1.52
27	j1	201	CYC	CAD-C3D	-2.19	1.48	1.52
28	l3	202	PUB	C4C-NC	2.19	1.39	1.35
28	D7	203	PUB	C4C-NC	2.19	1.39	1.35
28	e7	203	PUB	C4C-NC	2.19	1.39	1.35
28	c9	305	PUB	C4C-NC	2.19	1.39	1.35
29	aY	403	PVN	C15-C16	2.19	1.43	1.38
29	bY	1004	PVN	C15-C16	2.19	1.43	1.38
28	e6	203	PUB	C4C-NC	2.19	1.39	1.35
28	G8	203	PUB	C4C-NC	2.19	1.39	1.35
28	av	203	PUB	C4C-NC	2.19	1.39	1.35
28	bp	202	PUB	C4C-NC	2.19	1.39	1.35
28	bs	1004	PUB	C4C-NC	2.19	1.39	1.35
28	gz	305	PUB	C4C-NC	2.19	1.39	1.35
28	E8	203	PUB	C4C-NC	2.19	1.39	1.35
28	dD	203	PUB	C4C-NC	2.19	1.39	1.35
28	n2	203	PUB	C4C-NC	2.19	1.39	1.35
28	p7	202	PUB	C4C-NC	2.19	1.39	1.35
28	fs	203	PUB	C4C-NC	2.19	1.39	1.35
28	iD	1003	PUB	C4C-NC	2.19	1.39	1.35
28	aY	405	PUB	C4C-NC	2.19	1.39	1.35
28	dN	203	PUB	C4C-NC	2.19	1.39	1.35
28	gi	203	PUB	C4C-NC	2.19	1.39	1.35
28	hL	203	PUB	C4C-NC	2.19	1.39	1.35
28	aL	203	PUB	C4C-NC	2.19	1.39	1.35
28	ly	405	PUB	C4C-NC	2.19	1.39	1.35
28	lz	404	PUB	C4C-NC	2.19	1.39	1.35
28	jJ	1003	PUB	C4C-NC	2.19	1.39	1.35
29	ey	1004	PVN	C5-C4	-2.18	1.48	1.54
28	e9	306	PUB	C4C-NC	2.18	1.39	1.35
28	z9	203	PUB	C4C-NC	2.18	1.39	1.35
26	el	202	PEB	C3B-C2B	2.18	1.41	1.36
28	P7	203	PUB	C4C-NC	2.18	1.39	1.35
28	er	203	PUB	C4C-NC	2.18	1.39	1.35
29	T8	303	PVN	C19-C18	-2.18	1.44	1.48
28	aD	203	PUB	C4C-NC	2.18	1.39	1.35
27	c1	201	CYC	CAD-C3D	-2.18	1.48	1.52
28	eF	203	PUB	C4C-NC	2.18	1.39	1.35
27	M1	1001	CYC	CAD-C3D	-2.18	1.48	1.52
28	p2	203	PUB	C4C-NC	2.18	1.39	1.35
28	J7	202	PUB	C4C-NC	2.18	1.39	1.35
28	C8	203	PUB	C4C-NC	2.18	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	hY	405	PUB	C4C-NC	2.18	1.39	1.35
28	l7	203	PUB	C4C-NC	2.18	1.39	1.35
28	dj	203	PUB	C4C-NC	2.18	1.39	1.35
28	dt	203	PUB	C4C-NC	2.18	1.39	1.35
28	hG	202	PUB	C4C-NC	2.18	1.39	1.35
28	s7	203	PUB	C4C-NC	2.18	1.39	1.35
28	l2	203	PUB	C4C-NC	2.18	1.39	1.35
28	eJ	203	PUB	C4C-NC	2.18	1.39	1.35
27	t1	201	CYC	CAD-C3D	-2.18	1.48	1.52
28	L7	202	PUB	C4C-NC	2.18	1.39	1.35
28	ga	203	PUB	C4C-NC	2.18	1.39	1.35
27	S1	202	CYC	CAD-C3D	-2.18	1.48	1.52
28	dB	202	PUB	C4C-NC	2.18	1.39	1.35
28	r6	203	PUB	C4C-NC	2.18	1.39	1.35
28	T6	203	PUB	C4C-NC	2.18	1.39	1.35
28	b6	203	PUB	C4C-NC	2.18	1.39	1.35
28	hR	203	PUB	C4C-NC	2.18	1.39	1.35
28	T7	203	PUB	C4C-NC	2.18	1.39	1.35
28	P9	203	PUB	C4C-NC	2.17	1.39	1.35
27	r1	201	CYC	CAD-C3D	-2.17	1.48	1.52
28	b9	406	PUB	C4C-NC	2.17	1.39	1.35
29	44	303	PVN	C31-C3	2.17	1.56	1.51
28	p8	203	PUB	C4C-NC	2.17	1.39	1.35
28	e9	305	PUB	C4C-NC	2.17	1.39	1.35
28	Z3	203	PUB	C4C-NC	2.17	1.39	1.35
28	t5	203	PUB	C4C-NC	2.17	1.39	1.35
29	ey	1004	PVN	C15-C16	2.17	1.43	1.38
28	aR	203	PUB	C4C-NC	2.17	1.39	1.35
27	h1	201	CYC	CAD-C3D	-2.17	1.48	1.52
28	kX	1003	PUB	C4C-NC	2.17	1.39	1.35
28	lf	203	PUB	C4C-NC	2.16	1.39	1.35
27	a2	901	CYC	CAD-C3D	-2.16	1.48	1.52
27	Y1	201	CYC	CAD-C3D	-2.16	1.48	1.52
28	eR	203	PUB	CHB-C1C	2.16	1.36	1.35
29	aY	403	PVN	C41-C7	-2.16	1.47	1.51
28	fa	202	PUB	C4C-NC	2.15	1.39	1.35
29	bZ	304	PVN	C19-C18	-2.15	1.44	1.48
28	eR	203	PUB	C4C-NC	2.15	1.39	1.35
29	bY	1004	PVN	C41-C7	-2.15	1.47	1.51
28	ax	202	PUB	C4C-NC	2.15	1.39	1.35
27	v1	201	CYC	CAD-C3D	-2.14	1.48	1.52
29	Z5	304	PVN	C31-C3	2.14	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	ep	203	PUB	C4C-NC	2.14	1.39	1.35
29	Y9	303	PVN	C19-C18	-2.14	1.44	1.48
29	b8	1004	PVN	C11-C12	-2.13	1.42	1.45
29	b9	405	PVN	C11-C12	-2.13	1.42	1.45
28	dT	203	PUB	C4C-NC	2.12	1.38	1.35
29	bZ	304	PVN	O1-C1	-2.12	1.19	1.23
29	ly	404	PVN	C11-C12	-2.11	1.42	1.45
29	aZ	303	PVN	O1-C1	-2.10	1.19	1.23
26	bJ	202	PEB	C2C-C3C	2.10	1.43	1.37
29	dw	404	PVN	C11-C12	-2.10	1.42	1.45
26	J9	202	PEB	C2C-C3C	2.09	1.43	1.37
26	er	202	PEB	C2C-C3C	2.09	1.43	1.37
26	t3	202	PEB	C2C-C3C	2.09	1.43	1.37
27	a2	902	CYC	CBA-CGA	2.08	1.55	1.50
27	b2	1001	CYC	CBA-CGA	2.08	1.55	1.50
26	cs	202	PEB	C2C-C3C	2.08	1.43	1.37
26	i3	203	PEB	C2C-C3C	2.08	1.43	1.37
26	bV	202	PEB	C2C-C3C	2.08	1.43	1.37
26	ld	202	PEB	C2C-C3C	2.08	1.43	1.37
26	ln	202	PEB	C2C-C3C	2.08	1.43	1.37
26	et	202	PEB	C2C-C3C	2.08	1.43	1.37
26	kQ	1002	PEB	C2C-C3C	2.08	1.43	1.37
26	cY	202	PEB	C2C-C3C	2.08	1.43	1.37
26	iC	1002	PEB	C2C-C3C	2.08	1.43	1.37
26	P9	202	PEB	C2C-C3C	2.08	1.43	1.37
26	af	202	PEB	C2C-C3C	2.08	1.43	1.37
26	ec	202	PEB	C2C-C3C	2.08	1.43	1.37
26	gg	202	PEB	C2C-C3C	2.08	1.43	1.37
26	J3	202	PEB	C2C-C3C	2.08	1.43	1.37
26	cf	201	PEB	C2C-C3C	2.08	1.43	1.37
26	g5	202	PEB	C2C-C3C	2.08	1.43	1.37
26	X7	202	PEB	C2C-C3C	2.08	1.43	1.37
26	cJ	202	PEB	C2C-C3C	2.08	1.43	1.37
28	cO	203	PUB	C3B-C2B	2.08	1.43	1.37
26	p3	202	PEB	C2C-C3C	2.08	1.43	1.37
26	jJ	1002	PEB	C2C-C3C	2.08	1.43	1.37
26	ff	202	PEB	C2C-C3C	2.07	1.43	1.37
26	fo	202	PEB	C2C-C3C	2.07	1.43	1.37
26	W3	203	PEB	C2C-C3C	2.07	1.43	1.37
26	gt	202	PEB	C2C-C3C	2.07	1.43	1.37
26	T2	202	PEB	C2C-C3C	2.07	1.43	1.37
26	n7	202	PEB	C2C-C3C	2.07	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	eX	202	PUB	C3B-C2B	2.07	1.43	1.37
26	bQ	203	PEB	C2C-C3C	2.07	1.43	1.37
26	gk	202	PEB	C2C-C3C	2.07	1.43	1.37
26	n4	202	PEB	C2C-C3C	2.07	1.43	1.37
26	J5	202	PEB	C2C-C3C	2.07	1.43	1.37
27	S1	201	CYC	CBA-CGA	2.07	1.55	1.50
27	j1	201	CYC	CBA-CGA	2.07	1.55	1.50
28	n5	203	PUB	C3B-C2B	2.07	1.43	1.37
26	F3	202	PEB	C2C-C3C	2.07	1.43	1.37
26	cE	202	PEB	C2C-C3C	2.07	1.43	1.37
26	kX	1002	PEB	C2C-C3C	2.07	1.43	1.37
28	dX	203	PUB	C3B-C2B	2.07	1.43	1.37
26	bB	202	PEB	C2C-C3C	2.07	1.43	1.37
26	P5	201	PEB	C2C-C3C	2.07	1.43	1.37
26	ll	202	PEB	C2C-C3C	2.07	1.43	1.37
26	B5	202	PEB	C2C-C3C	2.07	1.43	1.37
26	v7	202	PEB	C2C-C3C	2.07	1.43	1.37
26	cL	202	PEB	C2C-C3C	2.07	1.43	1.37
26	dV	202	PEB	C2C-C3C	2.07	1.43	1.37
26	N5	202	PEB	C2C-C3C	2.07	1.43	1.37
26	B7	201	PEB	C2C-C3C	2.07	1.43	1.37
26	H7	202	PEB	C2C-C3C	2.07	1.43	1.37
26	f2	202	PEB	C2C-C3C	2.07	1.43	1.37
26	l2	202	PEB	C2C-C3C	2.07	1.43	1.37
27	a2	901	CYC	CBA-CGA	2.07	1.55	1.50
26	aD	202	PEB	C2C-C3C	2.07	1.43	1.37
26	ee	202	PEB	C2C-C3C	2.07	1.43	1.37
26	lo	203	PEB	C2C-C3C	2.07	1.43	1.37
28	C8	203	PUB	C3B-C2B	2.07	1.43	1.37
28	hG	202	PUB	C3B-C2B	2.07	1.43	1.37
26	j3	201	PEB	C2C-C3C	2.07	1.43	1.37
26	34	1001	PEB	C2C-C3C	2.07	1.43	1.37
26	r4	201	PEB	C2C-C3C	2.07	1.43	1.37
26	r5	202	PEB	C2C-C3C	2.07	1.43	1.37
26	V9	202	PEB	C2C-C3C	2.07	1.43	1.37
26	an	201	PEB	C2C-C3C	2.07	1.43	1.37
26	ep	202	PEB	C2C-C3C	2.07	1.43	1.37
28	at	203	PUB	C3B-C2B	2.07	1.43	1.37
29	hY	404	PVN	C11-C12	-2.07	1.42	1.45
26	z3	202	PEB	C2C-C3C	2.07	1.43	1.37
26	bN	202	PEB	C2C-C3C	2.07	1.43	1.37
26	jL	1002	PEB	C2C-C3C	2.07	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	P3	203	PUB	C3B-C2B	2.07	1.43	1.37
28	r3	203	PUB	C3B-C2B	2.07	1.43	1.37
26	l7	202	PEB	C2C-C3C	2.07	1.43	1.37
28	y6	204	PUB	C3B-C2B	2.07	1.43	1.37
28	dT	203	PUB	C3B-C2B	2.07	1.43	1.37
26	p4	202	PEB	C2C-C3C	2.07	1.43	1.37
26	hV	202	PEB	C2C-C3C	2.07	1.43	1.37
27	Y1	201	CYC	CBA-CGA	2.07	1.55	1.50
26	kR	1002	PEB	C2C-C3C	2.06	1.43	1.37
26	T9	202	PEB	C2C-C3C	2.06	1.43	1.37
28	aY	404	PUB	C3B-C2B	2.06	1.43	1.37
26	di	202	PEB	C2C-C3C	2.06	1.43	1.37
28	bY	1005	PUB	C3B-C2B	2.06	1.43	1.37
26	r3	202	PEB	C2C-C3C	2.06	1.43	1.37
26	df	202	PEB	C2C-C3C	2.06	1.43	1.37
28	b6	203	PUB	C3B-C2B	2.06	1.43	1.37
28	Y9	304	PUB	C3B-C2B	2.06	1.43	1.37
27	p1	201	CYC	CBA-CGA	2.06	1.55	1.50
26	34	1002	PEB	C2C-C3C	2.06	1.43	1.37
26	dL	202	PEB	C2C-C3C	2.06	1.43	1.37
26	X2	202	PEB	C2C-C3C	2.06	1.43	1.37
26	a7	202	PEB	C2C-C3C	2.06	1.43	1.37
28	dH	203	PUB	C3B-C2B	2.06	1.43	1.37
26	D5	202	PEB	C2C-C3C	2.06	1.43	1.37
26	L5	202	PEB	C2C-C3C	2.06	1.43	1.37
28	aD	203	PUB	C3B-C2B	2.06	1.43	1.37
26	Y7	1003	PEB	C2C-C3C	2.06	1.43	1.37
26	L9	202	PEB	C2C-C3C	2.06	1.43	1.37
26	av	202	PEB	C2C-C3C	2.06	1.43	1.37
26	lf	202	PEB	C2C-C3C	2.06	1.43	1.37
26	P3	202	PEB	C2C-C3C	2.06	1.43	1.37
26	bD	202	PEB	C2C-C3C	2.06	1.43	1.37
26	dY	202	PEB	C2C-C3C	2.06	1.43	1.37
26	fg	201	PEB	C2C-C3C	2.06	1.43	1.37
26	g4	202	PEB	C2C-C3C	2.06	1.43	1.37
26	n5	202	PEB	C2C-C3C	2.06	1.43	1.37
26	V7	202	PEB	C2C-C3C	2.06	1.43	1.37
26	t7	202	PEB	C2C-C3C	2.06	1.43	1.37
26	fu	201	PEB	C2C-C3C	2.06	1.43	1.37
29	bZ	304	PVN	C15-C14	2.06	1.45	1.40
26	az	202	PEB	C2C-C3C	2.06	1.43	1.37
26	lr	202	PEB	C2C-C3C	2.06	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	eX	201	PEB	C2C-C3C	2.06	1.43	1.37
26	y8	202	PEB	C2C-C3C	2.06	1.43	1.37
26	fw	202	PEB	C2C-C3C	2.06	1.43	1.37
28	B7	202	PUB	C3B-C2B	2.06	1.43	1.37
28	ge	203	PUB	C3B-C2B	2.06	1.43	1.37
26	T7	202	PEB	C2C-C3C	2.06	1.43	1.37
26	N9	202	PEB	C2C-C3C	2.06	1.43	1.37
26	lw	203	PEB	C2C-C3C	2.06	1.43	1.37
26	jM	1002	PEB	C2C-C3C	2.06	1.43	1.37
28	X3	202	PUB	C3B-C2B	2.06	1.43	1.37
26	hN	202	PEB	C2C-C3C	2.06	1.43	1.37
26	iE	1002	PEB	C2C-C3C	2.06	1.43	1.37
26	A5	203	PEB	C2C-C3C	2.06	1.43	1.37
26	ah	202	PEB	C2C-C3C	2.06	1.43	1.37
26	bH	202	PEB	C2C-C3C	2.06	1.43	1.37
26	co	201	PEB	C2C-C3C	2.06	1.43	1.37
26	kW	1002	PEB	C2C-C3C	2.06	1.43	1.37
28	Y9	305	PUB	C3B-C2B	2.06	1.43	1.37
26	fm	202	PEB	C2C-C3C	2.06	1.43	1.37
28	44	304	PUB	C3B-C2B	2.06	1.43	1.37
26	B4	202	PEB	C2C-C3C	2.06	1.43	1.37
26	al	202	PEB	C2C-C3C	2.06	1.43	1.37
26	dh	202	PEB	C2C-C3C	2.06	1.43	1.37
26	eL	202	PEB	C2C-C3C	2.06	1.43	1.37
26	f3	202	PEB	C2C-C3C	2.06	1.43	1.37
26	ap	202	PEB	C2C-C3C	2.06	1.43	1.37
26	ar	202	PEB	C2C-C3C	2.06	1.43	1.37
26	hJ	202	PEB	C2C-C3C	2.06	1.43	1.37
26	F9	202	PEB	C2C-C3C	2.06	1.43	1.37
26	cF	201	PEB	C2C-C3C	2.06	1.43	1.37
28	L6	202	PUB	C3B-C2B	2.06	1.43	1.37
26	c7	202	PEB	C2C-C3C	2.06	1.43	1.37
26	bL	202	PEB	C2C-C3C	2.06	1.43	1.37
26	jI	1002	PEB	C2C-C3C	2.06	1.43	1.37
28	n3	203	PUB	C3B-C2B	2.06	1.43	1.37
26	L2	202	PEB	C2C-C3C	2.06	1.43	1.37
26	ch	202	PEB	C2C-C3C	2.06	1.43	1.37
26	cn	201	PEB	C2C-C3C	2.06	1.43	1.37
26	cH	201	PEB	C2C-C3C	2.06	1.43	1.37
26	dl	202	PEB	C2C-C3C	2.06	1.43	1.37
28	bo	202	PUB	C3B-C2B	2.06	1.43	1.37
28	hB	203	PUB	C3B-C2B	2.06	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M1	1001	CYC	CBA-CGA	2.06	1.55	1.50
26	y7	202	PEB	C2C-C3C	2.06	1.43	1.37
28	V4	203	PUB	C3B-C2B	2.06	1.43	1.37
28	T6	203	PUB	C3B-C2B	2.06	1.43	1.37
28	g8	202	PUB	C3B-C2B	2.06	1.43	1.37
26	F5	202	PEB	C2C-C3C	2.06	1.43	1.37
28	y8	203	PUB	C3B-C2B	2.06	1.43	1.37
26	x3	202	PEB	C2C-C3C	2.05	1.43	1.37
26	ax	201	PEB	C2C-C3C	2.05	1.43	1.37
26	gp	202	PEB	C2C-C3C	2.05	1.43	1.37
28	a7	203	PUB	C3B-C2B	2.05	1.43	1.37
28	fi	203	PUB	C3B-C2B	2.05	1.43	1.37
27	r1	201	CYC	CBA-CGA	2.05	1.55	1.50
26	iD	1002	PEB	C2C-C3C	2.05	1.43	1.37
28	N6	203	PUB	C3B-C2B	2.05	1.43	1.37
28	bT	202	PUB	C3B-C2B	2.05	1.43	1.37
28	hD	203	PUB	C3B-C2B	2.05	1.43	1.37
26	fj	202	PEB	C2C-C3C	2.05	1.43	1.37
28	eY	405	PUB	C3B-C2B	2.05	1.43	1.37
28	eZ	404	PUB	C3B-C2B	2.05	1.43	1.37
26	li	203	PEB	C2C-C3C	2.05	1.43	1.37
28	P2	203	PUB	C3B-C2B	2.05	1.43	1.37
28	J4	203	PUB	C3B-C2B	2.05	1.43	1.37
28	cB	203	PUB	C3B-C2B	2.05	1.43	1.37
28	ly	406	PUB	C3B-C2B	2.05	1.43	1.37
28	lz	405	PUB	C3B-C2B	2.05	1.43	1.37
28	fy	202	PUB	C3B-C2B	2.05	1.43	1.37
27	c1	201	CYC	CBA-CGA	2.05	1.55	1.50
26	T3	202	PEB	C2C-C3C	2.05	1.43	1.37
28	H5	202	PUB	C3B-C2B	2.05	1.43	1.37
26	Z7	202	PEB	C2C-C3C	2.05	1.43	1.37
26	x7	202	PEB	C2C-C3C	2.05	1.43	1.37
28	H2	202	PUB	C3B-C2B	2.05	1.43	1.37
28	D5	203	PUB	C3B-C2B	2.05	1.43	1.37
28	jN	1003	PUB	C3B-C2B	2.05	1.43	1.37
26	h3	201	PEB	C2C-C3C	2.05	1.43	1.37
26	z5	202	PEB	C2C-C3C	2.05	1.43	1.37
26	P7	202	PEB	C2C-C3C	2.05	1.43	1.37
28	v4	203	PUB	C3B-C2B	2.05	1.43	1.37
28	v5	203	PUB	C3B-C2B	2.05	1.43	1.37
28	Z9	1005	PUB	C3B-C2B	2.05	1.43	1.37
28	jM	1003	PUB	C3B-C2B	2.05	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	v4	202	PEB	C2C-C3C	2.05	1.43	1.37
26	cp	202	PEB	C2C-C3C	2.05	1.43	1.37
28	eL	203	PUB	C3B-C2B	2.05	1.43	1.37
26	v9	202	PEB	C2C-C3C	2.05	1.43	1.37
26	ga	202	PEB	C2C-C3C	2.05	1.43	1.37
28	J6	203	PUB	C3B-C2B	2.05	1.43	1.37
28	dl	203	PUB	C3B-C2B	2.05	1.43	1.37
27	z1	201	CYC	CBA-CGA	2.05	1.55	1.50
26	ad	202	PEB	C2C-C3C	2.05	1.43	1.37
28	44	305	PUB	C3B-C2B	2.05	1.43	1.37
28	Z5	306	PUB	C3B-C2B	2.05	1.43	1.37
28	e6	203	PUB	C3B-C2B	2.05	1.43	1.37
26	D3	202	PEB	C2C-C3C	2.05	1.43	1.37
26	dd	202	PEB	C2C-C3C	2.05	1.43	1.37
26	ei	202	PEB	C2C-C3C	2.05	1.43	1.37
28	bp	202	PUB	C3B-C2B	2.05	1.43	1.37
28	bD	203	PUB	C3B-C2B	2.05	1.43	1.37
28	ey	1006	PUB	C3B-C2B	2.05	1.43	1.37
29	e8	303	PVN	C16-N4	2.05	1.41	1.37
28	jO	1003	PUB	C3B-C2B	2.05	1.43	1.37
28	h2	203	PUB	C3B-C2B	2.05	1.43	1.37
28	dx	407	PUB	C3B-C2B	2.05	1.43	1.37
26	kU	1002	PEB	C2C-C3C	2.05	1.43	1.37
28	ln	203	PUB	C3B-C2B	2.05	1.43	1.37
28	ly	405	PUB	C3B-C2B	2.05	1.43	1.37
28	lz	404	PUB	C3B-C2B	2.05	1.43	1.37
28	cP	203	PUB	C3B-C2B	2.05	1.43	1.37
28	et	203	PUB	C3B-C2B	2.05	1.43	1.37
28	gd	202	PUB	C3B-C2B	2.05	1.43	1.37
26	ev	202	PEB	C2C-C3C	2.05	1.43	1.37
26	fq	202	PEB	C2C-C3C	2.05	1.43	1.37
28	Z3	203	PUB	C3B-C2B	2.05	1.43	1.37
28	bJ	203	PUB	C3B-C2B	2.05	1.43	1.37
26	Z3	202	PEB	C2C-C3C	2.05	1.43	1.37
26	t5	202	PEB	C2C-C3C	2.05	1.43	1.37
26	ab	202	PEB	C2C-C3C	2.05	1.43	1.37
26	hR	202	PEB	C2C-C3C	2.05	1.43	1.37
28	f2	203	PUB	C3B-C2B	2.05	1.43	1.37
28	F3	203	PUB	C3B-C2B	2.05	1.43	1.37
28	fc	203	PUB	C3B-C2B	2.05	1.43	1.37
26	lp	202	PEB	C2C-C3C	2.05	1.43	1.37
26	gn	202	PEB	C2C-C3C	2.05	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y5	1006	PUB	C3B-C2B	2.05	1.43	1.37
28	ar	203	PUB	C3B-C2B	2.05	1.43	1.37
28	bN	203	PUB	C3B-C2B	2.05	1.43	1.37
28	kU	1003	PUB	C3B-C2B	2.05	1.43	1.37
28	R6	203	PUB	C3B-C2B	2.05	1.43	1.37
26	ea	203	PEB	C2C-C3C	2.05	1.43	1.37
26	N3	202	PEB	C2C-C3C	2.05	1.43	1.37
26	z7	202	PEB	C2C-C3C	2.05	1.43	1.37
26	C8	202	PEB	C2C-C3C	2.05	1.43	1.37
26	gv	202	PEB	C2C-C3C	2.05	1.43	1.37
26	R9	202	PEB	C2C-C3C	2.05	1.43	1.37
27	S1	202	CYC	CBA-CGA	2.05	1.55	1.50
26	cd	202	PEB	C2C-C3C	2.05	1.43	1.37
28	X2	203	PUB	C3B-C2B	2.05	1.43	1.37
28	dN	203	PUB	C3B-C2B	2.05	1.43	1.37
28	hT	203	PUB	C3B-C2B	2.05	1.43	1.37
26	gx	202	PEB	C2C-C3C	2.05	1.43	1.37
28	an	202	PUB	C3B-C2B	2.05	1.43	1.37
26	eV	202	PEB	C2C-C3C	2.05	1.43	1.37
26	kT	1002	PEB	C2C-C3C	2.05	1.43	1.37
28	j2	203	PUB	C3B-C2B	2.05	1.43	1.37
28	D6	202	PUB	C3B-C2B	2.05	1.43	1.37
28	I8	203	PUB	C3B-C2B	2.05	1.43	1.37
28	N9	203	PUB	C3B-C2B	2.05	1.43	1.37
28	dn	203	PUB	C3B-C2B	2.05	1.43	1.37
26	H9	202	PEB	C2C-C3C	2.05	1.43	1.37
26	hH	202	PEB	C2C-C3C	2.05	1.43	1.37
28	ep	203	PUB	C3B-C2B	2.05	1.43	1.37
28	eF	203	PUB	C3B-C2B	2.05	1.43	1.37
28	iF	1003	PUB	C3B-C2B	2.05	1.43	1.37
26	V3	202	PEB	C2C-C3C	2.05	1.43	1.37
28	aF	203	PUB	C3B-C2B	2.05	1.43	1.37
28	kW	1003	PUB	C3B-C2B	2.05	1.43	1.37
26	eB	203	PEB	C2C-C3C	2.05	1.43	1.37
28	cJ	203	PUB	C3B-C2B	2.05	1.43	1.37
28	dw	406	PUB	C3B-C2B	2.05	1.43	1.37
28	eH	203	PUB	C3B-C2B	2.05	1.43	1.37
27	t1	201	CYC	CBA-CGA	2.05	1.55	1.50
26	B6	202	PEB	C2C-C3C	2.05	1.43	1.37
28	aJ	203	PUB	C3B-C2B	2.05	1.43	1.37
28	aL	203	PUB	C3B-C2B	2.05	1.43	1.37
28	br	203	PUB	C3B-C2B	2.05	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	kR	1003	PUB	C3B-C2B	2.05	1.43	1.37
26	bT	201	PEB	C2C-C3C	2.04	1.43	1.37
26	cj	202	PEB	C2C-C3C	2.04	1.43	1.37
26	hB	202	PEB	C2C-C3C	2.04	1.43	1.37
26	hX	202	PEB	C2C-C3C	2.04	1.43	1.37
28	R2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	b9	406	PUB	C3B-C2B	2.04	1.43	1.37
28	cN	202	PUB	C3B-C2B	2.04	1.43	1.37
28	ez	1006	PUB	C3B-C2B	2.04	1.43	1.37
28	lf	203	PUB	C3B-C2B	2.04	1.43	1.37
28	fa	202	PUB	C3B-C2B	2.04	1.43	1.37
28	R9	203	PUB	C3B-C2B	2.04	1.43	1.37
29	T8	303	PVN	C11-C12	-2.04	1.42	1.45
29	Y9	303	PVN	C11-C12	-2.04	1.42	1.45
26	n3	202	PEB	C2C-C3C	2.04	1.43	1.37
26	p5	201	PEB	C2C-C3C	2.04	1.43	1.37
26	N7	202	PEB	C2C-C3C	2.04	1.43	1.37
28	t9	203	PUB	C3B-C2B	2.04	1.43	1.37
28	hR	203	PUB	C3B-C2B	2.04	1.43	1.37
27	h1	201	CYC	CBA-CGA	2.04	1.55	1.50
26	V2	202	PEB	C2C-C3C	2.04	1.43	1.37
26	R6	202	PEB	C2C-C3C	2.04	1.43	1.37
26	gr	201	PEB	C2C-C3C	2.04	1.43	1.37
28	V2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	Y5	1005	PUB	C3B-C2B	2.04	1.43	1.37
28	d6	203	PUB	C3B-C2B	2.04	1.43	1.37
26	j2	202	PEB	C2C-C3C	2.04	1.43	1.37
26	D7	202	PEB	C2C-C3C	2.04	1.43	1.37
28	fq	203	PUB	C3B-C2B	2.04	1.43	1.37
26	h2	202	PEB	C2C-C3C	2.04	1.43	1.37
26	X6	202	PEB	C2C-C3C	2.04	1.43	1.37
26	aj	202	PEB	C2C-C3C	2.04	1.43	1.37
26	lh	202	PEB	C2C-C3C	2.04	1.43	1.37
28	c8	305	PUB	C3B-C2B	2.04	1.43	1.37
28	L9	203	PUB	C3B-C2B	2.04	1.43	1.37
28	j3	202	PUB	C3B-C2B	2.04	1.43	1.37
28	L4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	bZ	305	PUB	C3B-C2B	2.04	1.43	1.37
28	dF	203	PUB	C3B-C2B	2.04	1.43	1.37
28	eR	203	PUB	C3B-C2B	2.04	1.43	1.37
27	H1	201	CYC	CBA-CGA	2.04	1.55	1.50
26	R3	202	PEB	C2C-C3C	2.04	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	l4	202	PEB	C2C-C3C	2.04	1.43	1.37
28	H3	203	PUB	C3B-C2B	2.04	1.43	1.37
28	Z4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	Z6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	J9	203	PUB	C3B-C2B	2.04	1.43	1.37
28	kQ	1003	PUB	C3B-C2B	2.04	1.43	1.37
26	B3	202	PEB	C2C-C3C	2.04	1.43	1.37
26	r7	202	PEB	C2C-C3C	2.04	1.43	1.37
26	jK	1002	PEB	C2C-C3C	2.04	1.43	1.37
28	n6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	c9	304	PUB	C3B-C2B	2.04	1.43	1.37
28	jL	1003	PUB	C3B-C2B	2.04	1.43	1.37
26	B1	301	PEB	C2C-C3C	2.04	1.43	1.37
28	c6	1004	PUB	C3B-C2B	2.04	1.43	1.37
28	l6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	e9	305	PUB	C3B-C2B	2.04	1.43	1.37
28	dj	203	PUB	C3B-C2B	2.04	1.43	1.37
28	dt	203	PUB	C3B-C2B	2.04	1.43	1.37
28	ec	203	PUB	C3B-C2B	2.04	1.43	1.37
28	fj	203	PUB	C3B-C2B	2.04	1.43	1.37
26	v3	202	PEB	C2C-C3C	2.04	1.43	1.37
26	gi	202	PEB	C2C-C3C	2.04	1.43	1.37
28	R5	203	PUB	C3B-C2B	2.04	1.43	1.37
28	co	202	PUB	C3B-C2B	2.04	1.43	1.37
28	dv	202	PUB	C3B-C2B	2.04	1.43	1.37
26	J6	202	PEB	C2C-C3C	2.04	1.43	1.37
26	cr	202	PEB	C2C-C3C	2.04	1.43	1.37
26	cz	202	PEB	C2C-C3C	2.04	1.43	1.37
26	dj	202	PEB	C2C-C3C	2.04	1.43	1.37
26	fy	201	PEB	C2C-C3C	2.04	1.43	1.37
26	ge	202	PEB	C2C-C3C	2.04	1.43	1.37
26	jN	1002	PEB	C2C-C3C	2.04	1.43	1.37
26	jP	1002	PEB	C2C-C3C	2.04	1.43	1.37
28	h3	202	PUB	C3B-C2B	2.04	1.43	1.37
28	D7	203	PUB	C3B-C2B	2.04	1.43	1.37
28	az	203	PUB	C3B-C2B	2.04	1.43	1.37
26	en	202	PEB	C2C-C3C	2.04	1.43	1.37
28	F4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	J7	202	PUB	C3B-C2B	2.04	1.43	1.37
28	V7	203	PUB	C3B-C2B	2.04	1.43	1.37
28	x7	203	PUB	C3B-C2B	2.04	1.43	1.37
28	ax	202	PUB	C3B-C2B	2.04	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h8	202	PEB	C2C-C3C	2.04	1.43	1.37
26	eJ	202	PEB	C2C-C3C	2.04	1.43	1.37
28	a3	1005	PUB	C3B-C2B	2.04	1.43	1.37
28	A8	203	PUB	C3B-C2B	2.04	1.43	1.37
28	cs	203	PUB	C3B-C2B	2.04	1.43	1.37
26	L3	202	PEB	C2C-C3C	2.04	1.43	1.37
26	cq	202	PEB	C2C-C3C	2.04	1.43	1.37
28	N2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	gp	203	PUB	C3B-C2B	2.04	1.43	1.37
28	jI	1003	PUB	C3B-C2B	2.04	1.43	1.37
28	jK	1003	PUB	C3B-C2B	2.04	1.43	1.37
26	H2	201	PEB	C2C-C3C	2.04	1.43	1.37
28	t2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	B4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	R4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	v7	203	PUB	C3B-C2B	2.04	1.43	1.37
28	Z9	1006	PUB	C3B-C2B	2.04	1.43	1.37
28	hL	203	PUB	C3B-C2B	2.04	1.43	1.37
26	p2	202	PEB	C2C-C3C	2.04	1.43	1.37
26	fs	202	PEB	C2C-C3C	2.04	1.43	1.37
28	cp	203	PUB	C3B-C2B	2.04	1.43	1.37
26	D4	202	PEB	C2C-C3C	2.04	1.43	1.37
28	aB	203	PUB	C3B-C2B	2.04	1.43	1.37
28	cn	202	PUB	C3B-C2B	2.04	1.43	1.37
28	cL	203	PUB	C3B-C2B	2.04	1.43	1.37
28	eJ	203	PUB	C3B-C2B	2.04	1.43	1.37
28	lb	203	PUB	C3B-C2B	2.04	1.43	1.37
28	gt	203	PUB	C3B-C2B	2.04	1.43	1.37
26	A1	301	PEB	C2C-C3C	2.04	1.43	1.37
26	eg	202	PEB	C2C-C3C	2.04	1.43	1.37
28	X4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	x4	202	PUB	C3B-C2B	2.04	1.43	1.37
28	p5	202	PUB	C3B-C2B	2.04	1.43	1.37
28	x5	202	PUB	C3B-C2B	2.04	1.43	1.37
28	p6	203	PUB	C3B-C2B	2.04	1.43	1.37
26	n6	202	PEB	C2C-C3C	2.04	1.43	1.37
28	x2	202	PUB	C3B-C2B	2.04	1.43	1.37
28	t4	203	PUB	C3B-C2B	2.04	1.43	1.37
28	Q8	203	PUB	C3B-C2B	2.04	1.43	1.37
28	H9	203	PUB	C3B-C2B	2.04	1.43	1.37
28	kX	1003	PUB	C3B-C2B	2.04	1.43	1.37
26	bP	202	PEB	C2C-C3C	2.04	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	hD	202	PEB	C2C-C3C	2.04	1.43	1.37
28	v2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	V3	203	PUB	C3B-C2B	2.04	1.43	1.37
28	a3	1006	PUB	C3B-C2B	2.04	1.43	1.37
28	e8	305	PUB	C3B-C2B	2.04	1.43	1.37
28	O8	203	PUB	C3B-C2B	2.04	1.43	1.37
28	cr	203	PUB	C3B-C2B	2.04	1.43	1.37
28	hY	405	PUB	C3B-C2B	2.04	1.43	1.37
26	n8	201	PEB	C2C-C3C	2.04	1.43	1.37
28	dY	203	PUB	C3B-C2B	2.04	1.43	1.37
26	L7	201	PEB	C2C-C3C	2.04	1.43	1.37
26	gd	201	PEB	C2C-C3C	2.04	1.43	1.37
28	H6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	cF	202	PUB	C3B-C2B	2.04	1.43	1.37
28	gx	203	PUB	C3B-C2B	2.04	1.43	1.37
26	j4	202	PEB	C2C-C3C	2.04	1.43	1.37
28	F6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	x6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	iH	1002	PUB	C3B-C2B	2.04	1.43	1.37
26	hL	202	PEB	C2C-C3C	2.04	1.43	1.37
28	p9	203	PUB	C3B-C2B	2.04	1.43	1.37
28	bP	203	PUB	C3B-C2B	2.04	1.43	1.37
28	gz	306	PUB	C3B-C2B	2.04	1.43	1.37
28	A2	1006	PUB	C3B-C2B	2.04	1.43	1.37
28	r4	202	PUB	C3B-C2B	2.04	1.43	1.37
28	r5	203	PUB	C3B-C2B	2.04	1.43	1.37
28	C2	304	PUB	C3B-C2B	2.04	1.43	1.37
28	z7	203	PUB	C3B-C2B	2.04	1.43	1.37
28	kS	1003	PUB	C3B-C2B	2.04	1.43	1.37
26	fc	202	PEB	C2C-C3C	2.04	1.43	1.37
26	hG	201	PEB	C2C-C3C	2.04	1.43	1.37
28	l2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	L2	203	PUB	C3B-C2B	2.04	1.43	1.37
28	L3	203	PUB	C3B-C2B	2.04	1.43	1.37
28	l3	202	PUB	C3B-C2B	2.04	1.43	1.37
28	u6	203	PUB	C3B-C2B	2.04	1.43	1.37
28	l7	203	PUB	C3B-C2B	2.04	1.43	1.37
28	F9	203	PUB	C3B-C2B	2.04	1.43	1.37
28	eg	203	PUB	C3B-C2B	2.04	1.43	1.37
28	fu	202	PUB	C3B-C2B	2.04	1.43	1.37
26	fi	202	PEB	C2C-C3C	2.04	1.43	1.37
26	kS	1002	PEB	C2C-C3C	2.04	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	v3	203	PUB	C3B-C2B	2.04	1.43	1.37
28	z3	203	PUB	C3B-C2B	2.04	1.43	1.37
28	34	1005	PUB	C3B-C2B	2.04	1.43	1.37
28	cY	203	PUB	C3B-C2B	2.04	1.43	1.37
28	eb	202	PUB	C3B-C2B	2.04	1.43	1.37
28	cR	203	PUB	C3B-C2B	2.03	1.43	1.37
26	n2	202	PEB	C2C-C3C	2.03	1.43	1.37
26	V5	202	PEB	C2C-C3C	2.03	1.43	1.37
26	kV	1002	PEB	C2C-C3C	2.03	1.43	1.37
28	D3	203	PUB	C3B-C2B	2.03	1.43	1.37
28	fw	203	PUB	C3B-C2B	2.03	1.43	1.37
26	v5	202	PEB	C2C-C3C	2.03	1.43	1.37
26	jO	1002	PEB	C2C-C3C	2.03	1.43	1.37
28	b7	202	PUB	C3B-C2B	2.03	1.43	1.37
28	dd	203	PUB	C3B-C2B	2.03	1.43	1.37
28	ff	203	PUB	C3B-C2B	2.03	1.43	1.37
28	fo	203	PUB	C3B-C2B	2.03	1.43	1.37
28	d3	303	PUB	C3B-C2B	2.03	1.43	1.37
28	H4	203	PUB	C3B-C2B	2.03	1.43	1.37
28	z6	203	PUB	C3B-C2B	2.03	1.43	1.37
28	aY	405	PUB	C3B-C2B	2.03	1.43	1.37
28	bY	1006	PUB	C3B-C2B	2.03	1.43	1.37
28	ei	203	PUB	C3B-C2B	2.03	1.43	1.37
28	C2	305	PUB	C3B-C2B	2.03	1.43	1.37
28	c3	305	PUB	C3B-C2B	2.03	1.43	1.37
28	aN	203	PUB	C3B-C2B	2.03	1.43	1.37
28	kT	1003	PUB	C3B-C2B	2.03	1.43	1.37
28	B3	203	PUB	C3B-C2B	2.03	1.43	1.37
28	x3	203	PUB	C3B-C2B	2.03	1.43	1.37
28	r6	203	PUB	C3B-C2B	2.03	1.43	1.37
28	hN	203	PUB	C3B-C2B	2.03	1.43	1.37
26	H3	202	PEB	C2C-C3C	2.03	1.43	1.37
26	F7	201	PEB	C2C-C3C	2.03	1.43	1.37
26	aF	202	PEB	C2C-C3C	2.03	1.43	1.37
26	bF	202	PEB	C2C-C3C	2.03	1.43	1.37
28	c3	304	PUB	C3B-C2B	2.03	1.43	1.37
28	P6	203	PUB	C3B-C2B	2.03	1.43	1.37
28	G8	203	PUB	C3B-C2B	2.03	1.43	1.37
28	U8	1005	PUB	C3B-C2B	2.03	1.43	1.37
28	n2	203	PUB	C3B-C2B	2.03	1.43	1.37
28	z4	203	PUB	C3B-C2B	2.03	1.43	1.37
28	z5	203	PUB	C3B-C2B	2.03	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	e4	202	PEB	C2C-C3C	2.03	1.43	1.37
28	r7	203	PUB	C3B-C2B	2.03	1.43	1.37
28	bZ	306	PUB	C3B-C2B	2.03	1.43	1.37
28	gz	305	PUB	C3B-C2B	2.03	1.43	1.37
26	el	202	PEB	C2C-C3C	2.03	1.43	1.37
28	D2	305	PUB	C3B-C2B	2.03	1.43	1.37
28	bR	202	PUB	C3B-C2B	2.03	1.43	1.37
26	e7	202	PEB	C2C-C3C	2.03	1.43	1.37
26	at	202	PEB	C2C-C3C	2.03	1.43	1.37
26	hT	202	PEB	C2C-C3C	2.03	1.43	1.37
28	dw	405	PUB	C3B-C2B	2.03	1.43	1.37
28	eN	203	PUB	C3B-C2B	2.03	1.43	1.37
28	d3	304	PUB	C3B-C2B	2.03	1.43	1.37
28	bn	202	PUB	C3B-C2B	2.03	1.43	1.37
28	T9	203	PUB	C3B-C2B	2.03	1.43	1.37
28	fs	203	PUB	C3B-C2B	2.03	1.43	1.37
26	B9	202	PEB	C2C-C3C	2.03	1.43	1.37
28	F2	203	PUB	C3B-C2B	2.03	1.43	1.37
28	f3	203	PUB	C3B-C2B	2.03	1.43	1.37
28	eY	404	PUB	C3B-C2B	2.03	1.43	1.37
28	eZ	403	PUB	C3B-C2B	2.03	1.43	1.37
26	A2	1003	PEB	C2C-C3C	2.03	1.43	1.37
26	cb	202	PEB	C2C-C3C	2.03	1.43	1.37
28	T8	304	PUB	C3B-C2B	2.03	1.43	1.37
28	gg	203	PUB	C3B-C2B	2.03	1.43	1.37
27	m1	201	CYC	C1C-NC	-2.03	1.35	1.37
26	cl	202	PEB	C2C-C3C	2.03	1.43	1.37
28	h8	203	PUB	C3B-C2B	2.03	1.43	1.37
28	b9	407	PUB	C3B-C2B	2.03	1.43	1.37
28	d9	305	PUB	C3B-C2B	2.03	1.43	1.37
28	T8	305	PUB	C3B-C2B	2.03	1.43	1.37
28	aP	203	PUB	C3B-C2B	2.03	1.43	1.37
27	v1	201	CYC	CBA-CGA	2.03	1.55	1.50
28	B6	203	PUB	C3B-C2B	2.03	1.43	1.37
28	aZ	305	PUB	C3B-C2B	2.03	1.43	1.37
27	J1	201	CYC	CBA-CGA	2.03	1.55	1.50
28	Z7	203	PUB	C3B-C2B	2.03	1.43	1.37
29	e9	304	PVN	C15-C14	2.03	1.45	1.40
28	D4	203	PUB	C3B-C2B	2.03	1.43	1.37
28	dx	406	PUB	C3B-C2B	2.03	1.43	1.37
28	ey	1005	PUB	C3B-C2B	2.03	1.43	1.37
28	A2	1005	PUB	C3B-C2B	2.03	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	t5	203	PUB	C3B-C2B	2.03	1.43	1.37
28	bq	203	PUB	C3B-C2B	2.03	1.43	1.37
28	eD	203	PUB	C3B-C2B	2.03	1.43	1.37
28	hY	406	PUB	C3B-C2B	2.03	1.43	1.37
28	N5	203	PUB	C3B-C2B	2.03	1.43	1.37
29	hZ	403	PVN	C11-C12	-2.03	1.42	1.45
26	R5	202	PEB	C2C-C3C	2.03	1.43	1.37
26	p8	202	PEB	C2C-C3C	2.03	1.43	1.37
28	z9	203	PUB	C3B-C2B	2.03	1.43	1.37
28	cq	203	PUB	C3B-C2B	2.03	1.43	1.37
28	b8	1006	PUB	C3B-C2B	2.03	1.43	1.37
28	dh	203	PUB	C3B-C2B	2.03	1.43	1.37
28	jJ	1003	PUB	C3B-C2B	2.03	1.43	1.37
28	K8	203	PUB	C3B-C2B	2.03	1.43	1.37
28	P9	203	PUB	C3B-C2B	2.03	1.43	1.37
28	aT	203	PUB	C3B-C2B	2.03	1.43	1.37
26	Z2	202	PEB	C2C-C3C	2.03	1.43	1.37
28	e8	304	PUB	C3B-C2B	2.03	1.43	1.37
28	df	203	PUB	C3B-C2B	2.03	1.43	1.37
28	di	203	PUB	C3B-C2B	2.03	1.43	1.37
28	dD	203	PUB	C3B-C2B	2.03	1.43	1.37
26	p7	201	PEB	C2C-C3C	2.03	1.43	1.37
28	T2	203	PUB	C3B-C2B	2.03	1.43	1.37
28	t3	203	PUB	C3B-C2B	2.03	1.43	1.37
28	V5	203	PUB	C3B-C2B	2.03	1.43	1.37
28	er	203	PUB	C3B-C2B	2.03	1.43	1.37
28	eV	203	PUB	C3B-C2B	2.03	1.43	1.37
27	I1	201	CYC	C1C-NC	-2.03	1.35	1.37
28	T3	203	PUB	C3B-C2B	2.03	1.43	1.37
28	P4	203	PUB	C3B-C2B	2.03	1.43	1.37
28	Z5	305	PUB	C3B-C2B	2.03	1.43	1.37
28	b8	1005	PUB	C3B-C2B	2.03	1.43	1.37
28	gk	203	PUB	C3B-C2B	2.03	1.43	1.37
26	S5	203	PEB	C2C-C3C	2.03	1.43	1.37
28	p2	203	PUB	C3B-C2B	2.03	1.43	1.37
28	F5	203	PUB	C3B-C2B	2.03	1.43	1.37
28	n7	203	PUB	C3B-C2B	2.03	1.43	1.37
28	hP	203	PUB	C3B-C2B	2.03	1.43	1.37
27	k1	201	CYC	C1C-NC	-2.02	1.35	1.37
26	cB	202	PEB	C2C-C3C	2.02	1.43	1.37
28	34	1006	PUB	C3B-C2B	2.02	1.43	1.37
28	v9	203	PUB	C3B-C2B	2.02	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	bV	203	PUB	C3B-C2B	2.02	1.43	1.37
28	hV	203	PUB	C3B-C2B	2.02	1.43	1.37
28	aV	203	PUB	C3B-C2B	2.02	1.43	1.37
28	bL	203	PUB	C3B-C2B	2.02	1.43	1.37
28	hZ	404	PUB	C3B-C2B	2.02	1.43	1.37
28	f8	203	PUB	C3B-C2B	2.02	1.43	1.37
26	hP	202	PEB	C2C-C3C	2.02	1.43	1.37
28	L5	203	PUB	C3B-C2B	2.02	1.43	1.37
28	T5	202	PUB	C3B-C2B	2.02	1.43	1.37
28	V6	203	PUB	C3B-C2B	2.02	1.43	1.37
28	t6	203	PUB	C3B-C2B	2.02	1.43	1.37
28	L7	202	PUB	C3B-C2B	2.02	1.43	1.37
28	U8	1006	PUB	C3B-C2B	2.02	1.43	1.37
28	eT	203	PUB	C3B-C2B	2.02	1.43	1.37
28	hH	203	PUB	C3B-C2B	2.02	1.43	1.37
28	iD	1003	PUB	C3B-C2B	2.02	1.43	1.37
28	v6	203	PUB	C3B-C2B	2.02	1.43	1.37
28	lr	203	PUB	C3B-C2B	2.02	1.43	1.37
28	M8	203	PUB	C3B-C2B	2.02	1.43	1.37
28	B9	203	PUB	C3B-C2B	2.02	1.43	1.37
28	dp	203	PUB	C3B-C2B	2.02	1.43	1.37
28	d7	203	PUB	C3B-C2B	2.02	1.43	1.37
28	ap	203	PUB	C3B-C2B	2.02	1.43	1.37
28	aZ	304	PUB	C3B-C2B	2.02	1.43	1.37
28	bH	203	PUB	C3B-C2B	2.02	1.43	1.37
28	lv	202	PUB	C3B-C2B	2.02	1.43	1.37
28	fw	203	PUB	CHB-C1C	2.02	1.36	1.35
26	R7	202	PEB	C2C-C3C	2.02	1.43	1.37
28	N4	203	PUB	C3B-C2B	2.02	1.43	1.37
28	J5	203	PUB	C3B-C2B	2.02	1.43	1.37
28	t7	203	PUB	C3B-C2B	2.02	1.43	1.37
28	aH	203	PUB	C3B-C2B	2.02	1.43	1.37
28	dB	202	PUB	C3B-C2B	2.02	1.43	1.37
28	dP	203	PUB	C3B-C2B	2.02	1.43	1.37
28	gy	305	PUB	C3B-C2B	2.02	1.43	1.37
28	n9	202	PUB	C3B-C2B	2.02	1.43	1.37
28	ga	203	PUB	C3B-C2B	2.02	1.43	1.37
28	iG	1002	PUB	C3B-C2B	2.02	1.43	1.37
28	P7	203	PUB	C3B-C2B	2.02	1.43	1.37
28	ld	203	PUB	C3B-C2B	2.02	1.43	1.37
28	r2	203	PUB	C3B-C2B	2.02	1.43	1.37
28	R3	203	PUB	C3B-C2B	2.02	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D2	304	PUB	C3B-C2B	2.02	1.43	1.37
28	N7	203	PUB	C3B-C2B	2.02	1.43	1.37
28	s7	203	PUB	C3B-C2B	2.02	1.43	1.37
28	n4	203	PUB	C3B-C2B	2.02	1.43	1.37
28	bz	203	PUB	C3B-C2B	2.02	1.43	1.37
28	o8	203	PUB	C3B-C2B	2.02	1.43	1.37
28	w8	203	PUB	C3B-C2B	2.02	1.43	1.37
28	hZ	405	PUB	C3B-C2B	2.02	1.43	1.37
28	dX	203	PUB	CHB-C1C	2.02	1.36	1.35
26	m5	1003	PEB	C2C-C3C	2.02	1.43	1.37
28	X6	203	PUB	C3B-C2B	2.02	1.43	1.37
28	T4	202	PUB	C3B-C2B	2.02	1.43	1.37
28	P5	202	PUB	C3B-C2B	2.02	1.43	1.37
28	c8	304	PUB	C3B-C2B	2.02	1.43	1.37
28	d8	304	PUB	C3B-C2B	2.02	1.43	1.37
28	J3	203	PUB	C3B-C2B	2.02	1.43	1.37
28	a6	203	PUB	C3B-C2B	2.02	1.43	1.37
28	n8	202	PUB	C3B-C2B	2.02	1.43	1.37
28	cH	202	PUB	C3B-C2B	2.02	1.43	1.37
28	dK	203	PUB	C3B-C2B	2.02	1.43	1.37
28	J2	202	PUB	C3B-C2B	2.02	1.43	1.37
28	c9	305	PUB	C3B-C2B	2.02	1.43	1.37
28	bs	1004	PUB	C3B-C2B	2.02	1.43	1.37
28	ez	1005	PUB	C3B-C2B	2.02	1.43	1.37
28	E8	203	PUB	C3B-C2B	2.02	1.43	1.37
28	bB	203	PUB	C3B-C2B	2.02	1.43	1.37
28	hX	203	PUB	C3B-C2B	2.02	1.43	1.37
28	iC	1003	PUB	C3B-C2B	2.02	1.43	1.37
28	ee	203	PUB	C3B-C2B	2.02	1.43	1.37
28	el	203	PUB	C3B-C2B	2.02	1.43	1.37
28	eP	204	PUB	C3B-C2B	2.02	1.43	1.37
28	av	203	PUB	C3B-C2B	2.02	1.43	1.37
28	aR	203	PUB	C3B-C2B	2.02	1.43	1.37
28	en	203	PUB	C3B-C2B	2.02	1.43	1.37
28	hJ	203	PUB	C3B-C2B	2.02	1.43	1.37
28	Z2	203	PUB	C3B-C2B	2.02	1.43	1.37
28	gy	306	PUB	C3B-C2B	2.02	1.43	1.37
28	iE	1003	PUB	C3B-C2B	2.02	1.43	1.37
28	H7	203	PUB	C3B-C2B	2.02	1.43	1.37
28	r9	203	PUB	C3B-C2B	2.02	1.43	1.37
26	d7	202	PEB	C2C-C3C	2.02	1.43	1.37
28	cM	203	PUB	C3B-C2B	2.02	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b1	1001	CYC	C1C-NC	-2.01	1.35	1.37
28	x9	203	PUB	C3B-C2B	2.01	1.43	1.37
28	D9	203	PUB	C3B-C2B	2.01	1.43	1.37
28	p8	203	PUB	C3B-C2B	2.01	1.43	1.37
28	cE	203	PUB	C3B-C2B	2.01	1.43	1.37
28	lh	203	PUB	C3B-C2B	2.01	1.43	1.37
28	gr	202	PUB	C3B-C2B	2.01	1.43	1.37
28	gi	203	PUB	C3B-C2B	2.01	1.43	1.37
28	ll	203	PUB	C3B-C2B	2.01	1.43	1.37
28	lt	203	PUB	C3B-C2B	2.01	1.43	1.37
28	p3	203	PUB	C3B-C2B	2.01	1.43	1.37
28	eB	204	PUB	C3B-C2B	2.01	1.43	1.37
28	X7	203	PUB	C3B-C2B	2.01	1.43	1.37
28	p4	203	PUB	C3B-C2B	2.01	1.43	1.37
28	z2	203	PUB	C3B-C2B	2.01	1.43	1.37
28	fm	203	PUB	C3B-C2B	2.01	1.43	1.37
28	R7	203	PUB	C3B-C2B	2.01	1.43	1.37
28	cz	203	PUB	C3B-C2B	2.01	1.43	1.37
28	kV	1003	PUB	C3B-C2B	2.01	1.43	1.37
27	f1	201	CYC	C1C-NC	-2.01	1.35	1.37
28	cQ	202	PUB	C3B-C2B	2.01	1.43	1.37
29	e8	303	PVN	C15-C14	2.01	1.45	1.40
26	J7	201	PEB	C2C-C3C	2.01	1.43	1.37
29	34	1004	PVN	C11-C12	-2.01	1.42	1.45
29	aZ	303	PVN	C15-C14	2.01	1.45	1.40
28	bZ	305	PUB	CHB-C1C	2.01	1.36	1.35
28	B5	203	PUB	C3B-C2B	2.01	1.43	1.37
28	e7	203	PUB	C3B-C2B	2.01	1.43	1.37
28	jP	1003	PUB	C3B-C2B	2.01	1.43	1.37
28	V9	203	PUB	C3B-C2B	2.01	1.43	1.37
28	dR	203	PUB	C3B-C2B	2.01	1.43	1.37
28	y7	203	PUB	C3B-C2B	2.01	1.43	1.37
28	F7	202	PUB	C3B-C2B	2.01	1.43	1.37
28	p7	202	PUB	C3B-C2B	2.01	1.43	1.37
28	ev	203	PUB	C3B-C2B	2.01	1.43	1.37
28	e9	306	PUB	C3B-C2B	2.01	1.43	1.37
28	bF	203	PUB	C3B-C2B	2.01	1.43	1.37
28	dr	203	PUB	C3B-C2B	2.01	1.43	1.37
28	dV	203	PUB	C3B-C2B	2.01	1.43	1.37
29	C2	303	PVN	O1-C1	-2.01	1.19	1.23
29	c3	303	PVN	O1-C1	-2.01	1.19	1.23
28	dL	203	PUB	C3B-C2B	2.01	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	lj	202	PUB	C3B-C2B	2.01	1.43	1.37
28	lx	201	PUB	C3B-C2B	2.01	1.43	1.37
28	gv	203	PUB	C3B-C2B	2.01	1.43	1.37
27	O1	201	CYC	C1C-NC	-2.00	1.35	1.37
28	gn	203	PUB	C3B-C2B	2.00	1.43	1.37
29	e9	304	PVN	C16-N4	2.00	1.41	1.37
28	D7	203	PUB	CHB-C1C	2.00	1.36	1.35
28	eZ	403	PUB	CHB-C1C	2.00	1.36	1.35
28	gr	202	PUB	CHB-C1C	2.00	1.36	1.35
26	eN	202	PEB	C2C-C3C	2.00	1.43	1.37
28	T7	203	PUB	C3B-C2B	2.00	1.43	1.37
28	N3	203	PUB	C3B-C2B	2.00	1.43	1.37

All (17239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z5	304	PVN	C5-C4-N1	16.81	133.47	113.95
29	44	303	PVN	C5-C4-N1	16.79	133.45	113.95
29	Z9	1004	PVN	C5-C4-N1	14.94	131.29	113.95
29	U8	1004	PVN	C5-C4-N1	14.90	131.24	113.95
29	dw	404	PVN	C5-C4-N1	14.20	130.44	113.95
29	aZ	303	PVN	C5-C4-N1	14.20	130.44	113.95
29	bZ	304	PVN	C5-C4-N1	14.14	130.37	113.95
29	eY	403	PVN	C5-C4-N1	14.02	130.22	113.95
29	eZ	402	PVN	C5-C4-N1	13.98	130.18	113.95
29	dx	405	PVN	C5-C4-N1	13.01	129.06	113.95
29	bY	1004	PVN	C5-C4-N1	12.67	128.66	113.95
29	aY	403	PVN	C5-C4-N1	12.64	128.63	113.95
29	eZ	402	PVN	C81-C17-C16	12.50	139.78	124.17
29	eY	403	PVN	C81-C17-C16	12.48	139.75	124.17
29	b9	405	PVN	C5-C4-N1	12.35	128.28	113.95
29	b8	1004	PVN	C5-C4-N1	12.29	128.22	113.95
28	B9	203	PUB	CHB-C1C-NC	-12.00	112.18	128.83
28	aJ	203	PUB	CHB-C1C-NC	-11.98	112.20	128.83
28	eT	203	PUB	CHB-C1C-NC	-11.98	112.21	128.83
28	K8	203	PUB	CHB-C1C-NC	-11.98	112.22	128.83
28	dv	202	PUB	CHB-C1C-NC	-11.98	112.22	128.83
28	bF	203	PUB	CHB-C1C-NC	-11.97	112.22	128.83
28	R6	203	PUB	CHB-C1C-NC	-11.97	112.22	128.83
28	X7	203	PUB	CHB-C1C-NC	-11.97	112.22	128.83
28	V3	203	PUB	CHB-C1C-NC	-11.97	112.22	128.83
28	bD	203	PUB	CHB-C1C-NC	-11.97	112.22	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	fj	203	PUB	CHB-C1C-NC	-11.97	112.22	128.83
28	r5	203	PUB	CHB-C1C-NC	-11.97	112.23	128.83
28	hJ	203	PUB	CHB-C1C-NC	-11.97	112.23	128.83
28	dw	405	PUB	CHB-C1C-NC	-11.97	112.23	128.83
28	fo	203	PUB	CHB-C1C-NC	-11.97	112.23	128.83
28	v6	203	PUB	CHB-C1C-NC	-11.97	112.23	128.83
28	H5	202	PUB	CHB-C1C-NC	-11.97	112.23	128.83
28	h3	202	PUB	CHB-C1C-NC	-11.96	112.23	128.83
28	n3	203	PUB	CHB-C1C-NC	-11.96	112.23	128.83
28	B3	203	PUB	CHB-C1C-NC	-11.96	112.23	128.83
28	bZ	305	PUB	CHB-C1C-NC	-11.96	112.23	128.83
28	jI	1003	PUB	CHB-C1C-NC	-11.96	112.23	128.83
28	R4	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	an	202	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	F4	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	r2	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	cn	202	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	eN	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	d3	304	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	bR	202	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	dF	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	cz	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	R7	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	N9	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	r9	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	Y9	304	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	dP	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	D7	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	aF	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	bZ	306	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	cE	203	PUB	CHB-C1C-NC	-11.96	112.24	128.83
28	t7	203	PUB	CHB-C1C-NC	-11.96	112.25	128.83
28	bL	203	PUB	CHB-C1C-NC	-11.96	112.25	128.83
28	z5	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	f8	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	fw	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	iE	1003	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	U8	1005	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	F9	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	L9	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	cH	202	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	lp	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	T2	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	d7	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	dK	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	eY	404	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	fq	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	iH	1002	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	C2	305	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	N3	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	c3	305	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	x3	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	F7	202	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	aP	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	bn	202	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	gr	202	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	kR	1003	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	F5	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	ga	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	hV	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	ey	1005	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	fy	202	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	hT	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	c3	304	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	I8	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	cM	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	dX	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	v2	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	N5	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	aH	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	aY	405	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	cP	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	lh	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	iD	1003	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	J6	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	H7	203	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	Y9	305	PUB	CHB-C1C-NC	-11.95	112.25	128.83
28	L4	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	w8	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	H9	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	V9	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	aT	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	cN	202	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	ly	405	PUB	CHB-C1C-NC	-11.95	112.26	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	lz	404	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	jJ	1003	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	jM	1003	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	n9	202	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	bB	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	gn	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	y7	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	T9	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	bT	202	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	lb	203	PUB	CHB-C1C-NC	-11.95	112.26	128.83
28	Z4	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	Z6	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	T8	304	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	eX	202	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	eY	405	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	eZ	404	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	iF	1003	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	34	1006	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	d9	305	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	J9	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	bY	1006	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	en	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	gz	305	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	P7	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	cs	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	ey	1006	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	hG	202	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	hZ	404	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	B4	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	x6	203	PUB	CHB-C1C-NC	-11.94	112.26	128.83
28	p4	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	B6	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	X6	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	o8	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	br	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	ez	1006	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	gt	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	R5	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	T7	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	p9	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	dl	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	44	304	PUB	CHB-C1C-NC	-11.94	112.27	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	bY	1005	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	L3	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	p7	202	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	R9	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	ar	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	eR	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	lf	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	iG	1002	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	jN	1003	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	F2	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	a3	1005	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	d3	303	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	l6	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	u6	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	z6	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	s7	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	M8	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	hR	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	D4	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	dw	406	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	dR	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	eH	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	hZ	405	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	R2	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	V2	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	r3	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	T6	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	ax	202	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	ly	406	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	v7	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	P9	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	lv	202	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	gz	306	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	t2	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	t5	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	D6	202	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	cR	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	dB	202	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	lr	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	hX	203	PUB	CHB-C1C-NC	-11.94	112.27	128.83
28	j2	203	PUB	CHB-C1C-NC	-11.93	112.27	128.83
28	J3	203	PUB	CHB-C1C-NC	-11.93	112.27	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	L7	202	PUB	CHB-C1C-NC	-11.93	112.27	128.83
28	iC	1003	PUB	CHB-C1C-NC	-11.93	112.27	128.83
28	kW	1003	PUB	CHB-C1C-NC	-11.93	112.27	128.83
28	a7	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	U8	1006	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	D9	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	aN	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	eV	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	A2	1006	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	D2	304	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	L2	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	y8	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	gi	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	hL	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	hP	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	Y5	1005	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	di	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	ev	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	ld	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	ln	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	n6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	z7	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	C2	304	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	D2	305	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	Z3	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	b7	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	O8	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	at	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	fu	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	hB	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	kQ	1003	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	kS	1003	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	P5	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	F6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	N6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	bz	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	gg	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	T3	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	N4	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	J5	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	V6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	x9	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	ap	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	dj	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	dt	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	eb	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	gd	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	34	1005	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	x4	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	Z9	1005	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	fs	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	r6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	x7	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	dx	406	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	dY	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	gv	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	kU	1003	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	z2	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	F3	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	d6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	r7	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	e9	306	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	E8	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	az	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	eF	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	x2	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	X3	202	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	v3	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	t6	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	cJ	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	dx	407	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	eB	204	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	eD	203	PUB	CHB-C1C-NC	-11.93	112.28	128.83
28	P4	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	H6	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	P6	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	c8	304	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	cQ	202	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	cY	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	eL	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	p2	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	X2	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	P3	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	c9	305	PUB	CHB-C1C-NC	-11.93	112.29	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	ee	203	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	ez	1005	PUB	CHB-C1C-NC	-11.93	112.29	128.83
28	h8	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	B7	202	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	aV	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	eZ	403	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	c7	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	e7	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	z9	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	A2	1005	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	z3	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	V7	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	aB	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	cF	202	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	H3	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	r4	202	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	Z5	305	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	c9	304	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	T8	305	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	cL	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	dn	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	h2	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	44	305	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	p5	202	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	x5	202	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	y6	204	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	e9	305	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	dh	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	d8	304	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	dp	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	jO	1003	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	Z7	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	C8	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	gk	203	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	gy	305	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	kT	1003	PUB	CHB-C1C-NC	-11.92	112.29	128.83
28	f2	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	X4	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	b6	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	cO	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	ff	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	J7	202	PUB	CHB-C1C-NC	-11.92	112.30	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	hN	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	N7	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	cB	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	lj	202	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	lx	201	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	n4	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	L6	202	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	l7	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	b8	1005	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	fa	202	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	gp	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	J2	202	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	j3	202	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	bs	1004	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	ec	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	eP	204	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	gx	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	hY	406	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	jK	1003	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	v4	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	v5	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	aR	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	eJ	203	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	jP	1003	PUB	CHB-C1C-NC	-11.92	112.30	128.83
28	N2	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	z4	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	e6	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	Q8	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	aZ	304	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	bo	202	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	ll	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	lt	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	R3	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	L5	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	ei	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	hD	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
29	ez	1004	PVN	C5-C4-N1	11.91	127.78	113.95
28	Z2	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	V4	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	fc	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	t9	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	fm	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	hH	203	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	kX	1003	PUB	CHB-C1C-NC	-11.91	112.30	128.83
28	l2	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	P2	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	p3	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	J4	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	c6	1004	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	b9	406	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	aZ	305	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	co	202	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	D3	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	t3	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	A8	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	bq	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	f3	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	Z9	1006	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	bV	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	cp	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	dd	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	lz	405	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	ge	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	n2	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	dr	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	hY	405	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	t4	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	n7	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	e8	305	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	b9	407	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	H4	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	T5	202	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	p6	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	b8	1006	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	cq	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	df	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	gy	306	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	a3	1006	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	Y5	1006	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	a6	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	aD	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	bH	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	dN	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	V5	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	p8	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	bJ	203	PUB	CHB-C1C-NC	-11.91	112.31	128.83
28	e8	304	PUB	CHB-C1C-NC	-11.90	112.31	128.83
28	v9	203	PUB	CHB-C1C-NC	-11.90	112.31	128.83
28	aL	203	PUB	CHB-C1C-NC	-11.90	112.31	128.83
28	eg	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	H2	202	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	el	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	dL	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	dH	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	bN	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	D5	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	bP	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	l3	202	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	G8	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	B5	203	PUB	CHB-C1C-NC	-11.90	112.32	128.83
28	av	203	PUB	CHB-C1C-NC	-11.90	112.33	128.83
28	aY	404	PUB	CHB-C1C-NC	-11.90	112.33	128.83
28	dD	203	PUB	CHB-C1C-NC	-11.90	112.33	128.83
28	er	203	PUB	CHB-C1C-NC	-11.90	112.33	128.83
28	Z5	306	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	jL	1003	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	cr	203	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	et	203	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	kV	1003	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	g8	202	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	n8	202	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	bp	202	PUB	CHB-C1C-NC	-11.89	112.33	128.83
28	n5	203	PUB	CHB-C1C-NC	-11.89	112.34	128.83
28	ep	203	PUB	CHB-C1C-NC	-11.89	112.34	128.83
28	fi	203	PUB	CHB-C1C-NC	-11.89	112.34	128.83
28	T4	202	PUB	CHB-C1C-NC	-11.89	112.34	128.83
28	dV	203	PUB	CHB-C1C-NC	-11.88	112.34	128.83
28	dT	203	PUB	CHB-C1C-NC	-11.88	112.35	128.83
28	c8	305	PUB	CHB-C1C-NC	-11.87	112.36	128.83
29	d8	303	PVN	C5-C4-N1	11.69	127.53	113.95
29	d9	304	PVN	C5-C4-N1	11.65	127.47	113.95
29	ey	1004	PVN	C5-C4-N1	11.62	127.44	113.95
29	hZ	403	PVN	C5-C4-N1	11.60	127.42	113.95
29	hY	404	PVN	C5-C4-N1	11.59	127.41	113.95
29	34	1004	PVN	C5-C4-N1	11.59	127.40	113.95
29	Y5	1004	PVN	C5-C4-N1	11.58	127.40	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	r1	201	CYC	CMA-C3A-C4A	11.32	142.50	125.06
27	z1	201	CYC	CMA-C3A-C4A	11.31	142.48	125.06
27	J1	201	CYC	CMA-C3A-C4A	11.29	142.45	125.06
27	S1	201	CYC	CMA-C3A-C4A	11.29	142.44	125.06
27	j1	201	CYC	CMA-C3A-C4A	11.29	142.44	125.06
27	c1	201	CYC	CMA-C3A-C4A	11.28	142.44	125.06
27	Y1	201	CYC	CMA-C3A-C4A	11.28	142.44	125.06
27	t1	201	CYC	CMA-C3A-C4A	11.28	142.44	125.06
27	M1	1001	CYC	CMA-C3A-C4A	11.28	142.44	125.06
27	a2	901	CYC	CMA-C3A-C4A	11.28	142.43	125.06
27	h1	201	CYC	CMA-C3A-C4A	11.27	142.42	125.06
27	H1	201	CYC	CMA-C3A-C4A	11.26	142.40	125.06
27	v1	201	CYC	CMA-C3A-C4A	11.26	142.40	125.06
27	p1	201	CYC	CMA-C3A-C4A	11.25	142.39	125.06
27	a2	902	CYC	CMA-C3A-C4A	11.24	142.37	125.06
27	b2	1001	CYC	CMA-C3A-C4A	11.24	142.37	125.06
27	S1	202	CYC	CMA-C3A-C4A	11.24	142.37	125.06
29	c3	303	PVN	C5-C4-N1	10.70	126.38	113.95
29	C2	303	PVN	C5-C4-N1	10.67	126.34	113.95
27	L1	201	CYC	C3B-C4B-NB	10.49	115.25	106.78
27	a1	201	CYC	C3B-C4B-NB	10.49	115.25	106.78
27	b1	1001	CYC	C3B-C4B-NB	10.48	115.25	106.78
27	g1	201	CYC	C3B-C4B-NB	10.48	115.24	106.78
27	f1	201	CYC	C3B-C4B-NB	10.47	115.24	106.78
27	K1	201	CYC	C3B-C4B-NB	10.47	115.23	106.78
27	X1	201	CYC	C3B-C4B-NB	10.46	115.23	106.78
27	I1	201	CYC	C3B-C4B-NB	10.46	115.23	106.78
29	d3	302	PVN	C5-C4-N1	10.45	126.08	113.95
27	k1	201	CYC	C3B-C4B-NB	10.45	115.22	106.78
27	e1	201	CYC	C3B-C4B-NB	10.45	115.22	106.78
27	w1	201	CYC	C3B-C4B-NB	10.45	115.22	106.78
27	Q1	201	CYC	C3B-C4B-NB	10.44	115.22	106.78
27	P1	201	CYC	C3B-C4B-NB	10.44	115.21	106.78
27	o1	1001	CYC	C3B-C4B-NB	10.44	115.21	106.78
27	u1	1001	CYC	C3B-C4B-NB	10.44	115.21	106.78
27	O1	201	CYC	C3B-C4B-NB	10.43	115.21	106.78
29	D2	303	PVN	C5-C4-N1	10.42	126.05	113.95
27	q1	201	CYC	C3B-C4B-NB	10.41	115.19	106.78
27	W1	201	CYC	C3B-C4B-NB	10.41	115.19	106.78
27	d1	1001	CYC	C3B-C4B-NB	10.41	115.19	106.78
27	G1	1001	CYC	C3B-C4B-NB	10.40	115.18	106.78
27	V1	201	CYC	C3B-C4B-NB	10.40	115.18	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	s1	201	CYC	C3B-C4B-NB	10.40	115.18	106.78
27	y1	201	CYC	C3B-C4B-NB	10.40	115.18	106.78
27	m1	201	CYC	C3B-C4B-NB	10.39	115.17	106.78
27	N1	201	CYC	C3B-C4B-NB	10.39	115.17	106.78
27	R1	1001	CYC	C3B-C4B-NB	10.39	115.17	106.78
27	i1	1001	CYC	C3B-C4B-NB	10.39	115.17	106.78
27	U1	201	CYC	C3B-C4B-NB	10.38	115.16	106.78
27	d2	101	CYC	C3B-C4B-NB	10.38	115.16	106.78
27	Z1	201	CYC	C3B-C4B-NB	10.38	115.16	106.78
27	n1	201	CYC	C3B-C4B-NB	10.36	115.14	106.78
29	e8	303	PVN	C5-C4-N1	10.00	125.56	113.95
29	e9	304	PVN	C5-C4-N1	9.96	125.52	113.95
29	Y5	1004	PVN	C32-C31-C3	9.33	127.13	112.98
29	34	1004	PVN	C32-C31-C3	9.33	127.12	112.98
29	hZ	403	PVN	C32-C31-C3	9.30	127.08	112.98
29	hY	404	PVN	C32-C31-C3	9.29	127.07	112.98
29	T8	303	PVN	C5-C4-N1	9.19	124.62	113.95
29	Y9	303	PVN	C5-C4-N1	9.19	124.62	113.95
29	c8	303	PVN	C5-C4-N1	9.00	124.39	113.95
29	c9	303	PVN	C5-C4-N1	8.97	124.37	113.95
29	C2	303	PVN	C32-C31-C3	8.90	126.47	112.98
29	c3	303	PVN	C32-C31-C3	8.90	126.47	112.98
27	J1	201	CYC	OC-C1C-C2C	-8.77	119.20	126.17
27	S1	202	CYC	OC-C1C-C2C	-8.77	119.20	126.17
27	M1	1001	CYC	OC-C1C-C2C	-8.76	119.21	126.17
27	Y1	201	CYC	OC-C1C-C2C	-8.74	119.22	126.17
27	v1	201	CYC	OC-C1C-C2C	-8.74	119.22	126.17
27	H1	201	CYC	OC-C1C-C2C	-8.74	119.22	126.17
27	r1	201	CYC	OC-C1C-C2C	-8.73	119.23	126.17
27	c1	201	CYC	OC-C1C-C2C	-8.73	119.23	126.17
27	a2	901	CYC	OC-C1C-C2C	-8.73	119.23	126.17
27	z1	201	CYC	OC-C1C-C2C	-8.73	119.23	126.17
27	p1	201	CYC	OC-C1C-C2C	-8.72	119.24	126.17
27	S1	201	CYC	OC-C1C-C2C	-8.69	119.27	126.17
27	j1	201	CYC	OC-C1C-C2C	-8.69	119.27	126.17
27	a2	902	CYC	OC-C1C-C2C	-8.69	119.27	126.17
27	b2	1001	CYC	OC-C1C-C2C	-8.69	119.27	126.17
29	U8	1004	PVN	C81-C17-C16	8.68	135.01	124.17
29	Z9	1004	PVN	C81-C17-C16	8.68	135.00	124.17
27	h1	201	CYC	OC-C1C-C2C	-8.67	119.28	126.17
27	t1	201	CYC	OC-C1C-C2C	-8.67	119.28	126.17
29	c3	303	PVN	C18-C19-N4	8.61	113.73	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	hY	404	PVN	C81-C17-C16	8.61	134.92	124.17
29	34	1004	PVN	C81-C17-C16	8.61	134.92	124.17
29	hZ	403	PVN	C81-C17-C16	8.60	134.91	124.17
29	Y5	1004	PVN	C81-C17-C16	8.59	134.90	124.17
29	C2	303	PVN	C18-C19-N4	8.58	113.71	106.78
29	C2	303	PVN	C52-C51-C8	8.55	127.20	112.62
29	c3	303	PVN	C52-C51-C8	8.54	127.20	112.62
27	Y1	201	CYC	C3B-C4B-NB	8.27	113.46	106.78
27	S1	201	CYC	C3B-C4B-NB	8.26	113.45	106.78
27	j1	201	CYC	C3B-C4B-NB	8.26	113.45	106.78
27	J1	201	CYC	C3B-C4B-NB	8.24	113.44	106.78
27	h1	201	CYC	C3B-C4B-NB	8.24	113.44	106.78
27	S1	202	CYC	C3B-C4B-NB	8.23	113.43	106.78
29	aY	403	PVN	C81-C17-C16	8.23	134.44	124.17
27	M1	1001	CYC	C3B-C4B-NB	8.23	113.42	106.78
27	a2	902	CYC	C3B-C4B-NB	8.23	113.42	106.78
27	b2	1001	CYC	C3B-C4B-NB	8.23	113.42	106.78
27	c1	201	CYC	C3B-C4B-NB	8.21	113.41	106.78
27	t1	201	CYC	C3B-C4B-NB	8.21	113.41	106.78
27	z1	201	CYC	C3B-C4B-NB	8.21	113.41	106.78
27	a2	901	CYC	C3B-C4B-NB	8.20	113.41	106.78
29	bY	1004	PVN	C81-C17-C16	8.20	134.41	124.17
27	r1	201	CYC	C3B-C4B-NB	8.20	113.40	106.78
27	p1	201	CYC	C3B-C4B-NB	8.19	113.40	106.78
27	H1	201	CYC	C3B-C4B-NB	8.18	113.38	106.78
27	v1	201	CYC	C3B-C4B-NB	8.17	113.38	106.78
29	A2	1004	PVN	C18-C19-N4	8.16	113.37	106.78
29	a3	1004	PVN	C18-C19-N4	8.16	113.37	106.78
29	hY	404	PVN	C2-C1-N1	7.99	114.30	107.21
29	Z5	304	PVN	C9-C10-C11	-7.96	119.30	128.81
29	hZ	403	PVN	C2-C1-N1	7.95	114.26	107.21
29	34	1004	PVN	C2-C1-N1	7.95	114.26	107.21
29	Y5	1004	PVN	C2-C1-N1	7.95	114.26	107.21
29	eY	403	PVN	C16-C15-C14	-7.94	108.69	128.08
29	eZ	402	PVN	C16-C15-C14	-7.93	108.70	128.08
29	44	303	PVN	C9-C10-C11	-7.93	119.34	128.81
29	bZ	304	PVN	C91-C18-C19	7.71	133.55	121.38
29	aZ	303	PVN	C91-C18-C19	7.67	133.49	121.38
29	dx	405	PVN	C81-C17-C16	7.66	133.73	124.17
29	bY	1004	PVN	C91-C18-C19	7.60	133.39	121.38
29	aY	403	PVN	C91-C18-C19	7.59	133.37	121.38
29	dw	404	PVN	C81-C17-C16	7.35	133.35	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	ez	1004	PVN	C81-C17-C16	7.20	133.16	124.17
29	eY	403	PVN	O19-C19-C18	-7.14	120.29	128.04
29	eZ	402	PVN	O19-C19-C18	-7.12	120.31	128.04
29	gz	304	PVN	C5-C4-N1	-7.12	105.68	113.95
29	eY	403	PVN	C2-C1-N1	7.07	113.48	107.21
29	d8	303	PVN	C81-C17-C16	7.07	132.99	124.17
29	eZ	402	PVN	C2-C1-N1	7.06	113.47	107.21
29	ey	1004	PVN	C81-C17-C16	7.02	132.93	124.17
27	g1	201	CYC	OB-C4B-C3B	-6.99	120.46	128.04
27	f1	201	CYC	OB-C4B-C3B	-6.99	120.46	128.04
29	d9	304	PVN	C81-C17-C16	6.97	132.88	124.17
29	T8	303	PVN	C18-C19-N4	6.97	112.41	106.78
27	k1	201	CYC	OB-C4B-C3B	-6.96	120.48	128.04
27	K1	201	CYC	OB-C4B-C3B	-6.96	120.49	128.04
27	P1	201	CYC	OB-C4B-C3B	-6.95	120.49	128.04
29	Y9	303	PVN	C18-C19-N4	6.95	112.39	106.78
27	s1	201	CYC	OB-C4B-C3B	-6.95	120.50	128.04
27	Q1	201	CYC	OB-C4B-C3B	-6.94	120.50	128.04
27	u1	1001	CYC	OB-C4B-C3B	-6.94	120.50	128.04
29	Z9	1004	PVN	C18-C19-N4	6.94	112.38	106.78
27	W1	201	CYC	OB-C4B-C3B	-6.94	120.51	128.04
27	X1	201	CYC	OB-C4B-C3B	-6.94	120.51	128.04
27	L1	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	a1	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	b1	1001	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	e1	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	G1	1001	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	V1	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	N1	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	I1	201	CYC	OB-C4B-C3B	-6.93	120.52	128.04
27	w1	201	CYC	OB-C4B-C3B	-6.92	120.53	128.04
29	U8	1004	PVN	C18-C19-N4	6.92	112.37	106.78
27	q1	201	CYC	OB-C4B-C3B	-6.92	120.53	128.04
27	d1	1001	CYC	OB-C4B-C3B	-6.91	120.54	128.04
27	U1	201	CYC	OB-C4B-C3B	-6.91	120.54	128.04
27	d2	101	CYC	OB-C4B-C3B	-6.91	120.54	128.04
27	Z1	201	CYC	OB-C4B-C3B	-6.91	120.54	128.04
27	O1	201	CYC	OB-C4B-C3B	-6.90	120.56	128.04
27	o1	1001	CYC	OB-C4B-C3B	-6.89	120.56	128.04
27	R1	1001	CYC	OB-C4B-C3B	-6.89	120.56	128.04
27	i1	1001	CYC	OB-C4B-C3B	-6.89	120.56	128.04
27	n1	201	CYC	OB-C4B-C3B	-6.89	120.56	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	y1	201	CYC	OB-C4B-C3B	-6.89	120.56	128.04
29	T8	303	PVN	C91-C18-C19	6.89	132.26	121.38
27	m1	201	CYC	OB-C4B-C3B	-6.88	120.57	128.04
29	Y9	303	PVN	C91-C18-C19	6.88	132.24	121.38
29	C2	303	PVN	C2-C1-N1	6.87	113.30	107.21
29	c3	303	PVN	C2-C1-N1	6.87	113.30	107.21
29	bZ	304	PVN	C2-C1-N1	6.86	113.30	107.21
29	D2	303	PVN	C18-C19-N4	6.86	112.32	106.78
29	d3	302	PVN	C18-C19-N4	6.86	112.32	106.78
29	aZ	303	PVN	C2-C1-N1	6.84	113.27	107.21
29	ey	1004	PVN	C2-C1-N1	6.78	113.22	107.21
29	aZ	303	PVN	C81-C17-C16	6.76	132.60	124.17
29	bZ	304	PVN	C81-C17-C16	6.75	132.59	124.17
29	T8	303	PVN	C32-C31-C3	6.70	123.14	112.98
29	Y9	303	PVN	C32-C31-C3	6.69	123.12	112.98
29	bY	1004	PVN	C32-C31-C3	6.65	123.06	112.98
29	aY	403	PVN	C32-C31-C3	6.63	123.03	112.98
29	gz	304	PVN	C81-C17-C16	6.60	132.41	124.17
29	eY	403	PVN	C18-C19-N4	6.59	112.11	106.78
29	ez	1004	PVN	C18-C19-N4	6.59	112.10	106.78
29	dx	405	PVN	C2-C1-N1	6.59	113.05	107.21
29	d9	304	PVN	C18-C19-N4	6.59	112.10	106.78
29	lz	403	PVN	C18-C19-N4	6.58	112.09	106.78
29	eZ	402	PVN	C18-C19-N4	6.57	112.08	106.78
29	b9	405	PVN	C18-C19-N4	6.56	112.08	106.78
29	ly	404	PVN	C18-C19-N4	6.56	112.08	106.78
29	c9	303	PVN	C81-C17-C16	6.55	132.35	124.17
29	b8	1004	PVN	C18-C19-N4	6.54	112.06	106.78
29	c8	303	PVN	C81-C17-C16	6.53	132.32	124.17
29	ey	1004	PVN	C18-C19-N4	6.53	112.05	106.78
29	ez	1004	PVN	C91-C18-C19	6.51	131.67	121.38
29	44	303	PVN	C91-C18-C19	6.51	131.66	121.38
29	Z5	304	PVN	C91-C18-C19	6.51	131.66	121.38
27	k1	201	CYC	CMA-C3A-C4A	6.50	135.08	125.06
29	d8	303	PVN	C18-C19-N4	6.49	112.02	106.78
29	hZ	403	PVN	C18-C19-N4	6.48	112.02	106.78
27	u1	1001	CYC	CMA-C3A-C4A	6.48	135.05	125.06
27	d2	101	CYC	CMA-C3A-C4A	6.48	135.05	125.06
27	q1	201	CYC	CMA-C3A-C4A	6.48	135.04	125.06
27	R1	1001	CYC	CMA-C3A-C4A	6.48	135.04	125.06
27	i1	1001	CYC	CMA-C3A-C4A	6.48	135.04	125.06
27	K1	201	CYC	CMA-C3A-C4A	6.48	135.04	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	W1	201	CYC	CMA-C3A-C4A	6.48	135.04	125.06
27	G1	1001	CYC	CMA-C3A-C4A	6.48	135.04	125.06
27	N1	201	CYC	CMA-C3A-C4A	6.48	135.04	125.06
27	Z1	201	CYC	CMA-C3A-C4A	6.48	135.04	125.06
29	dw	404	PVN	C18-C19-N4	6.47	112.01	106.78
27	w1	201	CYC	CMA-C3A-C4A	6.47	135.03	125.06
29	ey	1004	PVN	C91-C18-C19	6.47	131.60	121.38
27	U1	201	CYC	CMA-C3A-C4A	6.47	135.03	125.06
27	V1	201	CYC	CMA-C3A-C4A	6.47	135.03	125.06
27	s1	201	CYC	CMA-C3A-C4A	6.47	135.03	125.06
29	hY	404	PVN	C18-C19-N4	6.47	112.00	106.78
27	e1	201	CYC	CMA-C3A-C4A	6.47	135.02	125.06
27	I1	201	CYC	CMA-C3A-C4A	6.46	135.02	125.06
27	b1	1001	CYC	CMA-C3A-C4A	6.46	135.02	125.06
29	b8	1004	PVN	C81-C17-C16	6.46	132.24	124.17
27	m1	201	CYC	CMA-C3A-C4A	6.46	135.01	125.06
27	y1	201	CYC	CMA-C3A-C4A	6.46	135.01	125.06
27	Q1	201	CYC	CMA-C3A-C4A	6.46	135.01	125.06
27	g1	201	CYC	CMA-C3A-C4A	6.46	135.01	125.06
27	o1	1001	CYC	CMA-C3A-C4A	6.46	135.01	125.06
29	b9	405	PVN	C91-C18-C19	6.46	131.58	121.38
27	O1	201	CYC	CMA-C3A-C4A	6.46	135.00	125.06
27	P1	201	CYC	CMA-C3A-C4A	6.45	135.00	125.06
29	b9	405	PVN	C81-C17-C16	6.45	132.23	124.17
27	n1	201	CYC	CMA-C3A-C4A	6.45	135.00	125.06
27	X1	201	CYC	CMA-C3A-C4A	6.45	135.00	125.06
29	dx	405	PVN	C18-C19-N4	6.45	111.99	106.78
29	b8	1004	PVN	C91-C18-C19	6.45	131.56	121.38
27	L1	201	CYC	CMA-C3A-C4A	6.44	134.99	125.06
27	a1	201	CYC	CMA-C3A-C4A	6.44	134.99	125.06
27	f1	201	CYC	CMA-C3A-C4A	6.44	134.99	125.06
27	d1	1001	CYC	CMA-C3A-C4A	6.43	134.97	125.06
29	c8	303	PVN	C2-C1-N1	6.42	112.90	107.21
29	34	1004	PVN	C18-C19-N4	6.40	111.95	106.78
29	c9	303	PVN	C2-C1-N1	6.39	112.88	107.21
29	ez	1004	PVN	C2-C1-N1	6.38	112.87	107.21
27	o1	1001	CYC	OC-C1C-C2C	-6.37	121.11	126.17
29	Y5	1004	PVN	C18-C19-N4	6.36	111.92	106.78
27	b1	1001	CYC	OC-C1C-C2C	-6.34	121.13	126.17
27	P1	201	CYC	OC-C1C-C2C	-6.33	121.14	126.17
27	f1	201	CYC	OC-C1C-C2C	-6.33	121.14	126.17
27	V1	201	CYC	OC-C1C-C2C	-6.32	121.14	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	K1	201	CYC	OC-C1C-C2C	-6.32	121.15	126.17
27	q1	201	CYC	OC-C1C-C2C	-6.32	121.15	126.17
27	Q1	201	CYC	OC-C1C-C2C	-6.32	121.15	126.17
27	w1	201	CYC	OC-C1C-C2C	-6.31	121.15	126.17
27	I1	201	CYC	OC-C1C-C2C	-6.31	121.16	126.17
27	d1	1001	CYC	OC-C1C-C2C	-6.30	121.16	126.17
29	c8	303	PVN	C18-C19-N4	6.30	111.87	106.78
27	m1	201	CYC	OC-C1C-C2C	-6.30	121.17	126.17
27	O1	201	CYC	OC-C1C-C2C	-6.29	121.17	126.17
27	N1	201	CYC	OC-C1C-C2C	-6.29	121.17	126.17
27	e1	201	CYC	OC-C1C-C2C	-6.29	121.17	126.17
27	n1	201	CYC	OC-C1C-C2C	-6.28	121.18	126.17
27	R1	1001	CYC	OC-C1C-C2C	-6.28	121.18	126.17
27	W1	201	CYC	OC-C1C-C2C	-6.28	121.18	126.17
27	i1	1001	CYC	OC-C1C-C2C	-6.28	121.18	126.17
27	k1	201	CYC	OC-C1C-C2C	-6.28	121.18	126.17
27	L1	201	CYC	OC-C1C-C2C	-6.27	121.19	126.17
27	a1	201	CYC	OC-C1C-C2C	-6.27	121.19	126.17
27	s1	201	CYC	OC-C1C-C2C	-6.27	121.19	126.17
27	X1	201	CYC	OC-C1C-C2C	-6.26	121.19	126.17
27	G1	1001	CYC	OC-C1C-C2C	-6.26	121.19	126.17
27	Z1	201	CYC	OC-C1C-C2C	-6.26	121.20	126.17
27	u1	1001	CYC	OC-C1C-C2C	-6.25	121.20	126.17
29	c9	303	PVN	C18-C19-N4	6.25	111.83	106.78
27	y1	201	CYC	OC-C1C-C2C	-6.24	121.21	126.17
29	dw	404	PVN	C2-C1-N1	6.24	112.75	107.21
27	U1	201	CYC	OC-C1C-C2C	-6.24	121.21	126.17
27	d2	101	CYC	OC-C1C-C2C	-6.24	121.21	126.17
27	g1	201	CYC	OC-C1C-C2C	-6.22	121.23	126.17
29	e9	304	PVN	C18-C19-N4	6.18	111.77	106.78
29	44	303	PVN	C18-C19-N4	6.17	111.76	106.78
29	Z5	304	PVN	C18-C19-N4	6.17	111.76	106.78
29	e8	303	PVN	C18-C19-N4	6.17	111.76	106.78
29	gy	304	PVN	C5-C4-N1	-6.13	106.83	113.95
29	A2	1004	PVN	C5-C4-N1	6.12	121.06	113.95
29	a3	1004	PVN	C5-C4-N1	6.12	121.06	113.95
29	bY	1004	PVN	C18-C19-N4	6.11	111.72	106.78
29	e9	304	PVN	C2-C1-N1	6.10	112.62	107.21
29	aY	403	PVN	C18-C19-N4	6.04	111.66	106.78
29	e8	303	PVN	C2-C1-N1	6.04	112.56	107.21
29	eY	403	PVN	C16-C17-C18	-6.04	101.57	107.87
29	eZ	402	PVN	C16-C17-C18	-6.02	101.59	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a2	902	CYC	OB-C4B-C3B	-6.02	121.50	128.04
27	b2	1001	CYC	OB-C4B-C3B	-6.02	121.50	128.04
27	S1	201	CYC	OB-C4B-C3B	-6.01	121.51	128.04
27	j1	201	CYC	OB-C4B-C3B	-6.01	121.51	128.04
27	M1	1001	CYC	OB-C4B-C3B	-6.01	121.52	128.04
27	c1	201	CYC	OB-C4B-C3B	-6.01	121.52	128.04
29	44	303	PVN	C81-C17-C16	6.00	131.66	124.17
29	Z5	304	PVN	C81-C17-C16	6.00	131.66	124.17
27	h1	201	CYC	OB-C4B-C3B	-6.00	121.53	128.04
27	S1	202	CYC	OB-C4B-C3B	-5.99	121.54	128.04
27	a2	901	CYC	OB-C4B-C3B	-5.99	121.54	128.04
27	z1	201	CYC	OB-C4B-C3B	-5.98	121.55	128.04
27	t1	201	CYC	OB-C4B-C3B	-5.97	121.56	128.04
27	Y1	201	CYC	OB-C4B-C3B	-5.97	121.56	128.04
27	v1	201	CYC	OB-C4B-C3B	-5.96	121.57	128.04
27	H1	201	CYC	OB-C4B-C3B	-5.96	121.57	128.04
27	r1	201	CYC	OB-C4B-C3B	-5.96	121.57	128.04
27	p1	201	CYC	OB-C4B-C3B	-5.95	121.58	128.04
27	J1	201	CYC	OB-C4B-C3B	-5.95	121.58	128.04
29	lz	403	PVN	C2-C1-N1	5.91	112.45	107.21
29	ly	404	PVN	C2-C1-N1	5.85	112.40	107.21
29	lz	403	PVN	C5-C4-N1	5.85	120.74	113.95
29	ey	1004	PVN	C32-C31-C3	5.84	121.83	112.98
29	hZ	403	PVN	C91-C18-C19	5.84	130.60	121.38
29	ly	404	PVN	C5-C4-N1	5.83	120.71	113.95
29	hY	404	PVN	C91-C18-C19	5.82	130.58	121.38
29	b9	405	PVN	C2-C1-N1	5.80	112.35	107.21
29	34	1004	PVN	C91-C18-C19	5.79	130.52	121.38
29	Y5	1004	PVN	C91-C18-C19	5.79	130.52	121.38
29	b8	1004	PVN	C2-C1-N1	5.76	112.32	107.21
29	U8	1004	PVN	C91-C18-C19	5.75	130.46	121.38
29	Z9	1004	PVN	C91-C18-C19	5.74	130.45	121.38
26	r5	202	PEB	C1C-CHB-C4B	5.67	135.58	128.81
26	f3	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
26	eV	202	PEB	C1C-CHB-C4B	5.66	135.57	128.81
26	an	201	PEB	C1C-CHB-C4B	5.65	135.56	128.81
26	eN	202	PEB	C1C-CHB-C4B	5.65	135.56	128.81
26	ah	202	PEB	C1C-CHB-C4B	5.64	135.55	128.81
26	jO	1002	PEB	C1C-CHB-C4B	5.64	135.55	128.81
26	fm	202	PEB	C1C-CHB-C4B	5.64	135.55	128.81
26	n5	202	PEB	C1C-CHB-C4B	5.64	135.55	128.81
26	B4	202	PEB	C1C-CHB-C4B	5.64	135.54	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D7	202	PEB	C1C-CHB-C4B	5.64	135.54	128.81
26	iC	1002	PEB	C1C-CHB-C4B	5.64	135.54	128.81
26	fc	202	PEB	C1C-CHB-C4B	5.64	135.54	128.81
26	li	203	PEB	C1C-CHB-C4B	5.64	135.54	128.81
26	fs	202	PEB	C1C-CHB-C4B	5.64	135.54	128.81
26	r3	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	R6	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	ab	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	gr	201	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	hV	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	H2	201	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	cr	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	D3	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	N7	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	dl	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	ev	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	Z2	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	x3	202	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	kT	1002	PEB	C1C-CHB-C4B	5.63	135.54	128.81
26	dj	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	fi	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	kQ	1002	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	t3	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	c7	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	R3	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	y8	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	cn	201	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	F7	201	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	J9	202	PEB	C1C-CHB-C4B	5.63	135.53	128.81
26	bJ	202	PEB	C1C-CHB-C4B	5.62	135.53	128.81
26	ea	203	PEB	C1C-CHB-C4B	5.62	135.53	128.81
26	hJ	202	PEB	C1C-CHB-C4B	5.62	135.53	128.81
26	h2	202	PEB	C1C-CHB-C4B	5.62	135.53	128.81
26	F5	202	PEB	C1C-CHB-C4B	5.62	135.53	128.81
26	gp	202	PEB	C1C-CHB-C4B	5.62	135.53	128.81
26	L3	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	P3	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	34	1001	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	P5	201	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	D9	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	v4	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	ee	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ec	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	j4	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	lf	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	H9	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	af	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	fy	201	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	gx	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	iD	1002	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	kU	1002	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	ad	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	V2	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	X2	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	fo	202	PEB	C1C-CHB-C4B	5.62	135.52	128.81
26	l2	202	PEB	C1C-CHB-C4B	5.61	135.52	128.81
26	bH	202	PEB	C1C-CHB-C4B	5.61	135.52	128.81
26	cL	202	PEB	C1C-CHB-C4B	5.61	135.52	128.81
26	ei	202	PEB	C1C-CHB-C4B	5.61	135.52	128.81
26	jN	1002	PEB	C1C-CHB-C4B	5.61	135.52	128.81
26	kS	1002	PEB	C1C-CHB-C4B	5.61	135.52	128.81
26	cl	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	cq	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	cY	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	n3	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	cp	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	A2	1003	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	j3	201	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	cs	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	hL	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	V9	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	cE	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	fq	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	kW	1002	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	a7	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	L9	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	J5	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	C8	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	cb	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	eJ	202	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	J7	201	PEB	C1C-CHB-C4B	5.61	135.51	128.81
26	Z3	202	PEB	C1C-CHB-C4B	5.61	135.50	128.81
26	ga	202	PEB	C1C-CHB-C4B	5.61	135.50	128.81
26	x7	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	z3	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	R9	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	at	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	bQ	203	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	dh	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	h8	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	R7	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	co	201	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	l4	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	T7	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	ar	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	al	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	df	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	z7	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	bV	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	gg	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	hB	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	av	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	gd	201	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	kV	1002	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	n2	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	N3	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	T2	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	V7	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	ep	202	PEB	C1C-CHB-C4B	5.60	135.50	128.81
26	L2	202	PEB	C1C-CHB-C4B	5.60	135.49	128.81
26	fw	202	PEB	C1C-CHB-C4B	5.60	135.49	128.81
26	lh	202	PEB	C1C-CHB-C4B	5.60	135.49	128.81
26	n7	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	lr	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	gv	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	jJ	1002	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	p5	201	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	T9	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	ch	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	eg	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	fu	201	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	jI	1002	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	r7	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	hP	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	iE	1002	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	f2	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L5	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	g5	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	X6	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	bT	201	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	jM	1002	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	T3	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	az	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	kR	1002	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	A1	301	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	B1	301	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	e4	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	ll	202	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	kX	1002	PEB	C1C-CHB-C4B	5.59	135.49	128.81
26	bL	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	hR	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	F3	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	B5	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	R5	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	bD	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	cj	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	hG	201	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	p2	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	34	1002	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	D5	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	v7	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	v9	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	N9	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	cJ	202	PEB	C1C-CHB-C4B	5.59	135.48	128.81
26	g4	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	S5	203	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	n6	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	eL	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	ld	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	ln	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	jP	1002	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	z5	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	B6	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	X7	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	p8	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	L7	201	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	ax	201	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	dL	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	hT	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	hN	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	j2	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	V3	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	cB	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	di	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	eX	201	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	fj	202	PEB	C1C-CHB-C4B	5.58	135.48	128.81
26	Y7	1003	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	gt	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	el	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	jL	1002	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	N5	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	B9	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	H3	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	bN	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	P7	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	lp	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	gi	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	B3	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	H7	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	ap	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	fg	201	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	J6	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	bP	202	PEB	C1C-CHB-C4B	5.58	135.47	128.81
26	v5	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	F9	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	er	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	J3	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	t5	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	bB	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	aD	202	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	eB	203	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	lo	203	PEB	C1C-CHB-C4B	5.57	135.47	128.81
26	ff	202	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	t7	202	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	P9	202	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	dd	202	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	lw	203	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	r4	201	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	cF	201	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	W3	203	PEB	C1C-CHB-C4B	5.57	135.46	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p4	202	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	V5	202	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	A5	203	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	m5	1003	PEB	C1C-CHB-C4B	5.57	135.46	128.81
26	Z7	202	PEB	C1C-CHB-C4B	5.56	135.46	128.81
26	cH	201	PEB	C1C-CHB-C4B	5.56	135.46	128.81
26	h3	201	PEB	C1C-CHB-C4B	5.56	135.46	128.81
26	bF	202	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	D4	202	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	n8	201	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	en	202	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	l7	202	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	hH	202	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	y7	202	PEB	C1C-CHB-C4B	5.56	135.45	128.81
26	et	202	PEB	C1C-CHB-C4B	5.56	135.44	128.81
26	p7	201	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	dY	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	aF	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	cd	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	cf	201	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	hX	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	gk	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	hD	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	aj	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	dV	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	gn	202	PEB	C1C-CHB-C4B	5.55	135.44	128.81
26	e7	202	PEB	C1C-CHB-C4B	5.55	135.43	128.81
26	jK	1002	PEB	C1C-CHB-C4B	5.55	135.43	128.81
29	a3	1004	PVN	C81-C17-C16	5.54	131.09	124.17
26	i3	203	PEB	C1C-CHB-C4B	5.54	135.43	128.81
26	ge	202	PEB	C1C-CHB-C4B	5.54	135.43	128.81
26	n4	202	PEB	C1C-CHB-C4B	5.54	135.43	128.81
29	A2	1004	PVN	C81-C17-C16	5.54	131.08	124.17
26	v3	202	PEB	C1C-CHB-C4B	5.54	135.42	128.81
26	d7	202	PEB	C1C-CHB-C4B	5.53	135.41	128.81
26	p3	202	PEB	C1C-CHB-C4B	5.52	135.40	128.81
26	B7	201	PEB	C1C-CHB-C4B	5.50	135.38	128.81
29	bZ	304	PVN	C18-C19-N4	5.50	111.22	106.78
29	d8	303	PVN	C2-C1-N1	5.49	112.08	107.21
26	cz	202	PEB	C1C-CHB-C4B	5.49	135.37	128.81
29	dw	404	PVN	C91-C18-C19	5.48	130.04	121.38
29	ez	1004	PVN	C32-C31-C3	5.48	121.29	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	U8	1004	PVN	C2-C1-N1	5.48	112.07	107.21
29	aZ	303	PVN	C18-C19-N4	5.45	111.18	106.78
29	d9	304	PVN	C2-C1-N1	5.44	112.03	107.21
29	Z9	1004	PVN	C2-C1-N1	5.43	112.03	107.21
29	d3	302	PVN	C81-C17-C16	5.42	130.93	124.17
29	D2	303	PVN	C81-C17-C16	5.39	130.90	124.17
29	Y5	1004	PVN	C21-C2-C3	5.39	140.74	129.67
29	hZ	403	PVN	C21-C2-C3	5.38	140.73	129.67
29	hY	404	PVN	C21-C2-C3	5.38	140.72	129.67
29	34	1004	PVN	C21-C2-C3	5.37	140.72	129.67
29	c3	303	PVN	O19-C19-C18	-5.36	122.22	128.04
29	gy	304	PVN	C81-C17-C16	5.35	130.84	124.17
29	C2	303	PVN	O19-C19-C18	-5.34	122.25	128.04
29	C2	303	PVN	C91-C18-C17	5.32	136.63	127.53
29	c3	303	PVN	C91-C18-C17	5.31	136.62	127.53
27	M1	1001	CYC	CMB-C2B-C1B	5.31	130.79	124.17
27	a2	901	CYC	CMB-C2B-C1B	5.30	130.79	124.17
27	p1	201	CYC	CMB-C2B-C1B	5.30	130.78	124.17
27	J1	201	CYC	CMB-C2B-C1B	5.29	130.78	124.17
27	H1	201	CYC	CMB-C2B-C1B	5.28	130.76	124.17
27	S1	202	CYC	CMB-C2B-C1B	5.28	130.76	124.17
27	Y1	201	CYC	CMB-C2B-C1B	5.27	130.75	124.17
27	c1	201	CYC	CMB-C2B-C1B	5.27	130.75	124.17
27	h1	201	CYC	CMB-C2B-C1B	5.27	130.75	124.17
27	a2	902	CYC	CMB-C2B-C1B	5.27	130.75	124.17
27	b2	1001	CYC	CMB-C2B-C1B	5.27	130.75	124.17
27	S1	201	CYC	CMB-C2B-C1B	5.26	130.74	124.17
27	j1	201	CYC	CMB-C2B-C1B	5.26	130.74	124.17
27	r1	201	CYC	CMB-C2B-C1B	5.26	130.74	124.17
27	z1	201	CYC	CMB-C2B-C1B	5.26	130.73	124.17
27	t1	201	CYC	CMB-C2B-C1B	5.25	130.73	124.17
27	n1	201	CYC	CHB-C4A-NA	-5.24	113.96	124.93
27	v1	201	CYC	CMB-C2B-C1B	5.24	130.71	124.17
27	d1	1001	CYC	CHB-C4A-NA	-5.24	113.98	124.93
29	gz	304	PVN	C32-C31-C3	-5.23	105.04	112.98
27	P1	201	CYC	CHB-C4A-NA	-5.23	113.99	124.93
27	X1	201	CYC	CHB-C4A-NA	-5.23	113.99	124.93
27	Z1	201	CYC	CHB-C4A-NA	-5.23	114.00	124.93
27	o1	1001	CYC	CHB-C4A-NA	-5.23	114.00	124.93
27	W1	201	CYC	CHB-C4A-NA	-5.22	114.01	124.93
27	G1	1001	CYC	CHB-C4A-NA	-5.22	114.01	124.93
27	f1	201	CYC	CHB-C4A-NA	-5.22	114.01	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	L1	201	CYC	CHB-C4A-NA	-5.22	114.02	124.93
27	a1	201	CYC	CHB-C4A-NA	-5.22	114.02	124.93
27	s1	201	CYC	CHB-C4A-NA	-5.22	114.02	124.93
27	w1	201	CYC	CHB-C4A-NA	-5.22	114.02	124.93
27	u1	1001	CYC	CHB-C4A-NA	-5.22	114.02	124.93
27	O1	201	CYC	CHB-C4A-NA	-5.21	114.03	124.93
27	g1	201	CYC	CHB-C4A-NA	-5.21	114.03	124.93
27	q1	201	CYC	CHB-C4A-NA	-5.21	114.04	124.93
27	V1	201	CYC	CHB-C4A-NA	-5.21	114.04	124.93
27	e1	201	CYC	CHB-C4A-NA	-5.21	114.04	124.93
27	R1	1001	CYC	CHB-C4A-NA	-5.21	114.04	124.93
27	i1	1001	CYC	CHB-C4A-NA	-5.21	114.04	124.93
27	K1	201	CYC	CHB-C4A-NA	-5.21	114.04	124.93
27	U1	201	CYC	CHB-C4A-NA	-5.20	114.05	124.93
27	b1	1001	CYC	CHB-C4A-NA	-5.20	114.05	124.93
27	d2	101	CYC	CHB-C4A-NA	-5.20	114.05	124.93
27	N1	201	CYC	CHB-C4A-NA	-5.20	114.05	124.93
27	I1	201	CYC	CHB-C4A-NA	-5.20	114.06	124.93
27	k1	201	CYC	CHB-C4A-NA	-5.19	114.07	124.93
27	m1	201	CYC	CHB-C4A-NA	-5.19	114.07	124.93
27	y1	201	CYC	CHB-C4A-NA	-5.19	114.07	124.93
29	e9	304	PVN	C81-C17-C16	5.19	130.65	124.17
27	Q1	201	CYC	CHB-C4A-NA	-5.19	114.08	124.93
29	bY	1004	PVN	C2-C1-N1	5.17	111.80	107.21
27	Q1	201	CYC	CAB-C3B-C4B	5.16	129.52	121.38
27	g1	201	CYC	CAB-C3B-C4B	5.15	129.51	121.38
29	e8	303	PVN	C81-C17-C16	5.15	130.59	124.17
27	u1	1001	CYC	CAB-C3B-C4B	5.14	129.50	121.38
27	I1	201	CYC	CAB-C3B-C4B	5.14	129.50	121.38
29	aY	403	PVN	C2-C1-N1	5.14	111.77	107.21
27	P1	201	CYC	CAB-C3B-C4B	5.14	129.49	121.38
27	k1	201	CYC	CAB-C3B-C4B	5.14	129.49	121.38
27	L1	201	CYC	CAB-C3B-C4B	5.14	129.49	121.38
27	a1	201	CYC	CAB-C3B-C4B	5.14	129.49	121.38
27	f1	201	CYC	CAB-C3B-C4B	5.13	129.49	121.38
29	lz	403	PVN	C81-C17-C16	5.13	130.58	124.17
27	U1	201	CYC	CAB-C3B-C4B	5.13	129.48	121.38
27	b1	1001	CYC	CAB-C3B-C4B	5.13	129.48	121.38
27	V1	201	CYC	CAB-C3B-C4B	5.13	129.48	121.38
27	X1	201	CYC	CAB-C3B-C4B	5.13	129.48	121.38
27	K1	201	CYC	CAB-C3B-C4B	5.13	129.48	121.38
27	s1	201	CYC	CAB-C3B-C4B	5.13	129.47	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N1	201	CYC	CAB-C3B-C4B	5.12	129.47	121.38
27	W1	201	CYC	CAB-C3B-C4B	5.12	129.47	121.38
27	d1	1001	CYC	CAB-C3B-C4B	5.12	129.47	121.38
27	O1	201	CYC	CAB-C3B-C4B	5.12	129.47	121.38
27	Z1	201	CYC	CAB-C3B-C4B	5.11	129.46	121.38
27	R1	1001	CYC	CAB-C3B-C4B	5.11	129.46	121.38
27	i1	1001	CYC	CAB-C3B-C4B	5.11	129.46	121.38
27	o1	1001	CYC	CAB-C3B-C4B	5.11	129.46	121.38
27	w1	201	CYC	CAB-C3B-C4B	5.11	129.46	121.38
27	m1	201	CYC	CAB-C3B-C4B	5.11	129.45	121.38
27	q1	201	CYC	CAB-C3B-C4B	5.11	129.45	121.38
29	dx	405	PVN	C91-C18-C19	5.11	129.45	121.38
27	d2	101	CYC	CAB-C3B-C4B	5.11	129.45	121.38
27	G1	1001	CYC	CAB-C3B-C4B	5.11	129.45	121.38
27	e1	201	CYC	CAB-C3B-C4B	5.10	129.44	121.38
27	n1	201	CYC	CAB-C3B-C4B	5.09	129.42	121.38
27	y1	201	CYC	CAB-C3B-C4B	5.09	129.42	121.38
29	D2	303	PVN	C91-C18-C19	5.08	129.41	121.38
29	ly	404	PVN	C81-C17-C16	5.08	130.51	124.17
27	r1	201	CYC	CMA-C3A-C2A	-5.07	112.36	126.12
29	d3	302	PVN	C91-C18-C19	5.06	129.38	121.38
29	T8	303	PVN	C81-C17-C16	5.06	130.49	124.17
27	h1	201	CYC	CMA-C3A-C2A	-5.05	112.41	126.12
27	S1	201	CYC	CMA-C3A-C2A	-5.05	112.41	126.12
27	c1	201	CYC	CMA-C3A-C2A	-5.05	112.41	126.12
27	j1	201	CYC	CMA-C3A-C2A	-5.05	112.41	126.12
27	p1	201	CYC	CMA-C3A-C2A	-5.05	112.41	126.12
27	a2	901	CYC	CMA-C3A-C2A	-5.05	112.42	126.12
27	M1	1001	CYC	CMA-C3A-C2A	-5.04	112.42	126.12
27	z1	201	CYC	CMA-C3A-C2A	-5.04	112.43	126.12
27	J1	201	CYC	CMA-C3A-C2A	-5.04	112.43	126.12
27	v1	201	CYC	CMA-C3A-C2A	-5.04	112.43	126.12
27	S1	202	CYC	CMA-C3A-C2A	-5.04	112.44	126.12
27	a2	902	CYC	CMA-C3A-C2A	-5.04	112.44	126.12
27	b2	1001	CYC	CMA-C3A-C2A	-5.04	112.44	126.12
27	Y1	201	CYC	CMA-C3A-C2A	-5.04	112.44	126.12
27	t1	201	CYC	CMA-C3A-C2A	-5.04	112.45	126.12
29	Y9	303	PVN	C81-C17-C16	5.03	130.45	124.17
27	H1	201	CYC	CMA-C3A-C2A	-5.03	112.46	126.12
27	S1	202	CYC	OC-C1C-NC	4.89	130.87	124.94
27	J1	201	CYC	OC-C1C-NC	4.87	130.84	124.94
27	v1	201	CYC	OC-C1C-NC	4.87	130.84	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	p1	201	CYC	OC-C1C-NC	4.87	130.83	124.94
27	H1	201	CYC	OC-C1C-NC	4.86	130.83	124.94
27	r1	201	CYC	OC-C1C-NC	4.86	130.83	124.94
27	t1	201	CYC	OC-C1C-NC	4.86	130.83	124.94
27	q1	201	CYC	CHD-C4C-NC	4.86	130.98	125.20
27	Y1	201	CYC	OC-C1C-NC	4.86	130.82	124.94
27	c1	201	CYC	OC-C1C-NC	4.86	130.82	124.94
29	hZ	403	PVN	C5-C6-C7	-4.85	122.06	130.34
29	hY	404	PVN	C5-C6-C7	-4.85	122.06	130.34
27	G1	1001	CYC	CHD-C4C-NC	4.85	130.97	125.20
27	z1	201	CYC	OC-C1C-NC	4.84	130.81	124.94
27	O1	201	CYC	CHD-C4C-NC	4.84	130.96	125.20
27	a2	902	CYC	OC-C1C-NC	4.84	130.80	124.94
27	b2	1001	CYC	OC-C1C-NC	4.84	130.80	124.94
27	y1	201	CYC	CHD-C4C-NC	4.84	130.96	125.20
27	a2	901	CYC	OC-C1C-NC	4.84	130.80	124.94
27	S1	201	CYC	OC-C1C-NC	4.83	130.79	124.94
27	j1	201	CYC	OC-C1C-NC	4.83	130.79	124.94
27	Q1	201	CYC	CHD-C4C-NC	4.83	130.95	125.20
27	m1	201	CYC	CHD-C4C-NC	4.83	130.95	125.20
29	34	1004	PVN	C5-C6-C7	-4.83	122.09	130.34
29	Y5	1004	PVN	C5-C6-C7	-4.83	122.10	130.34
27	M1	1001	CYC	OC-C1C-NC	4.83	130.79	124.94
27	V1	201	CYC	CHD-C4C-NC	4.83	130.94	125.20
27	k1	201	CYC	CHD-C4C-NC	4.83	130.94	125.20
27	w1	201	CYC	CHD-C4C-NC	4.82	130.94	125.20
27	b1	1001	CYC	CHD-C4C-NC	4.82	130.93	125.20
27	f1	201	CYC	CHD-C4C-NC	4.82	130.93	125.20
27	L1	201	CYC	CHD-C4C-NC	4.82	130.93	125.20
27	a1	201	CYC	CHD-C4C-NC	4.82	130.93	125.20
27	U1	201	CYC	CHD-C4C-NC	4.81	130.93	125.20
27	n1	201	CYC	CHD-C4C-NC	4.81	130.93	125.20
27	d2	101	CYC	CHD-C4C-NC	4.81	130.93	125.20
27	g1	201	CYC	CHD-C4C-NC	4.81	130.93	125.20
27	h1	201	CYC	OC-C1C-NC	4.81	130.77	124.94
27	s1	201	CYC	CHD-C4C-NC	4.81	130.93	125.20
27	I1	201	CYC	CHD-C4C-NC	4.81	130.92	125.20
27	d1	1001	CYC	CHD-C4C-NC	4.80	130.92	125.20
27	o1	1001	CYC	CHD-C4C-NC	4.80	130.92	125.20
27	X1	201	CYC	CHD-C4C-NC	4.80	130.91	125.20
27	K1	201	CYC	CHD-C4C-NC	4.80	130.91	125.20
27	P1	201	CYC	CHD-C4C-NC	4.80	130.91	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	R1	1001	CYC	CHD-C4C-NC	4.79	130.91	125.20
27	e1	201	CYC	CHD-C4C-NC	4.79	130.91	125.20
27	i1	1001	CYC	CHD-C4C-NC	4.79	130.91	125.20
27	W1	201	CYC	CHD-C4C-NC	4.79	130.91	125.20
27	Z1	201	CYC	CHD-C4C-NC	4.79	130.90	125.20
27	o1	1001	CYC	OC-C1C-NC	4.78	130.74	124.94
27	u1	1001	CYC	CHD-C4C-NC	4.78	130.89	125.20
27	N1	201	CYC	CHD-C4C-NC	4.78	130.89	125.20
27	K1	201	CYC	OC-C1C-NC	4.76	130.71	124.94
27	Q1	201	CYC	OC-C1C-NC	4.75	130.70	124.94
27	m1	201	CYC	OC-C1C-NC	4.74	130.69	124.94
27	w1	201	CYC	OC-C1C-NC	4.74	130.69	124.94
29	D2	303	PVN	C2-C1-N1	4.74	111.42	107.21
27	d1	1001	CYC	OC-C1C-NC	4.74	130.68	124.94
27	V1	201	CYC	OC-C1C-NC	4.74	130.68	124.94
27	P1	201	CYC	OC-C1C-NC	4.74	130.68	124.94
27	f1	201	CYC	OC-C1C-NC	4.74	130.68	124.94
27	b1	1001	CYC	OC-C1C-NC	4.73	130.68	124.94
27	G1	1001	CYC	OC-C1C-NC	4.73	130.67	124.94
29	eY	403	PVN	C15-C16-N4	-4.73	115.91	126.06
27	n1	201	CYC	OC-C1C-NC	4.73	130.66	124.94
27	R1	1001	CYC	OC-C1C-NC	4.72	130.66	124.94
27	i1	1001	CYC	OC-C1C-NC	4.72	130.66	124.94
27	I1	201	CYC	OC-C1C-NC	4.72	130.66	124.94
27	Z1	201	CYC	OC-C1C-NC	4.72	130.66	124.94
27	k1	201	CYC	OC-C1C-NC	4.72	130.66	124.94
27	q1	201	CYC	OC-C1C-NC	4.72	130.66	124.94
27	N1	201	CYC	OC-C1C-NC	4.72	130.66	124.94
27	X1	201	CYC	OC-C1C-NC	4.72	130.66	124.94
29	d3	302	PVN	C2-C1-N1	4.71	111.39	107.21
29	eZ	402	PVN	C15-C16-N4	-4.71	115.95	126.06
27	O1	201	CYC	OC-C1C-NC	4.70	130.64	124.94
27	y1	201	CYC	OC-C1C-NC	4.70	130.63	124.94
27	e1	201	CYC	OC-C1C-NC	4.70	130.63	124.94
27	L1	201	CYC	OC-C1C-NC	4.70	130.63	124.94
27	a1	201	CYC	OC-C1C-NC	4.70	130.63	124.94
27	s1	201	CYC	OC-C1C-NC	4.69	130.63	124.94
27	u1	1001	CYC	OC-C1C-NC	4.69	130.63	124.94
27	W1	201	CYC	OC-C1C-NC	4.68	130.61	124.94
27	g1	201	CYC	OC-C1C-NC	4.67	130.60	124.94
29	dx	405	PVN	C32-C31-C3	4.67	120.05	112.98
27	U1	201	CYC	OC-C1C-NC	4.66	130.59	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d2	101	CYC	OC-C1C-NC	4.66	130.59	124.94
29	A2	1004	PVN	O19-C19-C18	-4.66	122.99	128.04
29	a3	1004	PVN	O19-C19-C18	-4.66	122.99	128.04
29	eY	403	PVN	C16-N4-C19	-4.62	104.79	110.67
28	aH	203	PUB	C4B-CHB-C1C	4.61	134.32	128.81
28	iD	1003	PUB	C4B-CHB-C1C	4.61	134.32	128.81
28	R6	203	PUB	C4B-CHB-C1C	4.61	134.32	128.81
28	lf	203	PUB	C4B-CHB-C1C	4.61	134.32	128.81
28	dN	203	PUB	C4B-CHB-C1C	4.61	134.31	128.81
28	gv	203	PUB	C4B-CHB-C1C	4.61	134.31	128.81
28	ga	203	PUB	C4B-CHB-C1C	4.61	134.31	128.81
28	A2	1006	PUB	C4B-CHB-C1C	4.60	134.31	128.81
28	P7	203	PUB	C4B-CHB-C1C	4.60	134.30	128.81
28	aJ	203	PUB	C4B-CHB-C1C	4.60	134.30	128.81
28	J3	203	PUB	C4B-CHB-C1C	4.60	134.30	128.81
28	fm	203	PUB	C4B-CHB-C1C	4.60	134.30	128.81
28	eX	202	PUB	C4B-CHB-C1C	4.60	134.30	128.81
29	eZ	402	PVN	C16-N4-C19	-4.60	104.82	110.67
28	bD	203	PUB	C4B-CHB-C1C	4.60	134.30	128.81
29	Y9	303	PVN	C2-C1-N1	4.60	111.28	107.21
28	K8	203	PUB	C4B-CHB-C1C	4.59	134.30	128.81
28	bn	202	PUB	C4B-CHB-C1C	4.59	134.30	128.81
28	ev	203	PUB	C4B-CHB-C1C	4.59	134.30	128.81
28	dv	202	PUB	C4B-CHB-C1C	4.59	134.30	128.81
28	hJ	203	PUB	C4B-CHB-C1C	4.59	134.30	128.81
28	Y9	304	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	F6	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	b7	202	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	a3	1005	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	eT	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	lz	404	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	fj	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	P4	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	T6	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	ly	406	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	fy	202	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	X7	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	T2	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	T9	203	PUB	C4B-CHB-C1C	4.59	134.29	128.81
28	fa	202	PUB	C4B-CHB-C1C	4.58	134.29	128.81
28	hR	203	PUB	C4B-CHB-C1C	4.58	134.29	128.81
28	c3	304	PUB	C4B-CHB-C1C	4.58	134.28	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	dj	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	dt	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	ei	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	n6	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	hG	202	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	e7	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	B9	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	di	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	l3	202	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	v3	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	r5	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	z5	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	e6	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	d7	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	x7	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	p9	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	df	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	gz	305	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	V3	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	d3	303	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	t7	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	c9	304	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	bF	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	cn	202	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	cE	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	ey	1005	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	B3	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	s7	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	E8	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	eN	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	lh	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	kX	1003	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	p4	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	cN	202	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	eJ	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	eY	405	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	eZ	404	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	hP	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	hZ	405	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	aB	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	cR	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	iH	1002	PUB	C4B-CHB-C1C	4.58	134.28	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	N5	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	Z5	305	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	fo	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	eY	404	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	ly	405	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	iG	1002	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	t4	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	n9	202	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	lp	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
28	fs	203	PUB	C4B-CHB-C1C	4.58	134.28	128.81
29	T8	303	PVN	C2-C1-N1	4.58	111.27	107.21
28	o8	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	p8	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	O8	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	hL	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	N9	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	az	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	bZ	306	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	hZ	404	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	p2	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	l7	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	b9	407	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	L9	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	dF	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	kR	1003	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	F4	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	r6	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	b8	1005	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	e8	304	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	V9	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	lb	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	jN	1003	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	H9	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	dw	405	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	V2	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	d3	304	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	L4	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	n7	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	bR	202	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	aY	405	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	dK	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	gn	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	h3	202	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	b6	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	D7	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	cz	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	ez	1006	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	iE	1003	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	Z3	203	PUB	C4B-CHB-C1C	4.57	134.27	128.81
28	D2	305	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	L2	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	n3	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	gz	306	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	jM	1003	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	J6	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	H7	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	R7	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	bY	1006	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	dd	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	C2	304	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	N4	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	J5	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	d9	305	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	x9	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	J9	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	ax	202	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	dT	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	dY	203	PUB	C4B-CHB-C1C	4.57	134.26	128.81
28	44	305	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	c9	305	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	P9	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	cp	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	dn	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	dD	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	hN	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	hV	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	bZ	305	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	dx	407	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	fq	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	gt	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	iF	1003	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	jI	1003	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	f2	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	j2	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	l2	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	C2	305	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	L3	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	R4	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	y8	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	fw	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	F5	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	aL	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	r4	202	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	z6	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	bs	1004	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	bL	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	eZ	403	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	R2	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	B4	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	L6	202	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	a7	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	r7	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	hH	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	N3	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	F9	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	cQ	202	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	ll	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	lt	203	PUB	C4B-CHB-C1C	4.56	134.26	128.81
28	Q8	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	bY	1005	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	z2	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	Z4	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	Z7	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	v7	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	bT	202	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	cH	202	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	x3	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	V5	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	e9	305	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	w8	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	aZ	304	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	x6	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	b8	1006	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	d8	304	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	cP	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	dl	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	gp	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	x2	202	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	F2	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	X3	202	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	v4	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	Y5	1005	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	v5	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	P6	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	aF	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	dh	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	gg	203	PUB	C4B-CHB-C1C	4.56	134.25	128.81
28	h2	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	X6	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	t6	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	v6	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	lv	202	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	dP	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	gr	202	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	hT	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	t3	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	u6	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	B7	202	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	eD	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	hX	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
29	A2	1004	PVN	C9-C10-C11	-4.55	123.37	128.81
28	P3	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	eH	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	ff	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	gi	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	gk	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	jL	1003	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	D5	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	Z6	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	dH	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	ld	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	ln	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	v2	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	z4	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	f8	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	N6	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	I8	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	r9	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	aP	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	bo	202	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	cM	203	PUB	C4B-CHB-C1C	4.55	134.25	128.81
28	M8	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	dp	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	ez	1005	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	gx	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	34	1006	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	J7	202	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	p7	202	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	bH	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	kQ	1003	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	kW	1003	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	c3	305	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	t5	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	L7	202	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	A8	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	z9	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	cs	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	Z2	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	z3	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	X4	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	F7	202	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	C8	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	lr	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	jO	1003	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	kT	1003	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	D2	304	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	D4	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	l6	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	n8	202	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	cY	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	hB	203	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	b9	406	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	dw	406	PUB	C4B-CHB-C1C	4.55	134.24	128.81
28	aR	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	aZ	305	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	gd	202	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	kS	1003	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	B5	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	T8	304	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	cq	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	ey	1006	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	34	1005	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	ar	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	fc	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	f3	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	c6	1004	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	c7	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	y7	203	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	an	202	PUB	C4B-CHB-C1C	4.54	134.24	128.81
28	r2	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	R5	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	d6	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	bP	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	cB	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	dr	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	dL	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	kV	1003	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	a6	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	jJ	1003	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	n2	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	A2	1005	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	F3	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	Y5	1006	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	bV	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	er	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
27	X1	201	CYC	CHB-C4A-C3A	4.54	136.57	124.90
28	dx	406	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	fu	202	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	H3	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	T7	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	cJ	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	jP	1003	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	Y9	305	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	ge	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	44	304	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	h8	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	V6	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	aV	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	X2	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	D3	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	L5	203	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	P5	202	PUB	C4B-CHB-C1C	4.54	134.23	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Z9	1006	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	iC	1003	PUB	C4B-CHB-C1C	4.54	134.23	128.81
28	x4	202	PUB	C4B-CHB-C1C	4.53	134.23	128.81
28	x5	202	PUB	C4B-CHB-C1C	4.53	134.23	128.81
28	e9	306	PUB	C4B-CHB-C1C	4.53	134.23	128.81
28	Z9	1005	PUB	C4B-CHB-C1C	4.53	134.23	128.81
28	D6	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	ap	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
27	n1	201	CYC	CHB-C4A-C3A	4.53	136.56	124.90
28	N2	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	T3	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	H6	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	V7	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	T8	305	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	bB	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	bN	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	dX	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	el	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
27	d1	1001	CYC	CHB-C4A-C3A	4.53	136.56	124.90
28	at	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	cO	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	lz	405	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	hY	405	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	bp	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	bq	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	H5	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	br	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	eL	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	H2	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	V4	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	y6	204	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	D9	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	r3	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	z7	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	cF	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	fi	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	a3	1006	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	gy	305	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	gy	306	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	aN	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	eb	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	J2	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	j3	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	U8	1005	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	R9	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	dB	202	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	dV	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	eB	204	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	N7	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	aD	203	PUB	C4B-CHB-C1C	4.53	134.22	128.81
28	t2	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	g8	202	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	jK	1003	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	w1	201	CYC	CHB-C4A-C3A	4.52	136.53	124.90
28	v9	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	f1	201	CYC	CHB-C4A-C3A	4.52	136.53	124.90
28	R3	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	T5	202	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	B6	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	aT	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	eg	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	lj	202	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	lx	201	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	P1	201	CYC	CHB-C4A-C3A	4.52	136.53	124.90
27	g1	201	CYC	CHB-C4A-C3A	4.52	136.53	124.90
28	aY	404	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	ec	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
29	a3	1004	PVN	C9-C10-C11	-4.52	123.41	128.81
27	O1	201	CYC	CHB-C4A-C3A	4.52	136.53	124.90
28	e8	305	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	o1	1001	CYC	CHB-C4A-C3A	4.52	136.53	124.90
28	c8	304	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	av	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	L1	201	CYC	CHB-C4A-C3A	4.52	136.52	124.90
27	a1	201	CYC	CHB-C4A-C3A	4.52	136.52	124.90
28	n4	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	cL	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	b1	1001	CYC	CHB-C4A-C3A	4.52	136.52	124.90
28	en	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	eF	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
27	Z1	201	CYC	CHB-C4A-C3A	4.52	136.52	124.90
28	T4	202	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	p5	202	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	p6	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	dR	203	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	eP	204	PUB	C4B-CHB-C1C	4.52	134.21	128.81
28	ee	203	PUB	C4B-CHB-C1C	4.52	134.20	128.81
27	u1	1001	CYC	CHB-C4A-C3A	4.52	136.51	124.90
28	H4	203	PUB	C4B-CHB-C1C	4.51	134.20	128.81
28	n5	203	PUB	C4B-CHB-C1C	4.51	134.20	128.81
27	W1	201	CYC	CHB-C4A-C3A	4.51	136.51	124.90
27	Q1	201	CYC	CHB-C4A-C3A	4.51	136.51	124.90
28	c8	305	PUB	C4B-CHB-C1C	4.51	134.20	128.81
28	eV	203	PUB	C4B-CHB-C1C	4.51	134.20	128.81
27	G1	1001	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	V1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	q1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	y1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	U1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	d2	101	CYC	CHB-C4A-C3A	4.51	136.50	124.90
28	bz	203	PUB	C4B-CHB-C1C	4.51	134.20	128.81
27	I1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	N1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
27	m1	201	CYC	CHB-C4A-C3A	4.51	136.50	124.90
29	bY	1004	PVN	C52-C51-C8	-4.51	104.93	112.62
28	P2	203	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	p3	203	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	co	202	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	hD	203	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	U8	1006	PUB	C4B-CHB-C1C	4.51	134.19	128.81
27	s1	201	CYC	CHB-C4A-C3A	4.51	136.49	124.90
28	Z5	306	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	t9	203	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	bJ	203	PUB	C4B-CHB-C1C	4.51	134.19	128.81
28	hY	406	PUB	C4B-CHB-C1C	4.51	134.19	128.81
27	R1	1001	CYC	CHB-C4A-C3A	4.50	136.48	124.90
27	i1	1001	CYC	CHB-C4A-C3A	4.50	136.48	124.90
28	kU	1003	PUB	C4B-CHB-C1C	4.50	134.19	128.81
27	K1	201	CYC	CHB-C4A-C3A	4.50	136.48	124.90
28	J4	203	PUB	C4B-CHB-C1C	4.50	134.19	128.81
28	G8	203	PUB	C4B-CHB-C1C	4.50	134.19	128.81
27	e1	201	CYC	CHB-C4A-C3A	4.50	136.47	124.90
28	cr	203	PUB	C4B-CHB-C1C	4.50	134.18	128.81
27	k1	201	CYC	CHB-C4A-C3A	4.49	136.46	124.90
28	ep	203	PUB	C4B-CHB-C1C	4.49	134.17	128.81
28	eR	203	PUB	C4B-CHB-C1C	4.48	134.16	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	et	203	PUB	C4B-CHB-C1C	4.46	134.14	128.81
29	aY	403	PVN	C52-C51-C8	-4.46	105.02	112.62
29	gz	304	PVN	C5-C6-C7	-4.45	122.74	130.34
29	C2	303	PVN	C92-C91-C18	4.40	124.57	112.43
29	c3	303	PVN	C92-C91-C18	4.40	124.57	112.43
27	S1	201	CYC	CHB-C4A-NA	-4.38	115.77	124.93
27	j1	201	CYC	CHB-C4A-NA	-4.38	115.77	124.93
27	a2	902	CYC	CHB-C4A-NA	-4.38	115.77	124.93
27	b2	1001	CYC	CHB-C4A-NA	-4.38	115.77	124.93
27	p1	201	CYC	CHB-C4A-NA	-4.38	115.78	124.93
27	z1	201	CYC	CHB-C4A-NA	-4.37	115.78	124.93
27	J1	201	CYC	CHB-C4A-NA	-4.37	115.79	124.93
27	Y1	201	CYC	CHB-C4A-NA	-4.37	115.79	124.93
27	H1	201	CYC	CHB-C4A-NA	-4.37	115.79	124.93
27	r1	201	CYC	CHB-C4A-NA	-4.37	115.79	124.93
27	v1	201	CYC	CHB-C4A-NA	-4.37	115.80	124.93
27	a2	901	CYC	CHB-C4A-NA	-4.36	115.81	124.93
27	S1	202	CYC	CHB-C4A-NA	-4.36	115.82	124.93
27	t1	201	CYC	CHB-C4A-NA	-4.36	115.82	124.93
29	aY	403	PVN	C91-C18-C17	-4.36	120.08	127.53
27	c1	201	CYC	CHB-C4A-NA	-4.35	115.83	124.93
27	h1	201	CYC	CHB-C4A-NA	-4.35	115.84	124.93
29	bY	1004	PVN	C91-C18-C17	-4.34	120.10	127.53
27	M1	1001	CYC	CHB-C4A-NA	-4.34	115.86	124.93
29	D2	303	PVN	C51-C52-C53	-4.34	101.61	113.76
29	d3	302	PVN	C51-C52-C53	-4.34	101.61	113.76
29	aZ	303	PVN	C91-C18-C17	-4.31	120.16	127.53
29	bZ	304	PVN	C91-C18-C17	-4.30	120.18	127.53
29	A2	1004	PVN	C52-C51-C8	4.25	119.87	112.62
29	a3	1004	PVN	C52-C51-C8	4.25	119.87	112.62
29	A2	1004	PVN	C16-N4-C19	-4.25	105.26	110.67
29	a3	1004	PVN	C16-N4-C19	-4.25	105.26	110.67
29	U8	1004	PVN	C5-C6-C7	4.16	137.43	130.34
29	ly	404	PVN	C9-C10-C11	-4.16	123.84	128.81
29	Z9	1004	PVN	C5-C6-C7	4.15	137.42	130.34
29	lz	403	PVN	C9-C10-C11	-4.13	123.87	128.81
29	Z5	304	PVN	C2-C1-N1	4.13	110.87	107.21
29	44	303	PVN	C2-C1-N1	4.12	110.87	107.21
26	eQ	201	PEB	C1C-CHB-C4B	4.11	133.72	128.81
26	dP	201	PEB	C1C-CHB-C4B	4.10	133.71	128.81
26	r3	201	PEB	C1C-CHB-C4B	4.10	133.71	128.81
26	aZ	301	PEB	C1C-CHB-C4B	4.09	133.69	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H3	201	PEB	C1C-CHB-C4B	4.09	133.69	128.81
26	s9	202	PEB	C1C-CHB-C4B	4.09	133.69	128.81
26	aa	1001	PEB	C1C-CHB-C4B	4.09	133.69	128.81
26	X4	201	PEB	C1C-CHB-C4B	4.08	133.69	128.81
26	hM	1001	PEB	C1C-CHB-C4B	4.08	133.69	128.81
26	d8	302	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	q7	201	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	bC	201	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	m5	1001	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	w5	201	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	s6	202	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	bS	201	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	dM	1002	PEB	C1C-CHB-C4B	4.08	133.68	128.81
26	eN	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	ls	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	dK	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	M8	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	eZ	401	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	s9	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	dT	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	Z9	1001	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	fn	1001	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	B6	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	O7	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	ad	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	aL	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	dq	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	dx	401	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	o4	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	d5	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	v8	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	C8	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	hX	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	R2	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	j7	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	B8	202	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	j9	201	PEB	C1C-CHB-C4B	4.07	133.67	128.81
26	C5	201	PEB	C1C-CHB-C4B	4.07	133.66	128.81
26	Y5	1001	PEB	C1C-CHB-C4B	4.07	133.66	128.81
26	e5	201	PEB	C1C-CHB-C4B	4.07	133.66	128.81
26	z9	202	PEB	C1C-CHB-C4B	4.07	133.66	128.81
26	eR	202	PEB	C1C-CHB-C4B	4.07	133.66	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	lq	202	PEB	C1C-CHB-C4B	4.07	133.66	128.81
26	y2	202	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	C7	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	li	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	T4	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	gk	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	a8	601	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	Q9	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	aP	202	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	eo	202	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	go	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	X4	202	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	k8	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	x6	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	G7	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	ae	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	cV	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	dS	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	P4	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	Y5	1003	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	a8	602	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	D8	202	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	K8	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	q2	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	y3	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	w6	1001	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	dJ	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	r5	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	bZ	301	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	dv	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	jL	1001	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	Q2	1001	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	K4	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	p4	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	Y6	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	bm	1002	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	ch	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	dR	201	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	hZ	402	PEB	C1C-CHB-C4B	4.06	133.66	128.81
26	h4	202	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	q3	1001	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	s3	201	PEB	C1C-CHB-C4B	4.06	133.65	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h6	202	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	T8	302	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	aX	401	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	bX	401	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	lz	401	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	fd	301	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	kX	1001	PEB	C1C-CHB-C4B	4.06	133.65	128.81
26	O4	1001	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	i8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	F8	1001	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	W8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	dx	404	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	d9	301	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	v8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	O8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	cj	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	dI	1002	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	fp	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	v4	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	I5	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	aZ	302	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	eB	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	ly	402	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	iE	1001	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	A4	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	G4	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	z5	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	W6	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	D9	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	P9	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	gz	303	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	J3	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	W7	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	N8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	ck	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	K2	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	D3	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	M3	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	T7	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	w8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	X9	401	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	ah	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bx	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	W2	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	t4	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	z4	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	O6	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	W6	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	e8	301	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	b9	403	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	E8	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	cP	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	dg	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	fx	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	f2	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	G2	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	Z2	201	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	bw	202	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	bK	1001	PEB	C1C-CHB-C4B	4.05	133.65	128.81
26	U2	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	B3	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	aH	202	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	cL	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	cR	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	ff	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	T6	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	r9	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	dU	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	eP	203	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	hA	201	PEB	C1C-CHB-C4B	4.05	133.64	128.81
26	O4	1002	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	e6	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	U7	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	bz	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	E3	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	Z6	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	c8	302	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	aY	406	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	dB	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	eU	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	gh	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	S4	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	b7	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	x7	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	i9	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	u9	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	v9	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	bA	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	dG	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	eG	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	eT	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	hI	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	k2	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	B2	502	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	H5	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	m6	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	r6	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	y6	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	aT	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	bo	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	cp	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	hW	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	u4	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	j5	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	c6	1001	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	o6	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	g7	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	U8	1001	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	aw	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	cN	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	cU	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	dj	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	fw	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	gb	1001	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	gs	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	e2	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	S3	203	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	t8	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	r9	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	B9	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	cY	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	do	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	dA	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	eS	202	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	gn	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	gu	201	PEB	C1C-CHB-C4B	4.04	133.64	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	kU	1001	PEB	C1C-CHB-C4B	4.04	133.64	128.81
26	g3	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	F5	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	c5	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	D6	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	G6	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	s8	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	R9	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	cJ	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	do	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dp	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	eF	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	hQ	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	Z4	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	E5	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	f8	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	i7	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	bt	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	ds	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	ed	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	eJ	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
29	44	303	PVN	C32-C31-C3	-4.04	106.85	112.98
26	l2	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	V2	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	M6	1001	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	b8	1001	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	aD	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	aJ	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	cX	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
29	Z5	304	PVN	C32-C31-C3	-4.04	106.86	112.98
26	b3	502	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	B4	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	m8	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	E6	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	r6	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	aW	302	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dp	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dQ	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	gq	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	r2	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	w2	203	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	Z3	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	x3	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	C4	1001	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	h9	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	p9	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	aG	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	by	1002	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	bz	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	cd	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dV	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	er	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	ly	403	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	lz	402	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	a3	1001	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	I4	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	J6	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	j6	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	o6	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	D7	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	A8	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	Q8	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	z9	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	ai	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	aV	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	bd	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dm	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dX	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	dX	202	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	eo	201	PEB	C1C-CHB-C4B	4.04	133.63	128.81
26	J2	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	j8	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	E7	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	dC	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	jJ	1001	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	a3	1003	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	A5	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	s5	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	H8	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	O8	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	dr	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	dt	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	gt	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	jP	1001	PEB	C1C-CHB-C4B	4.03	133.63	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	kT	1001	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	q2	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	s2	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	R6	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	Q7	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	t7	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	H8	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	av	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	aR	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	bl	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	bU	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	eV	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	lp	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	gv	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	hD	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	iF	1001	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	jO	1001	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	t2	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	l3	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	c4	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	k5	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	u5	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	y7	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	q9	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	u9	202	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	I9	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	bW	301	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	dw	403	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	en	201	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	ly	401	PEB	C1C-CHB-C4B	4.03	133.63	128.81
26	z2	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	I2	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	X3	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	u3	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	P4	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	L5	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	Z5	303	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	h6	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	A8	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	eP	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	S2	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	k3	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p3	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	I8	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	aW	301	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bu	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bL	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	dr	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	dw	402	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	fo	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	iC	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	g2	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	O3	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	y4	1002	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	V5	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	M7	1002	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	u7	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	b8	1003	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	x8	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	E8	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bc	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bE	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	cV	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	el	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	fs	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	b6	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	b6	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	l6	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	s6	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	u6	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	w8	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	P8	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	t9	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bd	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bu	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	cq	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	cR	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	L2	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	q8	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	e7	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	J8	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	h9	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	ay	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	ct	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cv	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	fl	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	iH	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	kV	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	D4	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	i4	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	y6	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	Z8	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	q9	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	aM	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	ba	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bv	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	du	203	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	ew	301	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	gm	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	hB	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	hT	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	J4	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	M4	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	d4	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	q4	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	x4	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	h8	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	S6	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	q6	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	z6	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	P7	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	o9	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	ab	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	dF	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	lc	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	jI	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	v2	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	F2	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	N2	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	F3	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	m3	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	24	401	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	H6	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	aT	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	aU	201	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	bh	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bs	1002	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	cC	1003	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	da	1001	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	dF	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	eD	202	PEB	C1C-CHB-C4B	4.03	133.62	128.81
26	N4	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	C6	202	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	f7	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	o7	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	t9	202	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	E9	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	cX	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	dY	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	lb	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	gz	301	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	A3	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	I3	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	j8	202	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	K6	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	c9	302	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	Z9	1007	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	aO	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	bZ	303	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	df	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	R3	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	j4	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	j5	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	U6	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	d6	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	X7	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	r7	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	d9	303	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	L8	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	bD	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	dd	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	gi	201	PEB	C1C-CHB-C4B	4.02	133.62	128.81
26	A6	1002	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bg	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dn	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dN	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ea	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ek	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fi	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	jM	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	e2	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	m4	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	t4	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	b5	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	y5	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	k8	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	V6	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	S8	401	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	aE	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	aK	1002	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	aS	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bl	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bw	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bV	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	cl	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	cm	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dA	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	hO	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	Y2	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	L3	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	P6	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	c9	301	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	e9	302	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	U9	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	V9	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	aS	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bj	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dt	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	du	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dC	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	eE	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	hK	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	W4	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	A6	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	l6	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	k7	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	a9	602	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	x8	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	U8	1002	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	H9	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z9	1003	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	be	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ce	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	cG	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	eC	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	lf	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	fj	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	gx	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	hC	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	u2	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	Y4	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	g4	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	l8	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	Q6	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	v7	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	T8	301	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bY	1003	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dn	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dz	401	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	eU	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ll	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	hH	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	X2	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	Q5	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	q5	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	m8	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	U8	1003	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ag	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	cQ	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ds	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dx	403	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ea	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ep	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	Y3	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	K6	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	X6	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	c7	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	I8	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	as	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	bQ	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	di	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dG	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eq	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	eM	1002	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	fh	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	hT	204	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	O2	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	T2	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	34	1007	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	l8	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	Z7	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	fc	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	fr	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	ge	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	m2	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	o3	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	34	1003	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	F6	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	t6	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	g9	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	az	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	aB	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dc	203	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	dZ	1001	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	eG	202	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	lq	201	PEB	C1C-CHB-C4B	4.02	133.61	128.81
26	A2	1002	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	M2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	F4	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	L4	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	44	302	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	C6	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	J8	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	Y8	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	M9	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	T9	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aJ	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aM	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bB	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cc	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cP	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cT	1002	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	dO	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	em	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	es	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	fm	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	f8	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	w7	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	b9	402	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	e9	303	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	y9	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	y9	1002	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	A9	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aU	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aY	402	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eC	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eK	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	fk	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	hF	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	hR	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	S3	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	l7	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	J9	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aB	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bs	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bY	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cE	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	fa	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	gl	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	k2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	t2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	C3	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	Y4	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	b4	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	l5	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	F6	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	M6	1002	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	m9	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	al	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	dz	402	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eb	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eA	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	fb	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	ga	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	gj	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	hJ	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	kW	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	o2	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	G2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	R5	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	d7	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bp	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bJ	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bR	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bX	402	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cW	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	dH	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	lm	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	v2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	N3	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	y6	203	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	ao	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aE	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bf	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	br	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cC	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cT	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eg	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	i2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	F2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	w4	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	B5	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	w9	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aN	204	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	dM	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	ey	1003	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eD	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	lb	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	gp	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	hP	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	iD	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	E2	1001	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	O2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	v3	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	n7	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	W8	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	L9	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	ar	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aX	402	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bq	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cA	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cZ	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	du	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eF	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eR	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	z2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	U5	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	T6	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	F8	1002	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	Y8	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	x9	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	aH	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	bv	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	dl	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eI	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	gy	303	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	p2	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	T3	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	R4	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	S4	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	k4	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	N5	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	O6	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	ac	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cx	201	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	cM	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	eH	202	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	hY	403	PEB	C1C-CHB-C4B	4.01	133.60	128.81
26	w2	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	D2	302	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	c3	302	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	Q6	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	G8	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	l9	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	aP	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	ci	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	cS	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	gy	301	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	K3	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	G4	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	x6	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	b8	1002	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	ap	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	aC	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	aF	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	bI	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	cb	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	dc	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	dy	401	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	dN	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	eI	202	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	eS	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	ln	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	lr	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	fd	303	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	hL	201	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	kS	1001	PEB	C1C-CHB-C4B	4.01	133.59	128.81
26	a5	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	l9	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	af	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aI	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	bs	1003	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	de	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	dk	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	gf	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	M2	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	U3	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	q4	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	S5	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	c6	1002	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	p8	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	k9	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	Y9	302	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aL	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	dL	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	E4	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	M7	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	G8	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	V8	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	at	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aA	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aV	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cS	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	dI	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	ey	1002	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	g8	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	j6	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	q6	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	X8	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	bx	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	eW	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	lk	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	m2	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	D2	301	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	f3	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	z3	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	K4	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	o5	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	K8	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	n9	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aN	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	bb	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	ca	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	cw	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	cy	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	la	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	fq	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	B2	501	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	e4	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	I6	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	N6	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	u6	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	z8	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	K9	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	ez	1002	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	iG	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	a4	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	w6	1002	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	au	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	bj	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	dD	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	hV	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	C2	302	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	u4	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	x5	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	g6	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	S7	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	Y7	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	D8	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	M8	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	x9	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aY	401	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	bm	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	ee	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	ej	202	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	o2	1002	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	w2	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	E6	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	I6	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	k6	1002	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	V7	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	aq	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	cr	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	cO	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	dW	201	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	kQ	1001	PEB	C1C-CHB-C4B	4.00	133.59	128.81
26	P2	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	W2	202	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	I4	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	m7	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	z7	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	bG	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	hE	1001	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	y2	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	i3	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	w3	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	s4	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	S6	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	r8	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	a9	601	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	G9	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	O9	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	bn	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	cg	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	dh	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	ej	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eT	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	fd	302	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	iB	1001	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	kR	1001	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	H4	202	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	Q4	202	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	J5	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	W5	301	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	p9	202	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	N9	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	aC	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	ef	201	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	ez	1003	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	jK	1001	PEB	C1C-CHB-C4B	4.00	133.58	128.81
26	Y2	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	Q3	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	y4	1001	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	P6	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	Z6	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	i6	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	d9	302	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	bO	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	dx	402	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	dR	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	eq	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	fv	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	L4	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	U4	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	n5	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	c6	1003	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	e9	301	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	y8	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	aI	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	bq	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	dm	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	eE	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	hN	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	hY	401	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	n4	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	e8	302	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	L8	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	Q8	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f9	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	bh	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	cO	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	db	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	ff	204	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	v6	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	bk	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	jN	1001	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	aF	204	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	by	1001	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	eK	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	eY	402	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	le	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	Z4	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	44	301	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	i5	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	m6	202	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	z8	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	cu	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	cz	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	la	1002	PEB	C1C-CHB-C4B	3.99	133.58	128.81
26	hS	201	PEB	C1C-CHB-C4B	3.99	133.58	128.81
29	Z9	1004	PVN	C32-C31-C3	3.99	119.03	112.98
26	V3	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	Q4	203	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	D5	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	P8	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	E4	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	a6	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	i6	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	H7	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	b9	404	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	aA	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	bP	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	cW	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	dK	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	dW	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	Q4	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	g5	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	dk	1002	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	eH	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	P3	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f9	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	F9	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	am	1001	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	aN	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	cV	203	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	K2	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	L6	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	bt	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	ed	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	eQ	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	lu	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	J4	202	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	f4	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	T5	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	v5	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	lv	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	gc	201	PEB	C1C-CHB-C4B	3.99	133.57	128.81
26	U4	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	k6	1001	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	z6	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	r2	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	x2	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	aK	1001	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	bi	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	dH	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	eO	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	K5	1001	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	l5	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	g6	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	a7	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	dO	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	dQ	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	es	202	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	p6	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	v6	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	ak	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
26	dq	201	PEB	C1C-CHB-C4B	3.98	133.57	128.81
29	U8	1004	PVN	C32-C31-C3	3.98	119.02	112.98
26	I2	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	aR	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	cB	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	iA	1001	PEB	C1C-CHB-C4B	3.98	133.56	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g2	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	H4	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	k8	203	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	f6	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	N8	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	cs	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	s2	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	Z5	301	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	w9	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	bN	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	eh	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	ez	1001	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	V4	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	X5	401	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	N7	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	aQ	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	cM	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	fe	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	ft	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	i2	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	s7	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	gg	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	h5	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	b9	401	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	u2	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	o4	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	o8	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	gw	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	M4	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	z4	202	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	S9	201	PEB	C1C-CHB-C4B	3.98	133.56	128.81
26	n3	201	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	br	201	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	dT	201	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	W4	202	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	lt	201	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	F4	201	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	u8	201	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	j9	202	PEB	C1C-CHB-C4B	3.97	133.56	128.81
26	C2	301	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	V4	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	bM	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R4	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	C9	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	aQ	202	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	dE	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	li	202	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	j2	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	h7	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	cI	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	dD	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	B8	201	PEB	C1C-CHB-C4B	3.97	133.55	128.81
26	W3	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	G5	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	K7	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	O5	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	cU	202	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	cD	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	h2	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	e3	1001	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	R7	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	bH	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	M5	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	t5	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	n2	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	l4	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	I7	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	aj	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	t3	201	PEB	C1C-CHB-C4B	3.96	133.54	128.81
26	dw	401	PEB	C1C-CHB-C4B	3.95	133.53	128.81
26	a9	603	PEB	C1C-CHB-C4B	3.95	133.53	128.81
26	eu	201	PEB	C1C-CHB-C4B	3.95	133.53	128.81
26	G3	201	PEB	C1C-CHB-C4B	3.95	133.52	128.81
26	bF	201	PEB	C1C-CHB-C4B	3.94	133.52	128.81
26	cK	201	PEB	C1C-CHB-C4B	3.94	133.52	128.81
29	hZ	403	PVN	C52-C51-C8	-3.94	105.89	112.62
29	lz	403	PVN	C52-C51-C8	3.94	119.34	112.62
26	b3	501	PEB	C1C-CHB-C4B	3.94	133.51	128.81
29	hY	404	PVN	C52-C51-C8	-3.94	105.90	112.62
29	U8	1004	PVN	O19-C19-C18	-3.93	123.78	128.04
29	ly	404	PVN	C52-C51-C8	3.93	119.32	112.62
29	34	1004	PVN	C52-C51-C8	-3.93	105.92	112.62
29	gy	304	PVN	C21-C2-C3	-3.93	121.61	129.67
26	dP	202	PEB	C1C-CHB-C4B	3.92	133.50	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Z9	1004	PVN	C16-N4-C19	-3.92	105.67	110.67
26	eW	201	PEB	C1C-CHB-C4B	3.92	133.49	128.81
26	eO	201	PEB	C1C-CHB-C4B	3.92	133.49	128.81
29	gz	304	PVN	C21-C2-C3	-3.92	121.62	129.67
26	eM	1001	PEB	C1C-CHB-C4B	3.92	133.49	128.81
29	c8	303	PVN	O19-C19-C18	-3.91	123.79	128.04
29	Y5	1004	PVN	C52-C51-C8	-3.91	105.94	112.62
29	Z9	1004	PVN	O19-C19-C18	-3.91	123.79	128.04
29	c9	303	PVN	O19-C19-C18	-3.91	123.80	128.04
29	U8	1004	PVN	C16-N4-C19	-3.90	105.70	110.67
29	dw	404	PVN	C32-C31-C3	3.90	118.89	112.98
29	dx	405	PVN	C9-C10-C11	-3.89	124.16	128.81
29	gy	304	PVN	C5-C6-C7	-3.86	123.76	130.34
27	S1	202	CYC	CHD-C4C-NC	3.84	129.77	125.20
27	J1	201	CYC	CHD-C4C-NC	3.82	129.74	125.20
27	Y1	201	CYC	CHD-C4C-NC	3.82	129.74	125.20
27	v1	201	CYC	CHD-C4C-NC	3.81	129.74	125.20
29	hY	404	PVN	C16-N4-C19	-3.81	105.82	110.67
27	t1	201	CYC	CHD-C4C-NC	3.80	129.72	125.20
29	d9	304	PVN	C91-C18-C19	3.80	127.38	121.38
27	h1	201	CYC	CHD-C4C-NC	3.80	129.72	125.20
29	gy	304	PVN	C32-C31-C3	-3.79	107.22	112.98
27	S1	201	CYC	CHD-C4C-NC	3.79	129.72	125.20
27	j1	201	CYC	CHD-C4C-NC	3.79	129.72	125.20
29	d9	304	PVN	O19-C19-C18	-3.79	123.93	128.04
27	z1	201	CYC	CHD-C4C-NC	3.79	129.71	125.20
29	bY	1004	PVN	C5-C6-C7	3.79	136.79	130.34
29	hZ	403	PVN	C16-N4-C19	-3.78	105.85	110.67
27	H1	201	CYC	CHD-C4C-NC	3.78	129.70	125.20
27	c1	201	CYC	CHD-C4C-NC	3.78	129.70	125.20
27	a2	902	CYC	CHD-C4C-NC	3.78	129.69	125.20
27	b2	1001	CYC	CHD-C4C-NC	3.78	129.69	125.20
29	aY	403	PVN	C5-C6-C7	3.77	136.77	130.34
27	p1	201	CYC	CHD-C4C-NC	3.77	129.69	125.20
27	a2	901	CYC	CHD-C4C-NC	3.77	129.69	125.20
29	d8	303	PVN	O19-C19-C18	-3.76	123.96	128.04
29	d8	303	PVN	C91-C18-C19	3.76	127.31	121.38
27	M1	1001	CYC	CHD-C4C-NC	3.75	129.66	125.20
29	34	1004	PVN	C16-N4-C19	-3.74	105.91	110.67
27	z1	201	CYC	CAA-C2A-C1A	3.74	131.62	125.01
27	a2	901	CYC	CAA-C2A-C1A	3.74	131.62	125.01
27	r1	201	CYC	CHD-C4C-NC	3.73	129.64	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	J1	201	CYC	C1B-C2B-C3B	-3.72	103.99	107.87
27	S1	201	CYC	CAA-C2A-C1A	3.72	131.59	125.01
27	j1	201	CYC	CAA-C2A-C1A	3.72	131.59	125.01
29	Y5	1004	PVN	C16-N4-C19	-3.72	105.94	110.67
27	M1	1001	CYC	CAA-C2A-C1A	3.72	131.58	125.01
27	a2	902	CYC	CAA-C2A-C1A	3.71	131.58	125.01
27	b2	1001	CYC	CAA-C2A-C1A	3.71	131.58	125.01
29	bZ	304	PVN	C32-C31-C3	3.71	118.61	112.98
27	c1	201	CYC	CAA-C2A-C1A	3.71	131.57	125.01
27	p1	201	CYC	CAA-C2A-C1A	3.71	131.57	125.01
27	v1	201	CYC	CAA-C2A-C1A	3.71	131.57	125.01
27	J1	201	CYC	CAA-C2A-C1A	3.71	131.57	125.01
27	Y1	201	CYC	CAA-C2A-C1A	3.71	131.57	125.01
27	H1	201	CYC	CAA-C2A-C1A	3.71	131.57	125.01
29	dx	405	PVN	C16-N4-C19	-3.71	105.95	110.67
29	aZ	303	PVN	C32-C31-C3	3.71	118.60	112.98
29	e8	303	PVN	O19-C19-C18	-3.70	124.02	128.04
27	p1	201	CYC	C1B-C2B-C3B	-3.70	104.01	107.87
27	r1	201	CYC	CAA-C2A-C1A	3.69	131.55	125.01
27	v1	201	CYC	C1B-C2B-C3B	-3.69	104.02	107.87
27	t1	201	CYC	CAA-C2A-C1A	3.69	131.54	125.01
29	d9	304	PVN	C16-N4-C19	-3.69	105.97	110.67
27	S1	202	CYC	CAA-C2A-C1A	3.69	131.53	125.01
27	h1	201	CYC	CAA-C2A-C1A	3.68	131.53	125.01
27	a2	901	CYC	C1B-C2B-C3B	-3.68	104.03	107.87
27	h1	201	CYC	C1B-C2B-C3B	-3.67	104.04	107.87
27	r1	201	CYC	C1B-C2B-C3B	-3.67	104.04	107.87
29	e9	304	PVN	O19-C19-C18	-3.67	124.06	128.04
29	ly	404	PVN	C91-C18-C19	3.67	127.17	121.38
27	M1	1001	CYC	C1B-C2B-C3B	-3.67	104.05	107.87
29	C2	303	PVN	C16-N4-C19	-3.66	106.01	110.67
29	c3	303	PVN	C16-N4-C19	-3.66	106.01	110.67
27	Y1	201	CYC	C1B-C2B-C3B	-3.66	104.05	107.87
29	d8	303	PVN	C16-N4-C19	-3.66	106.01	110.67
27	c1	201	CYC	C1B-C2B-C3B	-3.66	104.06	107.87
27	H1	201	CYC	C1B-C2B-C3B	-3.65	104.06	107.87
29	gz	304	PVN	C91-C18-C19	3.65	127.14	121.38
27	t1	201	CYC	C1B-C2B-C3B	-3.65	104.06	107.87
27	S1	201	CYC	C1B-C2B-C3B	-3.65	104.07	107.87
27	j1	201	CYC	C1B-C2B-C3B	-3.65	104.07	107.87
27	z1	201	CYC	C1B-C2B-C3B	-3.64	104.07	107.87
27	a2	902	CYC	C1B-C2B-C3B	-3.64	104.07	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	b2	1001	CYC	C1B-C2B-C3B	-3.64	104.07	107.87
27	S1	202	CYC	C1B-C2B-C3B	-3.64	104.08	107.87
29	lz	403	PVN	C91-C18-C19	3.63	127.11	121.38
29	c8	303	PVN	C91-C18-C19	3.58	127.04	121.38
29	dw	404	PVN	C16-N4-C19	-3.58	106.11	110.67
29	gz	304	PVN	C15-C14-N3	3.57	132.40	124.93
29	c9	303	PVN	C91-C18-C19	3.56	127.00	121.38
29	A2	1004	PVN	C41-C7-C8	-3.54	118.27	124.94
29	a3	1004	PVN	C41-C7-C8	-3.54	118.27	124.94
29	c8	303	PVN	C16-N4-C19	-3.51	106.20	110.67
29	gz	304	PVN	C10-C11-N3	3.49	133.67	128.83
28	eX	202	PUB	CHB-C1C-C2C	3.48	133.37	125.32
29	c9	303	PVN	C16-N4-C19	-3.48	106.24	110.67
28	lf	203	PUB	CHB-C1C-C2C	3.48	133.36	125.32
28	ly	405	PUB	CHB-C1C-C2C	3.48	133.35	125.32
28	lz	404	PUB	CHB-C1C-C2C	3.48	133.35	125.32
28	dN	203	PUB	CHB-C1C-C2C	3.48	133.35	125.32
28	gt	203	PUB	CHB-C1C-C2C	3.48	133.35	125.32
28	jI	1003	PUB	CHB-C1C-C2C	3.48	133.35	125.32
28	aY	405	PUB	CHB-C1C-C2C	3.47	133.35	125.32
28	dT	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	R4	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	dR	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	t7	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	ev	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	V3	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	R6	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	bH	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	dl	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	eT	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	ga	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	bZ	306	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	ly	406	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	a3	1005	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	F9	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	fq	203	PUB	CHB-C1C-C2C	3.47	133.34	125.32
28	cn	202	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	gv	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	x7	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	dv	202	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	J3	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	O8	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	C2	305	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	c3	305	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	34	1006	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	K8	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32
27	a2	902	CYC	CHB-C4A-C3A	3.47	133.81	124.90
27	b2	1001	CYC	CHB-C4A-C3A	3.47	133.81	124.90
28	r5	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32
28	hR	203	PUB	CHB-C1C-C2C	3.47	133.33	125.32
27	p1	201	CYC	CHB-C4A-C3A	3.46	133.81	124.90
28	z5	203	PUB	CHB-C1C-C2C	3.46	133.33	125.32
28	p8	203	PUB	CHB-C1C-C2C	3.46	133.33	125.32
28	lp	203	PUB	CHB-C1C-C2C	3.46	133.33	125.32
28	hX	203	PUB	CHB-C1C-C2C	3.46	133.33	125.32
28	r7	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	eN	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	lr	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	cE	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	dF	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	df	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	bF	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	hP	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	A2	1006	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	T6	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	n9	202	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	di	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	iE	1003	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	jK	1003	PUB	CHB-C1C-C2C	3.46	133.32	125.32
27	U1	201	CYC	CHA-C1A-NA	-3.46	124.03	128.83
27	d2	101	CYC	CHA-C1A-NA	-3.46	124.03	128.83
28	d3	304	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	z9	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	bL	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	iF	1003	PUB	CHB-C1C-C2C	3.46	133.32	125.32
27	b1	1001	CYC	CHA-C1A-NA	-3.46	124.03	128.83
28	T2	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	D3	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	d3	303	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	x3	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	l7	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	bn	202	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	ge	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	h3	202	PUB	CHB-C1C-C2C	3.46	133.32	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B9	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	bB	203	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	bR	202	PUB	CHB-C1C-C2C	3.46	133.32	125.32
28	f2	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	N5	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	n6	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	e7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	cP	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	fm	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	jM	1003	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	P7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	d7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	aH	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	D2	304	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	u6	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	eY	404	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	fy	202	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	hJ	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
27	X1	201	CYC	CHA-C1A-NA	-3.46	124.03	128.83
28	j2	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	B3	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	R7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
27	S1	202	CYC	CHB-C4A-C3A	3.46	133.79	124.90
28	h8	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	H7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	bD	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	fj	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
29	bY	1004	PVN	C71-C13-C14	-3.46	119.74	125.06
28	34	1005	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	iH	1002	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	l2	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	v2	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	L3	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	c3	304	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	x4	202	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	x5	202	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	cN	202	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	l3	202	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	f8	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	bY	1006	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	L4	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	a7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y9	304	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	dx	407	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	fa	202	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	hT	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	n2	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	N3	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	Z4	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	N7	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	d9	305	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	N9	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	ei	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	ey	1005	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	kU	1003	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	C2	304	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	z6	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	o8	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	V9	203	PUB	CHB-C1C-C2C	3.46	133.31	125.32
28	kV	1003	PUB	CHB-C1C-C2C	3.46	133.31	125.32
27	K1	201	CYC	CHA-C1A-NA	-3.46	124.03	128.83
28	N2	203	PUB	CHB-C1C-C2C	3.46	133.30	125.32
28	v3	203	PUB	CHB-C1C-C2C	3.46	133.30	125.32
28	F6	203	PUB	CHB-C1C-C2C	3.46	133.30	125.32
28	eY	405	PUB	CHB-C1C-C2C	3.46	133.30	125.32
28	eZ	404	PUB	CHB-C1C-C2C	3.46	133.30	125.32
28	N4	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	J5	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	Q8	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	ez	1006	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	eD	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	hL	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
27	q1	201	CYC	CHA-C1A-NA	-3.45	124.03	128.83
28	Z5	305	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	P9	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	Z9	1005	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	dB	202	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	jN	1003	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	dp	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
27	Q1	201	CYC	CHA-C1A-NA	-3.45	124.04	128.83
28	Y5	1005	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	T7	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	b7	202	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	e8	304	PUB	CHB-C1C-C2C	3.45	133.30	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	aD	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	aJ	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	dd	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	iG	1002	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	z3	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	cz	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	dr	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	lz	405	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	hZ	405	PUB	CHB-C1C-C2C	3.45	133.30	125.32
27	H1	201	CYC	CHB-C4A-C3A	3.45	133.78	124.90
28	P4	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	n4	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	r4	202	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	E8	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	an	202	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	hG	202	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	kS	1003	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	Z2	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	n3	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	J9	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	aT	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	bZ	305	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	cp	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	lb	203	PUB	CHB-C1C-C2C	3.45	133.30	125.32
28	L2	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	V6	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	b6	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	aR	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	cH	202	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	ez	1005	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	fw	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
27	L1	201	CYC	CHA-C1A-NA	-3.45	124.04	128.83
27	a1	201	CYC	CHA-C1A-NA	-3.45	124.04	128.83
28	aL	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	ld	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	lh	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	ln	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	jO	1003	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	r3	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	F4	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	x6	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	I8	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	dj	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	dn	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	dt	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	dx	406	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	h2	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	t4	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	aN	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	dh	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	ll	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	lt	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	hZ	404	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	jJ	1003	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	v4	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	v5	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	b9	407	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	gi	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
27	J1	201	CYC	CHB-C4A-C3A	3.45	133.77	124.90
27	Y1	201	CYC	CHB-C4A-C3A	3.45	133.77	124.90
28	n7	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	dH	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	r2	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	z2	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	H5	202	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	d8	304	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	v9	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	aV	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	aZ	304	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	cY	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	fu	202	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	gx	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	V2	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	F3	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	B7	202	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	C8	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	r9	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	ar	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	aP	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	dD	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	lv	202	PUB	CHB-C1C-C2C	3.45	133.29	125.32
27	k1	201	CYC	CHA-C1A-NA	-3.45	124.04	128.83
28	t3	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	X7	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	c7	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	c9	304	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	A8	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	x9	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	kT	1003	PUB	CHB-C1C-C2C	3.45	133.29	125.32
27	S1	201	CYC	CHB-C4A-C3A	3.45	133.76	124.90
27	j1	201	CYC	CHB-C4A-C3A	3.45	133.76	124.90
28	e9	305	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	eL	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	hB	203	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	kW	1003	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	kX	1003	PUB	CHB-C1C-C2C	3.45	133.29	125.32
28	V5	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	D7	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	aB	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	dY	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	gz	305	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	F7	202	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	y8	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	cR	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	eB	204	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	hV	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	44	304	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	r6	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	t6	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	M8	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	ey	1006	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	s7	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	p9	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	N6	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	v7	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
28	fc	203	PUB	CHB-C1C-C2C	3.45	133.28	125.32
27	I1	201	CYC	CHA-C1A-NA	-3.45	124.05	128.83
27	d1	1001	CYC	CHA-C1A-NA	-3.45	124.05	128.83
28	A2	1005	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	L5	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	bY	1005	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	dw	406	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	gn	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
27	h1	201	CYC	CHB-C4A-C3A	3.44	133.76	124.90
27	O1	201	CYC	CHA-C1A-NA	-3.44	124.05	128.83
28	c6	1004	PUB	CHB-C1C-C2C	3.44	133.28	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	w8	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	bN	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	bP	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	iD	1003	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	jP	1003	PUB	CHB-C1C-C2C	3.44	133.28	125.32
27	a2	901	CYC	CHB-C4A-C3A	3.44	133.76	124.90
28	D6	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	L9	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	aF	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	dw	405	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	dL	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	dP	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	fo	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
27	t1	201	CYC	CHB-C4A-C3A	3.44	133.76	124.90
27	v1	201	CYC	CHB-C4A-C3A	3.44	133.76	124.90
28	D2	305	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	J2	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	j3	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	B4	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	X4	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	y7	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	U8	1005	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	ap	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	eb	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	eH	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	ff	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	gy	306	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	x2	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	X3	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	B6	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	c8	304	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	e8	305	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	c9	305	PUB	CHB-C1C-C2C	3.44	133.28	125.32
27	n1	201	CYC	CHA-C1A-NA	-3.44	124.05	128.83
28	J6	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	v6	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	ax	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	az	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	cF	202	PUB	CHB-C1C-C2C	3.44	133.28	125.32
28	eJ	203	PUB	CHB-C1C-C2C	3.44	133.28	125.32
29	C2	303	PVN	C15-C16-N4	-3.44	118.67	126.06
29	c3	303	PVN	C15-C16-N4	-3.44	118.67	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D4	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	B5	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	p7	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	cO	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	hH	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	F5	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	l6	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	kR	1003	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	a3	1006	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	T5	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	H6	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	b8	1005	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	e9	306	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	44	305	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	p5	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	Z6	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	cJ	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	dK	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	dX	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	F2	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	H3	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	L7	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	aZ	305	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	bo	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	gd	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	jL	1003	PUB	CHB-C1C-C2C	3.44	133.27	125.32
27	P1	201	CYC	CHA-C1A-NA	-3.44	124.06	128.83
28	Z3	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	gz	306	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	H9	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	fi	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	gk	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	hN	203	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	g8	202	PUB	CHB-C1C-C2C	3.44	133.27	125.32
28	Z9	1006	PUB	CHB-C1C-C2C	3.44	133.27	125.32
29	hZ	403	PVN	C21-C2-C1	-3.44	113.31	121.39
28	b9	406	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	D9	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	bV	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	c8	305	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	Y9	305	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	kQ	1003	PUB	CHB-C1C-C2C	3.44	133.26	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	T9	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	bz	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	cq	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	cM	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
27	c1	201	CYC	CHB-C4A-C3A	3.44	133.74	124.90
28	P2	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	co	202	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	cB	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	H4	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	p4	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	P5	202	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	n8	202	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	V7	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	bT	202	PUB	CHB-C1C-C2C	3.44	133.26	125.32
27	o1	1001	CYC	CHA-C1A-NA	-3.44	124.06	128.83
28	T8	305	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	U8	1006	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	bs	1004	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	ee	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	fs	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	gr	202	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	L6	202	PUB	CHB-C1C-C2C	3.44	133.26	125.32
28	Z7	203	PUB	CHB-C1C-C2C	3.44	133.26	125.32
27	V1	201	CYC	CHA-C1A-NA	-3.43	124.06	128.83
27	z1	201	CYC	CHB-C4A-C3A	3.43	133.73	124.90
28	p2	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	P3	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	z7	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	at	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	cL	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	eF	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	J7	202	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	gg	203	PUB	CHB-C1C-C2C	3.43	133.26	125.32
28	y6	204	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	b8	1006	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	eR	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	eZ	403	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	hY	405	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	iC	1003	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	a6	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	bp	202	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	eP	204	PUB	CHB-C1C-C2C	3.43	133.25	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	gy	305	PUB	CHB-C1C-C2C	3.43	133.25	125.32
29	34	1004	PVN	C21-C2-C1	-3.43	113.32	121.39
29	Y5	1004	PVN	C21-C2-C1	-3.43	113.32	121.39
27	g1	201	CYC	CHA-C1A-NA	-3.43	124.06	128.83
28	T8	304	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	cr	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	er	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	hY	406	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	P6	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	e6	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
29	e9	304	PVN	C16-N4-C19	-3.43	106.30	110.67
28	T4	202	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	cs	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	ec	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	hD	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
27	u1	1001	CYC	CHA-C1A-NA	-3.43	124.07	128.83
28	p6	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
27	M1	1001	CYC	CHB-C4A-C3A	3.43	133.72	124.90
28	f3	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	gp	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	t2	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	R3	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	T3	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	z4	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	Y5	1006	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	aY	404	PUB	CHB-C1C-C2C	3.43	133.25	125.32
27	r1	201	CYC	CHB-C4A-C3A	3.43	133.72	124.90
28	J4	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
28	br	203	PUB	CHB-C1C-C2C	3.43	133.25	125.32
27	R1	1001	CYC	CHA-C1A-NA	-3.43	124.07	128.83
27	i1	1001	CYC	CHA-C1A-NA	-3.43	124.07	128.83
28	el	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	ep	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	X6	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	cQ	202	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	D5	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	t5	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
29	d3	302	PVN	C9-C10-C11	-3.43	124.71	128.81
28	R2	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	V4	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	av	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	X2	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G8	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
27	W1	201	CYC	CHA-C1A-NA	-3.43	124.07	128.83
28	H2	202	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	t9	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	R5	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	dV	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
28	eg	203	PUB	CHB-C1C-C2C	3.43	133.24	125.32
27	G1	1001	CYC	CHA-C1A-NA	-3.43	124.08	128.83
27	y1	201	CYC	CHA-C1A-NA	-3.42	124.08	128.83
28	n5	203	PUB	CHB-C1C-C2C	3.42	133.23	125.32
28	R9	203	PUB	CHB-C1C-C2C	3.42	133.23	125.32
28	et	203	PUB	CHB-C1C-C2C	3.42	133.23	125.32
29	e8	303	PVN	C16-N4-C19	-3.42	106.31	110.67
28	lj	202	PUB	CHB-C1C-C2C	3.42	133.23	125.32
28	lx	201	PUB	CHB-C1C-C2C	3.42	133.23	125.32
27	s1	201	CYC	CHA-C1A-NA	-3.42	124.08	128.83
29	A2	1004	PVN	C5-C6-C7	3.42	136.17	130.34
29	a3	1004	PVN	C5-C6-C7	3.42	136.17	130.34
28	eV	203	PUB	CHB-C1C-C2C	3.42	133.23	125.32
28	Z5	306	PUB	CHB-C1C-C2C	3.42	133.23	125.32
28	d6	203	PUB	CHB-C1C-C2C	3.42	133.23	125.32
28	bq	203	PUB	CHB-C1C-C2C	3.42	133.23	125.32
29	ey	1004	PVN	C52-C51-C8	-3.42	106.78	112.62
27	e1	201	CYC	CHA-C1A-NA	-3.42	124.08	128.83
29	hY	404	PVN	C21-C2-C1	-3.42	113.35	121.39
28	p3	203	PUB	CHB-C1C-C2C	3.42	133.22	125.32
28	en	203	PUB	CHB-C1C-C2C	3.42	133.22	125.32
27	m1	201	CYC	CHA-C1A-NA	-3.42	124.08	128.83
29	aY	403	PVN	C71-C13-C14	-3.42	119.80	125.06
27	f1	201	CYC	CHA-C1A-NA	-3.42	124.09	128.83
28	bJ	203	PUB	CHB-C1C-C2C	3.42	133.22	125.32
27	Z1	201	CYC	CHA-C1A-NA	-3.42	124.09	128.83
27	w1	201	CYC	CHA-C1A-NA	-3.41	124.09	128.83
27	N1	201	CYC	CHA-C1A-NA	-3.41	124.09	128.83
29	ey	1004	PVN	C16-N4-C19	-3.41	106.33	110.67
29	e9	304	PVN	C5-C6-C7	-3.41	124.52	130.34
29	d3	302	PVN	C16-N4-C19	-3.41	106.33	110.67
29	eY	403	PVN	C15-C16-C17	3.41	133.70	126.95
29	D2	303	PVN	C9-C10-C11	-3.40	124.74	128.81
29	gy	304	PVN	C15-C14-N3	3.40	132.05	124.93
29	Y9	303	PVN	C41-C7-C8	-3.40	118.54	124.94
29	b8	1004	PVN	C16-N4-C19	-3.40	106.35	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b9	405	PVN	C16-N4-C19	-3.40	106.35	110.67
29	D2	303	PVN	C16-N4-C19	-3.39	106.35	110.67
29	dw	404	PVN	C9-C10-C11	-3.39	124.76	128.81
29	aY	403	PVN	C16-N4-C19	-3.39	106.35	110.67
29	D2	303	PVN	C21-C2-C3	3.39	136.64	129.67
29	d3	302	PVN	C21-C2-C3	3.39	136.64	129.67
29	eZ	402	PVN	C15-C16-C17	3.39	133.66	126.95
29	T8	303	PVN	C41-C7-C8	-3.38	118.56	124.94
29	e8	303	PVN	C5-C6-C7	-3.38	124.57	130.34
29	eY	403	PVN	C10-C11-N3	-3.38	124.14	128.83
29	Y9	303	PVN	C9-C10-C11	-3.37	124.78	128.81
29	eZ	402	PVN	C10-C11-N3	-3.37	124.15	128.83
29	bY	1004	PVN	C16-N4-C19	-3.37	106.38	110.67
29	dx	405	PVN	O19-C19-C18	-3.35	124.41	128.04
29	T8	303	PVN	C9-C10-C11	-3.35	124.81	128.81
29	T8	303	PVN	C16-N4-C19	-3.34	106.41	110.67
29	Y9	303	PVN	C16-N4-C19	-3.34	106.41	110.67
29	ez	1004	PVN	C16-N4-C19	-3.34	106.41	110.67
29	ly	404	PVN	C16-N4-C19	-3.30	106.47	110.67
29	lz	403	PVN	C16-N4-C19	-3.30	106.47	110.67
29	D2	303	PVN	C51-C8-C7	-3.28	117.81	127.25
29	d3	302	PVN	C51-C8-C7	-3.28	117.81	127.25
26	dO	202	PEB	OA-C1A-C2A	-3.28	123.56	126.17
26	M7	1001	PEB	OA-C1A-C2A	-3.28	123.57	126.17
26	dO	201	PEB	OA-C1A-C2A	-3.27	123.57	126.17
28	T7	203	PUB	OD-C4D-C3D	-3.26	124.50	128.04
26	q7	201	PEB	OA-C1A-C2A	-3.26	123.58	126.17
26	n9	201	PEB	OA-C1A-C2A	-3.26	123.58	126.17
28	eX	202	PUB	OD-C4D-C3D	-3.25	124.51	128.04
26	e7	201	PEB	OA-C1A-C2A	-3.25	123.59	126.17
28	eT	203	PUB	OD-C4D-C3D	-3.25	124.51	128.04
26	cg	201	PEB	OA-C1A-C2A	-3.25	123.59	126.17
26	Y5	1003	PEB	OA-C1A-C2A	-3.25	123.59	126.17
26	cB	201	PEB	OA-C1A-C2A	-3.25	123.59	126.17
26	bE	201	PEB	OA-C1A-C2A	-3.25	123.59	126.17
26	G5	201	PEB	OA-C1A-C2A	-3.24	123.59	126.17
26	el	201	PEB	OA-C1A-C2A	-3.24	123.59	126.17
28	bN	203	PUB	OD-C4D-C3D	-3.24	124.52	128.04
26	x3	201	PEB	OA-C1A-C2A	-3.24	123.59	126.17
26	u9	202	PEB	OA-C1A-C2A	-3.24	123.59	126.17
26	bz	202	PEB	OA-C1A-C2A	-3.24	123.59	126.17
26	dP	201	PEB	OA-C1A-C2A	-3.24	123.59	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	eY	403	PVN	C61-C62-C63	-3.24	106.62	113.60
26	lv	201	PEB	OA-C1A-C2A	-3.24	123.59	126.17
29	ly	404	PVN	C15-C16-N4	-3.24	119.10	126.06
26	cV	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	eT	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
28	y8	203	PUB	OD-C4D-C3D	-3.24	124.52	128.04
26	eQ	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	fn	1001	PEB	OA-C1A-C2A	-3.24	123.60	126.17
28	di	203	PUB	OD-C4D-C3D	-3.24	124.53	128.04
26	V3	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	G8	202	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	aU	202	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	i5	201	PEB	OA-C1A-C2A	-3.24	123.60	126.17
26	gt	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
28	y7	203	PUB	OD-C4D-C3D	-3.23	124.53	128.04
26	p2	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	r5	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	bQ	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	cd	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	dA	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	hF	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
28	B6	203	PUB	OD-C4D-C3D	-3.23	124.53	128.04
26	K7	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	O7	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	P7	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	cI	201	PEB	OA-C1A-C2A	-3.23	123.60	126.17
26	L9	201	PEB	OA-C1A-C2A	-3.23	123.61	126.17
28	bY	1006	PUB	OD-C4D-C3D	-3.23	124.54	128.04
26	H4	202	PEB	OA-C1A-C2A	-3.23	123.61	126.17
26	dv	201	PEB	OA-C1A-C2A	-3.23	123.61	126.17
29	eZ	402	PVN	C61-C62-C63	-3.23	106.66	113.60
26	B4	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	c6	1002	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	gf	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
28	p2	203	PUB	OD-C4D-C3D	-3.22	124.54	128.04
28	ax	202	PUB	OD-C4D-C3D	-3.22	124.54	128.04
28	J5	203	PUB	OD-C4D-C3D	-3.22	124.54	128.04
28	gt	203	PUB	OD-C4D-C3D	-3.22	124.54	128.04
26	V7	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	dx	403	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	dI	1002	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	o4	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K6	202	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	cU	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	fb	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
28	bD	203	PUB	OD-C4D-C3D	-3.22	124.55	128.04
26	h4	202	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	Z7	201	PEB	OA-C1A-C2A	-3.22	123.61	126.17
26	aY	402	PEB	OA-C1A-C2A	-3.22	123.61	126.17
28	H2	202	PUB	OD-C4D-C3D	-3.22	124.55	128.04
28	T8	305	PUB	OD-C4D-C3D	-3.22	124.55	128.04
28	aB	203	PUB	OD-C4D-C3D	-3.22	124.55	128.04
28	gd	202	PUB	OD-C4D-C3D	-3.22	124.55	128.04
26	s7	201	PEB	OA-C1A-C2A	-3.22	123.62	126.17
26	eS	201	PEB	OA-C1A-C2A	-3.22	123.62	126.17
26	jL	1001	PEB	OA-C1A-C2A	-3.22	123.62	126.17
28	aL	203	PUB	OD-C4D-C3D	-3.22	124.55	128.04
26	G8	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	cw	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	dK	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	dW	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	J4	203	PUB	OD-C4D-C3D	-3.21	124.55	128.04
28	34	1005	PUB	OD-C4D-C3D	-3.21	124.55	128.04
28	Z5	305	PUB	OD-C4D-C3D	-3.21	124.55	128.04
28	bL	203	PUB	OD-C4D-C3D	-3.21	124.55	128.04
26	e6	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	N9	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	bl	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	ly	405	PUB	OD-C4D-C3D	-3.21	124.55	128.04
28	lz	404	PUB	OD-C4D-C3D	-3.21	124.55	128.04
28	jO	1003	PUB	OD-C4D-C3D	-3.21	124.55	128.04
26	l3	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	I5	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	f8	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	T6	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	bB	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	R9	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	bJ	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
29	A2	1004	PVN	C10-C11-N3	-3.21	124.37	128.83
29	a3	1004	PVN	C10-C11-N3	-3.21	124.37	128.83
26	N5	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	j6	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	bu	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	lm	1001	PEB	OA-C1A-C2A	-3.21	123.62	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fc	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	F7	202	PUB	OD-C4D-C3D	-3.21	124.56	128.04
26	P3	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	t9	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	aJ	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	kQ	1003	PUB	OD-C4D-C3D	-3.21	124.56	128.04
26	S5	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	d7	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	Z9	1003	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	aM	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	aN	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	fs	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	Q8	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	cM	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	cN	202	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	lp	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	kS	1003	PUB	OD-C4D-C3D	-3.21	124.56	128.04
26	L8	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	by	1002	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	dm	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	dC	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	dY	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	ff	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	r4	202	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	r5	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	b8	1006	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	X6	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
28	bP	203	PUB	OD-C4D-C3D	-3.21	124.56	128.04
26	g2	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	M7	1002	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	v8	202	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	S9	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
26	aI	201	PEB	OA-C1A-C2A	-3.21	123.62	126.17
28	D2	305	PUB	OD-C4D-C3D	-3.21	124.56	128.04
26	G2	202	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	N2	202	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	W2	202	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	W6	201	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	p8	201	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	U7	201	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	aG	201	PEB	OA-C1A-C2A	-3.20	123.62	126.17
26	cC	1001	PEB	OA-C1A-C2A	-3.20	123.62	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eh	201	PEB	OA-C1A-C2A	-3.20	123.62	126.17
28	fq	203	PUB	OD-C4D-C3D	-3.20	124.56	128.04
28	gr	202	PUB	OD-C4D-C3D	-3.20	124.56	128.04
26	a4	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	E6	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	o6	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	S8	401	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	B9	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	eg	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	Z7	203	PUB	OD-C4D-C3D	-3.20	124.56	128.04
28	aH	203	PUB	OD-C4D-C3D	-3.20	124.56	128.04
28	dK	203	PUB	OD-C4D-C3D	-3.20	124.56	128.04
26	p6	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	r8	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	Y8	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	aO	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	cx	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	dQ	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	eb	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	ey	1003	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	bY	1005	PUB	OD-C4D-C3D	-3.20	124.57	128.04
29	lz	403	PVN	C15-C16-N4	-3.20	119.19	126.06
26	v6	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	d9	302	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	aF	204	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	ew	301	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	eO	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	fi	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	p7	202	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	dr	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	hR	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	Y9	305	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	gk	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
26	s2	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	z2	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	r6	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	l7	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	eN	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	eQ	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	lz	401	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	hW	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	p9	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	cQ	202	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	eR	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
26	z2	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	a5	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	g8	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	c6	1001	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	b9	403	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	Z9	1007	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	av	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	cS	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	es	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	c3	304	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	L6	202	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	X7	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
26	q2	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	R3	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	a3	1003	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	ah	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	bp	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	bW	301	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	dl	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	t4	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	aF	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	ei	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	C2	304	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	cp	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
26	44	301	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	W6	202	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	C7	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
26	bM	201	PEB	OA-C1A-C2A	-3.20	123.63	126.17
28	h3	202	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	r6	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
28	V7	203	PUB	OD-C4D-C3D	-3.20	124.57	128.04
26	s2	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	H3	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	w4	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	C5	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	d6	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	cz	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	dc	203	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	eS	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17
28	b7	202	PUB	OD-C4D-C3D	-3.19	124.57	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B2	502	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	Z3	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	n3	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	G4	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	J4	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	D8	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	K8	202	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	eu	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	lt	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	fh	1001	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	ft	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
26	hS	201	PEB	OA-C1A-C2A	-3.19	123.63	126.17
28	d9	305	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	eH	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	eY	405	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	eZ	404	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	hY	405	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	D2	304	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	T3	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	x6	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	ap	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	ge	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
26	I2	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	Y2	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	d8	302	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	aZ	301	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	hP	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	hV	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
28	L2	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	R4	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	T4	202	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	E8	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	V9	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
26	L3	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	W3	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	u8	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	T7	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	d9	301	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	P8	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	ez	1002	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	eW	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
28	H3	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	bB	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	fm	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	hV	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	iG	1002	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	Z5	306	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	a6	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	n6	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	c7	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	dv	202	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	hG	202	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	hJ	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
26	y6	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	e9	303	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	ez	1001	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	fx	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	gm	1001	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	gu	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
28	v3	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	H7	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	b9	406	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	cB	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	eV	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
26	k4	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	R5	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	R6	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	X8	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	aV	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	bd	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	bh	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	dR	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	lf	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
28	L5	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	n5	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	f8	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	Z6	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	dT	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	fj	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
26	Z4	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	h6	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	j9	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	cq	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	cs	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eA	1001	PEB	OA-C1A-C2A	-3.19	123.64	126.17
28	D3	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	M8	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	fu	202	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	J2	202	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	R6	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	u6	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	d7	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	s7	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	J9	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
28	aN	203	PUB	OD-C4D-C3D	-3.19	124.58	128.04
26	k2	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	D2	302	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	E4	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	Q7	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	v7	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	aE	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	aT	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	bj	201	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	cR	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	dp	202	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	eM	1001	PEB	OA-C1A-C2A	-3.19	123.64	126.17
26	kV	1001	PEB	OA-C1A-C2A	-3.19	123.64	126.17
28	Y5	1005	PUB	OD-C4D-C3D	-3.18	124.58	128.04
28	c8	305	PUB	OD-C4D-C3D	-3.18	124.58	128.04
28	el	203	PUB	OD-C4D-C3D	-3.18	124.58	128.04
28	gv	203	PUB	OD-C4D-C3D	-3.18	124.58	128.04
26	Y2	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	Q3	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	n4	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	E8	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	x9	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	ae	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bo	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	do	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	du	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	en	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
28	z3	203	PUB	OD-C4D-C3D	-3.18	124.58	128.04
28	ev	203	PUB	OD-C4D-C3D	-3.18	124.58	128.04
28	fi	203	PUB	OD-C4D-C3D	-3.18	124.58	128.04
28	gx	203	PUB	OD-C4D-C3D	-3.18	124.58	128.04
26	V2	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y5	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	i8	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	w7	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	e9	302	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	K8	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	ad	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	aK	1002	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bw	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	gj	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
28	P3	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	x4	202	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	x5	202	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	H6	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	D9	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	ee	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	lh	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	iE	1003	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	jM	1003	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	h8	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
26	F2	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	G2	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	C3	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	y3	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	c9	301	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	L8	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	aE	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bs	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bw	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bY	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
28	V2	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	T9	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	bn	202	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	bz	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	cn	202	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	cE	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	dX	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	iC	1003	PUB	OD-C4D-C3D	-3.18	124.59	128.04
26	O4	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	Y4	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	Z4	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	F6	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	i6	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	z7	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	c9	302	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	H8	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	U8	1002	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	E9	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	I9	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bt	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	iF	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
28	34	1006	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	Y5	1006	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	e6	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	c9	304	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	w8	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	dl	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	dH	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	hZ	405	PUB	OD-C4D-C3D	-3.18	124.59	128.04
26	z4	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	b5	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	F6	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	I7	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	X7	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	w8	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	x8	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	bi	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	ds	202	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	dw	402	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	le	201	PEB	OA-C1A-C2A	-3.18	123.64	126.17
26	iC	1001	PEB	OA-C1A-C2A	-3.18	123.64	126.17
28	f3	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	r7	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	A8	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	K8	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	aY	404	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	cz	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	eg	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	ez	1005	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	lr	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	A2	1006	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	N6	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	c6	1004	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	I8	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	N9	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	eF	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	hT	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	kR	1003	PUB	OD-C4D-C3D	-3.18	124.59	128.04
26	j2	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	a6	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	cD	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	eG	202	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	eY	402	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	iA	1001	PEB	OA-C1A-C2A	-3.18	123.65	126.17
28	N2	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	J3	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	T8	304	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	dF	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	jK	1003	PUB	OD-C4D-C3D	-3.18	124.59	128.04
26	X4	202	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	F5	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	N6	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	u6	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	k7	1001	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	y7	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	a8	602	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	q9	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	bm	1002	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	da	1001	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	hI	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
28	ey	1006	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	gy	305	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	hL	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	f2	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	h2	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	B4	203	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	fa	202	PUB	OD-C4D-C3D	-3.18	124.59	128.04
28	kX	1003	PUB	OD-C4D-C3D	-3.18	124.59	128.04
26	e2	202	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	D2	301	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	E2	1001	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	V4	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	A6	1002	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	b6	202	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	af	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	aN	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	bZ	303	PEB	OA-C1A-C2A	-3.18	123.65	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dd	201	PEB	OA-C1A-C2A	-3.18	123.65	126.17
26	ey	1002	PEB	OA-C1A-C2A	-3.18	123.65	126.17
28	P7	203	PUB	OD-C4D-C3D	-3.17	124.59	128.04
28	F9	203	PUB	OD-C4D-C3D	-3.17	124.59	128.04
28	dw	405	PUB	OD-C4D-C3D	-3.17	124.59	128.04
28	gz	306	PUB	OD-C4D-C3D	-3.17	124.59	128.04
26	k3	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	u3	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	aR	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	ej	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	lq	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
28	n8	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	Z9	1006	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	dx	406	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	ld	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	ln	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
27	g1	201	CYC	CMD-C2D-C3D	-3.17	118.96	124.94
26	n5	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	g6	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	K9	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	cl	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	ep	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	er	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
28	p8	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	v9	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	fo	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	H5	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	b9	407	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	eY	404	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	kW	1003	PUB	OD-C4D-C3D	-3.17	124.60	128.04
26	c3	302	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	L4	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	x4	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	H5	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	a7	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	x8	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	P8	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	t9	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	P9	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	V9	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	aP	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	bt	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dM	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	eD	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	eF	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	gy	303	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	iE	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
28	z4	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	T6	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	v7	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
26	r6	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	z6	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	Q9	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	bv	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	cQ	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	fe	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	fr	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	go	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
28	L7	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	b8	1005	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	bs	1004	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	lt	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	hN	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	hX	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
26	w2	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	C4	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	m4	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	u4	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	w6	1002	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	au	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	bV	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	gg	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	hB	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
29	C2	303	PVN	C9-C10-C11	-3.17	125.02	128.81
29	c3	303	PVN	C9-C10-C11	-3.17	125.02	128.81
28	e7	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	x7	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	n9	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	lb	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	n2	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	N3	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	a3	1005	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	x3	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	N4	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	R5	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	D7	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	bo	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	df	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	dj	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	dt	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	lj	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	lx	201	PUB	OD-C4D-C3D	-3.17	124.60	128.04
26	D4	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	H4	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	v4	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	C6	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	q6	202	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	t8	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	j7	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	cP	201	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	hY	401	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	jK	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
26	kR	1001	PEB	OA-C1A-C2A	-3.17	123.65	126.17
28	e9	306	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	aD	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	bT	202	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	kT	1003	PUB	OD-C4D-C3D	-3.17	124.60	128.04
26	U2	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	X3	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	q3	1001	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	l5	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	S6	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	W7	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	I8	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	aq	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	bJ	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	dn	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	dn	202	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	dQ	202	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	eW	202	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	li	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	hD	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	hR	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	iD	1001	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	iG	1001	PEB	OA-C1A-C2A	-3.17	123.66	126.17
28	Z2	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d3	303	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	v6	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	lf	203	PUB	OD-C4D-C3D	-3.17	124.60	128.04
28	iD	1003	PUB	OD-C4D-C3D	-3.17	124.60	128.04
26	K2	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	I3	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	O3	1001	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	b3	501	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	K5	1001	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	B8	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	Y9	302	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	ao	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	cA	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	cX	202	PEB	OA-C1A-C2A	-3.17	123.66	126.17
26	dE	201	PEB	OA-C1A-C2A	-3.17	123.66	126.17
28	v4	203	PUB	OD-C4D-C3D	-3.17	124.61	128.04
28	v5	203	PUB	OD-C4D-C3D	-3.17	124.61	128.04
28	o8	203	PUB	OD-C4D-C3D	-3.17	124.61	128.04
28	C8	203	PUB	OD-C4D-C3D	-3.17	124.61	128.04
28	eL	203	PUB	OD-C4D-C3D	-3.17	124.61	128.04
28	ll	203	PUB	OD-C4D-C3D	-3.17	124.61	128.04
28	X3	202	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	aY	405	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	hY	406	PUB	OD-C4D-C3D	-3.16	124.61	128.04
27	X1	201	CYC	CMD-C2D-C3D	-3.16	118.98	124.94
26	L2	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	s3	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	Q4	203	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	k5	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	D6	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	e9	301	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aF	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dM	1002	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	fo	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	kS	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	R2	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	V3	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	V5	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	ar	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	cr	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	f2	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	w2	203	PEB	OA-C1A-C2A	-3.16	123.66	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P2	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	p3	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	34	1003	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	t4	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	z4	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	c5	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	g7	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	a9	602	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	j9	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bd	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	de	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dk	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	eH	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	eK	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	la	1002	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	kW	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	O8	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	bZ	306	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	ec	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	v2	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	B7	202	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	J7	202	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	U8	1006	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	gg	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	iH	1002	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	jN	1003	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	O5	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	d5	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	P6	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	x7	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	Q8	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	l9	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	ca	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dF	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	gq	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	x2	202	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	N5	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	N7	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	F2	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	A5	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	h6	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	D7	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a8	601	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	a9	603	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aL	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aS	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bA	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	cc	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	cM	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dg	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dx	404	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	ea	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	ej	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	eG	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	fm	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	j2	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	P6	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	R7	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	aZ	305	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	ey	1005	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	fs	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	gi	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	hZ	404	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	F4	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	M4	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	V5	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	l6	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	t6	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	z8	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	az	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bv	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bF	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	cW	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dw	401	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dx	401	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	lb	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	fd	301	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	fp	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	gw	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	P4	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	t5	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	z5	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	gz	305	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	jL	1003	PUB	OD-C4D-C3D	-3.16	124.61	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	l2	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	t2	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	X2	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	p3	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	e9	305	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	cL	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	dL	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	kV	1003	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	S2	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	D3	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	L4	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	s8	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	S7	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	A8	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	q9	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	U9	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aY	401	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bX	402	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dN	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	ga	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	gx	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	hE	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	hT	204	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	hY	403	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	U8	1005	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	hH	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	jJ	1003	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	N4	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	S4	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	W4	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	u6	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	o7	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	M8	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	o9	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	R9	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aL	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aQ	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	cr	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	cZ	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	dj	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	hT	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	C2	305	PUB	OD-C4D-C3D	-3.16	124.61	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n3	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	D6	202	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	l7	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	n7	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
28	x9	203	PUB	OD-C4D-C3D	-3.16	124.61	128.04
26	k2	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	r2	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	u2	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	X2	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	z3	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	G6	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	q8	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	W8	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	m9	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	w9	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aw	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	aS	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bg	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	bu	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	cU	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	eC	202	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	fk	201	PEB	OA-C1A-C2A	-3.16	123.66	126.17
26	kU	1001	PEB	OA-C1A-C2A	-3.16	123.66	126.17
28	V6	203	PUB	OD-C4D-C3D	-3.16	124.62	128.04
28	z7	203	PUB	OD-C4D-C3D	-3.16	124.62	128.04
28	H9	203	PUB	OD-C4D-C3D	-3.16	124.62	128.04
27	K1	201	CYC	CMD-C2D-C3D	-3.16	118.99	124.94
27	n1	201	CYC	CMD-C2D-C3D	-3.16	118.99	124.94
28	A2	1005	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	t3	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	D4	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	dw	406	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	er	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	ly	406	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	o2	1002	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	I4	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	s4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	g5	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	h8	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	m6	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	s6	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	w6	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	H9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ay	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	aC	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ck	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cL	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	do	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	j3	202	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	F6	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	bR	202	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	ez	1006	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	lz	405	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	i2	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	Y3	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	R4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	X4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	c4	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	D5	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	M5	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	s5	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	k8	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ag	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	bc	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cu	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dm	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dG	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	eD	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ls	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	gn	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	T2	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	d8	304	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	cq	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	J6	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	bZ	305	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	cF	202	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	cO	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	m2	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	A3	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	W4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	y4	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	H7	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	c8	302	PEB	OA-C1A-C2A	-3.15	123.67	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F8	1002	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	f9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	aV	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	aZ	302	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	bk	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	bN	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cG	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cP	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dZ	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	eB	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	c3	305	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	g8	202	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	e8	305	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	S3	203	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	24	401	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	f8	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	b8	1003	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	b9	404	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	N8	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	aJ	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	bq	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cR	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ds	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	eE	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	hB	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	hP	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	e2	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	W2	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	v3	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	K4	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	Q5	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	Y5	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	P6	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	o6	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	r7	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	V8	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ai	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ap	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	eT	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	gp	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	hZ	402	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	a3	1006	PUB	OD-C4D-C3D	-3.15	124.62	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	r3	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	Z4	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	d6	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	l6	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	z6	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	c8	304	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	aP	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	cJ	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	F4	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	B5	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	p6	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	cP	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	dh	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	i4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	Q6	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	b8	1002	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	Y8	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cv	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	cO	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dJ	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	jO	1001	PEB	OA-C1A-C2A	-3.15	123.67	126.17
27	u1	1001	CYC	CMD-C2D-C3D	-3.15	119.01	124.94
28	n4	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	an	202	PUB	OD-C4D-C3D	-3.15	124.62	128.04
28	cR	203	PUB	OD-C4D-C3D	-3.15	124.62	128.04
26	O2	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	s9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	at	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	bG	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	bP	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dt	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dB	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	dC	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	ll	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	hC	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	av	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	bV	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	cY	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	en	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	eZ	403	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	ff	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	hD	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	w2	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	t3	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	K4	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	U4	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	V6	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	R7	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	d9	303	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	z9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	T9	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	eU	202	PEB	OA-C1A-C2A	-3.15	123.67	126.17
26	fj	201	PEB	OA-C1A-C2A	-3.15	123.67	126.17
28	P2	203	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	eb	202	PUB	OD-C4D-C3D	-3.15	124.63	128.04
28	z2	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	Z3	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	H4	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	D5	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	b6	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	r9	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
26	t2	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	N3	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	U3	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	r3	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	C8	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	aP	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	bq	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	bO	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	dx	402	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	dF	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	eM	1002	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	lr	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	gl	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	iH	1001	PEB	OA-C1A-C2A	-3.14	123.67	126.17
28	44	305	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	T5	202	PUB	OD-C4D-C3D	-3.14	124.63	128.04
26	Q4	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	q4	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	O8	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	y9	1002	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	bs	1002	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	cK	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	cS	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	db	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	du	203	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	dL	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	ez	1003	PEB	OA-C1A-C2A	-3.14	123.67	126.17
27	W1	201	CYC	CMD-C2D-C3D	-3.14	119.02	124.94
27	o1	1001	CYC	CMD-C2D-C3D	-3.14	119.02	124.94
28	p4	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	p5	202	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	aR	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	aV	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	dP	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	fc	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	jI	1003	PUB	OD-C4D-C3D	-3.14	124.63	128.04
26	r2	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	Q2	1001	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	M4	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	V4	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	f4	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	t5	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	B6	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	U8	1003	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	ar	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	aN	204	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	aW	301	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	ba	1001	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	cm	1001	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	dK	202	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	ee	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	gs	201	PEB	OA-C1A-C2A	-3.14	123.67	126.17
26	iB	1001	PEB	OA-C1A-C2A	-3.14	123.67	126.17
28	R3	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	t7	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	dx	407	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	fy	202	PUB	OD-C4D-C3D	-3.14	124.63	128.04
29	hZ	403	PVN	O19-C19-C18	-3.14	124.63	128.04
28	F2	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	B3	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	z9	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	az	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
27	N1	201	CYC	CMD-C2D-C3D	-3.14	119.02	124.94
26	O2	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	44	302	PEB	OA-C1A-C2A	-3.14	123.68	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u5	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	I6	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	L6	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	aA	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	aX	402	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	bm	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	du	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	fa	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	jN	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
28	F3	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	t6	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	G8	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	L9	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	bq	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	cH	202	PUB	OD-C4D-C3D	-3.14	124.63	128.04
27	Q1	201	CYC	CMD-C2D-C3D	-3.14	119.02	124.94
26	E3	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	J4	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	S4	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	b4	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	o4	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	Z6	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	y8	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	h9	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	v9	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	aR	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	bf	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	cV	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	cV	203	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	cW	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	eI	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	fw	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
27	V1	201	CYC	CMD-C2D-C3D	-3.14	119.02	124.94
28	Z9	1005	PUB	OD-C4D-C3D	-3.14	124.63	128.04
28	ga	203	PUB	OD-C4D-C3D	-3.14	124.63	128.04
26	Q4	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	y4	1002	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	k6	1002	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	N8	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	aJ	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	bh	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	bC	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cT	1002	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	dI	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	dX	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	eo	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	gz	301	PEB	OA-C1A-C2A	-3.14	123.68	126.17
27	G1	1001	CYC	CMD-C2D-C3D	-3.14	119.03	124.94
27	U1	201	CYC	CMD-C2D-C3D	-3.14	119.03	124.94
27	d2	101	CYC	CMD-C2D-C3D	-3.14	119.03	124.94
28	dD	203	PUB	OD-C4D-C3D	-3.14	124.64	128.04
29	gz	304	PVN	C52-C51-C8	-3.14	107.27	112.62
27	I1	201	CYC	CMD-C2D-C3D	-3.14	119.03	124.94
26	g2	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	q2	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	y2	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	J2	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	B3	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	U4	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	Y4	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	u4	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	v6	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	w9	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	A9	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	la	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	lb	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	ff	204	PEB	OA-C1A-C2A	-3.14	123.68	126.17
28	d3	304	PUB	OD-C4D-C3D	-3.14	124.64	128.04
28	F5	203	PUB	OD-C4D-C3D	-3.14	124.64	128.04
28	jP	1003	PUB	OD-C4D-C3D	-3.14	124.64	128.04
26	K3	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	e3	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	b6	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	i6	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	B8	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	D8	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	ce	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	cy	1001	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	dt	202	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	fv	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
26	hJ	201	PEB	OA-C1A-C2A	-3.14	123.68	126.17
28	Y9	304	PUB	OD-C4D-C3D	-3.14	124.64	128.04
28	aT	203	PUB	OD-C4D-C3D	-3.14	124.64	128.04
28	fw	203	PUB	OD-C4D-C3D	-3.14	124.64	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	l3	202	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	P5	202	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	a7	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
26	l2	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	m2	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	u2	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	M2	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	t7	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	M8	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	i9	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	p9	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	D9	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	dc	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	dA	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	fq	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
27	b1	1001	CYC	CMD-C2D-C3D	-3.13	119.03	124.94
28	gy	306	PUB	OD-C4D-C3D	-3.13	124.64	128.04
26	h2	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	i2	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	x2	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	I2	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	d4	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	B5	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	K6	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	M6	1002	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	O6	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	U6	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	e8	302	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	W8	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	t9	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	dT	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	ed	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	eI	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	eJ	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	gi	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
28	at	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	cs	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	dd	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	eD	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
26	X5	401	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	f7	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	y9	1001	PEB	OA-C1A-C2A	-3.13	123.68	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eK	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
28	L3	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	y6	204	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	dp	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
27	e1	201	CYC	CMD-C2D-C3D	-3.13	119.04	124.94
27	z1	201	CYC	C2A-C1A-NA	3.13	114.60	110.05
28	ep	203	PUB	OD-C4D-C3D	-3.13	124.64	128.04
26	o2	1001	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	A2	1002	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	o3	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	O4	1002	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	P4	202	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	l4	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	v5	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	w5	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	l9	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	al	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	ci	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
26	hQ	201	PEB	OA-C1A-C2A	-3.13	123.68	126.17
28	44	304	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	e8	304	PUB	OD-C4D-C3D	-3.13	124.64	128.04
28	lv	202	PUB	OD-C4D-C3D	-3.13	124.64	128.04
27	s1	201	CYC	CMD-C2D-C3D	-3.13	119.04	124.94
26	C2	302	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	I4	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	Z5	303	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	I8	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	bK	1001	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	dP	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	dU	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	ly	401	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	hN	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	kX	1001	PEB	OA-C1A-C2A	-3.13	123.69	126.17
28	co	202	PUB	OD-C4D-C3D	-3.13	124.64	128.04
26	B2	501	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	M3	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	g3	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	R4	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	Z5	301	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	l8	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	x6	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	Z8	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p9	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	aa	1001	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	ab	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	cM	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	dq	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	fd	302	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	gb	1001	PEB	OA-C1A-C2A	-3.13	123.69	126.17
28	gp	203	PUB	OD-C4D-C3D	-3.13	124.65	128.04
27	R1	1001	CYC	CMD-C2D-C3D	-3.13	119.05	124.94
27	i1	1001	CYC	CMD-C2D-C3D	-3.13	119.05	124.94
28	eB	204	PUB	OD-C4D-C3D	-3.13	124.65	128.04
26	m8	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	m6	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	z8	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	s9	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	aj	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	am	1001	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	bx	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	bD	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	cE	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	eV	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	lu	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	ge	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
29	A2	1004	PVN	C15-C16-N4	-3.13	119.35	126.06
29	a3	1004	PVN	C15-C16-N4	-3.13	119.35	126.06
26	y2	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	m5	1001	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	l8	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	H8	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	J8	202	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	u9	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	aA	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
26	es	201	PEB	OA-C1A-C2A	-3.13	123.69	126.17
28	r2	203	PUB	OD-C4D-C3D	-3.13	124.65	128.04
28	iF	1003	PUB	OD-C4D-C3D	-3.13	124.65	128.04
27	Z1	201	CYC	CMD-C2D-C3D	-3.12	119.05	124.94
26	g4	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	j4	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	L5	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	j5	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	j5	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	x5	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A6	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	g6	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aB	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	dD	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	hL	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	hX	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
27	q1	201	CYC	CMD-C2D-C3D	-3.12	119.05	124.94
27	k1	201	CYC	CMD-C2D-C3D	-3.12	119.05	124.94
27	y1	201	CYC	CMD-C2D-C3D	-3.12	119.05	124.94
26	e4	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	W5	301	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	k8	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	z6	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	cT	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	di	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	dH	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
27	O1	201	CYC	CMD-C2D-C3D	-3.12	119.06	124.94
26	34	1007	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aM	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aU	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	bs	1003	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	dy	401	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	ed	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	eZ	401	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	hA	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
27	P1	201	CYC	CMD-C2D-C3D	-3.12	119.06	124.94
27	d1	1001	CYC	CMD-C2D-C3D	-3.12	119.06	124.94
27	w1	201	CYC	CMD-C2D-C3D	-3.12	119.06	124.94
28	aZ	304	PUB	OD-C4D-C3D	-3.12	124.65	128.04
27	f1	201	CYC	CMD-C2D-C3D	-3.12	119.06	124.94
26	S3	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	T3	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	k8	203	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	E6	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	M6	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	k6	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	F8	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	bS	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	jJ	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
27	v1	201	CYC	C2A-C1A-NA	3.12	114.59	110.05
28	bp	202	PUB	OD-C4D-C3D	-3.12	124.66	128.04
26	R2	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	m3	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	y6	203	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	w8	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aC	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aK	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	br	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	by	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	cX	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	dr	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	eH	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	lp	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	ly	403	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	lz	402	PEB	OA-C1A-C2A	-3.12	123.69	126.17
27	H1	201	CYC	C2A-C1A-NA	3.12	114.59	110.05
27	L1	201	CYC	CMD-C2D-C3D	-3.12	119.06	124.94
28	dn	203	PUB	OD-C4D-C3D	-3.12	124.66	128.04
26	F3	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	f3	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	E4	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	t4	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	T5	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	G7	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	n7	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	z9	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	cO	202	PEB	OA-C1A-C2A	-3.12	123.69	126.17
28	X4	203	PUB	OD-C4D-C3D	-3.12	124.66	128.04
28	c9	305	PUB	OD-C4D-C3D	-3.12	124.66	128.04
28	dY	203	PUB	OD-C4D-C3D	-3.12	124.66	128.04
27	a1	201	CYC	CMD-C2D-C3D	-3.12	119.07	124.94
26	v2	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	e5	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	m7	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	J8	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aB	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	aQ	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	eq	201	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	ly	402	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	gy	301	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	hM	1001	PEB	OA-C1A-C2A	-3.12	123.69	126.17
26	n2	201	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	J6	201	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	f6	201	PEB	OA-C1A-C2A	-3.12	123.70	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	i7	201	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	T8	301	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	bn	201	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	bZ	301	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	dN	201	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	dW	202	PEB	OA-C1A-C2A	-3.12	123.70	126.17
26	K2	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	b3	502	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	U5	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	o8	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	N7	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	v8	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	cN	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	dz	401	PEB	OA-C1A-C2A	-3.11	123.70	126.17
28	dV	203	PUB	OD-C4D-C3D	-3.11	124.66	128.04
28	gn	203	PUB	OD-C4D-C3D	-3.11	124.66	128.04
26	T4	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	G9	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	aY	406	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	be	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	bR	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	dG	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	ea	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	hO	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	A4	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	x6	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	aH	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	cb	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	ch	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	ek	1001	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	eR	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	eU	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	li	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	gc	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	gh	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
28	V4	203	PUB	OD-C4D-C3D	-3.11	124.66	128.04
28	eN	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
27	m1	201	CYC	CMD-C2D-C3D	-3.11	119.08	124.94
26	i3	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	j8	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	m8	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	S6	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T8	302	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	dz	402	PEB	OA-C1A-C2A	-3.11	123.70	126.17
28	L4	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
28	dR	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
26	T2	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	o5	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	q6	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	F9	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	dk	1002	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	gv	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
28	P9	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
28	br	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
28	kU	1003	PUB	OD-C4D-C3D	-3.11	124.67	128.04
26	H6	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	Z6	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	g9	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	J9	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	bl	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	eC	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	gz	303	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	jM	1001	PEB	OA-C1A-C2A	-3.11	123.70	126.17
28	B9	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
28	eJ	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
26	p4	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	C6	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	u7	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	U8	1001	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	dw	403	PEB	OA-C1A-C2A	-3.11	123.70	126.17
28	bH	203	PUB	OD-C4D-C3D	-3.11	124.67	128.04
26	l5	202	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	r9	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	dq	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	ef	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	lq	201	PEB	OA-C1A-C2A	-3.11	123.70	126.17
26	fd	303	PEB	OA-C1A-C2A	-3.11	123.70	126.17
27	a2	901	CYC	C2A-C1A-NA	3.10	114.56	110.05
26	y6	201	PEB	OA-C1A-C2A	-3.10	123.70	126.17
26	h7	201	PEB	OA-C1A-C2A	-3.10	123.70	126.17
26	b8	1001	PEB	OA-C1A-C2A	-3.10	123.70	126.17
26	a9	601	PEB	OA-C1A-C2A	-3.10	123.70	126.17
26	b9	402	PEB	OA-C1A-C2A	-3.10	123.70	126.17
26	Q8	201	PEB	OA-C1A-C2A	-3.10	123.70	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	df	201	PEB	OA-C1A-C2A	-3.10	123.70	126.17
28	bF	203	PUB	OD-C4D-C3D	-3.10	124.67	128.04
28	dB	202	PUB	OD-C4D-C3D	-3.10	124.67	128.04
27	c1	201	CYC	C2A-C1A-NA	3.10	114.56	110.05
26	Y7	1001	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	e8	301	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	E8	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	O8	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
27	S1	201	CYC	C2A-C1A-NA	3.10	114.56	110.05
27	j1	201	CYC	C2A-C1A-NA	3.10	114.56	110.05
26	C2	301	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	w3	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	bY	1003	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	dp	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	dH	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	eP	203	PEB	OA-C1A-C2A	-3.10	123.71	126.17
29	D2	303	PVN	C41-C7-C8	-3.10	119.09	124.94
29	d3	302	PVN	C41-C7-C8	-3.10	119.09	124.94
26	Z9	1001	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	aH	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	aI	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	bz	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	cC	1003	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	eq	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	lc	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	fl	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
28	eP	204	PUB	OD-C4D-C3D	-3.10	124.68	128.04
27	S1	202	CYC	C2A-C1A-NA	3.10	114.56	110.05
26	J3	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	P4	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	X6	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	aD	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	C9	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	M9	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	ln	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
28	et	203	PUB	OD-C4D-C3D	-3.10	124.68	128.04
26	cj	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
28	dN	203	PUB	OD-C4D-C3D	-3.10	124.68	128.04
26	Y6	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	A8	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	r9	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	aT	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eE	202	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	lk	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	gk	201	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	jP	1001	PEB	OA-C1A-C2A	-3.10	123.71	126.17
26	kQ	1001	PEB	OA-C1A-C2A	-3.10	123.71	126.17
27	Y1	201	CYC	CAB-C3B-C4B	3.09	126.27	121.38
26	q5	201	PEB	OA-C1A-C2A	-3.09	123.71	126.17
26	aX	401	PEB	OA-C1A-C2A	-3.09	123.71	126.17
26	bX	401	PEB	OA-C1A-C2A	-3.09	123.71	126.17
26	hK	201	PEB	OA-C1A-C2A	-3.09	123.71	126.17
27	p1	201	CYC	C2A-C1A-NA	3.09	114.55	110.05
26	j8	201	PEB	OA-C1A-C2A	-3.09	123.71	126.17
26	as	201	PEB	OA-C1A-C2A	-3.09	123.71	126.17
26	bb	201	PEB	OA-C1A-C2A	-3.09	123.71	126.17
26	dR	201	PEB	OA-C1A-C2A	-3.09	123.71	126.17
27	c1	201	CYC	CAB-C3B-C4B	3.09	126.26	121.38
27	t1	201	CYC	C2A-C1A-NA	3.09	114.55	110.05
26	J5	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	h5	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	dT	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	jI	1001	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	kT	1001	PEB	OA-C1A-C2A	-3.09	123.72	126.17
27	a2	902	CYC	CAB-C3B-C4B	3.09	126.26	121.38
27	b2	1001	CYC	CAB-C3B-C4B	3.09	126.26	121.38
26	c6	1003	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	s6	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	b7	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
29	b9	405	PVN	C9-C10-C11	-3.09	125.12	128.81
26	t2	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	M2	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	q4	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	h9	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	br	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	cY	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
27	J1	201	CYC	CAB-C3B-C4B	3.09	126.26	121.38
26	bH	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	bI	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	cp	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
29	ez	1004	PVN	C91-C18-C17	-3.09	122.25	127.53
27	M1	1001	CYC	C2A-C1A-NA	3.09	114.54	110.05
27	S1	201	CYC	CAB-C3B-C4B	3.09	126.25	121.38
27	j1	201	CYC	CAB-C3B-C4B	3.09	126.25	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	j6	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	O9	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	dr	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	eP	202	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	hH	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
29	T8	303	PVN	C21-C2-C3	3.09	136.01	129.67
26	Q6	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
26	dS	201	PEB	OA-C1A-C2A	-3.09	123.72	126.17
29	b8	1004	PVN	C9-C10-C11	-3.08	125.12	128.81
27	a2	902	CYC	C2A-C1A-NA	3.08	114.53	110.05
27	b2	1001	CYC	C2A-C1A-NA	3.08	114.53	110.05
26	T6	201	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	dD	201	PEB	OA-C1A-C2A	-3.08	123.72	126.17
27	h1	201	CYC	C2A-C1A-NA	3.08	114.53	110.05
26	f9	202	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	b3	501	PEB	CMD-C2D-C3D	-3.08	125.72	130.06
27	v1	201	CYC	CAB-C3B-C4B	3.08	126.25	121.38
26	E7	201	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	c7	201	PEB	OA-C1A-C2A	-3.08	123.72	126.17
26	eR	202	PEB	OA-C1A-C2A	-3.08	123.72	126.17
29	hY	404	PVN	O19-C19-C18	-3.08	124.70	128.04
29	gy	304	PVN	C71-C13-C14	-3.08	120.32	125.06
26	bj	202	PEB	OA-C1A-C2A	-3.08	123.72	126.17
27	J1	201	CYC	C2A-C1A-NA	3.08	114.53	110.05
27	Y1	201	CYC	C2A-C1A-NA	3.08	114.53	110.05
29	b9	405	PVN	C91-C18-C17	-3.08	122.27	127.53
26	G4	201	PEB	OA-C1A-C2A	-3.08	123.73	126.17
26	bx	202	PEB	OA-C1A-C2A	-3.08	123.73	126.17
29	Y9	303	PVN	C21-C2-C3	3.08	135.99	129.67
29	ey	1004	PVN	C91-C18-C17	-3.08	122.27	127.53
27	S1	202	CYC	CAB-C3B-C4B	3.08	126.24	121.38
27	h1	201	CYC	CAB-C3B-C4B	3.08	126.24	121.38
26	o8	202	PEB	CMD-C2D-C3D	-3.07	125.73	130.06
26	F4	202	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	Z2	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	a3	1001	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	x9	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	eF	202	PEB	OA-C1A-C2A	-3.07	123.73	126.17
27	r1	201	CYC	C2A-C1A-NA	3.07	114.52	110.05
26	em	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	ct	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	cG	201	PEB	CMD-C2D-C3D	-3.07	125.73	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ai	201	PEB	CMD-C2D-C3D	-3.07	125.74	130.06
26	dV	201	PEB	OA-C1A-C2A	-3.07	123.73	126.17
27	t1	201	CYC	CAB-C3B-C4B	3.07	126.22	121.38
27	M1	1001	CYC	CAB-C3B-C4B	3.07	126.22	121.38
29	34	1004	PVN	O19-C19-C18	-3.07	124.71	128.04
29	Y5	1004	PVN	O19-C19-C18	-3.07	124.71	128.04
27	r1	201	CYC	CAB-C3B-C4B	3.07	126.22	121.38
27	a2	901	CYC	CAB-C3B-C4B	3.07	126.22	121.38
26	b9	401	PEB	OA-C1A-C2A	-3.07	123.73	126.17
26	aW	302	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	dX	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	eo	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	b8	1002	PEB	CMD-C2D-C3D	-3.06	125.74	130.06
26	j7	201	PEB	CMD-C2D-C3D	-3.06	125.74	130.06
26	bS	201	PEB	CMD-C2D-C3D	-3.06	125.74	130.06
26	O6	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
27	p1	201	CYC	CAB-C3B-C4B	3.06	126.22	121.38
26	bJ	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
27	H1	201	CYC	CAB-C3B-C4B	3.06	126.22	121.38
26	eT	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
27	z1	201	CYC	CAB-C3B-C4B	3.06	126.21	121.38
26	t5	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	eM	1001	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	p8	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	v2	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	I6	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	l6	202	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	dh	201	PEB	OA-C1A-C2A	-3.06	123.74	126.17
26	F4	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	ep	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	v5	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	T7	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	cJ	201	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	l5	202	PEB	CMD-C2D-C3D	-3.06	125.75	130.06
26	E5	201	PEB	OA-C1A-C2A	-3.05	123.74	126.17
26	cJ	201	PEB	OA-C1A-C2A	-3.05	123.74	126.17
26	y6	202	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	N8	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	iF	1001	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	ac	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	dn	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	dR	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L9	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	gu	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	bL	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	bU	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	l8	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	E6	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	aT	201	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	dC	202	PEB	CMD-C2D-C3D	-3.05	125.76	130.06
26	ez	1001	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	G4	202	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	W6	201	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	I9	201	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	cA	201	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	G3	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	e3	1001	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	ew	301	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	jN	1001	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	kX	1001	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	z5	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	ak	201	PEB	OA-C1A-C2A	-3.05	123.75	126.17
26	cS	202	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	dO	201	PEB	CMD-C2D-C3D	-3.05	125.77	130.06
26	t2	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	cr	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	fr	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
29	gy	304	PVN	C15-C16-C17	3.04	132.98	126.95
26	bG	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	X4	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	x5	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	bH	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	dx	401	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	eO	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	fl	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	af	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	aK	1001	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	bE	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	bO	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	ct	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	S9	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	eq	202	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
26	hL	201	PEB	CMD-C2D-C3D	-3.04	125.77	130.06
29	b8	1004	PVN	C91-C18-C17	-3.04	122.33	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B3	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	d9	301	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eD	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	gz	303	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	s4	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	c9	302	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	al	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bg	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bD	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	dM	1001	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	h2	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	y4	1002	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	F6	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	w8	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bw	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	ck	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	cR	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	V4	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	O5	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	V5	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	J6	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	P8	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	ea	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eu	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	ff	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	fo	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	S4	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	H5	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	m6	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	A8	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bZ	303	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eH	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bM	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	du	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eE	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	U3	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	o6	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	y8	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bW	301	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	iB	1001	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
27	H1	201	CYC	CMD-C2D-C3D	-3.04	119.22	124.94
26	k7	1001	PEB	CMD-C2D-C3D	-3.04	125.78	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	I8	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	ar	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bu	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	cC	1001	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eo	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eG	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	A4	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	L5	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	t7	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	Q8	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	ad	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bh	202	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	bQ	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	cN	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	eQ	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	fs	201	PEB	CMD-C2D-C3D	-3.04	125.78	130.06
26	l3	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	e6	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	u9	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	V3	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	G7	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	o7	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	bi	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	cY	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	eb	201	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	gb	1001	PEB	CMD-C2D-C3D	-3.03	125.78	130.06
26	G2	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	x4	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	Y5	1003	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	p9	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dG	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	eg	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	eP	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	U4	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	k8	203	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	l8	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	U7	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	f9	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bb	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bv	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dx	403	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dN	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	hY	404	PVN	C91-C18-C17	-3.03	122.34	127.53
27	J1	201	CYC	CMD-C2D-C3D	-3.03	119.22	124.94
27	Y1	201	CYC	CMD-C2D-C3D	-3.03	119.22	124.94
26	K4	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	d5	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	k5	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	t8	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	T8	301	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bN	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	Q4	203	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	b6	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	E7	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	H7	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	W7	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	c8	302	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bn	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	ef	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	ez	1003	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
27	p1	201	CYC	CMD-C2D-C3D	-3.03	119.23	124.94
26	n5	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	F8	1002	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	I8	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	aX	402	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bz	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	cd	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dh	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	kV	1001	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	v2	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	q6	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	s6	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	y6	203	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	z8	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	F8	1001	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	P9	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	aQ	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	eR	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	M2	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	aV	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dK	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dM	1002	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	gz	301	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	iE	1001	PEB	CMD-C2D-C3D	-3.03	125.79	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	i2	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	I2	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	C3	1001	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	X6	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	L8	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bp	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	bX	401	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	gy	301	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
27	z1	201	CYC	CMD-C2D-C3D	-3.03	119.23	124.94
26	t4	202	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	z7	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	M9	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	aU	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	cq	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	dC	201	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	ly	401	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	hE	1001	PEB	CMD-C2D-C3D	-3.03	125.79	130.06
26	N3	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	44	301	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	e5	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	D7	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	Q7	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	E8	202	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	aL	202	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	cm	1001	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	er	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	eF	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	gy	303	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	o2	1002	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	i3	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	J4	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	B5	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	g5	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	x6	202	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	N9	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	dV	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	ln	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	fj	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	gi	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	gs	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	O2	202	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	v6	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	by	1002	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	lf	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	fw	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	gv	201	PEB	CMD-C2D-C3D	-3.03	125.80	130.06
26	X4	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	i6	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	C8	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aN	204	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	cu	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dX	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	eh	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	eI	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	fp	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	jM	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	M3	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	F4	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	k4	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	M6	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	G8	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	U8	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	Y8	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aY	401	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	bA	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dx	404	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dY	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	hT	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	J4	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	R5	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	A6	1002	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	T6	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aA	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dz	401	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	eW	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	j2	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	n2	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	C7	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	j9	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	J9	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aH	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aH	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aK	1002	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	bV	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cO	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	eQ	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	a3	1003	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	l5	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	G6	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	Z6	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	b9	403	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	w8	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	B8	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	bF	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	bI	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	ch	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dD	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	fk	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
27	a2	902	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
27	b2	1001	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
26	p2	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	X3	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	Z5	303	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	t6	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	w6	1002	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	T8	302	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	G9	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	V9	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	aJ	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	bs	1002	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	cx	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	cP	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	cV	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	hC	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
27	r1	201	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
26	z2	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	r3	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	z3	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	L4	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	O4	1002	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	b4	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	h4	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	m4	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	y4	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	F5	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	Z5	301	PEB	CMD-C2D-C3D	-3.02	125.80	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k6	1002	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	z9	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	bL	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	ci	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	cV	203	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dn	202	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dE	201	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	dI	1001	PEB	CMD-C2D-C3D	-3.02	125.80	130.06
26	B2	502	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	R3	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	T3	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	a6	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	h6	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	a9	601	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	H8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	q9	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	aR	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	aS	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	be	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	cc	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dW	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	gn	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	gt	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
27	c1	201	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
27	a2	901	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
26	D3	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	W8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ao	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bd	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dm	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dq	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dw	401	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dQ	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	es	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	iH	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	kU	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	q4	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	S5	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	w5	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	j8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	k8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	K6	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	l6	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	v6	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	G8	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	aA	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bt	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	do	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ej	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	eY	402	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	fa	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ga	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	P4	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	g4	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	l4	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	S6	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	P7	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	O8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	Y9	302	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	aB	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	cl	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ek	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	la	1002	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	gc	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	X9	401	PEB	OA-C1A-C2A	-3.02	123.77	126.17
26	P2	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	v3	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	N4	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	t9	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	cg	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	df	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dX	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ed	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ly	402	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
27	M1	1001	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
26	C2	302	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	U2	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	i4	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	j5	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	I6	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	I6	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	c9	301	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	x8	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	aR	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cz	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	da	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dO	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
27	t1	201	CYC	CMD-C2D-C3D	-3.02	119.25	124.94
29	hZ	403	PVN	C91-C18-C17	-3.02	122.37	127.53
26	Y2	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	34	1007	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	L6	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	N6	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	D8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	o9	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	A9	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bc	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dc	203	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dZ	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	eC	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	eN	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	ll	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	fc	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	iD	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	r2	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	R4	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	m8	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	S6	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	c6	1002	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	i7	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	Q8	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bl	202	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bm	1001	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bC	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	bP	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	cL	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	cR	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	dB	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	eC	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	li	201	PEB	CMD-C2D-C3D	-3.02	125.81	130.06
26	eO	201	PEB	OA-C1A-C2A	-3.01	123.78	126.17
26	o4	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	P6	202	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	W6	202	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	b8	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	b9	402	PEB	CMD-C2D-C3D	-3.01	125.81	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bj	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	bl	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	cp	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	ee	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	hY	401	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	o2	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	w2	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	o3	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	K5	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	X5	401	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	M6	1002	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	s6	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	K7	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	y7	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	v8	202	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	aE	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	aE	202	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	ba	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	bk	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	cI	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	dd	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	dr	202	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	dF	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	dI	1002	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	eP	203	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	lm	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	hV	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	k2	202	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	A2	1002	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	D2	302	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	E2	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	O7	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	e9	302	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	O9	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	aP	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	br	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	bK	1001	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	dt	201	PEB	CMD-C2D-C3D	-3.01	125.81	130.06
26	g2	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	s2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	j4	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	j5	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y5	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	w7	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	a8	602	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	b8	1003	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	Y8	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	j9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	am	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bY	1003	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dA	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eH	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
27	h1	201	CYC	CMD-C2D-C3D	-3.01	119.26	124.94
26	q2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	Z3	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	O4	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	Q4	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	l6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	u6	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	w6	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	b9	401	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dy	401	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ea	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	en	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eE	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	q2	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	F2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	j6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	n9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aW	302	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bZ	301	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dk	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eo	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eG	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eR	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eS	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
27	v1	201	CYC	CMD-C2D-C3D	-3.01	119.27	124.94
26	m3	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	W4	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	Y4	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	H6	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	U6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	b6	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	q7	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J8	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	f9	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	l9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	cy	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dD	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dK	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	gh	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	hY	403	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
29	dw	404	PVN	O19-C19-C18	-3.01	124.77	128.04
26	s2	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	x2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	W3	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	T6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	z6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	e9	303	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	w9	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	as	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aJ	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bx	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ce	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dL	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	el	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	em	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ey	1002	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	lp	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ls	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ly	403	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	lz	402	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	O2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	n3	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	P4	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	q5	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	C6	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	d6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	x6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	z8	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	M8	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	h9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	v9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	x9	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	H9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dj	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dP	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eB	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	lb	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	lt	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	gp	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	hD	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	hJ	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	jP	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	C2	301	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	L2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	S2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	H4	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	w4	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	z4	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	C6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	j6	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	b7	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	l7	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	U8	1002	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	g9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	t9	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ag	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aj	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ap	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aM	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aS	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bd	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bs	1003	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	cj	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	cW	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	ds	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	hK	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	i2	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	O3	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	p3	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	S4	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	u9	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	X9	401	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aM	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aN	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bU	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dk	1002	PEB	CMD-C2D-C3D	-3.01	125.82	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dF	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	eS	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	fm	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	fv	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	w3	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	G5	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	f8	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	B6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	D6	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	q9	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	aY	406	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	bj	202	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	cC	1003	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	di	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	dx	402	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	lr	201	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	jO	1001	PEB	CMD-C2D-C3D	-3.01	125.82	130.06
26	k2	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	u2	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	t3	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	H4	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	W4	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	c5	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	i6	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	r6	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	d9	302	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	ak	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	aP	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	aU	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	dc	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	do	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	dT	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	gq	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	D2	301	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	V2	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	B4	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	Z4	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	u4	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	f8	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	j8	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	m8	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	f6	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	n7	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	a9	602	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	h9	202	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	x9	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	cU	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	dp	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	dG	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	le	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	gx	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	hO	201	PEB	CMD-C2D-C3D	-3.01	125.83	130.06
26	s3	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	E4	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	a4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	M5	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	O6	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	q8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	a7	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	W8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	z9	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	F9	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	T9	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ab	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	aI	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dz	402	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	gf	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	kS	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	F2	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	I3	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	M4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	c4	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	N5	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	u6	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	e8	302	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	r9	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	B9	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	az	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bh	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bm	1002	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bu	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cB	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cO	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	la	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	hW	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	jJ	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	kR	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
27	S1	201	CYC	CMD-C2D-C3D	-3.00	119.28	124.94
27	j1	201	CYC	CMD-C2D-C3D	-3.00	119.28	124.94
26	q3	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	V4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	p4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	a5	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	Q6	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	f7	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	D8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	M8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	R9	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bo	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cv	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cE	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cK	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cM	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cT	1002	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	lq	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	hH	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	kQ	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	v2	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	W2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	W2	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	C4	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	aq	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dA	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	fb	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	fd	301	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	m2	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	K4	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	Z4	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	q4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	Y5	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	u5	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	s9	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dr	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	hZ	402	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
27	R1	1001	CYC	C1A-C2A-C3A	-3.00	103.46	106.78
27	i1	1001	CYC	C1A-C2A-C3A	-3.00	103.46	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	R4	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	t4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	r5	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	m6	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	K8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ac	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bf	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	br	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bw	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bR	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cP	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	cZ	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dm	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	du	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ej	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	eF	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	lk	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ff	204	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	fh	1001	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	hF	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	hT	204	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
27	u1	1001	CYC	C1A-C2A-C3A	-3.00	103.46	106.78
26	J2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	K2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	Y3	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	u3	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	e4	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	N7	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	T2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	k8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	K6	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	y6	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	bt	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dp	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ed	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	hB	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	z2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	Z2	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	d8	302	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	O8	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	aF	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	de	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dg	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ds	202	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	dS	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ey	1003	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ez	1002	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	eD	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	ge	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	gj	201	PEB	CMD-C2D-C3D	-3.00	125.83	130.06
26	u2	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	Y2	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	A3	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	44	302	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	W5	301	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	o5	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	O6	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	b9	404	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	k9	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	aN	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	dq	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	hR	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	E4	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	I4	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	T5	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	c7	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	e9	301	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	m9	1001	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	aC	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	bB	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	cX	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	lc	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	gw	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	hI	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
27	S1	202	CYC	CMD-C2D-C3D	-3.00	119.29	124.94
26	l2	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	34	1003	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	b5	1001	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	i8	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	P6	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	V6	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	o6	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	R7	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a8	601	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	U8	1003	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	p9	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	U9	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	at	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	lz	401	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	f3	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	Y4	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	o4	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	v4	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	g8	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	A8	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	V8	1001	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	i9	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	Z9	1001	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	cD	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	hN	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
29	34	1004	PVN	C91-C18-C17	-3.00	122.41	127.53
29	Y5	1004	PVN	C91-C18-C17	-3.00	122.41	127.53
29	gz	304	PVN	C9-C10-C11	3.00	132.39	128.81
26	e2	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	y2	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	C5	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	H8	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	N8	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	Z8	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	y9	1002	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	ah	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	bq	202	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	by	1001	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	cw	201	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	iA	1001	PEB	CMD-C2D-C3D	-3.00	125.84	130.06
26	G4	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	I5	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	Z6	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	c6	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	dt	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	s8	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	M7	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	d9	303	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	s9	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	Z9	1007	PEB	CMD-C2D-C3D	-2.99	125.84	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aT	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	cX	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	dQ	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	fe	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	ft	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	hS	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
27	I1	201	CYC	C1A-C2A-C3A	-2.99	103.47	106.78
26	u4	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	g6	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	I7	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	B8	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	aa	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	ay	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	bq	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	bx	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	fx	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	gg	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	E5	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	g6	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	Y7	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	E8	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	Q9	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	dv	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	dR	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	eq	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	eA	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	y3	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	h5	201	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	A6	1001	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	E6	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	M7	1002	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	aW	301	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	cM	202	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	eZ	401	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
26	fd	302	PEB	CMD-C2D-C3D	-2.99	125.84	130.06
27	X1	201	CYC	C1A-C2A-C3A	-2.99	103.47	106.78
26	c3	302	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	n4	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	Q5	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	r8	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	x8	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	aX	401	PEB	CMD-C2D-C3D	-2.99	125.85	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dw	403	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	eU	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	gl	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	x3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	e8	301	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	a9	603	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	L8	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	bY	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	cb	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
29	44	303	PVN	C91-C18-C17	-2.99	122.42	127.53
29	Z5	304	PVN	C91-C18-C17	-2.99	122.42	127.53
26	I2	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	S3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	g3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	k3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	d4	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	ca	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	dH	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	eI	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	eK	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	iG	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	F3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	Q3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	M4	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	J5	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	cW	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	dJ	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	lu	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	M2	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	G3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	Q4	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	z4	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	F6	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	r6	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	x7	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	eJ	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	lq	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
29	d3	302	PVN	C5-C6-C7	2.99	135.43	130.34
26	P3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	U5	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	Y6	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	e7	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z9	1003	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	aF	204	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	aZ	301	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	dH	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	dN	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	dT	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	eT	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	lb	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	hA	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	hQ	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	jI	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	jK	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
28	en	203	PUB	C2C-C1C-NC	2.99	114.39	110.05
26	G2	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	E3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	J3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	S3	203	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	b3	502	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	S8	401	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	E9	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	aB	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	bX	402	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	eK	202	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	hP	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	jL	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	X2	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	K3	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	p6	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	V7	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	hM	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	ae	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	gm	1001	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	go	201	PEB	CMD-C2D-C3D	-2.99	125.85	130.06
26	w2	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	L3	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	X8	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	cQ	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	eU	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	L4	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	f4	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	A5	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	z6	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K8	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	bz	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	kW	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
28	B9	203	PUB	C2C-C1C-NC	2.98	114.39	110.05
26	T4	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	k6	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	P8	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	aV	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	bv	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	du	203	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	c6	1003	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	cS	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	li	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	B2	501	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	h8	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	g7	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	v7	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	y9	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	aC	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	aZ	302	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	eO	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	kT	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	R2	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	i5	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	Q6	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	cT	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	cU	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	cV	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	es	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	lv	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	hX	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
29	T8	303	PVN	C91-C18-C17	-2.98	122.43	127.53
27	y1	201	CYC	C1A-C2A-C3A	-2.98	103.48	106.78
26	Q2	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	Z7	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	v8	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	fq	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
27	k1	201	CYC	C1B-NB-C4B	-2.98	106.88	110.67
26	r7	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	dU	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	fn	1001	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	R6	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J8	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	y2	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	I4	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	u8	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	w9	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	aG	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	aL	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
28	dw	405	PUB	C2C-C1C-NC	2.98	114.38	110.05
26	e2	202	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
26	m2	201	PEB	CMD-C2D-C3D	-2.98	125.86	130.06
28	eV	203	PUB	C2C-C1C-NC	2.98	114.38	110.05
26	a3	1001	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	D4	201	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	aY	402	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
28	aJ	203	PUB	C2C-C1C-NC	2.98	114.38	110.05
29	e9	304	PVN	C91-C18-C19	2.98	126.08	121.38
26	w2	203	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	N2	202	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	aQ	201	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	eW	201	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	r2	201	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	D9	201	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	bs	1001	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
26	fi	201	PEB	CMD-C2D-C3D	-2.98	125.87	130.06
28	R9	203	PUB	C2C-C1C-NC	2.98	114.38	110.05
27	g1	201	CYC	C1A-C2A-C3A	-2.98	103.49	106.78
26	f2	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	X7	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	h7	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	aI	202	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
28	R5	203	PUB	C2C-C1C-NC	2.97	114.38	110.05
27	y1	201	CYC	C1B-NB-C4B	-2.97	106.88	110.67
26	C9	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
28	v6	203	PUB	C2C-C1C-NC	2.97	114.38	110.05
26	H3	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	aD	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	db	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	dP	202	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
28	X7	203	PUB	C2C-C1C-NC	2.97	114.37	110.05
28	fo	203	PUB	C2C-C1C-NC	2.97	114.37	110.05
28	gr	202	PUB	C2C-C1C-NC	2.97	114.37	110.05
28	X6	203	PUB	C2C-C1C-NC	2.97	114.37	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d6	203	PUB	C2C-C1C-NC	2.97	114.37	110.05
26	z5	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	m7	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	gk	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	q6	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	s7	201	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
26	fd	303	PEB	CMD-C2D-C3D	-2.97	125.87	130.06
27	w1	201	CYC	C1A-C2A-C3A	-2.97	103.50	106.78
26	l9	202	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	K9	1001	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	dw	402	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	eM	1002	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
29	A2	1004	PVN	C2-C1-N1	2.97	109.84	107.21
29	a3	1004	PVN	C2-C1-N1	2.97	109.84	107.21
28	br	203	PUB	C2C-C1C-NC	2.97	114.37	110.05
26	U4	202	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	h6	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
28	t5	203	PUB	C2C-C1C-NC	2.97	114.37	110.05
26	t2	202	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	s5	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	aw	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
27	P1	201	CYC	C1B-NB-C4B	-2.97	106.89	110.67
28	T8	304	PUB	C2C-C1C-NC	2.97	114.37	110.05
26	K2	202	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	av	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	dW	202	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
28	R2	203	PUB	C2C-C1C-NC	2.97	114.37	110.05
26	eV	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
29	D2	303	PVN	C5-C6-C7	2.97	135.40	130.34
28	Y9	305	PUB	C2C-C1C-NC	2.97	114.36	110.05
26	24	401	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	D5	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
26	S7	201	PEB	CMD-C2D-C3D	-2.97	125.88	130.06
27	G1	1001	CYC	C1A-C2A-C3A	-2.97	103.50	106.78
27	Z1	201	CYC	C1A-C2A-C3A	-2.97	103.50	106.78
28	bT	202	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	cs	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	cM	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	dK	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	kR	1003	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	t2	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
26	dl	201	PEB	CMD-C2D-C3D	-2.96	125.88	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	dP	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
26	aO	201	PEB	CMD-C2D-C3D	-2.96	125.89	130.06
28	F5	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	H5	202	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	U8	1005	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	H9	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
29	Y9	303	PVN	C91-C18-C17	-2.96	122.46	127.53
27	q1	201	CYC	C1A-C2A-C3A	-2.96	103.50	106.78
28	eR	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
26	r9	201	PEB	CMD-C2D-C3D	-2.96	125.89	130.06
27	L1	201	CYC	C1B-NB-C4B	-2.96	106.90	110.67
27	a1	201	CYC	C1B-NB-C4B	-2.96	106.90	110.67
27	e1	201	CYC	C1B-NB-C4B	-2.96	106.90	110.67
28	aF	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
26	u7	201	PEB	CMD-C2D-C3D	-2.96	125.89	130.06
27	G1	1001	CYC	C1B-NB-C4B	-2.96	106.90	110.67
28	L9	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	r2	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	T3	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
28	T9	203	PUB	C2C-C1C-NC	2.96	114.36	110.05
27	w1	201	CYC	C1B-NB-C4B	-2.96	106.90	110.67
26	iC	1001	PEB	CMD-C2D-C3D	-2.96	125.89	130.06
28	X2	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	n3	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	dX	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	p4	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	J6	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	lj	202	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	lx	201	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	bJ	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	bZ	305	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	iD	1003	PUB	C2C-C1C-NC	2.96	114.35	110.05
27	V1	201	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
26	d7	201	PEB	CMD-C2D-C3D	-2.96	125.89	130.06
28	cQ	202	PUB	C2C-C1C-NC	2.96	114.35	110.05
27	b1	1001	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
28	p3	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	Z6	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	D7	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	y7	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	iC	1003	PUB	C2C-C1C-NC	2.96	114.35	110.05
27	o1	1001	CYC	C1B-NB-C4B	-2.96	106.91	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	q1	201	CYC	C1B-NB-C4B	-2.96	106.91	110.67
27	U1	201	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
27	d2	101	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
28	gg	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	gz	306	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	F4	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	z7	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
28	w8	203	PUB	C2C-C1C-NC	2.96	114.35	110.05
27	k1	201	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
27	n1	201	CYC	C1A-C2A-C3A	-2.96	103.51	106.78
28	r9	203	PUB	C2C-C1C-NC	2.95	114.35	110.05
28	bq	203	PUB	C2C-C1C-NC	2.95	114.35	110.05
27	d1	1001	CYC	C1A-C2A-C3A	-2.95	103.51	106.78
28	P5	202	PUB	C2C-C1C-NC	2.95	114.35	110.05
28	at	203	PUB	C2C-C1C-NC	2.95	114.35	110.05
28	fj	203	PUB	C2C-C1C-NC	2.95	114.35	110.05
28	gn	203	PUB	C2C-C1C-NC	2.95	114.35	110.05
27	g1	201	CYC	C1B-NB-C4B	-2.95	106.91	110.67
28	P6	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	bF	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
26	m5	1001	PEB	CMD-C2D-C3D	-2.95	125.90	130.06
27	K1	201	CYC	C1B-NB-C4B	-2.95	106.91	110.67
27	X1	201	CYC	C1B-NB-C4B	-2.95	106.91	110.67
28	B4	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	U8	1006	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	an	202	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	fw	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	hV	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
26	cs	201	PEB	CMD-C2D-C3D	-2.95	125.90	130.06
28	F7	202	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	bD	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	cz	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	eZ	403	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	kQ	1003	PUB	C2C-C1C-NC	2.95	114.34	110.05
27	b1	1001	CYC	C1B-NB-C4B	-2.95	106.91	110.67
28	t9	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	aP	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
27	d1	1001	CYC	C1B-NB-C4B	-2.95	106.91	110.67
28	D9	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	eF	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	fs	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	hJ	203	PUB	C2C-C1C-NC	2.95	114.34	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	p2	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	P3	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	B6	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	L7	202	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	K8	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	bz	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	gz	305	PUB	C2C-C1C-NC	2.95	114.34	110.05
29	e8	303	PVN	C91-C18-C19	2.95	126.04	121.38
27	o1	1001	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
28	F2	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	z4	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	eH	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	gy	305	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	p9	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	ee	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	gp	203	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	jJ	1003	PUB	C2C-C1C-NC	2.95	114.34	110.05
27	I1	201	CYC	C1B-NB-C4B	-2.95	106.92	110.67
28	p7	202	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	ax	202	PUB	C2C-C1C-NC	2.95	114.34	110.05
28	hY	406	PUB	C2C-C1C-NC	2.95	114.34	110.05
26	au	201	PEB	CMD-C2D-C3D	-2.95	125.91	130.06
29	C2	303	PVN	C21-C2-C3	2.95	135.73	129.67
29	c3	303	PVN	C21-C2-C3	2.95	135.73	129.67
28	Z3	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	D4	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	Z7	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	dv	202	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	eP	204	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	B3	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	D6	202	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	l6	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	s7	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	cH	202	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	cL	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	ec	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
27	O1	201	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
27	P1	201	CYC	C1A-C2A-C3A	-2.95	103.52	106.78
28	h3	202	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	V4	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	y6	204	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	R7	203	PUB	C2C-C1C-NC	2.95	114.33	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	I8	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	N9	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	dw	406	PUB	C2C-C1C-NC	2.95	114.33	110.05
28	lh	203	PUB	C2C-C1C-NC	2.95	114.33	110.05
27	z1	201	CYC	CHA-C1A-C2A	-2.94	118.52	125.32
27	O1	201	CYC	C1B-NB-C4B	-2.94	106.92	110.67
28	V7	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	T8	305	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	ar	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	ey	1006	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	M8	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	eg	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
27	N1	201	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
28	aT	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	bY	1005	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	gd	202	PUB	C2C-C1C-NC	2.94	114.33	110.05
27	R1	1001	CYC	C1B-NB-C4B	-2.94	106.92	110.67
27	i1	1001	CYC	C1B-NB-C4B	-2.94	106.92	110.67
27	a2	901	CYC	CHA-C1A-C2A	-2.94	118.52	125.32
28	D2	305	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	N3	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	f3	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	f8	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	J7	202	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	Y9	304	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	bR	202	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	eT	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
27	S1	201	CYC	CHA-C1A-C2A	-2.94	118.52	125.32
27	j1	201	CYC	CHA-C1A-C2A	-2.94	118.52	125.32
28	J4	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	44	304	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	x6	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	ap	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
27	u1	1001	CYC	C1B-NB-C4B	-2.94	106.92	110.67
28	H2	202	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	d3	304	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	hT	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	V2	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	R3	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	c3	304	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	H6	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	L6	202	PUB	C2C-C1C-NC	2.94	114.33	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	cR	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	eY	404	PUB	C2C-C1C-NC	2.94	114.33	110.05
27	K1	201	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
28	r5	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	e6	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	v7	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	V9	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	lb	203	PUB	C2C-C1C-NC	2.94	114.33	110.05
28	Z5	306	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	eb	202	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	gk	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	H3	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	D5	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	e9	306	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	cJ	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	hG	202	PUB	C2C-C1C-NC	2.94	114.32	110.05
27	s1	201	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
28	r6	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	bs	1004	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	ey	1005	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	hD	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	iH	1002	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	kW	1003	PUB	C2C-C1C-NC	2.94	114.32	110.05
27	Q1	201	CYC	C1A-C2A-C3A	-2.94	103.53	106.78
28	R6	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	c9	305	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	J9	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	hZ	404	PUB	C2C-C1C-NC	2.94	114.32	110.05
27	f1	201	CYC	C1B-NB-C4B	-2.94	106.93	110.67
28	y8	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	cB	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	Y5	1006	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	N6	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	p6	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	av	203	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	cF	202	PUB	C2C-C1C-NC	2.94	114.32	110.05
28	hY	405	PUB	C2C-C1C-NC	2.94	114.32	110.05
27	n1	201	CYC	C1B-NB-C4B	-2.93	106.93	110.67
28	T2	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	44	305	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	p5	202	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	d7	203	PUB	C2C-C1C-NC	2.93	114.32	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d9	305	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	az	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	dF	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	el	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	ez	1006	PUB	C2C-C1C-NC	2.93	114.32	110.05
27	s1	201	CYC	C1B-NB-C4B	-2.93	106.93	110.67
28	x2	202	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	X3	202	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	L4	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	dY	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	eY	405	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	eZ	404	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	fy	202	PUB	C2C-C1C-NC	2.93	114.32	110.05
27	a2	901	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
28	r3	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	Z4	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	N5	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	aH	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	bL	203	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	co	202	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	lv	202	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	iG	1002	PUB	C2C-C1C-NC	2.93	114.32	110.05
28	jN	1003	PUB	C2C-C1C-NC	2.93	114.32	110.05
27	a2	902	CYC	CHA-C1A-C2A	-2.93	118.54	125.32
27	b2	1001	CYC	CHA-C1A-C2A	-2.93	118.54	125.32
28	v2	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	V3	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	x3	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	c8	304	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	bn	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	gi	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	Q1	201	CYC	C1B-NB-C4B	-2.93	106.94	110.67
28	t6	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	T7	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	G8	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	bB	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	ff	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	iE	1003	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	m1	201	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
28	a6	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	H7	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	b8	1005	PUB	C2C-C1C-NC	2.93	114.31	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	x9	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	cN	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	hZ	405	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	M1	1001	CYC	CHA-C1A-C2A	-2.93	118.55	125.32
27	e1	201	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
27	f1	201	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
28	b9	406	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	hB	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	hN	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	p1	201	CYC	CHA-C1A-C2A	-2.93	118.55	125.32
28	L2	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	P2	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	b8	1006	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	c9	304	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	aN	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	cE	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	jP	1003	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	S1	201	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
27	j1	201	CYC	C1A-C2A-C3A	-2.93	103.54	106.78
27	V1	201	CYC	C1B-NB-C4B	-2.93	106.94	110.67
28	A2	1005	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	n5	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	z5	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	aB	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	cO	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	eL	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	z2	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	F3	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	X4	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	o8	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	et	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	Z1	201	CYC	C1B-NB-C4B	-2.93	106.94	110.67
28	b7	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	bV	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	cP	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	eB	204	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	eJ	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	eN	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	H4	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	aY	404	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	bo	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	ld	203	PUB	C2C-C1C-NC	2.93	114.31	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	ln	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	fu	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	jM	1003	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	H1	201	CYC	CHA-C1A-C2A	-2.93	118.56	125.32
28	Z9	1006	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	bY	1006	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	dx	406	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	hH	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	kS	1003	PUB	C2C-C1C-NC	2.93	114.31	110.05
27	W1	201	CYC	C1B-NB-C4B	-2.93	106.94	110.67
27	S1	202	CYC	CHA-C1A-C2A	-2.93	118.56	125.32
28	J2	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	j3	202	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	Y5	1005	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	dj	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	dt	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	lp	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	hL	203	PUB	C2C-C1C-NC	2.93	114.31	110.05
28	C2	304	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	L3	203	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	T5	202	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	z6	203	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	P7	203	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	c7	203	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	P9	203	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	dB	202	PUB	C2C-C1C-NC	2.93	114.30	110.05
28	kT	1003	PUB	C2C-C1C-NC	2.93	114.30	110.05
27	r1	201	CYC	CHA-C1A-C2A	-2.92	118.56	125.32
27	c1	201	CYC	CHA-C1A-C2A	-2.92	118.56	125.32
27	W1	201	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
28	V6	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	cn	202	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	jI	1003	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	C2	305	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	c3	305	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	u6	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	E8	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	aZ	305	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	bZ	306	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	cY	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	ez	1005	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	iF	1003	PUB	C2C-C1C-NC	2.92	114.30	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	n9	202	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	cq	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	dh	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	er	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
27	m1	201	CYC	C1B-NB-C4B	-2.92	106.95	110.67
28	j2	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	P4	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	L5	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
27	p1	201	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
27	r1	201	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
28	F6	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	B7	202	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	d8	304	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	e9	305	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	C8	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	aV	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	cr	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	h2	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	R4	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	r4	202	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	a7	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	dV	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
27	a2	902	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
27	b2	1001	CYC	C1A-C2A-C3A	-2.92	103.55	106.78
28	c6	1004	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	t7	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	F9	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	Z9	1005	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	eD	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	fc	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	a3	1006	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	aZ	304	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	dn	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	ep	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	fq	203	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	gy	306	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	jO	1003	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	kX	1003	PUB	C2C-C1C-NC	2.92	114.30	110.05
28	x4	202	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	bp	202	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	v3	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	34	1006	PUB	C2C-C1C-NC	2.92	114.29	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Z5	305	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	b6	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	n6	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	hR	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	D2	304	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	d3	303	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	N4	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	J5	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	e8	305	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	A8	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	ll	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	lt	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	ga	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	kU	1003	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	v4	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
28	v5	203	PUB	C2C-C1C-NC	2.92	114.29	110.05
27	N1	201	CYC	C1B-NB-C4B	-2.92	106.96	110.67
27	v1	201	CYC	CHA-C1A-C2A	-2.91	118.59	125.32
28	z3	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	T4	202	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	34	1005	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	n8	202	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	gx	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	n4	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	T6	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	A2	1006	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	t3	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	B5	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	h8	203	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	jL	1003	PUB	C2C-C1C-NC	2.91	114.29	110.05
28	b9	407	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	di	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	dp	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	dx	407	PUB	C2C-C1C-NC	2.91	114.28	110.05
27	L1	201	CYC	C1A-C2A-C3A	-2.91	103.56	106.78
27	a1	201	CYC	C1A-C2A-C3A	-2.91	103.56	106.78
28	n7	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	dL	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	g8	202	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	aY	405	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	lr	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	hX	203	PUB	C2C-C1C-NC	2.91	114.28	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	h1	201	CYC	CHA-C1A-C2A	-2.91	118.60	125.32
28	V5	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	x5	202	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	aR	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	hP	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
27	U1	201	CYC	C1B-NB-C4B	-2.91	106.96	110.67
27	d2	101	CYC	C1B-NB-C4B	-2.91	106.96	110.67
28	Z2	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	e7	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	N2	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	J3	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	Q8	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	bP	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
27	t1	201	CYC	CHA-C1A-C2A	-2.91	118.60	125.32
28	N7	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	bN	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	t4	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	dr	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	f2	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	a3	1005	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	cp	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	dd	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	dH	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	fa	202	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	v9	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	ei	203	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	ly	406	PUB	C2C-C1C-NC	2.91	114.28	110.05
28	lz	405	PUB	C2C-C1C-NC	2.91	114.28	110.05
27	c1	201	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
27	h1	201	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
28	r7	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	z9	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	aL	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	dD	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	fi	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
27	S1	202	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
28	dR	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
27	J1	201	CYC	CHA-C1A-C2A	-2.90	118.61	125.32
27	Y1	201	CYC	CHA-C1A-C2A	-2.90	118.61	125.32
28	dl	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	aD	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	ly	405	PUB	C2C-C1C-NC	2.90	114.27	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	lz	404	PUB	C2C-C1C-NC	2.90	114.27	110.05
27	M1	1001	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
27	v1	201	CYC	C1A-C2A-C3A	-2.90	103.57	106.78
28	l7	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	x7	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	e8	304	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	gv	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	n2	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	O8	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	fm	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	l2	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
28	gt	203	PUB	C2C-C1C-NC	2.90	114.27	110.05
27	z1	201	CYC	C1A-C2A-C3A	-2.90	103.58	106.78
28	c8	305	PUB	C2C-C1C-NC	2.90	114.26	110.05
29	Z9	1004	PVN	C81-C17-C18	-2.90	118.26	126.12
28	jK	1003	PUB	C2C-C1C-NC	2.89	114.26	110.05
28	D3	203	PUB	C2C-C1C-NC	2.89	114.26	110.05
28	ev	203	PUB	C2C-C1C-NC	2.89	114.26	110.05
28	ge	203	PUB	C2C-C1C-NC	2.89	114.26	110.05
28	df	203	PUB	C2C-C1C-NC	2.89	114.25	110.05
28	lf	203	PUB	C2C-C1C-NC	2.89	114.25	110.05
28	l3	202	PUB	C2C-C1C-NC	2.89	114.25	110.05
29	Z9	1004	PVN	C71-C13-C14	-2.89	120.62	125.06
28	eX	202	PUB	C2C-C1C-NC	2.89	114.25	110.05
29	e9	304	PVN	C15-C16-N4	-2.89	119.86	126.06
28	kV	1003	PUB	C2C-C1C-NC	2.89	114.25	110.05
28	p8	203	PUB	C2C-C1C-NC	2.88	114.24	110.05
27	H1	201	CYC	C1A-C2A-C3A	-2.88	103.59	106.78
29	d3	302	PVN	C15-C16-N4	-2.88	119.88	126.06
29	e8	303	PVN	C15-C16-N4	-2.88	119.88	126.06
29	44	303	PVN	C15-C16-N4	-2.88	119.88	126.06
29	Z5	304	PVN	C15-C16-N4	-2.88	119.88	126.06
29	b8	1004	PVN	C15-C16-N4	-2.88	119.88	126.06
28	bH	203	PUB	C2C-C1C-NC	2.88	114.23	110.05
29	D2	303	PVN	C32-C31-C3	2.88	117.34	112.98
29	d3	302	PVN	C32-C31-C3	2.88	117.34	112.98
29	U8	1004	PVN	C81-C17-C18	-2.87	118.32	126.12
29	D2	303	PVN	C15-C16-N4	-2.87	119.89	126.06
29	U8	1004	PVN	C71-C13-C14	-2.87	120.64	125.06
28	dN	203	PUB	C2C-C1C-NC	2.87	114.22	110.05
29	44	303	PVN	C16-N4-C19	-2.86	107.02	110.67
29	Z5	304	PVN	C16-N4-C19	-2.86	107.02	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	b9	405	PVN	C15-C16-N4	-2.86	119.92	126.06
27	J1	201	CYC	C1A-C2A-C3A	-2.86	103.62	106.78
27	Y1	201	CYC	C1A-C2A-C3A	-2.86	103.62	106.78
29	d9	304	PVN	C15-C16-N4	-2.86	119.93	126.06
29	gy	304	PVN	C15-C16-N4	-2.85	119.93	126.06
29	d8	303	PVN	C15-C16-N4	-2.85	119.93	126.06
27	t1	201	CYC	C1A-C2A-C3A	-2.85	103.63	106.78
28	bN	203	PUB	CHC-C1D-ND	-2.85	110.12	113.72
28	dT	203	PUB	C2C-C1C-NC	2.84	114.19	110.05
29	bZ	304	PVN	C16-N4-C19	-2.84	107.05	110.67
28	ev	203	PUB	CHC-C1D-ND	-2.83	110.14	113.72
28	ll	203	PUB	CHC-C1D-ND	-2.83	110.15	113.72
28	P7	203	PUB	CHC-C1D-ND	-2.82	110.15	113.72
27	G1	1001	CYC	CBA-CAA-C2A	2.82	120.46	112.63
28	el	203	PUB	CHC-C1D-ND	-2.82	110.16	113.72
28	z7	203	PUB	CHC-C1D-ND	-2.82	110.16	113.72
28	ez	1006	PUB	CHC-C1D-ND	-2.82	110.16	113.72
28	lx	201	PUB	CHC-C1D-ND	-2.82	110.16	113.72
28	hV	203	PUB	CHC-C1D-ND	-2.82	110.16	113.72
27	k1	201	CYC	C4A-C3A-C2A	-2.82	103.27	106.51
28	aP	203	PUB	CHC-C1D-ND	-2.82	110.16	113.72
28	lb	203	PUB	CHC-C1D-ND	-2.82	110.16	113.72
28	ep	203	PUB	CHC-C1D-ND	-2.82	110.16	113.72
27	f1	201	CYC	CBA-CAA-C2A	2.82	120.45	112.63
27	K1	201	CYC	C4A-C3A-C2A	-2.82	103.28	106.51
28	ee	203	PUB	CHC-C1D-ND	-2.81	110.16	113.72
27	W1	201	CYC	C4A-C3A-C2A	-2.81	103.28	106.51
27	e1	201	CYC	C4A-C3A-C2A	-2.81	103.28	106.51
28	a3	1005	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	cQ	202	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	s1	201	CYC	C4A-C3A-C2A	-2.81	103.28	106.51
28	aJ	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	gp	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
29	aZ	303	PVN	C16-N4-C19	-2.81	107.09	110.67
28	B6	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	N7	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	Q8	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	w1	201	CYC	CBA-CAA-C2A	2.81	120.44	112.63
28	34	1006	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	J9	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	gi	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	Y9	304	PUB	CHC-C1D-ND	-2.81	110.17	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	gg	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	K1	201	CYC	CBA-CAA-C2A	2.81	120.43	112.63
28	A8	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	hR	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
29	gz	304	PVN	C10-C11-C12	-2.81	118.83	125.32
28	H2	202	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	t9	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	aD	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	Q1	201	CYC	CBA-CAA-C2A	2.81	120.43	112.63
27	n1	201	CYC	CBA-CAA-C2A	2.81	120.43	112.63
28	D3	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	z6	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	gz	305	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	iE	1003	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	G1	1001	CYC	C4A-C3A-C2A	-2.81	103.28	106.51
27	m1	201	CYC	CBA-CAA-C2A	2.81	120.42	112.63
28	N3	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	n5	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	eY	404	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	W1	201	CYC	CBA-CAA-C2A	2.81	120.42	112.63
27	L1	201	CYC	CBA-CAA-C2A	2.81	120.42	112.63
27	a1	201	CYC	CBA-CAA-C2A	2.81	120.42	112.63
28	ap	203	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	bY	1005	PUB	CHC-C1D-ND	-2.81	110.17	113.72
28	fy	202	PUB	CHC-C1D-ND	-2.81	110.17	113.72
27	X1	201	CYC	CBA-CAA-C2A	2.80	120.42	112.63
28	aZ	305	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	cJ	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
27	y1	201	CYC	CBA-CAA-C2A	2.80	120.42	112.63
28	c8	304	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	aF	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	bF	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	iD	1003	PUB	CHC-C1D-ND	-2.80	110.18	113.72
27	u1	1001	CYC	CBA-CAA-C2A	2.80	120.41	112.63
27	q1	201	CYC	CBA-CAA-C2A	2.80	120.41	112.63
28	p2	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	J2	202	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	X4	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	L7	202	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	eT	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	hG	202	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	bJ	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	bT	202	PUB	CHC-C1D-ND	-2.80	110.18	113.72
27	N1	201	CYC	CBA-CAA-C2A	2.80	120.41	112.63
28	v4	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	v5	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	T8	305	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	dl	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	ec	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	eD	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	eH	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	eY	405	PUB	CHC-C1D-ND	-2.80	110.18	113.72
27	V1	201	CYC	CBA-CAA-C2A	2.80	120.41	112.63
27	o1	1001	CYC	CBA-CAA-C2A	2.80	120.41	112.63
27	L1	201	CYC	C4A-C3A-C2A	-2.80	103.29	106.51
27	a1	201	CYC	C4A-C3A-C2A	-2.80	103.29	106.51
28	z5	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	e9	306	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	K8	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	lp	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	gk	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
27	P1	201	CYC	CBA-CAA-C2A	2.80	120.41	112.63
28	D5	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	H5	202	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	t5	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	H9	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	bp	202	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	bL	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	dx	407	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	dL	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	lf	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	fq	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
27	d1	1001	CYC	CBA-CAA-C2A	2.80	120.40	112.63
28	H6	203	PUB	CHC-C1D-ND	-2.80	110.18	113.72
28	U8	1005	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	B5	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	P5	202	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	c9	305	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	cq	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	ey	1005	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	eZ	404	PUB	CHC-C1D-ND	-2.80	110.19	113.72
27	f1	201	CYC	C4A-C3A-C2A	-2.80	103.30	106.51
28	R4	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	N5	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	G8	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	V9	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
27	S1	202	CYC	O2A-CGA-CBA	2.80	123.01	114.03
27	b1	1001	CYC	CBA-CAA-C2A	2.80	120.39	112.63
28	f3	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	B9	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	az	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
28	er	203	PUB	CHC-C1D-ND	-2.80	110.19	113.72
27	O1	201	CYC	CBA-CAA-C2A	2.80	120.39	112.63
27	s1	201	CYC	CBA-CAA-C2A	2.79	120.39	112.63
28	n2	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	34	1005	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	t4	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	F7	202	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	aY	405	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	bP	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	dV	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	ln	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
27	e1	201	CYC	CBA-CAA-C2A	2.79	120.39	112.63
27	N1	201	CYC	C4A-C3A-C2A	-2.79	103.30	106.51
28	h8	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	dh	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	eg	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	lv	202	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	c6	1004	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	y7	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	b8	1005	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	ax	202	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	eb	202	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	eP	204	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	kQ	1003	PUB	CHC-C1D-ND	-2.79	110.19	113.72
27	Z1	201	CYC	CBA-CAA-C2A	2.79	120.39	112.63
28	C2	304	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	F3	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	R6	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	d8	304	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	aB	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	gz	306	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	hX	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
27	n1	201	CYC	C4A-C3A-C2A	-2.79	103.30	106.51
28	r2	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	R3	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	j3	202	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	N6	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	bY	1006	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	ey	1006	PUB	CHC-C1D-ND	-2.79	110.19	113.72
26	fs	202	PEB	CMD-C2D-C3D	-2.79	126.13	130.06
28	c7	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	ar	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	df	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	fw	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	gv	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	iF	1003	PUB	CHC-C1D-ND	-2.79	110.19	113.72
27	Z1	201	CYC	C4A-C3A-C2A	-2.79	103.30	106.51
26	X2	202	PEB	CMD-C2D-C3D	-2.79	126.13	130.06
29	ey	1004	PVN	C15-C16-N4	-2.79	120.07	126.06
27	k1	201	CYC	CBA-CAA-C2A	2.79	120.38	112.63
28	F6	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	V6	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	bz	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	cn	202	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	dp	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	hJ	203	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	hZ	404	PUB	CHC-C1D-ND	-2.79	110.19	113.72
28	kX	1003	PUB	CHC-C1D-ND	-2.79	110.19	113.72
27	V1	201	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
27	z1	201	CYC	O2A-CGA-CBA	2.79	122.99	114.03
28	E8	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	av	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	ga	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	gt	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	hT	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
27	g1	201	CYC	CBA-CAA-C2A	2.79	120.38	112.63
28	C2	305	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	r3	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	t3	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	d9	305	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	ld	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
27	I1	201	CYC	CBA-CAA-C2A	2.79	120.37	112.63
26	t7	202	PEB	CMD-C2D-C3D	-2.79	126.13	130.06
26	bL	202	PEB	CMD-C2D-C3D	-2.79	126.13	130.06
28	l2	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	L3	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	L4	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	v6	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	Z9	1005	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	fj	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
27	M1	1001	CYC	O2A-CGA-CBA	2.79	122.98	114.03
27	R1	1001	CYC	CBA-CAA-C2A	2.79	120.37	112.63
27	i1	1001	CYC	CBA-CAA-C2A	2.79	120.37	112.63
28	f8	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	b7	202	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	cE	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	eF	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	eR	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
27	R1	1001	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
27	i1	1001	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
27	q1	201	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
26	gd	201	PEB	CMD-C2D-C3D	-2.79	126.14	130.06
28	h3	202	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	n6	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
28	dY	203	PUB	CHC-C1D-ND	-2.79	110.20	113.72
27	o1	1001	CYC	C4A-C3A-C2A	-2.79	103.31	106.51
27	U1	201	CYC	CBA-CAA-C2A	2.79	120.36	112.63
27	d2	101	CYC	CBA-CAA-C2A	2.79	120.36	112.63
28	t2	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	R2	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	T3	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	X3	202	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	y6	204	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	I8	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	z9	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
26	av	202	PEB	CMD-C2D-C3D	-2.78	126.14	130.06
27	t1	201	CYC	O2A-CGA-CBA	2.78	122.98	114.03
28	L2	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	b9	407	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	hP	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	kU	1003	PUB	CHC-C1D-ND	-2.78	110.20	113.72
26	N3	202	PEB	CMD-C2D-C3D	-2.78	126.14	130.06
28	r9	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	aV	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	bn	202	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	gd	202	PUB	CHC-C1D-ND	-2.78	110.20	113.72
26	kU	1002	PEB	CMD-C2D-C3D	-2.78	126.14	130.06
27	d1	1001	CYC	C4A-C3A-C2A	-2.78	103.31	106.51
28	T2	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	U8	1006	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	P4	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	44	304	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	L6	202	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	at	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	aY	404	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	bR	202	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	ly	406	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	lz	405	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	fc	203	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	hY	405	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	iC	1003	PUB	CHC-C1D-ND	-2.78	110.20	113.72
28	kW	1003	PUB	CHC-C1D-ND	-2.78	110.20	113.72
27	U1	201	CYC	C4A-C3A-C2A	-2.78	103.31	106.51
27	d2	101	CYC	C4A-C3A-C2A	-2.78	103.31	106.51
27	h1	201	CYC	O2A-CGA-CBA	2.78	122.97	114.03
29	a3	1004	PVN	C71-C13-C14	-2.78	120.78	125.06
27	r1	201	CYC	O2A-CGA-CBA	2.78	122.97	114.03
28	D2	304	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	bZ	306	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	cL	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	cM	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	jN	1003	PUB	CHC-C1D-ND	-2.78	110.21	113.72
26	bH	202	PEB	CMD-C2D-C3D	-2.78	126.14	130.06
26	gi	202	PEB	CMD-C2D-C3D	-2.78	126.14	130.06
28	B3	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	J6	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	c8	305	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	bq	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	cp	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	cO	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	dd	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	ei	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
26	dU	202	PEB	C1C-CHB-C4B	2.78	132.13	128.81
28	C8	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	gn	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
29	A2	1004	PVN	C71-C13-C14	-2.78	120.78	125.06
28	A2	1005	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	e9	305	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	br	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	hZ	405	PUB	CHC-C1D-ND	-2.78	110.21	113.72
27	J1	201	CYC	O2A-CGA-CBA	2.78	122.95	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	f2	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	N2	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	P2	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	n3	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	Z6	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	eZ	403	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	lj	202	PUB	CHC-C1D-ND	-2.78	110.21	113.72
26	J3	202	PEB	CMD-C2D-C3D	-2.78	126.15	130.06
27	P1	201	CYC	C4A-C3A-C2A	-2.78	103.32	106.51
28	a6	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	dX	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	hL	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	hN	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
27	I1	201	CYC	C4A-C3A-C2A	-2.78	103.32	106.51
28	Z5	305	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	d6	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	l6	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	x7	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	b9	406	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	an	202	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	bV	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	lr	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	gr	202	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	jO	1003	PUB	CHC-C1D-ND	-2.78	110.21	113.72
27	S1	201	CYC	O2A-CGA-CBA	2.78	122.95	114.03
27	j1	201	CYC	O2A-CGA-CBA	2.78	122.95	114.03
27	Q1	201	CYC	C4A-C3A-C2A	-2.78	103.32	106.51
27	m1	201	CYC	C4A-C3A-C2A	-2.78	103.32	106.51
28	z2	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	H3	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	c3	305	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	v3	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	T4	202	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	J7	202	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	V7	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
28	R9	203	PUB	CHC-C1D-ND	-2.78	110.21	113.72
26	n2	202	PEB	CMD-C2D-C3D	-2.78	126.15	130.06
26	dY	202	PEB	CMD-C2D-C3D	-2.78	126.15	130.06
27	k1	201	CYC	C2B-C1B-NB	2.77	111.05	106.99
27	y1	201	CYC	C4A-C3A-C2A	-2.77	103.32	106.51
26	lf	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
28	n4	203	PUB	CHC-C1D-ND	-2.77	110.21	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	t6	203	PUB	CHC-C1D-ND	-2.77	110.21	113.72
28	e7	203	PUB	CHC-C1D-ND	-2.77	110.21	113.72
28	y8	203	PUB	CHC-C1D-ND	-2.77	110.21	113.72
28	lh	203	PUB	CHC-C1D-ND	-2.77	110.21	113.72
28	fm	203	PUB	CHC-C1D-ND	-2.77	110.21	113.72
29	U8	1004	PVN	C91-C18-C17	-2.77	122.78	127.53
27	Y1	201	CYC	O2A-CGA-CBA	2.77	122.94	114.03
26	r7	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	cr	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
27	g1	201	CYC	O2A-CGA-CBA	2.77	122.94	114.03
28	Z2	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	x3	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	b6	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	O8	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	n9	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	bZ	305	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	co	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	en	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
26	z3	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	A5	203	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	B6	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	D7	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	ap	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	cl	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
28	r4	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	r5	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	L9	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	bs	1004	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	di	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
27	p1	201	CYC	O2A-CGA-CBA	2.77	122.94	114.03
26	cz	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	gn	202	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
26	kV	1002	PEB	CMD-C2D-C3D	-2.77	126.15	130.06
28	h2	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	a7	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	c9	304	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	jM	1003	PUB	CHC-C1D-ND	-2.77	110.22	113.72
27	g1	201	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
26	V5	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	fw	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
28	Z7	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	p7	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	b8	1006	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	aZ	304	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	dw	406	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	eX	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	ly	405	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	lz	404	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	hH	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	hY	406	PUB	CHC-C1D-ND	-2.77	110.22	113.72
27	H1	201	CYC	O2A-CGA-CBA	2.77	122.93	114.03
26	l2	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	y7	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	bI	202	PEB	C1C-CHB-C4B	2.77	132.12	128.81
29	ey	1004	PVN	C9-C10-C11	-2.77	125.50	128.81
28	l3	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	p3	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	X6	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	p6	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	e8	304	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	F9	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	Z9	1006	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	cB	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	cN	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	gx	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
26	iE	1002	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
27	b1	1001	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
28	J4	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	X7	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	e8	305	PUB	CHC-C1D-ND	-2.77	110.22	113.72
27	a2	901	CYC	O2A-CGA-CBA	2.77	122.93	114.03
26	B9	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
27	w1	201	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
28	cr	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	dn	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	ez	1005	PUB	CHC-C1D-ND	-2.77	110.22	113.72
26	fm	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
27	U1	201	CYC	O2A-CGA-CBA	2.77	122.92	114.03
27	d2	101	CYC	O2A-CGA-CBA	2.77	122.92	114.03
26	r4	201	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	cp	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
28	J3	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	z4	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	V5	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	g8	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	bH	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	cF	202	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	gy	305	PUB	CHC-C1D-ND	-2.77	110.22	113.72
27	c1	201	CYC	O2A-CGA-CBA	2.77	122.92	114.03
28	X2	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	Z3	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	V4	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	44	305	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	Y5	1006	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	Z5	306	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	T6	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	aR	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
26	ar	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	cY	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	iC	1002	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
28	p4	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	Y9	305	PUB	CHC-C1D-ND	-2.77	110.22	113.72
27	a2	902	CYC	O2A-CGA-CBA	2.77	122.92	114.03
27	b2	1001	CYC	O2A-CGA-CBA	2.77	122.92	114.03
27	O1	201	CYC	C4A-C3A-C2A	-2.77	103.33	106.51
28	d3	303	PUB	CHC-C1D-ND	-2.77	110.22	113.72
28	x9	203	PUB	CHC-C1D-ND	-2.77	110.22	113.72
26	bD	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	cb	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	fi	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
26	hT	202	PEB	CMD-C2D-C3D	-2.77	126.16	130.06
28	F2	203	PUB	CHC-C1D-ND	-2.77	110.23	113.72
28	d3	304	PUB	CHC-C1D-ND	-2.77	110.23	113.72
28	v7	203	PUB	CHC-C1D-ND	-2.77	110.23	113.72
28	cs	203	PUB	CHC-C1D-ND	-2.77	110.23	113.72
28	iH	1002	PUB	CHC-C1D-ND	-2.77	110.23	113.72
27	N1	201	CYC	O2A-CGA-CBA	2.76	122.91	114.03
27	O1	201	CYC	O2A-CGA-CBA	2.76	122.91	114.03
27	W1	201	CYC	O2A-CGA-CBA	2.76	122.91	114.03
28	R7	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	eB	204	PUB	CHC-C1D-ND	-2.76	110.23	113.72
27	u1	1001	CYC	C4A-C3A-C2A	-2.76	103.33	106.51
27	P1	201	CYC	O2A-CGA-CBA	2.76	122.91	114.03
27	f1	201	CYC	O2A-CGA-CBA	2.76	122.91	114.03
26	hW	202	PEB	C1C-CHB-C4B	2.76	132.11	128.81
26	er	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	u1	1001	CYC	O2A-CGA-CBA	2.76	122.91	114.03
28	o8	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	r7	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	cz	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	cR	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	eJ	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	jL	1003	PUB	CHC-C1D-ND	-2.76	110.23	113.72
26	ao	202	PEB	C1C-CHB-C4B	2.76	132.11	128.81
26	cj	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	kX	1002	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
27	v1	201	CYC	O2A-CGA-CBA	2.76	122.91	114.03
28	j2	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	H7	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	bB	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dT	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	fo	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
27	o1	1001	CYC	O2A-CGA-CBA	2.76	122.91	114.03
26	v5	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	cs	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	fr	202	PEB	C1C-CHB-C4B	2.76	132.11	128.81
28	V2	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	u6	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	t7	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	T9	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dv	202	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dD	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	jP	1003	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	kT	1003	PUB	CHC-C1D-ND	-2.76	110.23	113.72
26	ad	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	hP	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	ep	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
28	v2	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	R5	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dr	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
27	y1	201	CYC	O2A-CGA-CBA	2.76	122.90	114.03
29	eZ	402	PVN	C81-C17-C18	-2.76	118.62	126.12
26	P5	201	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
28	c3	304	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	x4	202	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	x5	202	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	l7	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	N9	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	aL	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	cP	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
27	m1	201	CYC	O2A-CGA-CBA	2.76	122.90	114.03
27	s1	201	CYC	O2A-CGA-CBA	2.76	122.90	114.03
26	A1	301	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	B1	301	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	D5	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
28	P6	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	e6	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	T8	304	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	aH	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	fi	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
27	q1	201	CYC	O2A-CGA-CBA	2.76	122.89	114.03
26	p7	201	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	v9	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
28	T5	202	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	aN	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dx	406	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	et	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
26	C8	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
28	p5	202	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dw	405	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	dF	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
28	eV	203	PUB	CHC-C1D-ND	-2.76	110.23	113.72
27	I1	201	CYC	O2A-CGA-CBA	2.76	122.89	114.03
27	P1	201	CYC	C2B-C1B-NB	2.76	111.03	106.99
27	y1	201	CYC	C2B-C1B-NB	2.76	111.03	106.99
26	p2	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	x3	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	e7	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
26	lh	202	PEB	CMD-C2D-C3D	-2.76	126.17	130.06
27	X1	201	CYC	O2A-CGA-CBA	2.76	122.89	114.03
27	d1	1001	CYC	O2A-CGA-CBA	2.76	122.89	114.03
28	V3	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	N4	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	J5	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	r6	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
27	e1	201	CYC	O2A-CGA-CBA	2.76	122.89	114.03
26	l7	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	cd	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	lr	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	kT	1002	PEB	CMD-C2D-C3D	-2.76	126.18	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d1	1001	CYC	C2B-C1B-NB	2.76	111.02	106.99
28	F5	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	P9	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	cH	202	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	dH	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	dK	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	jJ	1003	PUB	CHC-C1D-ND	-2.76	110.24	113.72
26	v3	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	J6	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	R6	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	bF	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	di	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	fq	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
27	w1	201	CYC	O2A-CGA-CBA	2.76	122.88	114.03
28	a3	1006	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	B7	202	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	M8	203	PUB	CHC-C1D-ND	-2.76	110.24	113.72
28	fu	202	PUB	CHC-C1D-ND	-2.76	110.24	113.72
26	fo	202	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
26	kR	1002	PEB	CMD-C2D-C3D	-2.76	126.18	130.06
27	G1	1001	CYC	O2A-CGA-CBA	2.76	122.88	114.03
28	P3	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	B4	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	s7	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	v9	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	ge	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	hB	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
26	ee	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	ec	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	eL	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
28	p8	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	jK	1003	PUB	CHC-C1D-ND	-2.75	110.24	113.72
27	K1	201	CYC	O2A-CGA-CBA	2.75	122.88	114.03
27	R1	1001	CYC	O2A-CGA-CBA	2.75	122.88	114.03
27	i1	1001	CYC	O2A-CGA-CBA	2.75	122.88	114.03
27	K1	201	CYC	C2B-C1B-NB	2.75	111.02	106.99
28	w8	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	dP	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
26	hR	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	H9	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	ll	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
28	cY	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k3	202	PEB	C1C-CHB-C4B	2.75	132.10	128.81
27	b1	1001	CYC	O2A-CGA-CBA	2.75	122.87	114.03
26	T2	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	Z2	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	F3	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	v4	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	F9	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
26	P9	202	PEB	CMD-C2D-C3D	-2.75	126.18	130.06
27	n1	201	CYC	C2B-C1B-NB	2.75	111.02	106.99
28	D2	305	PUB	CHC-C1D-ND	-2.75	110.24	113.72
28	D4	203	PUB	CHC-C1D-ND	-2.75	110.24	113.72
26	V2	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	N7	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
27	Z1	201	CYC	O2A-CGA-CBA	2.75	122.87	114.03
27	n1	201	CYC	O2A-CGA-CBA	2.75	122.87	114.03
28	aT	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	gy	306	PUB	CHC-C1D-ND	-2.75	110.25	113.72
26	jP	1002	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
28	A2	1006	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	F4	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	d7	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	kR	1003	PUB	CHC-C1D-ND	-2.75	110.25	113.72
26	L5	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	v7	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	dh	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	et	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	ff	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	f2	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	j2	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	m5	1003	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	Z7	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
28	x2	202	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	fa	202	PUB	CHC-C1D-ND	-2.75	110.25	113.72
26	34	1001	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	F5	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
27	R1	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
27	i1	1001	CYC	C2B-C1B-NB	2.75	111.01	106.99
29	aY	403	PVN	C15-C16-N4	-2.75	120.16	126.06
26	H3	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	p4	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
28	z3	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	Y5	1005	PUB	CHC-C1D-ND	-2.75	110.25	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	x6	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
27	k1	201	CYC	O2A-CGA-CBA	2.75	122.85	114.03
26	N5	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	d7	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
27	X1	201	CYC	C2B-C1B-NB	2.75	111.01	106.99
28	Z4	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	T7	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
27	V1	201	CYC	O2A-CGA-CBA	2.75	122.85	114.03
26	cq	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	cF	201	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	cL	202	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
26	hG	201	PEB	CMD-C2D-C3D	-2.75	126.19	130.06
28	dj	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	dt	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	hD	203	PUB	CHC-C1D-ND	-2.75	110.25	113.72
28	kS	1003	PUB	CHC-C1D-ND	-2.75	110.25	113.72
26	U5	202	PEB	C1C-CHB-C4B	2.74	132.09	128.81
27	Q1	201	CYC	O2A-CGA-CBA	2.74	122.85	114.03
26	j4	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	N9	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
28	n8	202	PUB	CHC-C1D-ND	-2.74	110.25	113.72
28	iG	1002	PUB	CHC-C1D-ND	-2.74	110.25	113.72
29	eY	403	PVN	C81-C17-C18	-2.74	118.67	126.12
27	u1	1001	CYC	C2B-C1B-NB	2.74	111.00	106.99
26	P3	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	L9	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	V9	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	kW	1002	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
28	D6	202	PUB	CHC-C1D-ND	-2.74	110.25	113.72
28	lt	203	PUB	CHC-C1D-ND	-2.74	110.25	113.72
27	G1	1001	CYC	C2B-C1B-NB	2.74	111.00	106.99
26	r3	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	R5	202	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	n8	201	PEB	CMD-C2D-C3D	-2.74	126.19	130.06
26	j7	202	PEB	C1C-CHB-C4B	2.74	132.09	128.81
26	le	202	PEB	C1C-CHB-C4B	2.74	132.09	128.81
26	g5	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	J9	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	bV	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	co	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	eg	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	ge	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D9	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	eJ	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	g4	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	B7	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	aD	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
27	w1	201	CYC	C2B-C1B-NB	2.74	111.00	106.99
26	E5	202	PEB	C1C-CHB-C4B	2.74	132.08	128.81
26	K9	1002	PEB	C1C-CHB-C4B	2.74	132.08	128.81
26	A2	1003	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	V3	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	X6	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	an	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	bN	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
28	bo	202	PUB	CHC-C1D-ND	-2.74	110.26	113.72
28	ff	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
26	h8	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	H7	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	X7	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	fg	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	hB	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	gy	302	PEB	C1C-CHB-C4B	2.74	132.08	128.81
28	n7	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
28	p9	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
28	jI	1003	PUB	CHC-C1D-ND	-2.74	110.26	113.72
26	x7	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	gv	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	V6	202	PEB	C1C-CHB-C4B	2.74	132.08	128.81
28	bD	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
26	ea	203	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	ga	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	A7	201	PEB	C1C-CHB-C4B	2.74	132.08	128.81
26	V7	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	ei	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	gp	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	jM	1002	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
28	eL	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
28	fs	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
28	kV	1003	PUB	CHC-C1D-ND	-2.74	110.26	113.72
26	U2	202	PEB	C1C-CHB-C4B	2.74	132.08	128.81
27	V1	201	CYC	C2B-C1B-NB	2.74	111.00	106.99
27	X1	201	CYC	C4A-C3A-C2A	-2.74	103.36	106.51
26	J7	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bP	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	cn	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	dd	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	hV	202	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	jJ	1002	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
27	a1	201	CYC	O2A-CGA-CBA	2.74	122.82	114.03
28	dN	203	PUB	CHC-C1D-ND	-2.74	110.26	113.72
26	ld	201	PEB	C1C-CHB-C4B	2.74	132.08	128.81
26	H2	201	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
26	jN	1002	PEB	CMD-C2D-C3D	-2.74	126.20	130.06
27	L1	201	CYC	O2A-CGA-CBA	2.74	122.82	114.03
28	dB	202	PUB	CHC-C1D-ND	-2.74	110.26	113.72
26	ei	201	PEB	C1C-CHB-C4B	2.74	132.08	128.81
26	h2	202	PEB	CMD-C2D-C3D	-2.74	126.21	130.06
26	ab	202	PEB	CMD-C2D-C3D	-2.74	126.21	130.06
26	ld	202	PEB	CMD-C2D-C3D	-2.74	126.21	130.06
26	hL	202	PEB	CMD-C2D-C3D	-2.74	126.21	130.06
27	q1	201	CYC	C2B-C1B-NB	2.74	110.99	106.99
26	R3	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	z5	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	at	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	cB	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	O3	1002	PEB	C1C-CHB-C4B	2.73	132.08	128.81
26	kS	1002	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	i3	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
27	I1	201	CYC	C2B-C1B-NB	2.73	110.99	106.99
26	l4	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
29	Z9	1004	PVN	C91-C18-C17	-2.73	122.85	127.53
26	Y7	1002	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	J5	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	ax	201	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	bJ	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	bQ	203	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	fy	201	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	hX	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	jK	1002	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	jO	1002	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
28	H4	203	PUB	CHC-C1D-ND	-2.73	110.27	113.72
26	cI	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	fl	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	el	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
27	b1	1001	CYC	C2B-C1B-NB	2.73	110.99	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K5	1002	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	I7	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	aF	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	fu	201	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
27	L1	201	CYC	C2B-C1B-NB	2.73	110.99	106.99
27	a1	201	CYC	C2B-C1B-NB	2.73	110.99	106.99
26	i3	203	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	cE	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	en	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	cx	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
27	m1	201	CYC	C2B-C1B-NB	2.73	110.98	106.99
26	n6	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
26	ch	202	PEB	CMD-C2D-C3D	-2.73	126.21	130.06
27	g1	201	CYC	C2B-C1B-NB	2.73	110.98	106.99
27	o1	1001	CYC	C2B-C1B-NB	2.73	110.98	106.99
26	bZ	302	PEB	C1C-CHB-C4B	2.73	132.07	128.81
28	L5	203	PUB	CHC-C1D-ND	-2.73	110.27	113.72
26	al	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	gk	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	p5	201	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	L7	201	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	as	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	eB	203	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	lw	203	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	hD	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
27	s1	201	CYC	C2B-C1B-NB	2.73	110.98	106.99
26	u3	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	G5	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	K7	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	eY	401	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	h3	201	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	Y5	1002	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	O7	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	A9	202	PEB	C1C-CHB-C4B	2.73	132.07	128.81
26	f3	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	r5	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	B4	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	e4	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	B5	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	F7	201	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	dl	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	fj	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	hJ	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	jI	1002	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	Z9	1002	PEB	C1C-CHB-C4B	2.73	132.06	128.81
28	dR	203	PUB	CHC-C1D-ND	-2.73	110.28	113.72
27	W1	201	CYC	C2B-C1B-NB	2.73	110.98	106.99
26	B3	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	n3	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	y8	202	PEB	CMD-C2D-C3D	-2.73	126.22	130.06
26	M3	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	S3	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	m7	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	G9	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	S9	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	fp	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
27	N1	201	CYC	C2B-C1B-NB	2.72	110.98	106.99
26	E2	1002	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	P7	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	R9	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	dL	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	gt	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	hH	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	hN	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	W7	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	iA	1002	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	D3	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	Z3	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	j3	201	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	ah	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	bT	201	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
29	44	303	PVN	C21-C2-C1	2.72	127.80	121.39
29	Z5	304	PVN	C21-C2-C1	2.72	127.80	121.39
27	e1	201	CYC	C2B-C1B-NB	2.72	110.97	106.99
26	R2	201	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	t5	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	cH	201	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	dj	202	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
26	li	203	PEB	CMD-C2D-C3D	-2.72	126.22	130.06
27	O1	201	CYC	C2B-C1B-NB	2.72	110.97	106.99
27	Z1	201	CYC	C2B-C1B-NB	2.72	110.97	106.99
29	bY	1004	PVN	C15-C16-N4	-2.72	120.22	126.06
26	L2	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	kQ	1002	PEB	CMD-C2D-C3D	-2.72	126.23	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d3	301	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	au	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	fv	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	t3	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	D4	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	gg	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	W3	203	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	p3	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	34	1002	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	gr	201	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	E3	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	c7	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	cJ	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	I3	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	dJ	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	ek	1002	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	lt	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	jL	1002	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
28	D7	203	PUB	CHC-C1D-ND	-2.72	110.28	113.72
27	Q1	201	CYC	C2B-C1B-NB	2.72	110.97	106.99
26	h7	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	I9	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	hF	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	hQ	202	PEB	C1C-CHB-C4B	2.72	132.06	128.81
26	z7	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	df	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
27	U1	201	CYC	C2B-C1B-NB	2.72	110.97	106.99
27	d2	101	CYC	C2B-C1B-NB	2.72	110.97	106.99
26	az	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
27	S1	202	CYC	CHB-C1B-NB	-2.72	120.22	126.06
26	R7	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
28	D9	203	PUB	CHC-C1D-ND	-2.72	110.29	113.72
27	a2	901	CYC	CHB-C1B-NB	-2.72	120.23	126.06
26	eX	201	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
27	f1	201	CYC	C2B-C1B-NB	2.72	110.96	106.99
26	T3	202	PEB	CMD-C2D-C3D	-2.72	126.23	130.06
26	e6	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	n6	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	f7	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	i7	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	em	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	eB	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y7	1003	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	lo	203	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	S2	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	s7	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	S5	203	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	cf	201	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	a7	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	lp	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	c4	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	S5	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	lm	1002	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	gz	302	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	hM	1002	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	ev	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	iD	1002	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	eN	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	gx	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	w7	1002	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	bK	1002	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	ef	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	lk	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	lw	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	gb	1002	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	hI	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
27	r1	201	CYC	CHB-C1B-NB	-2.71	120.24	126.06
27	M1	1001	CYC	CHB-C1B-NB	-2.71	120.24	126.06
26	af	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	U7	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	ey	1001	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	eL	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81
28	eN	203	PUB	CHC-C1D-ND	-2.71	110.30	113.72
26	o8	201	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	bC	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	eh	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	gc	202	PEB	C1C-CHB-C4B	2.71	132.05	128.81
26	p8	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06
26	t8	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	ev	201	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	fn	1002	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	gf	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	gu	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	n7	202	PEB	CMD-C2D-C3D	-2.71	126.24	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S1	201	CYC	CHB-C1B-NB	-2.71	120.24	126.06
27	j1	201	CYC	CHB-C1B-NB	-2.71	120.24	126.06
26	q7	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	dc	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	o7	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	dg	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	T9	202	PEB	CMD-C2D-C3D	-2.71	126.25	130.06
26	dT	202	PEB	C3B-C4B-NB	-2.71	106.11	110.05
26	W3	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	ct	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	db	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	de	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	lu	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	gq	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	c3	301	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	G6	202	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	cm	1002	PEB	C1C-CHB-C4B	2.71	132.04	128.81
26	n4	202	PEB	CMD-C2D-C3D	-2.71	126.25	130.06
26	T7	202	PEB	CMD-C2D-C3D	-2.71	126.25	130.06
27	t1	201	CYC	CHB-C1B-NB	-2.70	120.25	126.06
26	h5	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	p6	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	aw	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	hK	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	bB	202	PEB	CMD-C2D-C3D	-2.70	126.25	130.06
26	s3	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	M5	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	N6	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	bG	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	bQ	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	fz	301	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	ln	202	PEB	CMD-C2D-C3D	-2.70	126.25	130.06
26	u7	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	lc	202	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	B7	201	PEB	C4B-NB-C1B	2.70	111.60	106.51
26	d7	202	PEB	C4B-NB-C1B	2.70	111.60	106.51
26	dV	202	PEB	CMD-C2D-C3D	-2.70	126.25	130.06
26	hZ	401	PEB	C1C-CHB-C4B	2.70	132.04	128.81
26	cE	202	PEB	C4B-NB-C1B	2.70	111.60	106.51
26	N2	201	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	U3	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	g7	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cu	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	da	1002	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	gw	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	D4	202	PEB	C4B-NB-C1B	2.70	111.59	106.51
26	A2	1001	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	bS	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	cC	1002	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	lh	201	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	hE	1002	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	lq	203	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	lw	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	fc	202	PEB	CMD-C2D-C3D	-2.70	126.26	130.06
26	A5	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	C9	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	bY	1002	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	hC	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	hU	201	PEB	C1C-CHB-C4B	2.70	132.03	128.81
27	h1	201	CYC	CHB-C1B-NB	-2.70	120.27	126.06
26	L3	202	PEB	CMD-C2D-C3D	-2.70	126.26	130.06
26	eV	202	PEB	CMD-C2D-C3D	-2.70	126.26	130.06
26	h4	201	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	fx	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	iB	1002	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	el	202	PEB	C4B-NB-C1B	2.70	111.59	106.51
26	e3	1002	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	bO	202	PEB	C1C-CHB-C4B	2.70	132.03	128.81
26	N4	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	O5	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	q5	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	lo	201	PEB	C1C-CHB-C4B	2.69	132.03	128.81
27	v1	201	CYC	CHB-C1B-NB	-2.69	120.28	126.06
26	w3	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	a6	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	E7	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	Q7	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	fg	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
29	ez	1004	PVN	C15-C16-N4	-2.69	120.28	126.06
27	z1	201	CYC	CHB-C1B-NB	-2.69	120.28	126.06
26	g3	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	Z5	302	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	u8	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	cv	202	PEB	C1C-CHB-C4B	2.69	132.03	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cy	1002	PEB	C1C-CHB-C4B	2.69	132.03	128.81
26	cd	202	PEB	C4B-NB-C1B	2.69	111.58	106.51
26	f6	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	bE	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	cZ	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	ls	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	go	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	o3	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	I5	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	lg	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	ax	201	PEB	C4B-NB-C1B	2.69	111.58	106.51
26	cD	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
29	34	1004	PVN	C81-C17-C18	-2.69	118.82	126.12
29	Y5	1004	PVN	C81-C17-C18	-2.69	118.82	126.12
28	eN	203	PUB	CHA-C4A-NA	-2.69	110.83	113.95
26	m3	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	U6	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	q8	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	fe	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	hA	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
27	J1	201	CYC	CHB-C1B-NB	-2.69	120.29	126.06
27	Y1	201	CYC	CHB-C1B-NB	-2.69	120.29	126.06
26	C7	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	n5	202	PEB	CMD-C2D-C3D	-2.69	126.28	130.06
26	gj	202	PEB	C1C-CHB-C4B	2.69	132.02	128.81
26	ac	201	PEB	C3B-C4B-NB	-2.69	106.14	110.05
26	y5	1002	PEB	C1C-CHB-C4B	2.68	132.02	128.81
26	lo	202	PEB	C1C-CHB-C4B	2.68	132.02	128.81
26	fb	202	PEB	C1C-CHB-C4B	2.68	132.02	128.81
26	eS	202	PEB	C3B-C4B-NB	-2.68	106.14	110.05
27	H1	201	CYC	CHB-C1B-NB	-2.68	120.30	126.06
27	p1	201	CYC	CHB-C1B-NB	-2.68	120.30	126.06
26	aj	202	PEB	CMD-C2D-C3D	-2.68	126.28	130.06
26	A3	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	w5	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	M7	1003	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	eu	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	P2	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	Y3	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	k7	1002	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	M9	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	gm	1002	PEB	C1C-CHB-C4B	2.68	132.01	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	c1	201	CYC	CHB-C1B-NB	-2.68	120.30	126.06
29	hZ	403	PVN	C81-C17-C18	-2.68	118.84	126.12
26	K3	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	O9	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	t6	201	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	bU	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	es	201	PEB	C3B-C4B-NB	-2.68	106.15	110.05
26	eO	201	PEB	C3B-C4B-NB	-2.68	106.15	110.05
26	A5	203	PEB	C4B-NB-C1B	2.68	111.56	106.51
26	cq	202	PEB	C4B-NB-C1B	2.68	111.56	106.51
26	w4	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	ec	201	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	fh	1002	PEB	C1C-CHB-C4B	2.68	132.01	128.81
29	ez	1004	PVN	C9-C10-C11	-2.68	125.61	128.81
27	a2	902	CYC	CHB-C1B-NB	-2.68	120.31	126.06
27	b2	1001	CYC	CHB-C1B-NB	-2.68	120.31	126.06
26	y3	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	m5	1002	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	c8	301	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	dZ	1002	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	fk	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
29	Y9	303	PVN	C5-C6-C7	2.68	134.90	130.34
26	ft	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	gs	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	cf	201	PEB	C4B-NB-C1B	2.68	111.56	106.51
26	cj	202	PEB	C4B-NB-C1B	2.68	111.55	106.51
26	f5	201	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	D7	202	PEB	C4B-NB-C1B	2.68	111.55	106.51
26	cG	202	PEB	C1C-CHB-C4B	2.68	132.01	128.81
26	P7	202	PEB	C4B-NB-C1B	2.68	111.55	106.51
26	ah	202	PEB	C4B-NB-C1B	2.68	111.55	106.51
26	s8	202	PEB	C1C-CHB-C4B	2.68	132.00	128.81
29	T8	303	PVN	C5-C6-C7	2.68	134.90	130.34
26	lg	201	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	gh	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	A4	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	r8	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	p5	201	PEB	C4B-NB-C1B	2.67	111.55	106.51
26	Y9	301	PEB	C1C-CHB-C4B	2.67	132.00	128.81
29	hY	404	PVN	C81-C17-C18	-2.67	118.86	126.12
26	N3	202	PEB	C4B-NB-C1B	2.67	111.55	106.51
26	eV	202	PEB	C4B-NB-C1B	2.67	111.55	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t6	202	PEB	C3B-C4B-NB	-2.67	106.16	110.05
26	s4	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	Q5	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	cw	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	lj	201	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	iF	1002	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	p3	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	v3	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	d8	301	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	et	201	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	R9	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	co	201	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	gl	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	aj	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	ap	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	df	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	er	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	p7	201	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	X6	201	PEB	C3B-C4B-NB	-2.67	106.17	110.05
26	N7	201	PEB	C3B-C4B-NB	-2.67	106.17	110.05
26	bG	201	PEB	C3B-C4B-NB	-2.67	106.17	110.05
26	C4	1002	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	r7	202	PEB	C4B-NB-C1B	2.67	111.54	106.51
26	r3	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	hN	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	G3	202	PEB	C1C-CHB-C4B	2.67	132.00	128.81
26	B4	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	S5	203	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	g5	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	aD	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	eJ	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	o8	202	PEB	C3B-C4B-NB	-2.67	106.17	110.05
26	ce	201	PEB	C3B-C4B-NB	-2.67	106.17	110.05
26	o5	202	PEB	C1C-CHB-C4B	2.67	131.99	128.81
26	Q9	202	PEB	C1C-CHB-C4B	2.67	131.99	128.81
26	U9	202	PEB	C1C-CHB-C4B	2.67	131.99	128.81
26	cK	202	PEB	C1C-CHB-C4B	2.67	131.99	128.81
26	hO	202	PEB	C1C-CHB-C4B	2.67	131.99	128.81
26	x7	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	cz	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	n5	202	PEB	C4B-NB-C1B	2.67	111.53	106.51
26	y7	202	PEB	C4B-NB-C1B	2.67	111.53	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bM	202	PEB	C1C-CHB-C4B	2.67	131.99	128.81
29	eY	403	PVN	C21-C2-C3	2.67	135.15	129.67
26	a3	1002	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	cA	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
29	eZ	402	PVN	C21-C2-C3	2.66	135.15	129.67
26	aN	204	PEB	C3B-C4B-NB	-2.66	106.17	110.05
26	H2	201	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	dC	201	PEB	C3B-C4B-NB	-2.66	106.17	110.05
26	eP	202	PEB	C3B-C4B-NB	-2.66	106.17	110.05
26	Q3	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	c7	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	eN	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	J9	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	j2	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	P9	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	at	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	dV	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	aq	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	hY	402	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	R3	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	T9	202	PEB	C4B-NB-C1B	2.66	111.53	106.51
26	eq	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	eB	203	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	fj	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	hT	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	s5	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	d6	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	eA	1002	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	R3	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	L4	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	Q4	202	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	R5	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	aY	402	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	dM	1001	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	fr	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	eg	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	ep	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	hL	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	j8	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	q6	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	bl	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	dO	202	PEB	C3B-C4B-NB	-2.66	106.18	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eP	201	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	i3	203	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	F9	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	bQ	203	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	cF	201	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	dY	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	aZ	302	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	lt	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	B9	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	S7	202	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	R7	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	a7	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	Q8	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	Y9	302	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	dM	1002	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	ay	1002	PEB	C1C-CHB-C4B	2.66	131.99	128.81
26	X6	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	L5	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	n2	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	Z3	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	av	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	az	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	cp	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	cY	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	kS	1002	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	aq	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	B5	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	N9	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	cb	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	lr	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	T2	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	ch	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	lf	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	fc	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	ge	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	u5	202	PEB	C1C-CHB-C4B	2.66	131.98	128.81
26	q2	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	P4	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	E5	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	w6	1001	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	y9	1001	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	cZ	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	do	201	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	eq	202	PEB	C3B-C4B-NB	-2.66	106.18	110.05
26	dl	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	et	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	ll	202	PEB	C4B-NB-C1B	2.66	111.52	106.51
26	bA	202	PEB	C1C-CHB-C4B	2.66	131.98	128.81
26	p4	202	PEB	C4B-NB-C1B	2.66	111.51	106.51
26	hP	202	PEB	C4B-NB-C1B	2.66	111.51	106.51
26	y8	202	PEB	C4B-NB-C1B	2.66	111.51	106.51
26	H9	202	PEB	C4B-NB-C1B	2.66	111.51	106.51
26	iD	1002	PEB	C4B-NB-C1B	2.66	111.51	106.51
26	F6	202	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	F8	1001	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	gz	303	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	h2	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	bL	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	fi	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	J8	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	dx	404	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	X2	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	N5	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	fw	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	jI	1002	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	g5	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	l2	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	F3	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	z3	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	bJ	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	kV	1002	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	I3	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	g9	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	ag	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	aW	302	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	eC	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	B3	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	bV	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	cr	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	R6	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	V7	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	ff	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	fo	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	H5	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b8	1003	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	cr	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	eF	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	eO	202	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	lp	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	gt	202	PEB	C4B-NB-C1B	2.65	111.51	106.51
26	Q4	203	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	j6	202	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	u9	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	au	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	dg	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	gz	301	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	H3	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	j3	201	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	V5	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	ad	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	N9	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	aG	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	dq	202	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	dP	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	gq	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	hT	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	h3	201	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	z5	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	Y7	1003	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	ev	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	r4	201	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	hX	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	v4	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	m9	1001	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	dU	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	lp	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	hH	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	34	1001	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	cJ	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	fg	201	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	kU	1002	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	O8	201	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	U8	1002	PEB	C3B-C4B-NB	-2.65	106.19	110.05
26	e4	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	n6	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	gd	201	PEB	C4B-NB-C1B	2.65	111.50	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S8	401	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	aH	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	dI	1002	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	c5	201	PEB	C1C-CHB-C4B	2.65	131.97	128.81
26	hS	202	PEB	C1C-CHB-C4B	2.65	131.97	128.81
26	Z2	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	R5	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	B6	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	en	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	gx	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	hD	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	Q8	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	C9	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	G9	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	dr	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	iB	1001	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	di	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	ee	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
29	bY	1004	PVN	C51-C8-C7	-2.65	119.64	127.25
26	E9	202	PEB	C1C-CHB-C4B	2.65	131.97	128.81
26	aF	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	gk	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	y2	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	R4	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	k8	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	h7	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	C8	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	O8	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	P8	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	T8	302	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	J9	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	at	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	av	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	eW	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
28	eT	203	PUB	CHA-C4A-NA	-2.65	110.87	113.95
26	L3	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	fq	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	I2	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	E3	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	f6	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	k6	1001	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	r6	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	x7	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	b9	401	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	A9	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	X9	401	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	jL	1001	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	C8	202	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	jJ	1002	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	o2	1001	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	b3	502	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	T5	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	x9	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	dw	401	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	hY	403	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	bT	201	PEB	C4B-NB-C1B	2.65	111.50	106.51
26	hG	201	PEB	C4B-NB-C1B	2.65	111.50	106.51
28	dX	203	PUB	CHA-C4A-NA	-2.65	110.88	113.95
26	A2	1003	PEB	C4B-NB-C1B	2.65	111.49	106.51
26	g4	202	PEB	C4B-NB-C1B	2.65	111.49	106.51
26	D5	202	PEB	C4B-NB-C1B	2.65	111.49	106.51
26	iC	1002	PEB	C4B-NB-C1B	2.65	111.49	106.51
26	t2	202	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	b5	1001	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	w5	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	f8	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	a9	602	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	f9	201	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	aY	406	PEB	C3B-C4B-NB	-2.65	106.20	110.05
26	an	201	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	hR	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	jO	1002	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	j2	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	l8	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	aK	1001	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	aU	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	cB	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	eH	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	hT	204	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	p2	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	J7	201	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	li	203	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	hV	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	o5	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y6	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	I7	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	a9	603	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	aQ	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	bY	1003	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	dn	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	dS	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	dZ	1001	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	jI	1001	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	J3	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	T7	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	bF	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	C3	1002	PEB	C1C-CHB-C4B	2.64	131.97	128.81
26	A1	301	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	B1	301	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	D3	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	n3	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	s3	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	h6	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	S7	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	w8	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	bF	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	cO	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	dX	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	eh	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	gm	1001	PEB	C3B-C4B-NB	-2.64	106.20	110.05
28	ep	203	PUB	CHA-C4A-NA	-2.64	110.88	113.95
26	cB	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	dd	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	dL	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	ld	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	ln	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	gn	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	e5	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	h9	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	eB	202	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	eH	201	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	lm	1001	PEB	C3B-C4B-NB	-2.64	106.20	110.05
26	C5	202	PEB	C1C-CHB-C4B	2.64	131.97	128.81
26	H6	201	PEB	C1C-CHB-C4B	2.64	131.97	128.81
26	r3	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	N5	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g8	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	p9	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	aF	204	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dC	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	lq	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	ls	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	lu	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	fe	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	l4	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	eL	202	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	B2	501	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	V4	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	W4	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	M6	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	v6	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	C7	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	V9	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	bZ	301	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	ch	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	hS	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	iE	1002	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	kW	1002	PEB	C4B-NB-C1B	2.64	111.49	106.51
26	ea	203	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	fy	201	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	T3	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	B4	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	b4	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	z5	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	bm	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	bR	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dF	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	t7	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	v9	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	G2	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	g3	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	Y4	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	44	301	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	a6	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	e9	303	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	l9	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dN	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	eA	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	iG	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	v5	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	m2	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	L2	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	G5	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	cJ	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dl	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dx	402	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dD	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dG	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	hZ	402	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	n4	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	L2	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	e7	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	bN	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	hH	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	bd	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	cq	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	ea	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	eC	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	fq	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	hB	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	G7	202	PEB	C1C-CHB-C4B	2.64	131.96	128.81
26	w2	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	O3	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	U5	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	j5	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	T9	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	aI	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	cX	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dw	403	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dx	401	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	lv	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	fk	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	fp	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	P3	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	V3	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	L9	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	ec	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	l2	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	s2	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	F2	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Q2	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	a3	1003	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	q3	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	r6	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	v8	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	w8	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	aO	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dq	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	V2	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	J5	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	gr	201	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	gv	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	jN	1002	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	t5	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	h8	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	bD	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	cH	201	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	fu	201	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	jL	1002	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	X5	401	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	u5	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	I6	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	G8	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	F9	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	aD	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	aM	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	bQ	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	cg	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	cM	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	dt	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	li	202	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	gl	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	gs	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	gt	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	hM	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	hW	201	PEB	C3B-C4B-NB	-2.64	106.21	110.05
26	iF	1001	PEB	C3B-C4B-NB	-2.64	106.21	110.05
28	az	203	PUB	CHA-C4A-NA	-2.64	110.89	113.95
26	af	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	gg	202	PEB	C4B-NB-C1B	2.64	111.48	106.51
26	g2	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	u2	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F4	202	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	H4	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	o4	202	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	t4	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	j6	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	q6	202	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	z7	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	h9	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	bv	202	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	lq	201	PEB	C3B-C4B-NB	-2.64	106.22	110.05
26	J6	202	PEB	C4B-NB-C1B	2.64	111.47	106.51
26	ga	202	PEB	C4B-NB-C1B	2.64	111.47	106.51
26	H3	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	C5	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	x6	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	b8	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	aP	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eN	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	gg	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	kQ	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	cl	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	E2	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	b3	501	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	G8	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	j9	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	cE	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	de	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ej	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eY	402	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	hQ	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	n8	201	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	V9	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	E4	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	S4	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	Q5	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	y5	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	P6	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	S6	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	cU	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ez	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eM	1002	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	jM	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c3	303	PVN	C15-C16-C17	2.63	132.17	126.95
26	B2	502	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	O7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	g7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	P8	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	r9	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	bp	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	bH	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	cV	203	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	du	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eR	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ll	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	f3	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	gi	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	jP	1002	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	kR	1002	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	i2	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	n2	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	v3	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	J4	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	y6	203	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	H7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	A8	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	X8	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	i9	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ao	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dk	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ej	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eD	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	fo	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	N7	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	cL	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	kT	1002	PEB	C4B-NB-C1B	2.63	111.47	106.51
28	dF	203	PUB	CHA-C4A-NA	-2.63	110.89	113.95
26	F7	201	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	z7	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	R2	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	s6	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	l7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	n7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	B8	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	Y8	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	M9	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	U9	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	bb	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dp	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	j4	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	L5	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	hJ	202	PEB	C4B-NB-C1B	2.63	111.47	106.51
29	ly	404	PVN	C51-C8-C7	-2.63	119.69	127.25
26	s2	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	O2	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	T7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	b7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	e7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	e9	301	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	e9	302	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	s9	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	bf	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dA	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ge	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	hF	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	iE	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	kV	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	jK	1002	PEB	C4B-NB-C1B	2.63	111.47	106.51
26	x2	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	z6	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	R7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dH	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dN	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eb	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eo	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	eX	201	PEB	C4B-NB-C1B	2.63	111.47	106.51
29	lz	403	PVN	C51-C8-C7	-2.63	119.69	127.25
26	z2	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	l3	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	n3	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	B6	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	J6	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	b9	403	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	M8	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	aS	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	aX	401	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	bM	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cC	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dk	1002	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	ed	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	em	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	fw	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	kW	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	v4	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	dj	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	kX	1002	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	o2	1002	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	r2	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	R4	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	Z7	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	w7	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	a8	601	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	Z8	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	w9	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	aT	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	aV	202	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	br	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	bs	1002	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	dR	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	lc	201	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	fh	1001	PEB	C3B-C4B-NB	-2.63	106.22	110.05
26	T3	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	X7	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
28	x7	203	PUB	CHA-C4A-NA	-2.63	110.89	113.95
28	bN	203	PUB	CHA-C4A-NA	-2.63	110.89	113.95
26	v2	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	u3	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	O4	1001	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	O5	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	W5	301	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	a5	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	E6	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	Q6	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	e8	302	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bC	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	lb	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	fm	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	gn	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	l7	202	PEB	C4B-NB-C1B	2.63	111.46	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	lw	203	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	r2	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	F4	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	N4	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	34	1003	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	m8	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	T6	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	w9	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	aE	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	aH	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bP	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	di	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	dK	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	eD	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	ft	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	hR	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	x3	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	v7	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	bB	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	dh	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	ei	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	p2	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	J3	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	e3	1001	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	I4	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	e4	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	I6	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	P6	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	S6	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	l6	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	d9	301	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	H8	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	y9	1002	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	aX	402	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bd	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bu	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bv	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bw	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bZ	303	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	ct	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	cY	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	ew	301	PEB	C3B-C4B-NB	-2.63	106.23	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fa	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	gp	202	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	x5	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	T6	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	y6	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	j7	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	o7	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	D8	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	P9	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	bx	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	cl	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	eZ	401	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	gx	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	iA	1001	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	P5	201	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	m5	1003	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	C2	301	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	U2	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	P3	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	f4	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	m5	1001	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	G6	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	k6	1002	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	K7	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	m7	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	d9	303	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	f9	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	q9	202	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	df	201	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	du	203	PEB	C3B-C4B-NB	-2.63	106.23	110.05
26	kQ	1002	PEB	C4B-NB-C1B	2.63	111.46	106.51
26	lh	202	PEB	C4B-NB-C1B	2.62	111.45	106.51
26	y2	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	X2	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	a4	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	g6	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	w6	1002	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	V7	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	b8	1002	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	bA	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cQ	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	dL	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ln	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	fv	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	f2	202	PEB	C4B-NB-C1B	2.62	111.45	106.51
26	e2	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	L3	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	K4	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	Q4	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	d5	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	p8	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	az	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cG	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	dj	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	ds	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	er	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	gu	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	kX	1001	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	W4	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	m8	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	Z6	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	I8	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	z9	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	bi	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	dR	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	ee	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	eG	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	gc	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	jP	1001	PEB	C3B-C4B-NB	-2.62	106.23	110.05
28	l6	203	PUB	CHA-C4A-NA	-2.62	110.90	113.95
26	bH	202	PEB	C4B-NB-C1B	2.62	111.45	106.51
26	f2	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	C2	302	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	z3	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	c4	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	M5	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	l5	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	P7	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	c7	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	N8	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	aL	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	aL	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	br	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cw	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cP	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cR	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cT	1001	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cW	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	cX	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	gb	1001	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	gj	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	34	1002	PEB	C4B-NB-C1B	2.62	111.45	106.51
26	L7	201	PEB	C4B-NB-C1B	2.62	111.45	106.51
26	cs	202	PEB	C4B-NB-C1B	2.62	111.45	106.51
28	dT	203	PUB	CHA-C4A-NA	-2.62	110.90	113.95
26	D2	302	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	D4	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	l4	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	o4	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	n5	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	s7	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	a8	602	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	r9	202	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	dp	201	PEB	C3B-C4B-NB	-2.62	106.23	110.05
26	fd	303	PEB	C3B-C4B-NB	-2.62	106.23	110.05
28	J7	202	PUB	CHA-C4A-NA	-2.62	110.90	113.95
26	K2	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	w3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	k4	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	O6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	V6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	c6	1002	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	y6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	E7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	a9	601	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	K8	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	j9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	q9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	S9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	aN	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	aQ	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cS	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dV	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Y2	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	H4	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	x4	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v5	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	j8	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	k8	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	g6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	c9	301	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	v9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Q9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	be	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cv	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cI	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dB	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	eu	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	fc	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hK	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	q2	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	M2	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	P2	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	p3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	L4	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	A5	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	K5	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	o6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	U7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	aB	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	aW	301	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	ci	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cT	1002	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dY	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	lr	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hC	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	jO	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	kS	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
28	kV	1003	PUB	CHA-C4A-NA	-2.62	110.91	113.95
26	ar	202	PEB	C4B-NB-C1B	2.62	111.44	106.51
26	G4	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	M4	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	X4	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Z5	303	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	c5	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	u6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	v7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	v8	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aC	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	bt	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	bX	401	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cD	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
28	aR	203	PUB	CHA-C4A-NA	-2.62	110.91	113.95
28	hZ	404	PUB	CHA-C4A-NA	-2.62	110.91	113.95
26	al	202	PEB	C4B-NB-C1B	2.62	111.44	106.51
26	A2	1002	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	t3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	i5	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	L6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	s6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	z8	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	N8	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	ar	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	bm	1002	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dm	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	eI	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	eP	203	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	gh	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hN	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
28	B9	203	PUB	CHA-C4A-NA	-2.62	110.91	113.95
26	F2	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	D3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	y3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	G4	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	I4	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Q7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	W7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	f7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	U8	1003	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	s9	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	bl	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cW	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dr	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	lb	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	lf	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	go	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	gy	303	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hY	401	PEB	C3B-C4B-NB	-2.62	106.24	110.05
29	T8	303	PVN	C51-C52-C53	-2.62	106.42	113.76
29	Y9	303	PVN	C51-C52-C53	-2.62	106.42	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	jM	1002	PEB	C4B-NB-C1B	2.62	111.44	106.51
28	F9	203	PUB	CHA-C4A-NA	-2.62	110.91	113.95
26	W2	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	f3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	V4	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	E6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	b6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	l6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cM	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dt	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dG	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	dK	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	eE	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hJ	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hX	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	C3	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	G3	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	C4	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	y4	1002	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Y5	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	s5	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	i8	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Q6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	d6	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	R9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	aF	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cb	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	da	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	eU	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	eW	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	fx	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
28	c9	305	PUB	CHA-C4A-NA	-2.62	110.91	113.95
28	E8	203	PUB	CHA-C4A-NA	-2.62	110.91	113.95
26	fm	202	PEB	C4B-NB-C1B	2.62	111.44	106.51
26	e2	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	h2	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	v2	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	A6	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	Z6	202	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	t7	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	c8	302	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	U8	1001	PEB	C3B-C4B-NB	-2.62	106.24	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y8	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	n9	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	af	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	aV	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	bg	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	bV	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cc	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	cC	1003	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hB	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
26	hI	201	PEB	C3B-C4B-NB	-2.62	106.24	110.05
28	d3	303	PUB	CHA-C4A-NA	-2.62	110.91	113.95
29	C2	303	PVN	C15-C16-C17	2.62	132.13	126.95
26	p8	202	PEB	C4B-NB-C1B	2.62	111.44	106.51
26	K4	202	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	J5	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	b9	404	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	x8	202	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	J8	202	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	bs	1003	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	bt	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	bw	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	ds	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	dJ	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	eF	202	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	fb	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	hA	201	PEB	C3B-C4B-NB	-2.62	106.25	110.05
26	n7	202	PEB	C4B-NB-C1B	2.61	111.44	106.51
26	T2	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	S3	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	W6	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	c6	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	y7	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	W8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	al	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	aB	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	aM	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bK	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cL	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cR	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	dx	403	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	dQ	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	gy	301	PEB	C3B-C4B-NB	-2.61	106.25	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	jN	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
28	gy	305	PUB	CHA-C4A-NA	-2.61	110.91	113.95
26	D2	301	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	G2	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	U3	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	h4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	u4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	l8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	d8	302	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	F8	1002	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	L8	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	Z9	1007	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bs	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bY	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	dn	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	fs	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	gk	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	fs	202	PEB	C4B-NB-C1B	2.61	111.43	106.51
29	ly	404	PVN	C15-C16-C17	2.61	132.13	126.95
26	i2	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	S3	203	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	a3	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	S4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	Z4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	y8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	K8	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	T8	301	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	as	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bX	402	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ez	1002	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	gp	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
28	ar	203	PUB	CHA-C4A-NA	-2.61	110.91	113.95
26	W3	203	PEB	C4B-NB-C1B	2.61	111.43	106.51
29	aY	403	PVN	C51-C8-C7	-2.61	119.74	127.25
26	t2	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	w2	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	W2	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	M7	1002	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	a7	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	E8	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	L8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	l9	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	E9	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	K9	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	aY	401	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bn	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bo	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cz	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	dz	401	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	fd	301	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ga	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	gw	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	iH	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	w2	203	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	P4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	q5	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	C6	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	H6	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	M8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	aI	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bc	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cO	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	dT	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ep	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	r5	202	PEB	C4B-NB-C1B	2.61	111.43	106.51
26	Z7	202	PEB	C4B-NB-C1B	2.61	111.43	106.51
26	Z2	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	g4	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	j4	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	F6	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	q8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	Y7	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	H8	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	p9	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bB	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bL	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cj	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cS	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	eQ	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ab	202	PEB	C4B-NB-C1B	2.61	111.43	106.51
26	i3	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	O4	1002	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	X4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	24	401	PEB	C3B-C4B-NB	-2.61	106.25	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y5	1003	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	u9	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ai	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	aJ	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	aZ	301	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bu	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cu	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	db	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	dW	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ed	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	eT	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	fd	302	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	U4	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	j5	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	m6	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	o6	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	A8	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	V8	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ba	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bq	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bq	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bz	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	cs	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	eg	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	kU	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
28	p8	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	b9	407	PUB	CHA-C4A-NA	-2.61	110.92	113.95
26	k2	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	q4	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	K6	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	e8	301	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	c9	302	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ad	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	bh	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ca	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	eM	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	fn	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	gv	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	jK	1001	PEB	C3B-C4B-NB	-2.61	106.25	110.05
28	f2	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	F3	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	n3	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d9	305	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	H9	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	cp	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
26	M2	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	B5	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	u6	202	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	u7	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	x9	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	by	1002	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	eK	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	le	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	ly	401	PEB	C3B-C4B-NB	-2.61	106.25	110.05
26	fj	201	PEB	C3B-C4B-NB	-2.61	106.25	110.05
28	J9	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	cs	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
26	K2	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	34	1007	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	i4	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	y4	1001	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	e6	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	ap	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	aS	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	bz	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	bE	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	cK	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	ea	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	eE	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	ly	403	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	lz	402	PEB	C3B-C4B-NB	-2.61	106.26	110.05
28	t5	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
26	A3	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	A4	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	T4	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	W6	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	G7	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	D8	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	B9	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	O9	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	aN	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	bh	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	dw	402	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	eI	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	gf	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	bP	202	PEB	C4B-NB-C1B	2.61	111.42	106.51
26	I2	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	F3	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	b6	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	x6	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	t8	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	W8	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	aU	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	cP	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	ey	1002	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	eK	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	H7	202	PEB	C4B-NB-C1B	2.61	111.42	106.51
26	lo	203	PEB	C4B-NB-C1B	2.61	111.42	106.51
26	B3	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	K3	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	J4	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	V5	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	bk	201	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	du	202	PEB	C3B-C4B-NB	-2.61	106.26	110.05
26	ez	1003	PEB	C3B-C4B-NB	-2.61	106.26	110.05
28	z2	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	V6	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	b6	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
28	T9	203	PUB	CHA-C4A-NA	-2.61	110.92	113.95
26	k2	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	u2	202	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	x3	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	Y4	202	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	d4	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	k8	203	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	N6	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	aK	1002	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	dy	401	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	dz	402	PEB	C3B-C4B-NB	-2.60	106.26	110.05
28	el	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
26	V3	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	E4	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	n4	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	Z5	301	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	r5	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	h8	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U6	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	p6	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	u8	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	x8	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	D9	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	by	1001	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	lk	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	iD	1001	PEB	C3B-C4B-NB	-2.60	106.26	110.05
28	h2	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	J2	202	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	c3	305	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	o8	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	l7	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	n9	202	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	gz	305	PUB	CHA-C4A-NA	-2.60	110.92	113.95
26	Z3	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	44	302	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	K6	202	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	M6	1002	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	v6	202	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	ae	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	am	1001	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	aR	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	V2	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	k3	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	m4	1001	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	t5	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	h6	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	I8	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	o9	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	L9	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	cU	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	cV	202	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	do	202	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	dE	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	eU	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	hV	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
28	cr	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	dP	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
28	eJ	203	PUB	CHA-C4A-NA	-2.60	110.92	113.95
26	t3	202	PEB	C4B-NB-C1B	2.60	111.41	106.51
26	m3	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U4	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	D5	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	dc	203	PEB	C3B-C4B-NB	-2.60	106.26	110.05
26	dH	201	PEB	C3B-C4B-NB	-2.60	106.26	110.05
28	X7	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	C8	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	v9	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	aZ	304	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	eB	204	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	w4	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	l5	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	i6	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	z6	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	bj	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	bJ	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	dc	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	ef	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	la	1002	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	gi	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	H2	202	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	s7	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	D7	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	E8	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	Z9	1001	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	cx	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	dD	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	eQ	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
29	hY	404	PVN	C15-C16-N4	-2.60	120.47	126.06
26	M3	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	Z4	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	s4	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	t4	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	aE	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	hD	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	hE	1001	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	hP	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	jJ	1001	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	aV	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	ll	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	D9	202	PEB	C4B-NB-C1B	2.60	111.41	106.51
26	J2	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	S2	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p4	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	z4	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	D6	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	X7	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	H9	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	aP	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	aT	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	bI	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	F5	202	PEB	C4B-NB-C1B	2.60	111.41	106.51
28	L4	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	M8	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	x9	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	M7	1001	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	ff	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	B4	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	F4	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	34	1005	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	L6	202	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	w8	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	eZ	403	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	lv	202	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	jM	1003	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	N3	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	b9	402	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	t9	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	dm	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	v2	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	V3	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	r5	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	cM	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	gt	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
29	44	303	PVN	C15-C16-C17	2.60	132.09	126.95
29	Z5	304	PVN	C15-C16-C17	2.60	132.09	126.95
26	W3	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	z4	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	c6	1003	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	B8	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	z9	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	ay	1001	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	kT	1001	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	N2	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	c3	302	PEB	C3B-C4B-NB	-2.60	106.27	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	i6	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	t9	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	I9	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	dv	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	eJ	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	f3	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	J6	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	P6	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	H7	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	O8	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	bs	1004	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	hD	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	hX	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	ab	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	aR	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	dd	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	dA	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	eo	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	ff	204	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	C2	304	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	T2	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	aF	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
28	fw	203	PUB	CHA-C4A-NA	-2.60	110.93	113.95
26	m2	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	O2	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	q4	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	z8	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	Z9	1003	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	aC	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	bj	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	bN	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	cV	201	PEB	C3B-C4B-NB	-2.60	106.27	110.05
26	es	202	PEB	C3B-C4B-NB	-2.60	106.27	110.05
28	N3	203	PUB	CHA-C4A-NA	-2.59	110.93	113.95
28	B6	203	PUB	CHA-C4A-NA	-2.59	110.93	113.95
28	V9	203	PUB	CHA-C4A-NA	-2.59	110.93	113.95
28	ey	1005	PUB	CHA-C4A-NA	-2.59	110.93	113.95
26	X3	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	o3	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	C6	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	cA	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	eR	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	hO	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	iC	1001	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	C2	305	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	Z2	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	N6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	x6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	dw	405	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ff	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	jK	1003	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	Y2	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	d7	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	dQ	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	eS	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	fi	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	g2	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	cd	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	ly	402	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	lz	401	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	r2	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	X3	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	b7	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	cB	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	eY	405	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	eZ	404	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	cn	201	PEB	C4B-NB-C1B	2.59	111.39	106.51
26	cp	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	dP	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	kR	1001	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	c6	1004	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	bz	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	dd	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	hL	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	Y3	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	A6	1002	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	m6	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	cm	1001	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	dI	1001	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	fl	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	Z4	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	z6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	p7	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	iF	1003	PUB	CHA-C4A-NA	-2.59	110.94	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	M4	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	u4	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	r8	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	r7	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	k9	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	ak	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	aA	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	ey	1003	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	H6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	T6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	bV	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	cL	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	dl	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	dH	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	dK	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ly	405	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	iE	1003	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	aA	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	eV	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
29	C2	303	PVN	C5-C6-C7	2.59	134.75	130.34
29	c3	303	PVN	C5-C6-C7	2.59	134.75	130.34
26	I5	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	li	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	z4	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	d7	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	aZ	305	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ld	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ln	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ge	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	gy	306	PUB	CHA-C4A-NA	-2.59	110.94	113.95
29	aY	403	PVN	C81-C17-C18	-2.59	119.09	126.12
26	s8	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	i7	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	q7	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	aJ	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	bx	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	bU	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	e8	304	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	p9	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ap	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	dD	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	eT	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	la	1001	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	p2	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	P3	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	p4	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	F5	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	e8	305	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	Y9	305	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	hR	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	F5	201	PEB	C3B-C4B-NB	-2.59	106.28	110.05
26	f8	202	PEB	C3B-C4B-NB	-2.59	106.28	110.05
28	L7	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	an	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	lb	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	cy	1001	PEB	C3B-C4B-NB	-2.59	106.29	110.05
29	bY	1004	PVN	C81-C17-C18	-2.59	119.09	126.12
26	z2	201	PEB	C3B-C4B-NB	-2.59	106.29	110.05
28	x3	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	v6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	y8	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	eb	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	lz	404	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ga	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	iD	1003	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	hL	201	PEB	C3B-C4B-NB	-2.59	106.29	110.05
28	a3	1005	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	e6	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	cn	202	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	ei	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
28	gk	203	PUB	CHA-C4A-NA	-2.59	110.94	113.95
26	dF	202	PEB	C3B-C4B-NB	-2.58	106.29	110.05
28	D2	304	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	L2	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	L3	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	X4	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	Y5	1005	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	Q8	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	cR	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	eg	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	lr	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	gd	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	kS	1003	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	R6	201	PEB	C3B-C4B-NB	-2.58	106.29	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bD	201	PEB	C3B-C4B-NB	-2.58	106.29	110.05
28	r6	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	bq	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	cQ	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	ee	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	lp	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	d9	302	PEB	C3B-C4B-NB	-2.58	106.29	110.05
26	ek	1001	PEB	C3B-C4B-NB	-2.58	106.29	110.05
28	T5	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	T8	304	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	cP	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	R3	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	h3	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	J4	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	dN	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	eV	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	hV	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	iG	1002	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	eG	201	PEB	C3B-C4B-NB	-2.58	106.29	110.05
28	N4	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	R7	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	cq	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	eH	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	Q3	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
26	ah	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
26	aw	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
26	dh	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
29	gz	304	PVN	C15-C16-C17	2.58	132.06	126.95
28	F2	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	c3	304	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	H4	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	e9	305	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	aP	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	S5	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
26	bS	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
28	V4	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	L5	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	P5	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	R5	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	N7	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	r9	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	Z9	1005	PUB	CHA-C4A-NA	-2.58	110.95	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	bD	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	gz	306	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	N3	201	PEB	CHC-C4C-C3C	-2.58	125.94	130.34
28	n2	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	T3	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	n6	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	b8	1006	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	ev	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	hJ	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	kU	1003	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	bO	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
26	el	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
28	V2	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	z7	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	bn	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	bZ	305	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	gi	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	O6	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
29	hZ	403	PVN	C15-C16-N4	-2.58	120.53	126.06
28	D5	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	B7	202	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	r7	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	z9	203	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	aY	404	PUB	CHA-C4A-NA	-2.58	110.95	113.95
28	jP	1003	PUB	CHA-C4A-NA	-2.58	110.95	113.95
26	eS	201	PEB	CHC-C4C-C3C	-2.58	125.94	130.34
28	R4	203	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	44	304	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	ax	202	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	bP	203	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	er	203	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	ez	1005	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	ly	406	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	gg	203	PUB	CHA-C4A-NA	-2.58	110.96	113.95
28	hY	406	PUB	CHA-C4A-NA	-2.58	110.96	113.95
26	h5	201	PEB	C3B-C4B-NB	-2.58	106.30	110.05
26	dW	202	PEB	C3B-C4B-NB	-2.58	106.30	110.05
28	t6	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	bT	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	eL	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	fj	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	fq	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	jL	1003	PUB	CHA-C4A-NA	-2.57	110.96	113.95
26	k5	201	PEB	C3B-C4B-NB	-2.57	106.30	110.05
26	aj	201	PEB	C3B-C4B-NB	-2.57	106.30	110.05
28	j2	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	B3	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	t3	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	T8	305	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	co	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	cz	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	dp	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	kR	1003	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	34	1006	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	v7	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	hG	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
26	aa	1001	PEB	C3B-C4B-NB	-2.57	106.31	110.05
29	lz	403	PVN	C15-C16-C17	2.57	132.05	126.95
26	k7	1001	PEB	C3B-C4B-NB	-2.57	106.31	110.05
28	D3	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	X6	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	Z9	1006	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	cE	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
29	34	1004	PVN	C15-C16-N4	-2.57	120.54	126.06
29	Y5	1004	PVN	C15-C16-N4	-2.57	120.54	126.06
26	eQ	202	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
28	n7	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	dr	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	hT	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
26	al	201	PEB	CHC-C4C-C3C	-2.57	125.95	130.34
28	t4	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	Y5	1006	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	g8	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	av	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	bR	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	dv	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	eX	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	hZ	405	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	P2	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	p3	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	br	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
26	ck	201	PEB	C3B-C4B-NB	-2.57	106.31	110.05
28	Z6	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	cF	202	PUB	CHA-C4A-NA	-2.57	110.96	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	df	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	fc	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	gp	203	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	jO	1003	PUB	CHA-C4A-NA	-2.57	110.96	113.95
28	kW	1003	PUB	CHA-C4A-NA	-2.57	110.96	113.95
26	M4	201	PEB	CHC-C4C-C3C	-2.57	125.96	130.34
26	en	201	PEB	C3B-C4B-NB	-2.57	106.31	110.05
28	N2	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	R2	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	r3	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	F6	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	c9	304	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	dh	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	ez	1006	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	eY	404	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	lz	405	PUB	CHA-C4A-NA	-2.57	110.97	113.95
26	bW	301	PEB	C3B-C4B-NB	-2.57	106.31	110.05
28	v4	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	v5	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	aJ	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	bp	202	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	bF	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	cO	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
26	cq	201	PEB	CHC-C4C-C3C	-2.57	125.96	130.34
28	b8	1005	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	ey	1006	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	gn	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
26	F5	201	PEB	CHC-C4C-C3C	-2.57	125.96	130.34
26	dX	202	PEB	C3B-C4B-NB	-2.57	106.32	110.05
28	D4	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	at	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	bY	1005	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	ec	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	eD	203	PUB	CHA-C4A-NA	-2.57	110.97	113.95
28	D2	305	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	n5	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	aT	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	jJ	1003	PUB	CHA-C4A-NA	-2.56	110.97	113.95
26	b9	401	PEB	CHC-C4C-C3C	-2.56	125.96	130.34
26	aw	201	PEB	CHC-C4C-C3C	-2.56	125.96	130.34
26	bl	202	PEB	CHC-C4C-C3C	-2.56	125.96	130.34
28	t2	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	44	305	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	u6	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	et	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	lj	202	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	lx	201	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	iC	1003	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	jI	1003	PUB	CHA-C4A-NA	-2.56	110.97	113.95
26	aU	202	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	j3	202	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	V5	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	a7	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	c7	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	bH	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	cY	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
29	dx	405	PVN	C15-C16-N4	-2.56	120.56	126.06
26	cN	201	PEB	C3B-C4B-NB	-2.56	106.32	110.05
26	bH	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	dQ	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	dO	201	PEB	C3B-C4B-NB	-2.56	106.32	110.05
28	t7	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	dY	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	hB	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
26	C4	1001	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	ck	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	cD	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	ar	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	A2	1005	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	v3	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	n4	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	J5	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	D6	202	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	P7	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	c8	305	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	en	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	fi	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	gx	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	hP	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	kQ	1003	PUB	CHA-C4A-NA	-2.56	110.97	113.95
26	q5	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	aj	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	y6	204	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	e7	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eV	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	c8	304	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	I8	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
28	D9	203	PUB	CHA-C4A-NA	-2.56	110.97	113.95
26	n4	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	k5	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	v5	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	Z8	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	Z5	306	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	n8	202	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	y7	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	G8	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	L9	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	aL	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
26	u2	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
26	cj	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	x2	202	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	z3	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	aD	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
26	aG	201	PEB	CHC-C4C-C3C	-2.56	125.97	130.34
28	f8	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	D7	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	aN	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	aY	405	PUB	CHA-C4A-NA	-2.56	110.98	113.95
26	aC	202	PEB	CHC-C4C-C3C	-2.56	125.98	130.34
26	eN	201	PEB	CHC-C4C-C3C	-2.56	125.98	130.34
28	X2	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	l3	202	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	bJ	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	cN	202	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	A2	1006	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	N5	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	b9	406	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	dj	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	dt	203	PUB	CHA-C4A-NA	-2.56	110.98	113.95
28	fa	202	PUB	CHA-C4A-NA	-2.56	110.98	113.95
26	t5	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	ad	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	bV	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
28	D7	203	PUB	CHA-C1B-C2B	-2.55	125.98	130.34
26	E4	202	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	m8	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	kT	1001	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
28	J3	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	d3	304	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	x4	202	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	x5	202	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	e9	306	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	fs	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	iH	1002	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	kT	1003	PUB	CHA-C4A-NA	-2.55	110.98	113.95
26	W6	202	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	J8	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	L8	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	cY	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	fr	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	af	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
28	l2	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	H3	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	T4	202	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	A8	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	bZ	306	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	lh	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	eP	204	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	hN	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
26	i2	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	bO	201	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	eE	202	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	eP	203	PEB	CHC-C4C-C3C	-2.55	125.98	130.34
26	H8	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	f9	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	ai	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	cW	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	fd	301	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
28	eX	202	PUB	CHA-C1B-C2B	-2.55	125.99	130.34
28	B5	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	Z5	305	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	t9	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
28	gv	203	PUB	CHA-C4A-NA	-2.55	110.98	113.95
26	l3	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	j7	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
28	a3	1006	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	H5	202	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	bL	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	T3	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	bv	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	ff	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	fo	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	hN	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
28	r4	202	PUB	CHA-C4A-NA	-2.55	110.99	113.95
26	G2	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	R3	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	S2	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	S6	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	U8	1002	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	lp	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
28	d6	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	dn	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
26	Q4	203	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	Z5	301	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	i5	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	b7	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	X8	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	h9	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	dV	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	es	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
28	U8	1005	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	N9	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	bo	202	PUB	CHA-C4A-NA	-2.55	110.99	113.95
26	x2	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	aD	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	cz	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	cP	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	a3	1003	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	a5	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	M6	1002	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	bq	202	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
28	R6	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	R9	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	bB	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
28	lf	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
26	b4	1001	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	U5	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	K6	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	k6	1002	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
26	q7	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fe	201	PEB	CHC-C4C-C3C	-2.55	125.99	130.34
29	hY	404	PVN	C51-C8-C7	-2.55	119.93	127.25
28	aH	203	PUB	CHA-C4A-NA	-2.55	110.99	113.95
26	O3	1001	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	a4	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	l5	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	N9	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	aR	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	bj	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	bB	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	hB	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
28	cJ	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	dL	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
26	Z7	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	z8	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	cI	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	cU	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	dF	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	ed	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	eJ	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	fc	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
28	ly	406	PUB	CHA-C1B-C2B	-2.54	126.00	130.34
28	K8	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	P9	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	Y9	304	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	fm	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	hY	405	PUB	CHA-C4A-NA	-2.54	110.99	113.95
26	k2	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	n3	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	l8	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	q8	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	ay	1001	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	cS	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	fk	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	d9	301	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	dW	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
28	h8	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	di	203	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	dx	407	PUB	CHA-C4A-NA	-2.54	110.99	113.95
28	fy	202	PUB	CHA-C4A-NA	-2.54	110.99	113.95
26	o4	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	dp	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dy	401	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
29	hZ	403	PVN	C51-C8-C7	-2.54	119.94	127.25
28	z5	203	PUB	CHA-C4A-NA	-2.54	111.00	113.95
29	Y5	1004	PVN	C51-C8-C7	-2.54	119.94	127.25
26	M6	1001	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	cV	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	de	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	eH	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	H8	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	aa	1001	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	eS	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
28	V7	203	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	gr	202	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	kX	1003	PUB	CHA-C4A-NA	-2.54	111.00	113.95
26	h9	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	az	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	bI	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	dK	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	dX	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
28	Z4	203	PUB	CHA-C1B-C2B	-2.54	126.00	130.34
29	ey	1004	PVN	C51-C8-C7	-2.54	119.94	127.25
26	t2	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	J4	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	x6	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	g9	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	M9	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	aT	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	eE	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	lz	401	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	hV	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
28	jM	1003	PUB	CHA-C1B-C2B	-2.54	126.00	130.34
26	f3	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	Y4	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	j4	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	C5	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	j5	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	p6	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	z6	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	G7	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	b9	404	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	ag	201	PEB	CHC-C4C-C3C	-2.54	126.00	130.34
26	aP	202	PEB	CHC-C4C-C3C	-2.54	126.00	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	P4	203	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	p6	203	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	aB	203	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	dx	406	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	dB	202	PUB	CHA-C4A-NA	-2.54	111.00	113.95
26	I2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	i4	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	x5	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	u6	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	y7	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	r9	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	aA	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	aC	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	aK	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bl	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bm	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bs	1002	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	by	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	cl	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	eG	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	B3	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	c3	302	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	G4	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	e9	303	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	i9	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	aP	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bS	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dg	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dx	403	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dQ	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dT	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	ea	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	eD	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	gz	301	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	r2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	s2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	L2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	M5	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	n5	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	i6	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	g7	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	e8	301	PEB	CHC-C4C-C3C	-2.54	126.01	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B8	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	p9	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	z9	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	X9	401	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	cM	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	cO	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	ew	301	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
28	dX	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	hG	202	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	hP	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	U8	1006	PUB	CHA-C4A-NA	-2.54	111.00	113.95
26	z2	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	w6	1002	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	v8	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	w9	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	cp	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	eU	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	go	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	hE	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	kS	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
28	C8	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	jO	1003	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
26	m3	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	O4	1002	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	Z4	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	C6	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	aE	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bs	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dF	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
28	X2	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	ep	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
26	e2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	p2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	M2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	U2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	z3	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	F4	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	N4	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bZ	301	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	du	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
28	fo	203	PUB	CHA-C4A-NA	-2.54	111.00	113.95
28	fu	202	PUB	CHA-C4A-NA	-2.54	111.00	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O2	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	F3	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	X4	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	o5	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	V6	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	f6	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	b8	1003	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	ab	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bj	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	br	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	bZ	303	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	cy	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dw	403	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	lv	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
28	eT	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	kX	1003	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
26	q6	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	P9	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	aJ	202	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	dC	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	fv	201	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
26	jM	1001	PEB	CHC-C4C-C3C	-2.54	126.01	130.34
28	x7	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	hH	203	PUB	CHA-C1B-C2B	-2.54	126.01	130.34
28	eF	203	PUB	CHA-C4A-NA	-2.53	111.00	113.95
28	jN	1003	PUB	CHA-C4A-NA	-2.53	111.00	113.95
26	k4	201	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	K5	1001	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	t9	202	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	aN	201	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	aQ	202	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	bk	201	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
26	ly	402	PEB	CHC-C4C-C3C	-2.53	126.01	130.34
28	34	1005	PUB	CHA-C1B-C2B	-2.53	126.01	130.34
26	u2	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	J3	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	E4	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	b9	402	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	ao	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	aF	204	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	bR	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	cK	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dP	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	lr	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	N6	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	iG	1002	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	Z3	203	PUB	CHA-C4A-NA	-2.53	111.00	113.95
28	d8	304	PUB	CHA-C4A-NA	-2.53	111.00	113.95
28	bY	1006	PUB	CHA-C4A-NA	-2.53	111.00	113.95
28	cH	202	PUB	CHA-C4A-NA	-2.53	111.00	113.95
29	ez	1004	PVN	C51-C8-C7	-2.53	119.97	127.25
26	M7	1002	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	Q7	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	f7	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	A8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	j9	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	Z9	1003	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	cP	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	cT	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	el	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	hA	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	jK	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	R2	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	H4	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	l7	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	b9	406	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
26	Q2	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	C3	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	x4	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	P6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	g6	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	G8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	am	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	aV	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	bd	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	cB	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dz	402	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	lq	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	hC	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	dN	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
26	v2	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	D3	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	k8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	D6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h6	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	T9	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	cd	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	ct	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dw	401	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	m2	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	R2	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	V4	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	L5	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	g8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	y6	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	d9	302	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	p9	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dn	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	ff	204	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	F3	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	p5	202	PUB	CHA-C4A-NA	-2.53	111.01	113.95
28	T7	203	PUB	CHA-C4A-NA	-2.53	111.01	113.95
28	dw	406	PUB	CHA-C4A-NA	-2.53	111.01	113.95
26	j2	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	P3	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	R4	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	y4	1002	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	C7	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	s9	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	aW	302	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	bU	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	le	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	hS	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	P3	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	b6	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	L7	202	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	eL	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
26	M3	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	a6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	b6	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	m6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	w9	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	y9	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	I9	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	aR	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	bf	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dk	1002	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dm	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dp	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dx	402	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dA	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dL	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	eW	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	L6	202	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	dV	203	PUB	CHA-C4A-NA	-2.53	111.01	113.95
26	U4	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	L6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	O6	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	R6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	v8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	W8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	bt	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	bz	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	cT	1002	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dh	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	ey	1003	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	eW	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	gk	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	t4	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
28	J6	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34
29	34	1004	PVN	C51-C8-C7	-2.53	119.98	127.25
28	hH	203	PUB	CHA-C4A-NA	-2.53	111.01	113.95
26	r2	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	b3	501	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	V4	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	v4	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	O8	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	l9	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	s9	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	ly	401	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	F2	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	Y2	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	W3	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	a3	1001	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	j6	201	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	aI	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
26	dD	202	PEB	CHC-C4C-C3C	-2.53	126.02	130.34
28	d6	203	PUB	CHA-C1B-C2B	-2.53	126.02	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F7	202	PUB	CHA-C4A-NA	-2.53	111.01	113.95
28	Z7	203	PUB	CHA-C4A-NA	-2.53	111.01	113.95
28	lt	203	PUB	CHA-C4A-NA	-2.53	111.01	113.95
26	y2	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	f8	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	o6	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	d7	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	w8	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	y8	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	Q8	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	df	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dI	1002	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	eo	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	li	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	li	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	hD	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	jO	1001	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	c8	305	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	F9	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
26	z2	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	O2	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	R4	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	S5	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	w7	1001	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	d8	302	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	bX	402	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	cN	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	eR	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	ls	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	hJ	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	hR	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	n5	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
26	J2	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	Z5	303	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	O7	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	C8	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	T8	302	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	aW	301	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	bx	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	cV	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	eu	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	la	1002	PEB	CHC-C4C-C3C	-2.53	126.03	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fj	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	ft	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	hP	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	iD	1001	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	y8	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	cR	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
26	I2	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	z4	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	D5	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	x9	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	aF	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dO	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dS	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	eo	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	gz	303	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	d3	303	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	gt	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	iF	1003	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
26	S3	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	o6	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	r8	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	x7	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	a9	603	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	aK	1002	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	bK	1001	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dc	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dc	203	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dr	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	hI	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	hZ	402	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	ey	1006	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
26	n2	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	w3	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	J4	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	C6	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	c6	1001	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	z6	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	M7	1001	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	U8	1003	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	q9	202	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	y9	1002	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	Q9	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	be	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	br	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	dx	404	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	eQ	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
26	gu	201	PEB	CHC-C4C-C3C	-2.53	126.03	130.34
28	D5	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	B6	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	an	202	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	co	202	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	dD	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
28	ge	203	PUB	CHA-C1B-C2B	-2.53	126.03	130.34
29	T8	303	PVN	C15-C16-N4	-2.52	120.64	126.06
29	Y9	303	PVN	C15-C16-N4	-2.52	120.64	126.06
26	m2	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	S4	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	c4	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	G6	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	S6	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	T6	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	E9	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	V9	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	du	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	du	203	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	eg	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	ez	1003	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	eB	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	lm	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	gj	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	hL	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	iA	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	kQ	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	kV	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
28	bD	203	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
29	T8	303	PVN	C92-C91-C18	2.52	119.39	112.43
26	K4	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	P4	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	T4	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	N7	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	E8	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	m9	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	aq	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	aY	402	PEB	CHC-C4C-C3C	-2.52	126.03	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bh	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	eI	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	lt	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	kR	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
28	X4	203	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	dw	405	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	dF	203	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	lz	405	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
26	E2	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	K4	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	Y5	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	m7	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	a8	602	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	w8	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	U8	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	ak	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	au	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	aB	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	aO	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	bq	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	ce	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	dN	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
28	D2	304	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	D3	203	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	c9	304	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
26	g2	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	w2	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	y3	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	H4	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	T5	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	h8	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	m6	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	I8	202	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	U9	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	bE	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	dP	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	fp	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
28	R4	203	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	x6	203	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	a6	203	PUB	CHA-C4A-NA	-2.52	111.02	113.95
26	q3	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	34	1003	PEB	CHC-C4C-C3C	-2.52	126.03	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	y5	1001	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	d6	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	i6	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	p8	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	P7	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	dm	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	dv	201	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	dw	402	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
26	ez	1002	PEB	CHC-C4C-C3C	-2.52	126.03	130.34
28	g8	202	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	e8	305	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
28	Z9	1006	PUB	CHA-C1B-C2B	-2.52	126.03	130.34
29	Y9	303	PVN	C92-C91-C18	2.52	119.38	112.43
28	eR	203	PUB	CHA-C4A-NA	-2.52	111.02	113.95
26	h2	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	o3	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	u3	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	v3	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	t4	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	Y5	1003	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	O6	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	G8	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	u9	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	v9	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	av	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	bu	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cJ	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cW	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cX	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dK	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	eT	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	ge	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	hY	401	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	jN	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	kU	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	44	304	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	V6	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	Y9	305	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	aL	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	ee	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	C2	302	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	I3	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b3	502	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	H5	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	I6	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	i7	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	F8	1002	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	k9	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	aL	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dq	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dR	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	eG	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	fn	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	hW	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	t3	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	F4	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	I8	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	aF	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	dw	406	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	K2	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	T2	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	R5	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	I6	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	E7	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	e9	301	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	B8	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	K8	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	L8	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cC	1003	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	ly	403	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	lz	402	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	f8	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	N7	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	cF	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	gg	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	U4	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	m5	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	m8	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	u6	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	c8	302	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	c9	301	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	K8	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dA	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dX	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	gt	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	iE	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	j3	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	bz	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	eY	405	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	eZ	404	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	hB	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	q2	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	s2	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	O5	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	Y8	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	L9	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	aX	401	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	bC	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	d7	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	e9	305	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	E8	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	aZ	305	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	bp	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	Y2	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	Q4	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	l4	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	b5	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	s6	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	t8	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	E8	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	n9	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	aY	406	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	bx	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	ca	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	lf	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	gm	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	gx	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	l2	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	L3	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	H5	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	G8	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	bN	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	fq	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	jJ	1003	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	o2	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	e4	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	W5	301	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	F6	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	r6	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	s6	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	aS	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	bY	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cb	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cw	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dB	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	eT	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	lu	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	fi	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	hX	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	D6	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	ez	1006	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	C2	301	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	s3	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	A4	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	P4	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	N8	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	bh	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	cU	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	ds	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	eC	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	lq	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	Z3	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	h3	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	e7	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	br	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	bT	202	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	B2	501	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	S3	203	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	B4	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	m4	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	T6	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	v6	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	h7	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	s7	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	D8	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	J8	202	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	t9	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	Y9	302	PEB	CHC-C4C-C3C	-2.52	126.04	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bz	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	bL	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	dr	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	eb	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	fx	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	gb	1001	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
26	gg	201	PEB	CHC-C4C-C3C	-2.52	126.04	130.34
28	Y5	1005	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	X7	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	z7	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	L9	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	aD	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
28	fo	203	PUB	CHA-C1B-C2B	-2.52	126.04	130.34
26	e3	1001	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	i3	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	L4	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	V5	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	M8	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	O8	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	ap	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	aS	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	ez	1001	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	fd	302	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	gy	301	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
28	l3	202	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	O8	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	bV	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	cO	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	ln	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	hN	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
26	34	1007	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	Q6	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	q6	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	C9	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	aT	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	bv	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	cr	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	db	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	ea	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	eF	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	eP	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	lk	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fh	1001	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
28	n3	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
26	u4	202	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	z4	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	aE	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	aQ	201	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
26	gy	303	PEB	CHC-C4C-C3C	-2.52	126.05	130.34
28	t5	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	n6	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	K8	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	P9	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	Z9	1005	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	cp	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	eH	203	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
28	lz	404	PUB	CHA-C1B-C2B	-2.52	126.05	130.34
26	B2	502	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	G2	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	K2	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	P2	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	G3	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	F4	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	u4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	Q5	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	A6	1001	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	B6	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	A8	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	B9	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	Z9	1007	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	aZ	302	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bW	301	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dt	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	ej	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	eY	402	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	lc	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	v9	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	hD	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	jP	1003	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	kV	1003	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	D4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	M4	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	w4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	K6	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	e6	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	l6	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	r6	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	T7	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	e9	302	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	aU	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	aV	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bd	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cu	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cM	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	z3	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	B4	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	P6	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	V7	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	Z7	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	aT	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	k2	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	l2	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	q2	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	K3	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	L3	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	d5	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	s8	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bw	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bD	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bY	1003	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	eM	1002	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	a3	1006	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	Z5	305	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	at	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	kW	1003	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	t2	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	W2	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	Z4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	g4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	c6	1003	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	x9	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cs	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cO	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cV	203	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	eI	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	hF	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	hM	1001	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	hO	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	Z5	306	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	eg	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	lf	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	o2	1002	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	N2	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	Y3	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	r3	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	E6	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	aM	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	da	1001	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	do	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dx	401	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dH	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	ed	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	jI	1001	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	c3	305	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	r3	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	F5	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	d9	305	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	N9	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	bJ	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	bR	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	cr	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	el	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	M2	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	X4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	s4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	f8	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	A6	1002	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	X6	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	j6	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	I7	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	o7	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	D9	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bM	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	bQ	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cG	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	cX	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	hT	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	V2	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	34	1006	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	x4	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	x5	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	r7	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	d8	304	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	cH	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	ev	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	eF	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	W4	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	q4	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	R7	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	z7	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	aM	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dl	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dn	202	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dE	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
26	dH	201	PEB	CHC-C4C-C3C	-2.51	126.05	130.34
28	C2	305	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	b7	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	v7	203	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	bo	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
28	dv	202	PUB	CHA-C1B-C2B	-2.51	126.05	130.34
26	U3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	N5	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	E6	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	T8	301	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	l9	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	J9	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	K9	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cm	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	fa	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gl	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gn	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	44	305	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	e9	306	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	dr	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	dx	407	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	ey	1005	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	eD	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	ga	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	V3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	W4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A5	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	o8	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	x8	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bm	1002	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	by	1002	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cC	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	dR	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	eh	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	ej	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	eD	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	fq	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	x2	202	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	R3	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	X3	202	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	c3	304	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	n7	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	M8	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	Y9	304	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	G4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	y4	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	l5	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	M8	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	Z9	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	dG	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	ef	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	es	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	eA	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gq	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gv	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	l6	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	b8	1005	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	t9	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
29	44	303	PVN	C21-C2-C3	-2.51	124.52	129.67
26	H3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	H4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	k6	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	V8	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	ch	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cv	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	dC	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	en	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	fw	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y5	1006	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	s7	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	dH	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	eZ	403	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	fi	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	w2	203	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	g3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	p4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	t4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	B5	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	U6	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	Z6	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	c7	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	Y8	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	aI	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bb	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bg	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bG	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gf	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	j2	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	Z2	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	r9	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	aZ	304	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	bn	202	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	eJ	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	fa	202	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	fw	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	iD	1003	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	iH	1002	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	V2	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	X2	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	Z3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	x3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	44	302	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	y6	203	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	F8	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	f9	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	R9	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	aX	402	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cQ	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	ey	1002	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	eM	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	jP	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	v2	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	T2	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	V3	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	V4	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	ar	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	dK	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	Z2	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	K7	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	U7	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	n7	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	a8	601	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	aN	204	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cc	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	ds	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	dZ	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	hH	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	iF	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	x3	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	x9	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	cY	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	ly	405	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	k8	203	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	d9	303	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cL	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cR	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	eq	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gw	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	iG	1001	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	D2	305	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	J7	202	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	T8	305	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	D9	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	t3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	Y4	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	d4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	t7	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	v7	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	N8	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	u9	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bs	1003	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bw	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bA	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	di	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	fb	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	z2	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	bZ	305	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	cs	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	gp	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	E3	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	I4	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	Q4	202	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	s5	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	a9	601	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	S9	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	ac	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	bp	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	cx	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	dd	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	dY	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	eC	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
26	gp	201	PEB	CHC-C4C-C3C	-2.51	126.06	130.34
28	p8	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	c7	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	gx	203	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
28	kQ	1003	PUB	CHA-C1B-C2B	-2.51	126.06	130.34
26	D2	301	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
26	D2	302	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
26	j5	202	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
26	i8	201	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
26	j9	201	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
26	aZ	301	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
26	fl	201	PEB	CHC-C4C-C3C	-2.50	126.06	130.34
28	r2	203	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
28	t6	203	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
28	y6	204	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
28	aR	203	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
28	aY	404	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
28	cN	202	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
28	gy	305	PUB	CHA-C1B-C2B	-2.50	126.06	130.34
26	g2	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	H6	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	w6	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	dW	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J2	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	p9	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	ap	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	cM	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dj	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dt	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dP	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dT	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
26	A2	1002	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	44	301	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	I5	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	g5	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	N6	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	h6	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	P8	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	q9	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	dG	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	er	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	la	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	lb	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	C2	304	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	b9	407	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	c9	305	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	B9	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	hZ	404	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
26	S4	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	h5	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	u5	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	l6	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	b8	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	x8	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	G9	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	bN	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	cZ	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	dk	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	fm	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	U8	1005	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	ax	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	df	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
26	i2	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	y2	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	L4	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b6	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	e7	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	aA	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	eO	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	lb	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	gi	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	hK	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	kX	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	f3	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	N5	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	h8	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	B7	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dd	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	eB	204	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	hY	406	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	jL	1003	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dR	203	PUB	CHA-C4A-NA	-2.50	111.04	113.95
26	u8	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	aJ	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	aY	401	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	bt	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	bJ	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	gc	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	gs	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	jJ	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	kW	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	h2	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	D4	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	U8	1006	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	av	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	cE	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dh	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	gr	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	gv	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
29	T8	303	PVN	C51-C8-C7	-2.50	120.06	127.25
29	Y9	303	PVN	C51-C8-C7	-2.50	120.06	127.25
29	U8	1004	PVN	C9-C10-C11	-2.50	125.82	128.81
26	f2	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	z5	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	k8	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	ci	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	L2	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d3	304	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	L4	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	c6	1004	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	R9	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	eV	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	fc	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	hJ	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
26	j8	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	r7	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	P8	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	cR	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	dU	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	ee	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	hY	403	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	iC	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	A8	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
29	c8	303	PVN	C15-C16-N4	-2.50	120.69	126.06
26	W2	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	aB	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	aN	202	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	bi	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	eZ	401	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	J4	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	dl	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	hY	405	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
26	k3	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	24	401	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	k7	1001	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	at	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	dj	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	dM	1002	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
26	ll	201	PEB	CHC-C4C-C3C	-2.50	126.07	130.34
28	P2	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	T4	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	bY	1005	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	cQ	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	lr	203	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	fy	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	gd	202	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
28	iE	1003	PUB	CHA-C1B-C2B	-2.50	126.07	130.34
29	Z5	304	PVN	C21-C2-C3	-2.50	124.54	129.67
26	h4	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u7	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	bn	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	cS	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	dq	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	H3	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	T9	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	V9	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	aY	405	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	cn	202	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	dx	406	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	hZ	405	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	jK	1003	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	O4	1001	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	H7	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	D8	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	r9	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	bF	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	do	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	em	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	fs	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	gh	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	v3	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	N4	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	J5	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	e6	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	y7	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	cq	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	kS	1003	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	o4	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	j8	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	v6	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	z9	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	eK	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	H2	202	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	aJ	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	ff	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	e2	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	v2	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	F2	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	J5	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	l7	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	bo	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bu	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	iH	1001	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	A2	1006	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	cJ	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	kR	1003	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	q4	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	P6	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	e8	302	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	b9	403	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	O9	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	hQ	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	v6	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	bq	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	X5	401	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	e5	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	w5	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	l8	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	aH	202	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	hT	204	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	N3	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	n8	202	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	b8	1006	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	aV	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	iC	1003	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	Q6	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	V7	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	c9	302	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	aL	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	cE	201	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
26	dM	1001	PEB	CHC-C4C-C3C	-2.50	126.08	130.34
28	R5	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	aP	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	bB	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	cL	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	ei	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
28	ll	203	PUB	CHA-C1B-C2B	-2.50	126.08	130.34
26	c6	1002	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
26	dD	201	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
26	eH	202	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
28	n2	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	A2	1005	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	a3	1005	PUB	CHA-C1B-C2B	-2.49	126.08	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	v4	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	v5	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	R6	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	X6	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	di	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	ez	1005	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	lj	202	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	lx	201	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	gi	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	gz	306	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
26	J6	201	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
26	dN	201	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
28	t2	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	T3	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	lv	202	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
26	b8	1002	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
26	ae	201	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
26	eO	202	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
28	F6	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	H6	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	a7	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	bZ	306	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	kU	1003	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
29	Z9	1004	PVN	C9-C10-C11	-2.49	125.83	128.81
26	S8	401	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
26	dJ	201	PEB	CHC-C4C-C3C	-2.49	126.08	130.34
28	dn	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	dp	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	fs	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	hV	203	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
28	kT	1003	PUB	CHA-C1B-C2B	-2.49	126.08	130.34
26	W8	202	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	H9	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	ah	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	eq	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	T8	304	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	az	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	y6	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	A9	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	J3	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	J9	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	cB	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	dV	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	W6	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	X7	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	aH	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	ba	1001	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	dz	401	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	bP	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	Y6	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	bP	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	dO	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	f2	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	fu	202	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
27	z1	201	CYC	C4D-CHA-C1A	-2.49	125.83	128.81
26	Q3	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	f4	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	I8	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	z4	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	z5	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	dB	202	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	I4	202	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	z8	202	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	ep	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	eU	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	lb	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	ld	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	lp	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	jN	1003	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	w2	202	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	x6	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	o9	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	ga	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	N2	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	T6	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	o8	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	G5	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	cg	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	z6	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	a7	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	p4	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	V5	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	p6	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	e8	304	PUB	CHA-C1B-C2B	-2.49	126.09	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X3	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	Q8	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
26	dt	201	PEB	CHC-C4C-C3C	-2.49	126.09	130.34
28	F2	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	c8	304	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	Q8	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
28	cP	203	PUB	CHA-C1B-C2B	-2.49	126.09	130.34
26	p3	201	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
26	t6	202	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
26	jL	1001	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
28	B3	203	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
28	gz	305	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
26	Z6	202	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
26	fd	303	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
28	u6	203	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
28	bL	203	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
28	jI	1003	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
26	a9	602	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
26	bc	201	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
26	ln	201	PEB	CHC-C4C-C3C	-2.49	126.10	130.34
28	r4	202	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
28	r5	203	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
28	eY	404	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
28	gn	203	PUB	CHA-C1B-C2B	-2.49	126.10	130.34
29	dw	404	PVN	C91-C18-C17	-2.48	123.28	127.53
26	c5	202	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	D7	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	dI	1001	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
28	n4	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	w8	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	H9	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	bs	1004	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	lh	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
29	dw	404	PVN	C15-C16-N4	-2.48	120.72	126.06
26	r5	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	S7	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
28	p2	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	eb	202	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	gk	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
27	a2	901	CYC	C4D-CHA-C1A	-2.48	125.84	128.81
26	F6	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	eK	202	PEB	CHC-C4C-C3C	-2.48	126.10	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	fj	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	gy	306	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
26	A3	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	g6	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	Y7	1001	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
26	dT	202	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
28	dY	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	eP	204	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	eR	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	aH	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	cz	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
26	W7	201	PEB	CHC-C4C-C3C	-2.48	126.10	130.34
28	T5	202	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	fm	203	PUB	CHA-C1B-C2B	-2.48	126.10	130.34
28	B5	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	H7	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	p7	202	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	dL	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	hT	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	p3	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
26	cA	201	PEB	CHC-C4C-C3C	-2.48	126.11	130.34
26	eF	202	PEB	CHC-C4C-C3C	-2.48	126.11	130.34
28	P4	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	L5	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	p5	202	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	hL	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
27	S1	201	CYC	C4D-CHA-C1A	-2.48	125.85	128.81
27	j1	201	CYC	C4D-CHA-C1A	-2.48	125.85	128.81
26	E5	201	PEB	CHC-C4C-C3C	-2.48	126.11	130.34
28	Z6	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	r6	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	n9	202	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
29	bY	1004	PVN	C12-C11-N3	-2.48	106.44	110.05
28	ec	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	R7	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	lt	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
27	M1	1001	CYC	C4D-CHA-C1A	-2.48	125.85	128.81
26	iB	1001	PEB	CHC-C4C-C3C	-2.48	126.11	130.34
28	P5	202	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	P7	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	bH	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34
28	hR	203	PUB	CHA-C1B-C2B	-2.48	126.11	130.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eR	202	PEB	CHC-C4C-C3C	-2.47	126.12	130.34
28	t7	203	PUB	CHA-C1B-C2B	-2.47	126.12	130.34
28	bF	203	PUB	CHA-C1B-C2B	-2.47	126.12	130.34
28	aB	203	PUB	CHA-C1B-C2B	-2.47	126.12	130.34
28	hX	203	PUB	CHA-C1B-C2B	-2.47	126.12	130.34
27	H1	201	CYC	C4D-CHA-C1A	-2.47	125.85	128.81
26	F9	201	PEB	CHC-C4C-C3C	-2.47	126.12	130.34
26	bX	401	PEB	CHC-C4C-C3C	-2.47	126.12	130.34
28	bY	1006	PUB	CHA-C1B-C2B	-2.47	126.12	130.34
28	T7	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
28	er	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
28	a6	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
28	z9	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
28	aN	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
28	eN	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
28	et	203	PUB	CHA-C1B-C2B	-2.47	126.13	130.34
29	gy	304	PVN	C91-C18-C19	2.47	125.27	121.38
29	gy	304	PVN	C92-C91-C18	-2.47	105.64	112.43
28	dR	203	PUB	CHA-C1B-C2B	-2.46	126.13	130.34
28	F7	202	PUB	CHA-C1B-C2B	-2.46	126.13	130.34
28	en	203	PUB	CHA-C1B-C2B	-2.46	126.14	130.34
29	c9	303	PVN	C15-C16-N4	-2.46	120.78	126.06
27	r1	201	CYC	C4D-CHA-C1A	-2.46	125.87	128.81
27	a2	902	CYC	C4D-CHA-C1A	-2.46	125.87	128.81
27	b2	1001	CYC	C4D-CHA-C1A	-2.46	125.87	128.81
27	p1	201	CYC	C4D-CHA-C1A	-2.46	125.88	128.81
26	dO	201	PEB	CBB-CAB-C3B	-2.45	105.81	112.63
27	S1	202	CYC	C4D-CHA-C1A	-2.45	125.88	128.81
26	as	201	PEB	CHC-C4C-C3C	-2.45	126.15	130.34
29	aY	403	PVN	C12-C11-N3	-2.45	106.49	110.05
26	er	201	PEB	CBB-CAB-C3B	-2.45	105.83	112.63
27	v1	201	CYC	C4D-CHA-C1A	-2.45	125.89	128.81
26	dS	201	PEB	CBB-CAB-C3B	-2.45	105.83	112.63
26	ek	1001	PEB	CHC-C4C-C3C	-2.45	126.17	130.34
26	eP	203	PEB	CBB-CAB-C3B	-2.44	105.83	112.63
26	q5	201	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
26	dD	201	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
26	eW	201	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
27	c1	201	CYC	C4D-CHA-C1A	-2.44	125.89	128.81
26	dI	1001	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
26	au	201	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
26	dN	201	PEB	CBB-CAB-C3B	-2.44	105.84	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	iB	1001	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
26	aj	201	PEB	CBB-CAB-C3B	-2.44	105.84	112.63
26	bz	201	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	cK	201	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	dc	201	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	w2	203	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	cJ	201	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
27	t1	201	CYC	C4D-CHA-C1A	-2.44	125.89	128.81
26	H9	201	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	em	201	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	W6	202	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	Y5	1003	PEB	CBB-CAB-C3B	-2.44	105.85	112.63
26	U8	1003	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	dQ	201	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	dG	201	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	bS	201	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	hM	1001	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	t6	202	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	a9	603	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	U7	201	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	X7	201	PEB	CBB-CAB-C3B	-2.44	105.86	112.63
26	L4	202	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	d8	302	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	eR	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	n4	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	l8	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	q6	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	w8	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	dw	403	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	dz	402	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	z3	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	D6	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	cd	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	do	202	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	eH	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	f3	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	X4	202	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	aG	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	aP	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	en	201	PEB	CBB-CAB-C3B	-2.43	105.86	112.63
26	V8	1001	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	n9	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ck	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	cE	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	eT	202	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	H3	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	O4	1002	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	t7	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	c8	302	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	dm	202	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	fx	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	K2	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	C3	1001	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	E9	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	aY	401	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	bh	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	bV	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	dH	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
27	J1	201	CYC	C4D-CHA-C1A	-2.43	125.90	128.81
27	Y1	201	CYC	C4D-CHA-C1A	-2.43	125.90	128.81
26	e4	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	W5	301	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	f9	202	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	M9	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	ge	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	G5	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	Q4	203	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	f4	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	q4	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	v8	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	bw	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	iH	1001	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	jP	1001	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	Z9	1003	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	ch	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	dx	404	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	dW	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	eZ	401	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	o6	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	V9	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	eO	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	hC	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	t2	202	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	N2	202	PEB	CBB-CAB-C3B	-2.43	105.87	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	E5	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	V5	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	du	202	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	ek	1001	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	eF	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	lt	201	PEB	CBB-CAB-C3B	-2.43	105.87	112.63
26	s2	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	J4	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	ap	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	cV	203	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	dA	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	dX	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	kV	1001	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	a5	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	i9	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bb	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bd	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bX	401	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	cD	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	do	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	la	1002	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	e8	301	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	L8	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	r9	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	ae	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bs	1002	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	dX	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	g2	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	F2	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	Y4	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	t8	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	b9	404	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	af	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	aU	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bF	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	cs	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	q2	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	G2	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	B5	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	l9	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	O9	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	aF	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bm	1002	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	eU	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	L2	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	r3	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	24	401	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	l8	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	Y8	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	B9	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bE	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	dx	403	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	z7	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	aO	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	dZ	1001	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	gx	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bG	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	i2	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	34	1003	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	k5	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	o7	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	D9	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	lc	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	fb	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	fq	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	gc	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	gm	1001	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	hR	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	iD	1001	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	D2	301	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	D3	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	B6	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	d7	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	E8	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	U8	1001	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	ai	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	aN	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	bv	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	es	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	li	202	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	fr	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	hB	201	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	jI	1001	PEB	CBB-CAB-C3B	-2.43	105.88	112.63
26	p2	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u2	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	W2	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	i5	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	F6	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	B8	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	X9	401	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	dl	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	dx	401	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	gi	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	w4	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	O6	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	z8	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	bO	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	lp	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	F2	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	K3	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	Y3	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	H4	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	g6	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	z6	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	dy	401	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	dH	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	w2	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	p3	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	v3	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	D5	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	u8	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	I8	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	bg	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	eC	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	ff	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	y2	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	Y4	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	e5	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	L6	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	T6	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	g9	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	x9	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	bJ	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	cr	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	dE	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	eu	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eF	202	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	eT	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	eU	201	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	hZ	402	PEB	CBB-CAB-C3B	-2.43	105.89	112.63
26	N3	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	g5	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	j5	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	k8	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	A6	1002	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	ak	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	br	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	da	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	dC	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	ej	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	eS	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	fh	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	r2	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	O3	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	x3	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	l6	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	C9	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	dK	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	eb	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	l2	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	P2	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	n3	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	V4	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	a8	602	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	aM	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	cv	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	ej	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	eq	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	go	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	e2	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	V2	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	g3	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	N4	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	J5	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	S6	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	g6	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	M7	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	Y7	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b8	1002	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	a9	601	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	y9	1002	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	bX	402	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	eG	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	fk	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	fn	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	fs	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	hE	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	hK	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	kU	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
27	h1	201	CYC	C4D-CHA-C1A	-2.42	125.91	128.81
26	U2	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	W2	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	F3	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	e3	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	K4	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	Q6	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	d9	303	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	M8	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	bj	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	dp	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	dF	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	fd	303	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	ft	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	hI	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	hJ	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	r2	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	T2	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	h5	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	K6	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	N6	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	c6	1001	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	M7	1002	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	c9	301	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	Q8	201	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	aK	1002	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	lq	202	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	hY	403	PEB	CBB-CAB-C3B	-2.42	105.89	112.63
26	R2	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	V3	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	u3	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	u4	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	k8	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	u6	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	Q7	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	q7	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	q9	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aS	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	bl	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	eD	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	jJ	1001	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	f2	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	O2	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	u6	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	E7	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	P7	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	S8	401	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aN	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	be	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	eI	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	gp	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	L4	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	X4	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	R5	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	o6	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	k9	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aS	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	bn	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	by	1002	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cu	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	le	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	ly	402	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	gt	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	hA	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	u2	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	A4	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	g8	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	a8	601	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	b9	402	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	u9	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aL	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aW	302	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	bN	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ce	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cU	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cY	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dh	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dF	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	gw	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	hD	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	jL	1001	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	k2	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	d5	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	T6	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	k6	1002	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	e9	302	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	P8	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	v9	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	Q9	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	ah	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aD	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aT	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cT	1002	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dw	401	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	ez	1003	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	jK	1001	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	m2	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	v2	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	X3	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	v4	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	K6	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	y6	203	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	e9	301	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aC	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aJ	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	bv	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	bC	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cO	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dk	1001	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dT	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	gk	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	gz	301	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	A3	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	s3	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	v5	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	m6	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	s7	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	z8	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	B8	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	w9	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aR	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cM	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	du	203	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dD	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	lv	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	G2	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	o5	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	G6	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	M6	1001	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	v6	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	g7	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	T8	302	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	z9	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	Y9	302	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	ad	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	aQ	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	bi	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cW	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	jM	1001	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	X2	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	R3	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	s4	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	z4	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	c6	1003	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	q8	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	J9	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cq	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	cM	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	dR	202	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	eG	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	hX	201	PEB	CBB-CAB-C3B	-2.42	105.90	112.63
26	D2	302	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Z3	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	E4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Q4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	i8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	b8	1003	PEB	CBB-CAB-C3B	-2.42	105.91	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	j9	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	o9	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	y9	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Z9	1007	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aN	204	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aZ	301	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	eK	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	eM	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	ga	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	iA	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	l3	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	o3	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	R4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	H5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	k8	203	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	C6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	a6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	e9	303	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	y8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	A8	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	C8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	H8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	u9	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aJ	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	br	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	bA	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	dw	402	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	eq	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fd	302	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	gy	303	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	i2	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	x2	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	b3	501	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	w3	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	P4	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	x4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	E6	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	r6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	p8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	r8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	h7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	r7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	p9	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aZ	302	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	by	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	J4	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	M4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Z4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	A5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	I5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	x9	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	U9	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cj	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	dM	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fd	301	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	gl	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	kR	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	S4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	b9	401	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	d9	302	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	E8	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	t9	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	at	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aM	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	bw	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	bP	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	ct	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cx	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	db	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	de	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fw	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	a3	1003	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	D4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	O6	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	U6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	j6	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	y6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	D7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	j9	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	az	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	ci	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cL	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cR	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	df	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fc	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fj	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	gq	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	O2	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	M5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	h8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	c6	1002	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	f7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	O8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	bk	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cc	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cS	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	dd	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	lr	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	gn	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	J2	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	F4	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Q5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	e6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	h6	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	H7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	j7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	n7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	x7	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	A9	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Z9	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aC	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	bB	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	cA	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	dG	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	B2	502	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	S3	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	G4	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	44	301	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	j5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Z6	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	i6	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	b8	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	Z8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	dn	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	ea	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ey	1002	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	gb	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
27	m1	201	CYC	C2C-C3C-C4C	2.42	104.96	101.34
26	S3	203	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	q3	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	t3	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	x5	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	x8	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	l9	202	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aE	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	aX	401	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	ca	1001	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	dJ	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	ef	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fa	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
26	fe	201	PEB	CBB-CAB-C3B	-2.42	105.91	112.63
29	C2	303	PVN	C81-C17-C16	2.42	127.18	124.17
26	m2	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	B2	501	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	I3	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	o4	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	s5	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	W6	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	i6	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	G7	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	l7	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	u7	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	h9	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	bq	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	bU	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	dr	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	dR	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	ln	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	c4	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	W8	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	P9	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	T9	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	aL	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	bx	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	bR	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	cQ	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	cX	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dj	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	v2	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	P3	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	t4	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	j8	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	y6	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	I7	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	G8	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	aA	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	aB	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	aH	202	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	aV	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	dT	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	hH	201	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	kX	1001	PEB	CBB-CAB-C3B	-2.42	105.92	112.63
26	W3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	B4	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	o8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	G8	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	U8	1002	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	ab	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	am	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aw	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	dg	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	ds	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	dY	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	ey	1003	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	eW	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	eY	402	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	hT	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
29	hY	404	PVN	C16-C15-C14	-2.41	122.18	128.08
26	C2	301	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	a3	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	y4	1002	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	C5	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	T5	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	b6	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	w6	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	Y8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	al	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aE	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bs	1003	PEB	CBB-CAB-C3B	-2.41	105.92	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ee	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	eI	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	gv	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	jO	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	g2	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	E2	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	T3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	Z4	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	y7	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aA	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aB	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aR	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bo	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	cT	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	dk	1002	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	eA	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	eQ	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	gf	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	hS	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	I4	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	g4	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	j4	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	X5	401	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	f8	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	I9	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aX	402	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	hT	204	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	iC	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	M3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	o4	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	y4	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	P6	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	N8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aH	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bc	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bl	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	cC	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	fi	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	hO	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	hQ	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	hV	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	kW	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	j2	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	y2	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	z2	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	M2	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	E3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	y3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	I4	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	R4	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	S4	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	r6	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	K7	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	w8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	H8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aY	402	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bM	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bY	1003	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	cN	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	ed	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	lb	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	lm	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	n2	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	o2	1002	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	i3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	V4	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	m5	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	u5	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	H6	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	R6	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	h6	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	m6	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	V7	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	K8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	as	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aF	204	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bq	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bW	301	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	dr	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
29	34	1004	PVN	C16-C15-C14	-2.41	122.19	128.08
29	Y5	1004	PVN	C16-C15-C14	-2.41	122.19	128.08
26	w2	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	m3	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	44	302	PEB	CBB-CAB-C3B	-2.41	105.92	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K5	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	f8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	j8	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	j6	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	e7	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	w7	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	I8	202	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	R9	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	aK	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	bm	1001	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	dB	201	PEB	CBB-CAB-C3B	-2.41	105.92	112.63
26	k2	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Z2	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	T4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	z4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	n5	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	C6	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	x6	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	s8	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ac	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	aT	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ez	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ez	1002	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	lq	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	gu	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	P4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	34	1007	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	a4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	b6	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	v6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	W7	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	m7	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	f9	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	cX	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dL	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	hY	401	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	s2	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	d4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	h4	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	S5	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	U5	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Y6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q6	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	x6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	z6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	m9	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	r9	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dq	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dM	1002	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	eR	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	lb	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ly	403	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	lz	402	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	fl	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	iE	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	t2	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	b3	502	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	m8	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	d6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	l6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	i7	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	D8	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	K8	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	F9	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bp	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	cp	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dt	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dU	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	kT	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	G3	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	k4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Y5	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	a7	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	a9	602	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	v8	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	T8	301	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ao	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bj	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bx	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bZ	303	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dp	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	eK	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	lu	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	fo	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	m4	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	s6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	p9	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ar	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bs	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bY	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	cO	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	eJ	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	la	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	lf	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ls	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	hN	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	e2	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	E4	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	K4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Q4	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Z5	301	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	M6	1002	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	D8	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	J8	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	av	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	cz	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dP	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	li	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	lz	401	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	hL	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
27	o1	1001	CYC	C2C-C3C-C4C	2.41	104.95	101.34
26	o2	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Q3	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	M4	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	W4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	l5	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	t5	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	L8	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ay	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	aU	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bu	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	cS	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dm	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	eh	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	ly	401	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	M2	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S2	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	C4	1001	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	i4	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	Q6	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	S6	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	R7	201	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	e8	302	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	P8	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	bd	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	dO	202	PEB	CBB-CAB-C3B	-2.41	105.93	112.63
26	A2	1002	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	B3	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	m8	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	A8	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	aI	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	bI	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	bL	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cP	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	es	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	eM	1002	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	fv	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	hP	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	iG	1001	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	t4	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	L5	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	E6	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	p6	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	aQ	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cw	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cG	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	dt	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	ea	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	N8	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	z9	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	bh	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	bu	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	eE	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	eE	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	hW	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
29	gz	304	PVN	C71-C13-C14	-2.41	121.36	125.06
26	h2	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	J3	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	G4	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	c5	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	P6	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	s6	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	k7	1001	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	aa	1001	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cB	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cV	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	dn	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	N7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	Z7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	c7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	q9	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cW	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	ds	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	dC	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	lk	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	kQ	1001	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	kS	1001	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	W4	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	q4	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	N5	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	J6	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	dI	1002	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	ep	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	q2	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	U3	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	O5	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	V6	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	Q8	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cI	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	ff	204	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	hF	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
29	hZ	403	PVN	C16-C15-C14	-2.41	122.20	128.08
26	x8	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	X8	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	aP	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	dz	401	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	jN	1001	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	I2	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	U4	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	r5	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	aI	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	gs	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
29	44	303	PVN	C51-C8-C7	-2.41	120.33	127.25
29	Z5	304	PVN	C51-C8-C7	-2.41	120.33	127.25
26	I2	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	I6	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	O7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	S7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	T7	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	h9	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	bz	202	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	cV	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	gj	201	PEB	CBB-CAB-C3B	-2.41	105.94	112.63
26	O4	1001	PEB	CBB-CAB-C3B	-2.40	105.94	112.63
26	F6	201	PEB	CBB-CAB-C3B	-2.40	105.94	112.63
26	k6	1001	PEB	CBB-CAB-C3B	-2.40	105.94	112.63
26	c9	302	PEB	CBB-CAB-C3B	-2.40	105.94	112.63
26	G9	201	PEB	CBB-CAB-C3B	-2.40	105.94	112.63
26	S9	201	PEB	CBB-CAB-C3B	-2.40	105.94	112.63
26	z2	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	Y2	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	k3	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	H4	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	y5	1001	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	f6	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	w9	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	cR	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	cU	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	di	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	C2	302	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	p4	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	F8	1002	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	O8	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	ed	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	eH	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	eP	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	eS	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	gz	303	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	F4	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	b9	403	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	F8	1001	PEB	CBB-CAB-C3B	-2.40	105.95	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aV	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dq	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
27	h1	201	CYC	O2D-CGD-O1D	-2.40	117.31	123.30
27	t1	201	CYC	O2D-CGD-O1D	-2.40	117.31	123.30
26	w6	1002	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	bH	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	bK	1001	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dA	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dP	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	eo	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	gg	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	U4	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	b5	1001	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dc	203	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dv	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	ew	301	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	fp	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	bt	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	cg	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	w5	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	t9	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	bf	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	cP	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dK	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	l4	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	J8	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	L9	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	dN	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	Z5	303	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	l5	202	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	ba	1001	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	eD	201	PEB	CBB-CAB-C3B	-2.40	105.95	112.63
26	u4	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	b7	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	eo	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	A6	1001	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	N9	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	aW	301	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	bZ	301	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	cm	1001	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	eB	202	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	aY	406	PEB	CBB-CAB-C3B	-2.40	105.96	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eQ	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	ll	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	L3	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	z5	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	eg	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	Q2	1001	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	M8	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	s9	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	eC	202	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	gh	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	I6	202	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	d9	301	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	W8	202	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	dV	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	b4	1001	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	Z6	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	bt	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	bQ	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	dx	402	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
29	aY	403	PVN	C71-C13-C12	2.40	132.63	126.12
27	v1	201	CYC	O2D-CGD-O1D	-2.40	117.32	123.30
26	K2	202	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	cZ	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	du	201	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
26	dQ	202	PEB	CBB-CAB-C3B	-2.40	105.96	112.63
29	dw	404	PVN	C51-C8-C7	-2.40	120.36	127.25
26	X6	201	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	K9	1001	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	cy	1001	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	gy	301	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	s9	202	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	dW	202	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
27	S1	202	CYC	O2D-CGD-O1D	-2.40	117.33	123.30
26	Y2	202	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	iF	1001	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	aq	201	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	bD	201	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	cC	1003	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	fm	201	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
26	cl	201	PEB	CBB-CAB-C3B	-2.40	105.97	112.63
27	X1	201	CYC	C2C-C3C-C4C	2.40	104.93	101.34
26	eV	201	PEB	CBB-CAB-C3B	-2.39	105.97	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F5	201	PEB	CBB-CAB-C3B	-2.39	105.97	112.63
27	r1	201	CYC	O2D-CGD-O1D	-2.39	117.33	123.30
26	c3	302	PEB	CBB-CAB-C3B	-2.39	105.98	112.63
27	z1	201	CYC	O2D-CGD-O1D	-2.39	117.33	123.30
27	S1	201	CYC	O2D-CGD-O1D	-2.39	117.34	123.30
27	j1	201	CYC	O2D-CGD-O1D	-2.39	117.34	123.30
27	K1	201	CYC	C2C-C3C-C4C	2.39	104.92	101.34
27	a2	902	CYC	O2D-CGD-O1D	-2.39	117.34	123.30
27	b2	1001	CYC	O2D-CGD-O1D	-2.39	117.34	123.30
26	cb	201	PEB	CBB-CAB-C3B	-2.39	105.98	112.63
26	eO	202	PEB	CBB-CAB-C3B	-2.39	105.98	112.63
27	Y1	201	CYC	O2D-CGD-O1D	-2.39	117.34	123.30
26	eN	201	PEB	CBB-CAB-C3B	-2.39	105.99	112.63
29	c3	303	PVN	C81-C17-C16	2.39	127.15	124.17
27	a2	901	CYC	O2D-CGD-O1D	-2.39	117.35	123.30
27	p1	201	CYC	O2D-CGD-O1D	-2.39	117.35	123.30
27	t1	201	CYC	CAD-CBD-CGD	-2.38	107.08	113.76
27	L1	201	CYC	C2C-C3C-C4C	2.38	104.91	101.34
27	O1	201	CYC	C2C-C3C-C4C	2.38	104.91	101.34
27	k1	201	CYC	C2C-C3C-C4C	2.38	104.91	101.34
26	ag	201	PEB	CBB-CAB-C3B	-2.38	106.00	112.63
27	M1	1001	CYC	O2D-CGD-O1D	-2.38	117.36	123.30
27	G1	1001	CYC	C2C-C3C-C4C	2.38	104.91	101.34
29	bY	1004	PVN	C71-C13-C12	2.38	132.58	126.12
29	dx	405	PVN	C12-C11-N3	-2.38	106.59	110.05
27	v1	201	CYC	CAD-CBD-CGD	-2.38	107.08	113.76
27	s1	201	CYC	C2C-C3C-C4C	2.38	104.90	101.34
27	w1	201	CYC	C2C-C3C-C4C	2.38	104.90	101.34
26	Y9	302	PEB	C4B-NB-C1B	2.38	110.99	106.51
27	H1	201	CYC	CAD-CBD-CGD	-2.38	107.09	113.76
27	c1	201	CYC	O2D-CGD-O1D	-2.38	117.37	123.30
27	d1	1001	CYC	C2C-C3C-C4C	2.38	104.90	101.34
27	a2	901	CYC	CAD-CBD-CGD	-2.38	107.09	113.76
27	h1	201	CYC	CAD-CBD-CGD	-2.38	107.10	113.76
27	H1	201	CYC	O2D-CGD-O1D	-2.38	117.38	123.30
29	lz	403	PVN	O19-C19-C18	-2.38	125.46	128.04
27	p1	201	CYC	CAD-CBD-CGD	-2.38	107.10	113.76
26	el	201	PEB	CBB-CAB-C3B	-2.38	106.03	112.63
29	T8	303	PVN	C21-C2-C1	-2.37	115.81	121.39
27	Q1	201	CYC	C2C-C3C-C4C	2.37	104.89	101.34
26	bG	201	PEB	C4B-NB-C1B	2.37	110.98	106.51
26	eO	201	PEB	C4B-NB-C1B	2.37	110.98	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	iE	1001	PEB	C4B-NB-C1B	2.37	110.98	106.51
27	I1	201	CYC	C2C-C3C-C4C	2.37	104.89	101.34
27	P1	201	CYC	C2C-C3C-C4C	2.37	104.89	101.34
29	gz	304	PVN	C81-C17-C18	-2.37	119.68	126.12
29	Y9	303	PVN	C21-C2-C1	-2.37	115.82	121.39
26	cq	201	PEB	C4B-NB-C1B	2.37	110.98	106.51
27	y1	201	CYC	C2C-C3C-C4C	2.37	104.89	101.34
27	c1	201	CYC	CAD-CBD-CGD	-2.37	107.11	113.76
27	r1	201	CYC	CAD-CBD-CGD	-2.37	107.11	113.76
27	n1	201	CYC	C2C-C3C-C4C	2.37	104.89	101.34
26	dM	1001	PEB	C4B-NB-C1B	2.37	110.97	106.51
26	D5	201	PEB	C4B-NB-C1B	2.37	110.97	106.51
26	dN	201	PEB	C4B-NB-C1B	2.37	110.97	106.51
26	X6	201	PEB	C4B-NB-C1B	2.37	110.97	106.51
27	S1	201	CYC	CAD-CBD-CGD	-2.37	107.12	113.76
27	j1	201	CYC	CAD-CBD-CGD	-2.37	107.12	113.76
27	Z1	201	CYC	C2C-C3C-C4C	2.37	104.88	101.34
26	aD	201	PEB	C4B-NB-C1B	2.37	110.97	106.51
26	K7	201	PEB	C4B-NB-C1B	2.37	110.97	106.51
27	N1	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
27	e1	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
26	eq	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
27	h1	201	CYC	O2A-CGA-O1A	-2.36	117.41	123.30
27	S1	202	CYC	CAD-CBD-CGD	-2.36	107.13	113.76
26	S8	401	PEB	C4B-NB-C1B	2.36	110.96	106.51
27	q1	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
27	S1	201	CYC	O2A-CGA-O1A	-2.36	117.41	123.30
27	j1	201	CYC	O2A-CGA-O1A	-2.36	117.41	123.30
26	y5	1001	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	F6	202	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	p8	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	hH	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
27	R1	1001	CYC	C2C-C3C-C4C	2.36	104.88	101.34
27	i1	1001	CYC	C2C-C3C-C4C	2.36	104.88	101.34
26	R7	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	aZ	302	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	cr	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
29	ly	404	PVN	O19-C19-C18	-2.36	125.48	128.04
27	J1	201	CYC	O2A-CGA-O1A	-2.36	117.41	123.30
27	Y1	201	CYC	O2A-CGA-O1A	-2.36	117.41	123.30
26	E5	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	bH	201	PEB	C4B-NB-C1B	2.36	110.96	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ce	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	eC	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
27	f1	201	CYC	C2C-C3C-C4C	2.36	104.88	101.34
26	G9	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
27	M1	1001	CYC	CAD-CBD-CGD	-2.36	107.14	113.76
26	cC	1001	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	es	201	PEB	C4B-NB-C1B	2.36	110.96	106.51
26	iF	1001	PEB	C4B-NB-C1B	2.36	110.96	106.51
27	J1	201	CYC	O2D-CGD-O1D	-2.36	117.42	123.30
27	r1	201	CYC	O2A-CGA-O1A	-2.36	117.42	123.30
27	W1	201	CYC	C2C-C3C-C4C	2.36	104.87	101.34
27	b1	1001	CYC	C2C-C3C-C4C	2.36	104.87	101.34
27	u1	1001	CYC	C2C-C3C-C4C	2.36	104.87	101.34
26	B4	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	eP	203	PEB	C4B-NB-C1B	2.36	110.95	106.51
27	g1	201	CYC	C2C-C3C-C4C	2.36	104.87	101.34
26	cJ	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	eq	202	PEB	C4B-NB-C1B	2.36	110.95	106.51
27	J1	201	CYC	CAD-CBD-CGD	-2.36	107.15	113.76
27	a2	902	CYC	CAD-CBD-CGD	-2.36	107.15	113.76
27	b2	1001	CYC	CAD-CBD-CGD	-2.36	107.15	113.76
26	O5	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	lm	1001	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	b3	501	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	U5	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	k8	202	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	lp	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	hN	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
27	t1	201	CYC	O2A-CGA-O1A	-2.36	117.42	123.30
27	z1	201	CYC	O2A-CGA-O1A	-2.36	117.42	123.30
26	n5	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	w8	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	eo	202	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	jM	1001	PEB	C4B-NB-C1B	2.36	110.95	106.51
27	M1	1001	CYC	O2A-CGA-O1A	-2.36	117.43	123.30
26	L5	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	z6	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	N9	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	dW	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	b4	1001	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	j7	201	PEB	C4B-NB-C1B	2.36	110.95	106.51
26	v4	201	PEB	C4B-NB-C1B	2.36	110.95	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	Y1	201	CYC	CAD-CBD-CGD	-2.35	107.16	113.76
29	D2	303	PVN	O19-C19-C18	-2.35	125.48	128.04
29	d3	302	PVN	O19-C19-C18	-2.35	125.48	128.04
26	u3	201	PEB	C4B-NB-C1B	2.35	110.95	106.51
26	F4	201	PEB	C4B-NB-C1B	2.35	110.95	106.51
26	G5	201	PEB	C4B-NB-C1B	2.35	110.95	106.51
26	eb	201	PEB	C4B-NB-C1B	2.35	110.95	106.51
26	eH	201	PEB	C4B-NB-C1B	2.35	110.95	106.51
26	W3	203	PEB	CHC-C1D-ND	-2.35	111.21	113.95
26	I3	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	b3	502	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	34	1003	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	m7	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dp	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dD	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	eP	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	g5	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	e7	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	h7	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	T8	302	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	aH	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	cZ	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
27	S1	202	CYC	O2A-CGA-O1A	-2.35	117.43	123.30
26	Q4	203	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	l8	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	o8	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	F8	1001	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dC	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dU	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	gw	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	hT	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
27	z1	201	CYC	CAD-CBD-CGD	-2.35	107.16	113.76
26	t6	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	f9	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	T9	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	fm	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
29	gy	304	PVN	C15-C14-C13	-2.35	118.85	124.90
26	r2	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	B2	501	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dn	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dx	401	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dN	202	PEB	C4B-NB-C1B	2.35	110.94	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eu	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	F4	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	L4	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	K5	1001	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	k6	1001	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	N7	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	S7	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	ca	1001	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	q2	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	J5	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	C9	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dr	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	lt	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	iB	1001	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	V4	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	B8	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	C8	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	az	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	ln	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	hY	403	PEB	C4B-NB-C1B	2.35	110.94	106.51
27	U1	201	CYC	C2C-C3C-C4C	2.35	104.86	101.34
27	d2	101	CYC	C2C-C3C-C4C	2.35	104.86	101.34
27	p1	201	CYC	O2A-CGA-O1A	-2.35	117.44	123.30
26	o2	1001	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	b9	401	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	X9	401	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	aN	204	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	r6	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	e8	302	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	a9	603	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	bt	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	bF	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	dM	1002	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	fe	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	o7	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	bh	202	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	ee	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	gs	201	PEB	C4B-NB-C1B	2.35	110.94	106.51
26	L2	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	T3	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	N5	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	b9	403	PEB	C4B-NB-C1B	2.35	110.93	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O9	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	dk	1002	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	c4	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	R5	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	jI	1001	PEB	C4B-NB-C1B	2.35	110.93	106.51
27	a1	201	CYC	C2C-C3C-C4C	2.35	104.86	101.34
26	Q4	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	n7	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	aK	1001	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	cU	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	do	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	dq	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	eh	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	ez	1001	PEB	C4B-NB-C1B	2.35	110.93	106.51
27	v1	201	CYC	O2A-CGA-O1A	-2.35	117.45	123.30
26	f2	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	S3	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	C5	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	bu	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	eW	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	gq	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	hK	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
27	q1	201	CYC	CMC-C2C-C1C	2.35	117.46	112.40
26	G2	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	s3	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	c5	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	l5	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	b9	404	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	g9	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	q9	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	aY	402	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	ll	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	gl	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	l6	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	l6	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	P8	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	y9	1001	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	aW	302	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	bb	201	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	eS	202	PEB	C4B-NB-C1B	2.35	110.93	106.51
26	j4	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	j5	201	PEB	C4B-NB-C1B	2.34	110.93	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t5	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	i8	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	K6	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	j6	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	q6	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	O7	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	w9	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	H9	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	ac	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	bC	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	bV	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	gm	1001	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	M4	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	Q6	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	K8	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	aM	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	aU	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	bv	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	dC	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	dO	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	eO	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	gz	301	PEB	C4B-NB-C1B	2.34	110.93	106.51
29	C2	303	PVN	C16-C17-C18	-2.34	105.42	107.87
26	Z2	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	W4	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	Z5	303	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	f8	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	q6	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	v6	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	y6	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	K8	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	br	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	cX	202	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	ez	1002	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	eD	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
26	fr	201	PEB	C4B-NB-C1B	2.34	110.93	106.51
27	V1	201	CYC	C2C-C3C-C4C	2.34	104.85	101.34
26	I2	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	P3	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	x7	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	cO	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dQ	202	PEB	C4B-NB-C1B	2.34	110.92	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	lq	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bH	202	PEB	CHC-C1D-ND	-2.34	111.23	113.95
26	a3	1003	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	H5	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	q9	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	eD	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	lc	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	A5	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	o5	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	O8	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Q8	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	h9	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ae	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bi	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	br	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ci	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	cw	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dm	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dw	401	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ge	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	w2	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	34	1007	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	z7	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	D8	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Q8	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	be	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bQ	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	cG	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ed	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	eU	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	la	1002	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	C4	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	P4	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	w5	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	I6	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	s6	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	x6	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	e9	301	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	T8	301	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	w9	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Z9	1003	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	av	201	PEB	C4B-NB-C1B	2.34	110.92	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dl	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	e2	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	r2	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	x2	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	44	301	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Y6	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	h6	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	c7	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	j9	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	aG	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	de	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dx	404	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dE	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	eI	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
27	H1	201	CYC	O2A-CGA-O1A	-2.34	117.47	123.30
26	E3	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	G4	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	n4	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	j6	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	H7	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bp	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	iA	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	jP	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
27	b1	1001	CYC	CMC-C2C-C1C	2.34	117.45	112.40
26	F2	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Y4	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	f4	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	s9	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	u9	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	au	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	aS	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ch	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	o2	1002	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	q3	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	p6	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	n9	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	s9	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	V9	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ew	301	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	lr	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	hS	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	v3	201	PEB	C4B-NB-C1B	2.34	110.92	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X8	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Y8	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	cO	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dg	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dq	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dw	403	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dG	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	lb	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
27	a2	901	CYC	O2A-CGA-O1A	-2.34	117.47	123.30
26	w2	203	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	Z6	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	C7	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	g7	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	D8	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bs	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bx	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	bY	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dk	1001	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	dI	1002	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	ej	202	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	eN	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	fc	201	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	gy	303	PEB	C4B-NB-C1B	2.34	110.92	106.51
26	m8	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	U6	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	a8	602	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	M9	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	ar	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	aV	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	cp	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	dx	403	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	dK	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	dX	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	eR	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	gh	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	gz	303	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	jK	1001	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	P3	202	PEB	CHC-C1D-ND	-2.34	111.23	113.95
27	V1	201	CYC	CMC-C2C-C1C	2.34	117.44	112.40
26	l3	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	a4	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	m8	202	PEB	C4B-NB-C1B	2.34	110.91	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	o6	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	t7	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	O8	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	K9	1001	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	ai	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	cV	203	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	dV	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	eI	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	eZ	401	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	gg	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	D2	302	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	r3	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	M4	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	v5	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	a9	602	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	G8	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	aO	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	bd	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	eF	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
27	N1	201	CYC	CMC-C2C-C1C	2.34	117.44	112.40
26	R2	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	X2	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	D3	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	z3	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	Z4	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	P7	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	m9	1001	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	bt	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	dT	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	eC	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
27	K1	201	CYC	CMC-C2C-C1C	2.34	117.44	112.40
26	Z7	202	PEB	CHC-C1D-ND	-2.34	111.23	113.95
26	kU	1002	PEB	CHC-C1D-ND	-2.34	111.23	113.95
26	u2	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	H4	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	Z6	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	k6	1002	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	r6	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	A9	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	aA	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	ba	1001	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	bu	201	PEB	C4B-NB-C1B	2.34	110.91	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ds	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	dT	202	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	eg	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	lu	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
26	gv	201	PEB	C4B-NB-C1B	2.34	110.91	106.51
27	w1	201	CYC	CMC-C2C-C1C	2.34	117.44	112.40
26	I2	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	J4	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	f9	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	jL	1001	PEB	C4B-NB-C1B	2.33	110.91	106.51
27	o1	1001	CYC	CMC-C2C-C1C	2.33	117.44	112.40
26	h2	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	O3	1001	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	n3	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	x3	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	P6	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	e9	302	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	z8	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	J8	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	i9	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	bm	1002	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	cd	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	cK	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	V3	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	i5	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	j8	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	g6	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	p9	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	ao	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	bB	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	cl	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	cE	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	cW	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	dP	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	gn	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	gt	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
27	Q1	201	CYC	CMC-C2C-C1C	2.33	117.43	112.40
26	m2	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	s2	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	t2	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	m3	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	e5	201	PEB	C4B-NB-C1B	2.33	110.91	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	w7	1001	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	b8	1001	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	G8	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	v9	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	aE	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	aY	401	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	li	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	gc	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
27	X1	201	CYC	CMC-C2C-C1C	2.33	117.43	112.40
26	Q5	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	Z5	301	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	E6	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	S6	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	l9	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	al	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	aQ	202	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	ls	201	PEB	C4B-NB-C1B	2.33	110.91	106.51
26	hY	401	PEB	C4B-NB-C1B	2.33	110.91	106.51
27	c1	201	CYC	O2A-CGA-O1A	-2.33	117.48	123.30
26	B2	502	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	D2	301	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	I5	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	M5	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	I7	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	v8	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aN	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cX	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	eM	1002	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	eT	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	fk	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	ft	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hC	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hJ	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	gi	202	PEB	CHC-C1D-ND	-2.33	111.24	113.95
26	k2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	l2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	W4	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	T5	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	I6	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	S6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	l7	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	bl	201	PEB	C4B-NB-C1B	2.33	110.90	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cA	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cB	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	dH	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	eB	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hP	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	l4	202	PEB	CHC-C1D-ND	-2.33	111.24	113.95
27	W1	201	CYC	CMC-C2C-C1C	2.33	117.43	112.40
27	Z1	201	CYC	CMC-C2C-C1C	2.33	117.43	112.40
26	E2	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	T2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	R3	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	d5	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	x5	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	A6	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	G6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	y6	203	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	d9	301	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	k9	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	ab	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	ak	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aR	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	en	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hF	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hR	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
27	P1	201	CYC	CMC-C2C-C1C	2.33	117.43	112.40
26	q2	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	y2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	M2	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	i4	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	r5	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	M6	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	E7	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	e9	303	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	w8	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	I8	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hM	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	jO	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
27	y1	201	CYC	CMC-C2C-C1C	2.33	117.43	112.40
26	Y2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	X7	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aQ	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cm	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dF	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	eY	402	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	fw	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
29	gz	304	PVN	C15-C16-N4	-2.33	121.06	126.06
27	m1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
26	o4	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	T6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	f6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	c8	302	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	J8	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	x9	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	L9	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	bM	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	bZ	303	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cM	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cP	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	dz	401	PEB	C4B-NB-C1B	2.33	110.90	106.51
27	s1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
27	z1	201	CYC	CBD-CAD-C3D	2.33	116.59	112.62
26	i2	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	M2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	W3	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	f3	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	b5	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	j8	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	J6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	a6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	A8	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	D9	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	U9	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aK	1002	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	dA	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	ed	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	hI	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	iG	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
27	f1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
26	C2	301	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	T6	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	H8	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aI	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	bX	401	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cT	1002	PEB	C4B-NB-C1B	2.33	110.90	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dY	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	ea	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	eQ	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	jN	1001	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	F2	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	S4	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	i6	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	u6	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	T7	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aN	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	aZ	301	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cc	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	cM	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	dD	202	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	eF	201	PEB	C4B-NB-C1B	2.33	110.90	106.51
26	w3	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	U4	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	u7	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	z9	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	ag	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bs	1003	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	cT	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	cV	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	dm	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	dt	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	dZ	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	eH	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	lq	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	hW	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
27	g1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
27	c1	201	CYC	CBD-CAD-C3D	2.33	116.59	112.62
27	r1	201	CYC	CBD-CAD-C3D	2.33	116.59	112.62
26	K2	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	J3	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	e3	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	E4	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	m4	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	P6	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	p9	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	aH	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bj	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bs	1002	PEB	C4B-NB-C1B	2.33	110.89	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eA	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	ly	401	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	fi	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	fx	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	go	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	hQ	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	kQ	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
27	L1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
27	a1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
27	e1	201	CYC	CMC-C2C-C1C	2.33	117.42	112.40
26	m2	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	K4	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	q4	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	C6	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	N8	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	U8	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	h9	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	P9	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	ay	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	aF	204	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	aX	401	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	cY	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	ep	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	eK	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	fs	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	hE	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	jJ	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
27	S1	202	CYC	CBD-CAD-C3D	2.33	116.59	112.62
27	I1	201	CYC	O2A-CGA-O1A	-2.33	117.50	123.30
26	C2	302	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	U2	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	l4	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	w6	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	c9	301	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	L8	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	W8	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bd	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bw	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	di	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	dn	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	iD	1001	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	w2	202	PEB	C4B-NB-C1B	2.33	110.89	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J2	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	A3	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	K3	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	N3	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	G4	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	O4	1002	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	o6	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	z6	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	N8	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	P8	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	aI	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bA	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	bW	301	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	ea	202	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	le	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	gj	201	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	hT	204	PEB	C4B-NB-C1B	2.33	110.89	106.51
26	L2	202	PEB	CHC-C1D-ND	-2.33	111.25	113.95
26	v7	202	PEB	CHC-C1D-ND	-2.33	111.25	113.95
26	dl	202	PEB	CHC-C1D-ND	-2.33	111.25	113.95
26	n2	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	a5	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	b6	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	e6	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	v6	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	v8	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	Z8	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	E9	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	aW	301	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	ey	1002	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	lb	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	fq	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	hZ	402	PEB	C4B-NB-C1B	2.32	110.89	106.51
27	G1	1001	CYC	CMC-C2C-C1C	2.32	117.41	112.40
27	a2	902	CYC	O2A-CGA-O1A	-2.32	117.50	123.30
27	b2	1001	CYC	O2A-CGA-O1A	-2.32	117.50	123.30
26	Q4	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	s4	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	V5	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	f8	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	b8	1002	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	b8	1003	PEB	C4B-NB-C1B	2.32	110.89	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a9	601	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	I8	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	bk	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	cV	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	df	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	dL	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	gi	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
27	h1	201	CYC	CBD-CAD-C3D	2.32	116.59	112.62
27	n1	201	CYC	CMC-C2C-C1C	2.32	117.41	112.40
26	V2	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	H3	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	a3	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	R4	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	o4	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	u4	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	B6	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	H6	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	M6	1002	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	b7	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	U8	1002	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	x9	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	R9	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	dh	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	ej	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	cf	201	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	W2	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	Y2	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	B3	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	u4	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	y4	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	q5	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	t8	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	f7	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	s7	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	d9	302	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	bm	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	bw	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	by	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	bX	402	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	cx	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	da	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	fd	302	PEB	C4B-NB-C1B	2.32	110.89	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fh	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	fo	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	kW	1001	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	z5	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	r8	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	x8	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	y9	1002	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	bn	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	em	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	fb	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	t9	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	J9	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	af	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	aL	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	eW	202	PEB	C4B-NB-C1B	2.32	110.89	106.51
26	fp	201	PEB	C4B-NB-C1B	2.32	110.89	106.51
27	d1	1001	CYC	O2A-CGA-O1A	-2.32	117.51	123.30
26	Q2	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	t3	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	N4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	V6	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	x6	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	S9	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	Z9	1007	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	at	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aE	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	bj	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	cS	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	du	203	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	er	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
27	k1	201	CYC	CMC-C2C-C1C	2.32	117.41	112.40
27	M1	1001	CYC	CBD-CAD-C3D	2.32	116.58	112.62
27	a2	902	CYC	CBD-CAD-C3D	2.32	116.58	112.62
27	b2	1001	CYC	CBD-CAD-C3D	2.32	116.58	112.62
26	J4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	t4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	y7	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	A8	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	cj	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	ds	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	ef	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	eG	201	PEB	C4B-NB-C1B	2.32	110.88	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fj	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	D7	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	G3	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	g3	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	d4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	q8	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	M8	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dr	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dB	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
27	U1	201	CYC	O2A-CGA-O1A	-2.32	117.52	123.30
27	d2	101	CYC	O2A-CGA-O1A	-2.32	117.52	123.30
29	eY	403	PVN	C17-C16-N4	2.32	110.38	106.99
27	I1	201	CYC	CMC-C2C-C1C	2.32	117.40	112.40
26	ap	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	ax	201	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	cr	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	p2	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	u2	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	O2	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	t4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	s5	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	b6	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	u8	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	x8	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	r9	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	F9	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aw	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	bf	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dp	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	kX	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
29	c3	303	PVN	C16-C17-C18	-2.32	105.45	107.87
26	j2	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	k2	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	P2	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	p3	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	q4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	B5	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	g6	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	w6	1002	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	Z9	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aX	402	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dx	402	PEB	C4B-NB-C1B	2.32	110.88	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dI	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	eS	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	eU	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	fv	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	hX	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	n3	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	z5	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
27	P1	201	CYC	O2A-CGA-O1A	-2.32	117.52	123.30
26	z2	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	I4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	L4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	R4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	y8	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	F8	1002	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	W8	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	cI	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dc	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	kS	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
27	Y1	201	CYC	CBD-CAD-C3D	2.32	116.58	112.62
26	s2	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	X3	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	I4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	X4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	z4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	z4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	W5	301	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	y6	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	d9	303	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	l9	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	ad	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	as	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	cS	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dS	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	lv	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	gy	301	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	H3	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
26	hH	202	PEB	CHC-C1D-ND	-2.32	111.25	113.95
27	U1	201	CYC	CMC-C2C-C1C	2.32	117.40	112.40
27	d2	101	CYC	CMC-C2C-C1C	2.32	117.40	112.40
26	H4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	u5	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	i6	201	PEB	C4B-NB-C1B	2.32	110.88	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	m6	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	U8	1003	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aq	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aU	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	bK	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	bU	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	ct	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	cQ	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	eG	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	H9	202	PEB	CHC-C1D-ND	-2.32	111.26	113.95
26	cB	202	PEB	CHC-C1D-ND	-2.32	111.26	113.95
26	i2	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	v2	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	W2	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	E4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	O4	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aL	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dF	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	dH	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	ly	403	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	lz	402	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	hV	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
29	C2	303	PVN	C91-C18-C19	-2.32	117.72	121.38
29	eZ	402	PVN	C17-C16-N4	2.32	110.38	106.99
27	J1	201	CYC	CBD-CAD-C3D	2.32	116.57	112.62
26	h4	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	k4	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	c6	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	k7	1001	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aC	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	aM	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	bD	201	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	cR	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
26	eQ	202	PEB	C4B-NB-C1B	2.32	110.88	106.51
27	t1	201	CYC	CBD-CAD-C3D	2.32	116.57	112.62
26	Y4	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	N6	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	M8	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	j9	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	aP	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	bv	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	cv	201	PEB	C4B-NB-C1B	2.32	110.87	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dJ	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	ey	1003	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	gx	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	hL	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
27	d1	1001	CYC	CMC-C2C-C1C	2.32	117.39	112.40
26	G2	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	U3	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	e4	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	E6	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	K6	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	Z7	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	b9	402	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	H8	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	ah	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	p2	202	PEB	CHC-C1D-ND	-2.32	111.26	113.95
26	n5	202	PEB	CHC-C1D-ND	-2.32	111.26	113.95
26	Q3	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	K4	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	aB	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	aY	406	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	cW	202	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	eE	201	PEB	C4B-NB-C1B	2.32	110.87	106.51
26	m5	1003	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	S3	203	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	d6	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	I9	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	ap	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bP	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bZ	301	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	fa	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	hA	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
27	S1	201	CYC	CBD-CAD-C3D	2.31	116.57	112.62
27	j1	201	CYC	CBD-CAD-C3D	2.31	116.57	112.62
26	O2	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	V4	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	g4	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	x4	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	s6	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	ff	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	fn	1001	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	gb	1001	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	gu	201	PEB	C4B-NB-C1B	2.31	110.87	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	iH	1001	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	j5	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	D6	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	O6	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	c6	1002	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	Q7	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	r7	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bq	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bq	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	cP	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	dG	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	ez	1003	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	la	1001	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	kV	1001	PEB	C4B-NB-C1B	2.31	110.87	106.51
27	O1	201	CYC	CMC-C2C-C1C	2.31	117.39	112.40
26	al	202	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	g2	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	24	401	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	X5	401	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	h6	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	G7	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	z8	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	t9	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bc	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	cU	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	dR	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	lf	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	fd	303	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	kU	1001	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	t2	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	v2	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	c6	1003	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	s8	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	c9	302	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bR	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	gk	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
27	w1	201	CYC	O2A-CGA-O1A	-2.31	117.53	123.30
26	X6	202	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	gx	202	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	jJ	1002	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	kW	1002	PEB	CHC-C1D-ND	-2.31	111.26	113.95
27	s1	201	CYC	O2A-CGA-O1A	-2.31	117.54	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g2	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	i3	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	S4	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	T4	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	Z4	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	y4	1002	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	g8	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	d8	302	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	Y8	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	aR	202	PEB	C4B-NB-C1B	2.31	110.87	106.51
26	bO	201	PEB	C4B-NB-C1B	2.31	110.87	106.51
27	N1	201	CYC	O2A-CGA-O1A	-2.31	117.54	123.30
26	e2	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	k8	203	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	R6	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bg	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	cg	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	cu	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	eK	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	li	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	y2	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	D4	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	l5	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	h8	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	a7	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	aj	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	cb	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	dj	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	dR	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	eo	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	eR	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	fd	301	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	H7	202	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	F9	202	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	az	202	PEB	CHC-C1D-ND	-2.31	111.26	113.95
26	Y3	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	l8	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	L8	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	B9	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bh	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bz	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	du	202	PEB	C4B-NB-C1B	2.31	110.86	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dA	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	ly	402	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	lz	401	PEB	C4B-NB-C1B	2.31	110.86	106.51
27	O1	201	CYC	O2A-CGA-O1A	-2.31	117.54	123.30
26	Y5	1001	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	W6	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	a8	601	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	z9	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	lk	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	n4	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	fj	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	fy	201	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	L6	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	aT	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	do	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	N2	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	o3	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	Y5	1003	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	D7	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	v7	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	aB	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	aJ	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	aV	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bo	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	cC	1003	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	cD	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	dw	402	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	dK	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	fl	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	A2	1003	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	cs	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	hR	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	k3	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	E8	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bE	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
27	R1	1001	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
27	a1	201	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
27	i1	1001	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
26	h3	201	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	at	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	hL	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	aJ	201	PEB	C4B-NB-C1B	2.31	110.86	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bl	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bz	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
27	H1	201	CYC	CBD-CAD-C3D	2.31	116.56	112.62
27	p1	201	CYC	CBD-CAD-C3D	2.31	116.56	112.62
27	m1	201	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
26	C3	1001	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	M7	1002	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	cz	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	iC	1001	PEB	C4B-NB-C1B	2.31	110.86	106.51
27	v1	201	CYC	CBD-CAD-C3D	2.31	116.56	112.62
27	W1	201	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
26	aA	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	bx	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	by	1002	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	dd	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	el	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	gp	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
27	R1	1001	CYC	CMC-C2C-C1C	2.31	117.38	112.40
27	i1	1001	CYC	CMC-C2C-C1C	2.31	117.38	112.40
27	n1	201	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
26	an	201	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	L3	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	F5	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	A6	1002	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	C6	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	Q6	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	W6	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	B8	202	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	V8	1001	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	aF	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	eJ	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
26	hB	201	PEB	C4B-NB-C1B	2.31	110.86	106.51
29	D2	303	PVN	C15-C16-C17	2.31	131.52	126.95
29	d3	302	PVN	C15-C16-C17	2.31	131.52	126.95
26	A2	1002	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	m5	1001	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	k8	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	r9	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	u9	202	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	aP	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	du	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	dv	201	PEB	C4B-NB-C1B	2.31	110.85	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dW	202	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	R3	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	n8	201	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	y8	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	D9	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	bQ	203	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	bV	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	cp	202	PEB	CHC-C1D-ND	-2.31	111.27	113.95
26	hG	201	PEB	CHC-C1D-ND	-2.31	111.27	113.95
27	g1	201	CYC	O2A-CGA-O1A	-2.31	117.55	123.30
29	ez	1004	PVN	C81-C17-C18	-2.31	119.86	126.12
27	u1	1001	CYC	CMC-C2C-C1C	2.31	117.37	112.40
26	F3	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	y3	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	V7	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	e8	301	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	bI	201	PEB	C4B-NB-C1B	2.31	110.85	106.51
26	dc	203	PEB	C4B-NB-C1B	2.31	110.85	106.51
27	o1	1001	CYC	O2A-CGA-O1A	-2.30	117.55	123.30
26	K2	202	PEB	C4B-NB-C1B	2.30	110.85	106.51
27	Z1	201	CYC	O2A-CGA-O1A	-2.30	117.56	123.30
26	z3	202	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	cH	201	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	lp	202	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	w4	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	E8	202	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	db	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	cE	202	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	eB	203	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	z2	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	S2	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	Y7	1001	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	ga	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
27	V1	201	CYC	O2A-CGA-O1A	-2.30	117.56	123.30
26	S5	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	m6	202	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	M7	1001	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	bN	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	bL	202	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	fo	202	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	jK	1002	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	M3	201	PEB	C4B-NB-C1B	2.30	110.85	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	o9	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	aC	202	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	bY	1003	PEB	C4B-NB-C1B	2.30	110.85	106.51
29	c3	303	PVN	C91-C18-C19	-2.30	117.74	121.38
26	cs	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	eV	201	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	hB	202	PEB	CHC-C1D-ND	-2.30	111.27	113.95
26	44	302	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	aS	202	PEB	C4B-NB-C1B	2.30	110.85	106.51
26	n6	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
27	y1	201	CYC	O2A-CGA-O1A	-2.30	117.56	123.30
27	k1	201	CYC	O2A-CGA-O1A	-2.30	117.56	123.30
26	A4	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	p4	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	bJ	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	kT	1001	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	x3	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	ld	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	ln	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	hJ	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	P4	202	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	h5	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	Q9	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	aT	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	eT	202	PEB	C4B-NB-C1B	2.30	110.84	106.51
27	f1	201	CYC	O2A-CGA-O1A	-2.30	117.57	123.30
26	B7	201	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	F7	201	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	lo	203	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	Z3	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
27	u1	1001	CYC	O2A-CGA-O1A	-2.30	117.57	123.30
26	hO	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	D4	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	bJ	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	F6	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	X4	202	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	U7	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	ek	1001	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	H2	201	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	A5	203	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	D5	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	bT	201	PEB	CHC-C1D-ND	-2.30	111.28	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cF	201	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	fi	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	dy	401	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	dz	402	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	ff	204	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	T2	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	V2	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	i3	203	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	B5	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	t7	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	eX	201	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	U4	202	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	dt	201	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	kR	1001	PEB	C4B-NB-C1B	2.30	110.84	106.51
26	dj	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
27	q1	201	CYC	O2A-CGA-O1A	-2.30	117.58	123.30
26	u6	202	PEB	C4B-NB-C1B	2.30	110.83	106.51
26	eE	202	PEB	C4B-NB-C1B	2.30	110.83	106.51
27	K1	201	CYC	O2A-CGA-O1A	-2.30	117.58	123.30
26	c3	302	PEB	C4B-NB-C1B	2.30	110.83	106.51
26	i7	201	PEB	C4B-NB-C1B	2.30	110.83	106.51
26	dP	201	PEB	C4B-NB-C1B	2.30	110.83	106.51
26	f2	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	F3	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
26	gv	202	PEB	CHC-C1D-ND	-2.30	111.28	113.95
29	A2	1004	PVN	C91-C18-C19	2.29	125.00	121.38
29	a3	1004	PVN	C91-C18-C19	2.29	125.00	121.38
26	d7	201	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	L3	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	J5	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	av	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	jP	1002	PEB	CHC-C1D-ND	-2.29	111.28	113.95
27	e1	201	CYC	O2A-CGA-O1A	-2.29	117.58	123.30
26	gf	201	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	B3	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	f3	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	N7	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	r7	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	ad	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	bB	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	fu	201	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	jO	1002	PEB	CHC-C1D-ND	-2.29	111.28	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X1	201	CYC	O2A-CGA-O1A	-2.29	117.58	123.30
27	b1	1001	CYC	O2A-CGA-O1A	-2.29	117.58	123.30
26	X2	202	PEB	CHC-C1D-ND	-2.29	111.28	113.95
26	hD	201	PEB	C4B-NB-C1B	2.29	110.83	106.51
27	a2	901	CYC	CBD-CAD-C3D	2.29	116.53	112.62
26	dX	202	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	a7	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	p7	201	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	R9	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	ff	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	aa	1001	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	cL	201	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	cR	201	PEB	C4B-NB-C1B	2.29	110.83	106.51
27	Q1	201	CYC	O2A-CGA-O1A	-2.29	117.59	123.30
26	am	1001	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	n7	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	cd	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	bL	201	PEB	C4B-NB-C1B	2.29	110.83	106.51
26	es	202	PEB	C4B-NB-C1B	2.29	110.83	106.51
27	G1	1001	CYC	O2A-CGA-O1A	-2.29	117.59	123.30
26	h2	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	kS	1002	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	O6	201	PEB	C4B-NB-C1B	2.29	110.82	106.51
26	k5	201	PEB	C4B-NB-C1B	2.29	110.82	106.51
26	D3	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	B9	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	cz	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	lh	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	cN	201	PEB	C4B-NB-C1B	2.29	110.82	106.51
26	L5	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	N9	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	ch	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	gg	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	hV	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	j2	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	l2	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	B4	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	ah	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	aj	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	eV	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	iE	1002	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	34	1002	PEB	CHC-C1D-ND	-2.29	111.29	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J6	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	R6	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	cL	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	dY	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	iD	1002	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	bS	201	PEB	C4B-NB-C1B	2.29	110.82	106.51
26	ei	202	PEB	CHC-C1D-ND	-2.29	111.29	113.95
26	T3	202	PEB	CHC-C1D-ND	-2.28	111.29	113.95
26	v4	202	PEB	CHC-C1D-ND	-2.28	111.29	113.95
26	p8	202	PEB	CHC-C1D-ND	-2.28	111.29	113.95
26	kR	1002	PEB	CHC-C1D-ND	-2.28	111.29	113.95
26	q7	201	PEB	C4B-NB-C1B	2.28	110.81	106.51
26	dO	201	PEB	C4B-NB-C1B	2.28	110.81	106.51
26	eM	1001	PEB	C4B-NB-C1B	2.28	110.81	106.51
26	C8	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	bD	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	dh	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	F5	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	P9	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	T9	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	bF	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	hT	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	jL	1002	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	b8	1004	PVN	C15-C16-C17	2.28	131.47	126.95
26	V5	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	eJ	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	gn	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	p4	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	co	201	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	ck	201	PEB	C4B-NB-C1B	2.28	110.81	106.51
27	L1	201	CYC	O2A-CGA-O1A	-2.28	117.61	123.30
26	R7	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	cj	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	hP	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	X7	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	ga	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	ge	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	hD	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	j4	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	p5	201	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	v5	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	di	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	et	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	fg	201	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	fs	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	cy	1001	PEB	C4B-NB-C1B	2.28	110.80	106.51
26	r4	201	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	t5	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	lf	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	fm	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	hN	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	bZ	304	PVN	C81-C17-C18	-2.28	119.93	126.12
29	dx	405	PVN	C51-C8-C7	-2.28	120.70	127.25
26	V7	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	fq	202	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	kT	1002	PEB	CHC-C1D-ND	-2.28	111.30	113.95
26	P5	201	PEB	CHC-C1D-ND	-2.28	111.30	113.95
29	b9	405	PVN	C15-C16-C17	2.28	131.46	126.95
26	L7	201	PEB	CHC-C1D-ND	-2.28	111.31	113.95
26	aD	202	PEB	CHC-C1D-ND	-2.28	111.31	113.95
26	bN	202	PEB	CHC-C1D-ND	-2.28	111.31	113.95
26	gd	201	PEB	CHC-C1D-ND	-2.28	111.31	113.95
26	n2	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	Z2	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	j3	201	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	c7	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	lr	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	jI	1002	PEB	CHC-C1D-ND	-2.27	111.31	113.95
29	lz	403	PVN	C62-C61-C12	2.27	118.94	112.63
26	J7	201	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	v9	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	N5	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	kV	1002	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	W7	201	PEB	C4B-NB-C1B	2.27	110.79	106.51
26	g5	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	ll	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	gp	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	gt	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	r5	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	x7	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	jN	1002	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	kQ	1002	PEB	CHC-C1D-ND	-2.27	111.31	113.95
29	Z9	1004	PVN	C15-C16-N4	-2.27	121.19	126.06
26	v3	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cl	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	eN	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	B7	201	PEB	C3B-C4B-NB	-2.27	106.75	110.05
26	d7	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	dL	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	el	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	g4	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	z7	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	el	202	PEB	C3B-C4B-NB	-2.27	106.75	110.05
26	t3	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	R5	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	h8	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	cn	201	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	eg	202	PEB	CHC-C1D-ND	-2.27	111.31	113.95
26	V3	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	l7	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	cq	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	dQ	201	PEB	C4B-NB-C1B	2.26	110.78	106.51
29	dx	405	PVN	C81-C17-C18	-2.26	119.97	126.12
26	Z3	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	cb	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	n5	202	PEB	C3B-C4B-NB	-2.26	106.76	110.05
26	B1	301	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	34	1001	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	gr	201	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	J3	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	y7	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	L9	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	dd	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	cd	202	PEB	C3B-C4B-NB	-2.26	106.76	110.05
26	dV	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	ec	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	fw	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
29	ly	404	PVN	C62-C61-C12	2.26	118.91	112.63
26	ee	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	p3	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	cJ	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	ep	202	PEB	CHC-C1D-ND	-2.26	111.32	113.95
26	c7	202	PEB	C3B-C4B-NB	-2.26	106.76	110.05
29	aZ	303	PVN	C81-C17-C18	-2.26	119.99	126.12
26	A1	301	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	lw	203	PEB	CHC-C1D-ND	-2.26	111.33	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	eZ	402	PVN	C32-C31-C3	2.26	116.40	112.98
26	fc	202	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	kX	1002	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	i3	203	PEB	C3B-C4B-NB	-2.26	106.77	110.05
26	iC	1002	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	jM	1002	PEB	CHC-C1D-ND	-2.26	111.33	113.95
26	S5	203	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	B6	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	T7	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	ar	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	eL	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	gk	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	T2	202	PEB	C3B-C4B-NB	-2.25	106.77	110.05
26	t7	202	PEB	C3B-C4B-NB	-2.25	106.77	110.05
26	df	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	ea	203	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	D4	202	PEB	C3B-C4B-NB	-2.25	106.77	110.05
26	L3	201	PEB	C2A-C3A-C4A	2.25	104.71	101.34
29	dx	405	PVN	C91-C18-C17	-2.25	123.68	127.53
26	D7	202	PEB	C3B-C4B-NB	-2.25	106.77	110.05
26	a7	202	PEB	C3B-C4B-NB	-2.25	106.77	110.05
26	N3	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	V9	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	F3	202	PEB	C3B-C4B-NB	-2.25	106.77	110.05
26	ev	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	co	201	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	kS	1002	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	aF	202	PEB	CHC-C1D-ND	-2.25	111.33	113.95
26	B4	202	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	cf	201	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	cE	202	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	eQ	202	PEB	C2A-C3A-C4A	2.25	104.71	101.34
26	Y7	1003	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	er	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	x3	202	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	bP	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	en	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	d7	202	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	eV	202	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	P7	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	e7	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95
26	cY	202	PEB	CHC-C1D-ND	-2.25	111.34	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cy	1001	PEB	C2A-C3A-C4A	2.25	104.70	101.34
26	cF	201	PEB	C3B-C4B-NB	-2.25	106.78	110.05
26	y7	202	PEB	C3B-C4B-NB	-2.24	106.78	110.05
26	H9	202	PEB	C3B-C4B-NB	-2.24	106.78	110.05
26	hX	202	PEB	CHC-C1D-ND	-2.24	111.34	113.95
26	li	203	PEB	CHC-C1D-ND	-2.24	111.34	113.95
26	av	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
29	U8	1004	PVN	C15-C16-N4	-2.24	121.24	126.06
26	H2	201	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	ax	201	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	aD	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	dQ	202	PEB	C2A-C3A-C4A	2.24	104.70	101.34
26	B3	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	F9	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	kU	1002	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	r3	202	PEB	CHC-C1D-ND	-2.24	111.34	113.95
26	et	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	eU	201	PEB	C2A-C3A-C4A	2.24	104.69	101.34
26	N3	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	n6	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	E5	202	PEB	CHC-C1D-ND	-2.24	111.35	113.95
29	dw	404	PVN	C5-C6-C7	2.24	134.15	130.34
26	B9	202	PEB	C3B-C4B-NB	-2.24	106.79	110.05
26	e4	202	PEB	CHC-C1D-ND	-2.24	111.35	113.95
26	r3	202	PEB	C3B-C4B-NB	-2.24	106.80	110.05
26	lf	202	PEB	C3B-C4B-NB	-2.24	106.80	110.05
26	ab	202	PEB	CHC-C1D-ND	-2.24	111.35	113.95
26	p8	202	PEB	C3B-C4B-NB	-2.24	106.80	110.05
26	jI	1002	PEB	C3B-C4B-NB	-2.24	106.80	110.05
26	az	202	PEB	C3B-C4B-NB	-2.24	106.80	110.05
26	bB	202	PEB	C3B-C4B-NB	-2.24	106.80	110.05
26	p4	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	cp	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	hP	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	J9	202	PEB	CHC-C1D-ND	-2.23	111.35	113.95
26	f3	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	cr	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	af	202	PEB	CHC-C1D-ND	-2.23	111.36	113.95
26	v3	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	g4	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	hJ	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	B5	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R5	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	p5	201	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	P9	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	af	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	cq	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	h3	201	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	B6	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	ev	202	PEB	C3B-C4B-NB	-2.23	106.80	110.05
26	g5	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	T9	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	lp	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	r4	201	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	J7	201	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	ap	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	en	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	hN	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	V5	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	x7	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	eR	201	PEB	C2A-C3A-C4A	2.23	104.68	101.34
26	j3	201	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	aj	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	gt	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	L2	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	r7	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	hT	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	iD	1002	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	N9	202	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	S5	203	PEB	C3B-C4B-NB	-2.23	106.81	110.05
26	l2	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	eg	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	eJ	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	eQ	201	PEB	C2A-C3A-C4A	2.22	104.67	101.34
27	Q1	201	CYC	C1A-NA-C4A	2.22	110.70	106.51
26	bY	1002	PEB	CHC-C1D-ND	-2.22	111.36	113.95
26	A5	203	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	gd	201	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	iC	1002	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	q8	202	PEB	CHC-C1D-ND	-2.22	111.36	113.95
26	j7	202	PEB	CHC-C1D-ND	-2.22	111.36	113.95
26	P7	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	cj	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05
26	cz	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fc	202	PEB	C3B-C4B-NB	-2.22	106.81	110.05
27	N1	201	CYC	C1A-NA-C4A	2.22	110.70	106.51
27	y1	201	CYC	C1A-NA-C4A	2.22	110.70	106.51
26	eS	201	PEB	C2A-C3A-C4A	2.22	104.67	101.34
26	R9	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	cL	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	fq	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	eo	201	PEB	CMB-C2B-C1B	2.22	128.49	125.06
26	h4	201	PEB	CHC-C1D-ND	-2.22	111.37	113.95
26	L9	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
29	eY	403	PVN	C32-C31-C3	2.22	116.35	112.98
26	p3	201	PEB	C2A-C3A-C4A	2.22	104.67	101.34
26	fd	302	PEB	C2A-C3A-C4A	2.22	104.67	101.34
26	Z3	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	34	1001	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	T7	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	p7	201	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	fj	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
29	gz	304	PVN	C16-C15-C14	-2.22	122.66	128.08
26	R3	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	er	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	fi	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	jN	1002	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	L5	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	gk	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	V4	201	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	ek	1001	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	eT	201	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	h2	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	v4	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	bT	201	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	df	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	ea	203	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	n2	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	D5	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	bH	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	as	201	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	ly	403	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	lz	402	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	dL	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
27	g1	201	CYC	C1A-NA-C4A	2.22	110.69	106.51
26	R2	202	PEB	C2A-C3A-C4A	2.22	104.66	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	E9	201	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	bu	202	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	R6	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	y8	202	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	eB	203	PEB	C3B-C4B-NB	-2.22	106.82	110.05
26	gf	202	PEB	CHC-C1D-ND	-2.22	111.37	113.95
27	m1	201	CYC	C1A-NA-C4A	2.22	110.69	106.51
26	X2	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	N5	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	ff	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	fo	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	hR	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	em	201	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	e4	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	h8	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	X6	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	bV	202	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	li	203	PEB	C3B-C4B-NB	-2.22	106.83	110.05
26	S6	202	PEB	C2A-C3A-C4A	2.22	104.66	101.34
26	L3	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	eL	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	dl	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	dV	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	hL	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	A6	1001	PEB	C2A-C3A-C4A	2.21	104.66	101.34
26	Z6	201	PEB	C2A-C3A-C4A	2.21	104.66	101.34
26	C9	201	PEB	C2A-C3A-C4A	2.21	104.66	101.34
26	cb	201	PEB	C2A-C3A-C4A	2.21	104.66	101.34
26	fq	201	PEB	C2A-C3A-C4A	2.21	104.66	101.34
26	gf	201	PEB	C2A-C3A-C4A	2.21	104.66	101.34
29	aZ	303	PVN	C21-C2-C3	2.21	134.22	129.67
26	t3	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	di	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	j2	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	J3	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	bQ	203	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	lr	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	gx	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
27	f1	201	CYC	C1A-NA-C4A	2.21	110.68	106.51
27	w1	201	CYC	C1A-NA-C4A	2.21	110.68	106.51
26	u2	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	W3	203	PEB	C3B-C4B-NB	-2.21	106.83	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J9	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	ah	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	hH	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	iE	1002	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	F5	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	g6	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	f9	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	ci	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	ew	301	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	gx	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	C3	1002	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	fu	201	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	gg	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	kR	1002	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	P5	201	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	n8	201	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	eN	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
27	u1	1001	CYC	C1A-NA-C4A	2.21	110.67	106.51
26	V3	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	f8	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	d9	302	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	aa	1001	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	dX	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	hF	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	J5	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	z5	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	ll	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	K4	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	b9	401	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	D9	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	I9	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	aF	204	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	p3	202	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	34	1002	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	lw	203	PEB	C3B-C4B-NB	-2.21	106.83	110.05
26	bX	401	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	q5	202	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	n4	202	PEB	C3B-C4B-NB	-2.21	106.84	110.05
26	R7	202	PEB	C3B-C4B-NB	-2.21	106.84	110.05
26	kV	1002	PEB	C3B-C4B-NB	-2.21	106.84	110.05
26	T2	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	H6	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k6	1001	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	cE	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	ed	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	bF	202	PEB	C3B-C4B-NB	-2.21	106.84	110.05
27	e1	201	CYC	C1A-NA-C4A	2.21	110.67	106.51
26	i2	202	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	U7	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	fp	201	PEB	C2A-C3A-C4A	2.21	104.65	101.34
26	N4	202	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	as	202	PEB	CHC-C1D-ND	-2.21	111.38	113.95
26	q3	1001	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	Q5	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
27	R1	1001	CYC	C1A-NA-C4A	2.21	110.67	106.51
27	i1	1001	CYC	C1A-NA-C4A	2.21	110.67	106.51
26	cJ	202	PEB	C3B-C4B-NB	-2.21	106.84	110.05
26	cY	202	PEB	C3B-C4B-NB	-2.21	106.84	110.05
26	j2	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	G6	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	z8	202	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	dZ	1001	PEB	C2A-C3A-C4A	2.21	104.64	101.34
27	W1	201	CYC	C1A-NA-C4A	2.21	110.67	106.51
26	l4	202	PEB	C3B-C4B-NB	-2.21	106.84	110.05
27	I1	201	CYC	C1A-NA-C4A	2.21	110.67	106.51
26	t6	202	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	n7	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	bU	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	cx	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	dl	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	dI	1001	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	eE	202	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	J3	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	y4	1001	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	d5	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	l5	202	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	x5	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	E8	202	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	dU	201	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	jK	1001	PEB	C2A-C3A-C4A	2.21	104.64	101.34
26	F7	201	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	hD	202	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	kW	1002	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	L2	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b3	501	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	o3	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	V5	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	y5	1001	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	k6	1002	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	dz	401	PEB	C2A-C3A-C4A	2.20	104.64	101.34
27	s1	201	CYC	C1A-NA-C4A	2.20	110.66	106.51
26	L7	201	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	an	201	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	i5	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	d7	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	H8	202	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	I8	202	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	cZ	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	fo	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	ct	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	J6	202	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	V9	202	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	fw	202	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	C2	302	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	r7	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	z7	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	bd	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	cv	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	dh	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	D3	202	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	ga	202	PEB	C3B-C4B-NB	-2.20	106.84	110.05
26	bq	202	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	cc	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	cM	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	go	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
27	K1	201	CYC	C1A-NA-C4A	2.20	110.66	106.51
27	q1	201	CYC	C1A-NA-C4A	2.20	110.66	106.51
26	A4	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	eQ	201	PEB	CMB-C2B-C1B	2.20	128.46	125.06
26	C8	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	hV	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	jJ	1002	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	jK	1002	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	kX	1002	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	c3	302	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	d4	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aK	1001	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	bu	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	de	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	dP	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	jI	1001	PEB	C2A-C3A-C4A	2.20	104.64	101.34
27	b1	1001	CYC	C1A-NA-C4A	2.20	110.66	106.51
29	bZ	304	PVN	C21-C2-C3	2.20	134.19	129.67
26	j4	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	lh	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	jL	1002	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	K6	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	ff	204	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	gj	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	cx	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	cG	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	x3	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	M4	202	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	S4	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	Z6	202	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	gt	201	PEB	C2A-C3A-C4A	2.20	104.64	101.34
26	gv	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	jO	1002	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	l3	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	aX	401	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	cU	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	lz	401	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	fr	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	fv	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	Z2	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	dj	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	ec	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	aq	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	D3	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	z4	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	a8	602	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	ac	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bl	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	cV	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	A1	301	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	B1	301	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	A2	1003	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	gr	201	PEB	C3B-C4B-NB	-2.20	106.85	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	ez	1004	PVN	C15-C16-C17	2.20	131.31	126.95
27	G1	1001	CYC	C1A-NA-C4A	2.20	110.65	106.51
26	f2	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	J4	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	W7	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	R9	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	dF	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	dO	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	gb	1001	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	al	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	at	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
29	dw	404	PVN	C81-C17-C18	-2.20	120.15	126.12
26	Z4	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	o4	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	I5	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	p9	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	gm	1001	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	Y7	1003	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	aF	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	cB	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	fr	202	PEB	CHC-C1D-ND	-2.20	111.39	113.95
26	el	201	PEB	CMB-C2B-C1B	2.20	128.45	125.06
27	L1	201	CYC	C1A-NA-C4A	2.20	110.65	106.51
27	a1	201	CYC	C1A-NA-C4A	2.20	110.65	106.51
26	D5	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	C6	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	g6	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	n9	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	aH	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bm	1002	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bF	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bZ	301	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	ck	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	cA	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	dF	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	eI	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	z3	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	N7	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	ch	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	dd	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	dh	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	fg	201	PEB	C3B-C4B-NB	-2.20	106.85	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eL	201	PEB	CHC-C1D-ND	-2.20	111.40	113.95
26	H3	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	X3	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	V6	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	u6	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	h7	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bf	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bD	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	di	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	dW	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	eo	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bJ	202	PEB	C3B-C4B-NB	-2.20	106.85	110.05
26	t8	202	PEB	CHC-C1D-ND	-2.20	111.40	113.95
26	gl	202	PEB	CHC-C1D-ND	-2.20	111.40	113.95
26	hS	202	PEB	CHC-C1D-ND	-2.20	111.40	113.95
26	i2	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	I2	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	V4	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	p4	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	X8	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bq	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	dr	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	eh	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	lp	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	T3	202	PEB	C3B-C4B-NB	-2.20	106.86	110.05
26	n3	202	PEB	C3B-C4B-NB	-2.20	106.86	110.05
27	k1	201	CYC	C1A-NA-C4A	2.20	110.65	106.51
26	r2	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	s2	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	s3	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	F6	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	q6	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	X7	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	bl	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	cU	202	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	ls	201	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	jL	1001	PEB	C2A-C3A-C4A	2.20	104.63	101.34
26	d8	301	PEB	CHC-C1D-ND	-2.20	111.40	113.95
26	fv	202	PEB	CHC-C1D-ND	-2.20	111.40	113.95
26	V2	202	PEB	C3B-C4B-NB	-2.20	106.86	110.05
26	gi	202	PEB	C3B-C4B-NB	-2.20	106.86	110.05
26	f7	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	P1	201	CYC	C1A-NA-C4A	2.19	110.64	106.51
27	U1	201	CYC	C1A-NA-C4A	2.19	110.64	106.51
27	d2	101	CYC	C1A-NA-C4A	2.19	110.64	106.51
26	p2	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	U2	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	Z3	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	Q6	202	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	Y7	1001	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	Y8	202	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	U9	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	af	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	gl	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	hD	201	PEB	C2A-C3A-C4A	2.19	104.63	101.34
26	dY	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	N2	201	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	m5	1002	PEB	CHC-C1D-ND	-2.19	111.40	113.95
27	O1	201	CYC	C1A-NA-C4A	2.19	110.64	106.51
26	s5	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	c6	1003	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	l7	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	e8	301	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	f9	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	ay	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	az	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	en	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eE	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
27	Z1	201	CYC	C1A-NA-C4A	2.19	110.64	106.51
26	P3	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	V7	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	cl	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	hX	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	eu	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	hZ	401	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	s2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	O4	1002	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	h4	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	t4	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	O6	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	d8	302	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	v8	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	L8	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	O8	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ap	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	aG	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	cu	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	do	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	la	1002	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	gz	301	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	hE	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	kW	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	z7	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	fy	201	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	H7	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06
26	Y3	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	h7	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	g2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	34	1003	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	T6	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	c6	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	t9	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	bY	1003	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	cJ	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eq	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	fh	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	hA	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	hW	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	m2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	k4	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	n4	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	w4	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	L6	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	e7	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	T8	302	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	ba	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	bI	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	cK	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	eB	201	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	fb	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	ad	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	ld	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	ln	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	hG	201	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	m5	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	d6	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	s7	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	h9	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	aN	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	cm	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dD	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	fa	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dV	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06
26	f2	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	ee	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	S3	203	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	z3	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	Y4	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	j5	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	H8	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	P9	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dw	402	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dA	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	gc	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
27	V1	201	CYC	C1A-NA-C4A	2.19	110.64	106.51
27	o1	1001	CYC	C1A-NA-C4A	2.19	110.64	106.51
26	kT	1002	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	W7	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	bZ	302	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	lo	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	lu	202	PEB	CHC-C1D-ND	-2.19	111.40	113.95
26	I2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	J2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	P2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	r3	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	X5	401	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	h5	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	e9	303	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	aI	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	cX	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eJ	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	le	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	bC	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06
26	dQ	201	PEB	CMB-C2B-C1B	2.19	128.44	125.06
26	ar	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	fs	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	hB	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	34	1007	PEB	C2A-C3A-C4A	2.19	104.62	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	l4	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	t4	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	h6	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	W8	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	bt	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dx	402	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eV	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	hA	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	H3	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	X7	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	e7	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	ep	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	fm	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	gn	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	gp	202	PEB	C3B-C4B-NB	-2.19	106.86	110.05
26	X2	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	Y6	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	r6	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	T7	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	N8	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	A9	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	aN	204	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	bR	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	cd	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	cS	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dy	401	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dD	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	ea	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eq	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	lr	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	lt	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	gy	303	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eR	202	PEB	CMB-C2B-C1B	2.19	128.43	125.06
26	E2	1002	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	u5	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	w5	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	p6	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	ev	201	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	A5	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	k7	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	P8	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	Z9	1007	PEB	C2A-C3A-C4A	2.19	104.62	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aL	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	bJ	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	dW	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	eD	202	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	hP	201	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	jO	1001	PEB	C2A-C3A-C4A	2.19	104.62	101.34
26	t5	202	PEB	C3B-C4B-NB	-2.19	106.87	110.05
26	lo	203	PEB	C3B-C4B-NB	-2.19	106.87	110.05
26	A2	1001	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	Z5	302	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	I7	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	g7	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	E9	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	lw	201	PEB	CHC-C1D-ND	-2.19	111.41	113.95
27	X1	201	CYC	C1A-NA-C4A	2.19	110.63	106.51
26	v2	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	G4	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	m9	1001	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	x9	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	aX	402	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	aY	402	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	bx	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	cR	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	cR	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	df	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	eT	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	kV	1001	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	eM	1001	PEB	CMB-C2B-C1B	2.19	128.43	125.06
26	K3	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	w3	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	lm	1002	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	fp	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	t2	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	D2	302	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	S3	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	G4	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	Z4	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	v6	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	t7	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	x8	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	z9	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	G9	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bn	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	bz	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	cC	1003	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	cI	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	cK	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	dt	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	dz	402	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	dY	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	iF	1001	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	v5	202	PEB	C3B-C4B-NB	-2.19	106.87	110.05
26	jP	1002	PEB	C3B-C4B-NB	-2.19	106.87	110.05
26	e2	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	g2	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	s4	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	a6	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	p6	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	R7	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	k9	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	aB	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	be	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	es	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	lv	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	gn	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	Y5	1003	PEB	CMB-C2B-C1B	2.19	128.43	125.06
26	U6	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	q7	202	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	eY	401	PEB	CHC-C1D-ND	-2.19	111.41	113.95
26	W4	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	X4	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	j4	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	j5	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	k5	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	k8	203	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	y6	202	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	p8	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	D7	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	e8	302	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	x8	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	C8	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	av	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	aY	401	PEB	C2A-C3A-C4A	2.19	104.61	101.34
26	li	201	PEB	C2A-C3A-C4A	2.19	104.61	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	g3	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	s8	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	U9	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	bG	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	U4	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	q4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	W6	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	c9	301	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	M8	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	u9	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	v9	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	aR	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bZ	303	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	cB	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dm	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	fn	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	hQ	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	t3	201	PEB	CMB-C2B-C1B	2.18	128.43	125.06
26	bL	202	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	Y9	301	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	e2	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	n2	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	a3	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	M4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	Y5	1003	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	m8	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	c6	1002	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	G7	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	w7	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	d9	301	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	U8	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	i9	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	aR	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bH	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dp	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dx	404	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eS	202	PEB	CMB-C2B-C1B	2.18	128.43	125.06
26	V3	202	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	v9	202	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	cb	202	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	C4	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	a4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	l6	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	g7	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	b8	1002	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	K8	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	aZ	302	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bK	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	cT	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dc	203	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dO	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dX	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eW	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	ly	402	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	gy	302	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	l7	202	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	ei	202	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	kQ	1002	PEB	C3B-C4B-NB	-2.18	106.87	110.05
26	K7	201	PEB	CMB-C2B-C1B	2.18	128.43	125.06
26	G2	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	b3	502	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	m3	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	E4	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	z4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	a9	601	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	au	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	aL	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	aT	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bX	402	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	cO	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	ee	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	ej	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eD	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eG	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eY	402	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	gi	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	hK	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	e4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	W5	301	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	f8	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	m6	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	y6	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	b8	1003	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	K9	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	bk	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bo	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	cg	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eb	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	ep	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	fd	303	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	fl	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	ga	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	gs	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	S2	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	ay	1002	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	ey	1001	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	fe	202	PEB	CHC-C1D-ND	-2.18	111.41	113.95
26	n7	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	eX	201	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	E2	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	P3	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	K6	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	i6	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	q8	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	v8	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	I8	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	aI	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	cS	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eB	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	eG	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	gy	301	PEB	C2A-C3A-C4A	2.18	104.61	101.34
27	a2	901	CYC	C2B-C1B-NB	2.18	110.18	106.99
26	H7	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	dg	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	x2	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	W2	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	e3	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	u3	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	I4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	L4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	N4	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	X4	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	R5	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	Z5	303	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	j8	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	N6	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	j6	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	s6	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	y6	203	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	F8	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	s9	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	t9	202	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	u9	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	y9	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bs	1002	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	bP	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	db	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	dp	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	fb	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	ft	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	hM	1001	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	hO	201	PEB	C2A-C3A-C4A	2.18	104.61	101.34
26	w2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	C3	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	v3	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	K4	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	44	302	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	G5	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	T6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	b7	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	D8	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	J8	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	T9	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	X9	401	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aO	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	by	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ds	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ez	1003	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	hT	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	gj	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
27	d1	1001	CYC	C1A-NA-C4A	2.18	110.62	106.51
26	k6	1001	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	p2	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	bN	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	cs	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	l2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	O2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	F4	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	24	401	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	q4	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	M6	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	P6	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	a8	601	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aC	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	bw	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	cM	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dC	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dM	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	eP	203	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	fk	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
27	n1	201	CYC	C1A-NA-C4A	2.18	110.61	106.51
26	cI	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	dU	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	o4	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	o9	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	V2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	a5	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	m8	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	I6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	b6	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	z6	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aB	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aN	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ca	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	cV	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ds	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	du	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dv	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dG	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dJ	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ez	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	hC	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
27	u1	1001	CYC	CAA-C2A-C3A	2.18	131.94	127.88
26	ef	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	fg	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	o2	1002	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	y2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	z2	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	R4	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	g8	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	X6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	c7	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aY	406	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dn	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	hV	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	F5	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	M4	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	ed	201	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	jI	1001	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	q2	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	v2	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	T3	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	g3	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	S5	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	S6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	w6	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	N8	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	L9	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	Y9	302	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	bs	1003	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	da	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dn	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	do	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dq	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dw	401	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	el	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	eH	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ff	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	jJ	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	bP	202	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	cH	201	PEB	C3B-C4B-NB	-2.18	106.88	110.05
26	R2	201	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	A3	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	I3	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	O3	1002	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	Q7	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	bA	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	bC	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	eQ	202	PEB	CMB-C2B-C1B	2.18	128.42	125.06
26	u2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	Y2	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	J4	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q5	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	b6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	l6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	V7	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aJ	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aP	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	aS	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	bW	301	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	cP	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	cW	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dj	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	fe	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	fw	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	O7	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	cm	1002	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	lg	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	fh	1002	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	Z6	201	PEB	CMB-C2B-C1B	2.18	128.41	125.06
26	em	201	PEB	CMB-C2B-C1B	2.18	128.41	125.06
26	k3	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	E5	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	k8	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	A6	1002	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	Q6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	o8	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	I7	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	w8	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	l9	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	p9	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ao	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	bz	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	cY	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	ez	1002	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	eH	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	eU	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	lf	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	jM	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	bY	1003	PEB	CMB-C2B-C1B	2.18	128.41	125.06
26	dc	203	PEB	CMB-C2B-C1B	2.18	128.41	125.06
26	kV	1001	PEB	CMB-C2B-C1B	2.18	128.41	125.06
26	cD	202	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	et	201	PEB	CHC-C1D-ND	-2.18	111.42	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	lq	203	PEB	CHC-C1D-ND	-2.18	111.42	113.95
26	y2	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	K2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	W2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	Z2	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	N3	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	U4	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	h6	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	P8	202	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	br	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	cr	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	du	203	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	dS	201	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	iC	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	iH	1001	PEB	C2A-C3A-C4A	2.18	104.60	101.34
26	v7	202	PEB	C3B-C4B-NB	-2.18	106.89	110.05
26	T2	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	cg	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	o4	202	PEB	C2A-C3A-C4A	2.17	104.60	101.34
26	O6	201	PEB	C2A-C3A-C4A	2.17	104.60	101.34
26	cq	201	PEB	C2A-C3A-C4A	2.17	104.60	101.34
26	dP	202	PEB	C2A-C3A-C4A	2.17	104.60	101.34
26	lq	202	PEB	C2A-C3A-C4A	2.17	104.60	101.34
26	hR	201	PEB	C2A-C3A-C4A	2.17	104.60	101.34
26	fn	1002	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	dh	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	dP	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	i3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	D4	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	I4	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	N5	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	j8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	G8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	L8	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Q8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	z9	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	aU	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bh	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cC	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cW	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ey	1002	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hI	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	o7	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	Q9	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	lj	201	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	lt	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	y5	1001	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	u6	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	cR	202	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	q2	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	D2	301	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	O2	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	O3	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	F6	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	t8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	e9	302	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	l9	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	x9	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	y9	1002	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	al	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	aD	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	aM	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bc	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bg	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bj	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bs	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bx	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bY	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cj	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ej	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	eI	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	iA	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	kT	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ls	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	hO	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	iF	1002	PEB	CHC-C1D-ND	-2.17	111.42	113.95
29	aZ	303	PVN	C92-C91-C18	2.17	118.42	112.43
26	bD	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	C2	301	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	U5	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Y5	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	o5	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	l8	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	a9	603	PEB	C2A-C3A-C4A	2.17	104.59	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	o9	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ad	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	aM	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	dw	403	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hH	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hL	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hX	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	jN	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	s2	202	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	E7	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	bv	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	bQ	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	y3	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	G5	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	dc	202	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	lg	201	PEB	CHC-C1D-ND	-2.17	111.42	113.95
26	M5	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	b5	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	O7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	v7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	b9	402	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	w8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	N9	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	aS	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bv	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ce	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ln	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bq	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	i4	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	t5	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	q7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	b9	403	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	w9	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	B9	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	J9	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ag	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	aQ	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cX	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	dr	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	eF	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hJ	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hT	204	PEB	C2A-C3A-C4A	2.17	104.59	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	kU	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	jM	1002	PEB	C3B-C4B-NB	-2.17	106.89	110.05
26	m8	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	dw	401	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	hE	1001	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	M2	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	R3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Y4	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	h8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	M6	1002	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	u7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ai	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bv	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bN	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cT	1002	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	dg	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	dK	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	li	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	lq	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Z7	202	PEB	C3B-C4B-NB	-2.17	106.89	110.05
29	bZ	304	PVN	C92-C91-C18	2.17	118.41	112.43
26	d3	301	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	i7	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	ei	201	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	K2	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	m4	1001	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	B3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	F3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Q3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	R4	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	u5	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	D6	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	o6	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	o6	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	s6	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	H7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	V8	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cp	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	dx	401	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	es	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	eC	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	w2	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U2	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	ft	201	PEB	CMB-C2B-C1B	2.17	128.41	125.06
26	Q5	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	Y5	1002	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	e6	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	cw	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	fx	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	E4	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	r6	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	y7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	J8	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	K8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bS	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	cO	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	fj	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	fx	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hY	403	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	m5	1003	PEB	C3B-C4B-NB	-2.17	106.89	110.05
26	ge	202	PEB	C3B-C4B-NB	-2.17	106.89	110.05
26	k3	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	G4	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	d9	302	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	fp	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	R6	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	j6	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	B8	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	dk	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ey	1003	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	eF	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	lb	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	hZ	402	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	kS	1001	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	I5	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	dJ	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	hQ	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	g2	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	Z4	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	t9	202	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	cQ	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
27	U1	201	CYC	CAA-C2A-C3A	2.17	131.92	127.88
27	d2	101	CYC	CAA-C2A-C3A	2.17	131.92	127.88
26	h2	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	a3	1003	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	y3	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	B4	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	P4	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Q4	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	U6	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	Z7	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	B8	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ar	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	bj	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ch	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ct	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	eC	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	lb	202	PEB	C2A-C3A-C4A	2.17	104.59	101.34
26	ll	201	PEB	C2A-C3A-C4A	2.17	104.59	101.34
29	ey	1004	PVN	C15-C16-C17	2.17	131.24	126.95
26	C7	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	ft	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	gc	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	q2	202	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	C5	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	q7	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	r9	202	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	bJ	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	bV	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	cP	202	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	iH	1001	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	B2	501	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	Q4	203	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	T4	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	Z8	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	cP	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	du	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	dI	1002	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	ed	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	eg	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	er	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	fc	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	fi	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	Q3	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	Q4	203	PEB	CMB-C2B-C1B	2.17	128.40	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dj	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	dq	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	eM	1002	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	ab	202	PEB	C3B-C4B-NB	-2.17	106.90	110.05
26	h5	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	y5	1002	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	r8	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	le	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	Q2	1001	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	Z5	301	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	e5	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	l5	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	n5	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	F9	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	at	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	aC	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	aV	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	eP	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	y4	1001	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	b6	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	P7	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	r7	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	Q8	202	PEB	CMB-C2B-C1B	2.17	128.40	125.06
29	gz	304	PVN	C15-C14-C13	-2.17	119.33	124.90
26	W3	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	m3	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	bK	1002	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	F2	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	A3	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	c4	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	O5	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	f7	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	q9	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	aA	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	bB	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	dR	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	gp	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	v2	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	B4	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	j6	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	r6	201	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	c9	301	PEB	CMB-C2B-C1B	2.17	128.40	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aB	202	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	ba	1001	PEB	CMB-C2B-C1B	2.17	128.40	125.06
26	cC	1001	PEB	CMB-C2B-C1B	2.17	128.40	125.06
29	Z5	304	PVN	C41-C7-C8	-2.17	120.86	124.94
26	o2	1001	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	r2	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	B2	502	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	U3	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	u4	202	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	J6	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	M7	1002	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	E8	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	O9	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	bQ	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	cw	201	PEB	C2A-C3A-C4A	2.17	104.58	101.34
26	c4	201	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	C5	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	aw	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	cu	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	gw	202	PEB	CHC-C1D-ND	-2.17	111.43	113.95
26	S3	203	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	m5	1001	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	cY	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	z2	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	I3	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	W3	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	F4	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	S4	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	v4	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	e6	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	E7	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	P7	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	a7	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	G8	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	O8	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	by	1002	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bE	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	dd	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	hS	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	o2	1002	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	I2	202	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	x8	202	PEB	CMB-C2B-C1B	2.16	128.40	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ad	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	dw	403	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	K9	1002	PEB	CHC-C1D-ND	-2.16	111.43	113.95
26	hF	202	PEB	CHC-C1D-ND	-2.16	111.43	113.95
26	hU	201	PEB	CHC-C1D-ND	-2.16	111.43	113.95
26	hY	402	PEB	CHC-C1D-ND	-2.16	111.43	113.95
27	R1	1001	CYC	CAA-C2A-C3A	2.16	131.91	127.88
27	i1	1001	CYC	CAA-C2A-C3A	2.16	131.91	127.88
26	K2	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	N2	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	L4	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	H5	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	g5	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	v5	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	ab	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bd	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bi	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	cs	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	hN	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	C3	1001	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	Q4	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	S5	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	N6	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	af	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	bW	301	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	cN	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	dn	202	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	du	202	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	hD	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	iG	1001	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	O5	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	U5	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	eh	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	b4	1001	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	y4	1002	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	J5	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	K5	1001	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	E6	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	v6	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	w6	1002	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	h9	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	ah	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aE	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	br	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bV	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	cD	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	cQ	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	eN	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	gw	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	o3	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	N8	202	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	R9	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	bI	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	fx	201	PEB	CMB-C2B-C1B	2.16	128.40	125.06
26	O4	1001	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	f4	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	x4	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	C6	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	o7	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	Y8	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	r9	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	Q9	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aJ	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aV	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bA	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	dC	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	dN	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	ef	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	eu	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	eK	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	jP	1001	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	M3	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	u3	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	t6	201	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	f7	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	G9	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	cZ	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	i4	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	P6	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	lm	1001	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	D9	202	PEB	C3B-C4B-NB	-2.16	106.90	110.05
26	S2	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	G3	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	c5	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k8	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	W6	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	q6	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	j7	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	A8	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	s9	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aT	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	T5	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	V7	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	aQ	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	dK	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	dO	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	li	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
27	I1	201	CYC	CAA-C2A-C3A	2.16	131.90	127.88
26	H6	201	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	A9	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	ld	201	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	I6	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	P6	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	x6	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	S8	401	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	Z9	1003	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aW	302	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aZ	301	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	dB	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	lc	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	fm	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	gh	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	p2	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	y4	1002	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	H5	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	a7	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	bl	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	eE	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	eI	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	gh	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	n6	201	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	bS	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	iB	1002	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	W4	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	m4	1001	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	z5	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	w9	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aw	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	aE	202	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bI	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	bL	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	dE	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	eZ	401	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	gg	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	gk	201	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	kQ	1001	PEB	C2A-C3A-C4A	2.16	104.58	101.34
26	K3	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	aL	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	aT	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	be	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	bj	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	bq	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	en	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	ff	204	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	fh	1001	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	gy	301	PEB	CMB-C2B-C1B	2.16	128.39	125.06
29	d8	303	PVN	C16-C17-C18	-2.16	105.62	107.87
26	r5	202	PEB	C3B-C4B-NB	-2.16	106.91	110.05
26	G3	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	db	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	ek	1002	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	lc	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	fk	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	t2	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	L5	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	u8	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	S7	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	i7	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	m7	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	aH	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	cL	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	dG	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	eo	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	lk	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	hB	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	kR	1001	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	W2	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	44	302	PEB	CMB-C2B-C1B	2.16	128.39	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U9	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	Z9	1003	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	dD	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	eN	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	F2	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	B6	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	S9	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	dk	1002	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	dm	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	dA	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	fd	301	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	e2	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	t2	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	y2	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	c6	1002	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	b7	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	Y8	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	P9	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	aH	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	bN	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	dI	1002	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	eP	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	gl	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	k3	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	gm	1002	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	go	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	iA	1002	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	h2	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	E2	1001	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	O5	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	G6	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	W6	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	J9	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	cb	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	cJ	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	ed	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	hH	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	k2	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	G2	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	s8	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	C7	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	F8	1002	PEB	C2A-C3A-C4A	2.16	104.57	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	q9	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	V9	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	aq	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	aK	1002	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	dM	1002	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	hK	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	u8	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	ec	201	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	e2	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	G2	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	q3	1001	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	p4	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	s4	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	c5	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	d5	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	B6	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	I7	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	k9	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	aJ	202	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	cr	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	cT	1001	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	dA	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	lf	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	hQ	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	A2	1002	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	M2	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	w3	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	l8	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	A8	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	W8	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	eW	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
27	X1	201	CYC	CAA-C2A-C3A	2.16	131.90	127.88
29	eZ	402	PVN	C51-C52-C53	-2.16	107.71	113.76
26	M5	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	m7	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	s7	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	u7	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	cy	1002	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	fz	301	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	Q6	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	c6	1003	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	n9	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B9	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	br	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	cd	201	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	gz	303	PEB	CMB-C2B-C1B	2.16	128.39	125.06
26	Y2	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	B5	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	E6	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	x6	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	U8	1002	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	r9	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	bO	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	ea	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	eO	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
29	ey	1004	PVN	C81-C17-C18	-2.16	120.26	126.12
26	g2	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	r2	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	z2	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	S2	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	34	1003	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	j8	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	B8	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	ae	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	aV	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	bs	1003	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	bK	1001	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	cm	1001	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	eg	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	ez	1001	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	g4	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	r5	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	M9	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	ae	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	eR	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	lu	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	U2	202	PEB	CHC-C1D-ND	-2.16	111.44	113.95
26	o2	1001	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	C2	302	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	D2	301	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	c3	302	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	n3	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	G4	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	w5	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K6	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	p9	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	Z9	1007	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	dq	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	dF	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	ea	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
27	y1	201	CYC	CAA-C2A-C3A	2.16	131.89	127.88
26	m2	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	P4	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	Q4	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	N7	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	c9	302	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	M8	202	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	g9	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	cN	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	gq	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
29	gy	304	PVN	C9-C10-C11	-2.16	126.23	128.81
26	I4	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	G8	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	I8	202	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	am	1001	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	aN	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	eT	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	la	1001	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	gx	201	PEB	CMB-C2B-C1B	2.16	128.38	125.06
26	Y3	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	x7	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	bh	201	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	dx	403	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	iE	1001	PEB	C2A-C3A-C4A	2.16	104.57	101.34
26	s5	202	PEB	CHC-C1D-ND	-2.15	111.44	113.95
26	S3	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	Q4	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	d4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	l4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	r8	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	c7	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	q9	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aP	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	dc	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	eE	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	fk	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	w2	203	PEB	C2A-C3A-C4A	2.15	104.57	101.34
26	A4	201	PEB	C2A-C3A-C4A	2.15	104.57	101.34
26	Q7	201	PEB	C2A-C3A-C4A	2.15	104.57	101.34
26	e9	301	PEB	C2A-C3A-C4A	2.15	104.57	101.34
26	bb	201	PEB	C2A-C3A-C4A	2.15	104.57	101.34
26	iG	1001	PEB	C2A-C3A-C4A	2.15	104.57	101.34
29	T8	303	PVN	O19-C19-N4	-2.15	120.07	125.08
26	L4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	L8	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	bv	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	bZ	301	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	es	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	ly	402	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	fi	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	U3	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	t3	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	H4	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	H4	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	44	301	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	C5	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	T5	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	i6	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	d9	303	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dc	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dL	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	F2	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	n5	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	k7	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	A8	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	E8	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	ab	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aQ	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	bb	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	lr	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	iA	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	y8	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	z8	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	T8	301	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	U8	1003	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	lm	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	hC	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	hM	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	M1	1001	CYC	C2B-C1B-NB	2.15	110.14	106.99
26	Y2	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	K4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	R4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	V4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	x4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	I5	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	X5	401	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	w7	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aE	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aR	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aS	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	cM	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	lb	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	k2	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	M3	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	f3	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	b8	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	j9	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	bm	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dH	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dH	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	eM	1002	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	la	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	cn	201	PEB	C3B-C4B-NB	-2.15	106.92	110.05
26	B2	502	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	f8	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	C6	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	j6	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	u6	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	E8	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	J8	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	M8	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	V8	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	cT	1002	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	dJ	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	eu	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
29	44	303	PVN	C41-C7-C8	-2.15	120.89	124.94
26	M7	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	aP	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dt	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	gz	303	PEB	C2A-C3A-C4A	2.15	104.56	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	iB	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	w2	203	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	N2	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	O2	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	b3	502	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	F4	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	P4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	Z4	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	T8	301	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	s9	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	w9	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	bd	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	cD	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	cG	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	dx	404	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	dP	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	kX	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	S3	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	c3	301	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	U7	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	lh	201	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	gb	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	c8	302	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dN	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dV	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
27	q1	201	CYC	CAA-C2A-C3A	2.15	131.88	127.88
26	r2	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	y3	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	I6	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	g6	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	Y7	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	e8	301	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	e9	302	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	G8	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	O8	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aA	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aI	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	aI	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	bn	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	cq	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	cs	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	eA	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	fn	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	hB	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	hC	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	hV	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	hX	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	jM	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	u4	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	D8	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	aQ	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	eA	1001	PEB	C2A-C3A-C4A	2.15	104.56	101.34
27	N1	201	CYC	CAA-C2A-C3A	2.15	131.88	127.88
26	w4	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	S5	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	cv	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	G3	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	R4	202	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	T4	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	Y5	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	W6	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	w6	1001	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	w6	1002	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	U7	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	W8	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	bS	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	eD	201	PEB	CMB-C2B-C1B	2.15	128.38	125.06
26	Q8	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	bp	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	bt	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	bC	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	A5	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	G6	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	au	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	gu	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
29	eY	403	PVN	C51-C52-C53	-2.15	107.73	113.76
26	P3	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	B5	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	i6	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	X7	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	l7	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	q9	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bX	401	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	ey	1003	PEB	CMB-C2B-C1B	2.15	128.37	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	jJ	1001	PEB	CMB-C2B-C1B	2.15	128.37	125.06
27	P1	201	CYC	CAA-C2A-C3A	2.15	131.88	127.88
27	r1	201	CYC	C2B-C1B-NB	2.15	110.13	106.99
26	m6	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	cz	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dK	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dR	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	eK	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	eO	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	fs	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	t2	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	W4	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	o7	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	y8	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	w9	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bh	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	cV	203	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dg	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dm	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dx	401	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dX	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	eT	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	jP	1001	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	o3	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	ao	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	eA	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	gh	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
29	gz	304	PVN	C14-C13-C12	2.15	108.97	106.51
26	K7	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	z4	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	a5	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	I8	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	G9	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	av	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	aY	401	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	aZ	301	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bL	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	ce	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	eF	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	eG	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	Q3	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	N6	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C9	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	n3	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	aF	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	dq	202	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	ge	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	gv	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	A5	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	Y9	302	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bu	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bw	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	ds	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dv	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dR	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dZ	1001	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	ej	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	eF	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	fm	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
27	m1	201	CYC	CAA-C2A-C3A	2.15	131.88	127.88
26	aW	301	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	bM	201	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	hY	401	PEB	C2A-C3A-C4A	2.15	104.56	101.34
26	c5	201	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	d6	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	k7	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	Z9	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	da	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	gs	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	i3	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	x3	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	K4	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	N4	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	V6	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	b9	401	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	eH	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	lk	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
27	o1	1001	CYC	CAA-C2A-C3A	2.15	131.88	127.88
26	w2	202	PEB	C2A-C3A-C4A	2.15	104.55	101.34
26	i8	201	PEB	C2A-C3A-C4A	2.15	104.55	101.34
26	k2	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	A2	1002	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	P2	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	X2	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	p3	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	V5	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	k5	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	D6	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	S6	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	v6	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	x8	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	z8	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	p9	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	u9	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	y9	1001	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bA	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	bM	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	eb	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	fc	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	hS	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dZ	1002	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	lw	202	PEB	CHC-C1D-ND	-2.15	111.45	113.95
26	F2	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	w4	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	z5	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	m8	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	t8	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	Z7	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	C8	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	u9	201	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	aT	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	cS	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dm	202	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	dx	402	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	fd	302	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	hY	403	PEB	CMB-C2B-C1B	2.15	128.37	125.06
26	C4	1002	PEB	CHC-C1D-ND	-2.15	111.46	113.95
26	K5	1002	PEB	CHC-C1D-ND	-2.15	111.46	113.95
26	V6	202	PEB	CHC-C1D-ND	-2.15	111.46	113.95
26	G7	202	PEB	CHC-C1D-ND	-2.15	111.46	113.95
26	Y7	1002	PEB	CHC-C1D-ND	-2.15	111.46	113.95
26	r8	201	PEB	C2A-C3A-C4A	2.15	104.55	101.34
26	b9	404	PEB	C2A-C3A-C4A	2.15	104.55	101.34
26	aj	201	PEB	C2A-C3A-C4A	2.15	104.55	101.34
26	iD	1001	PEB	C2A-C3A-C4A	2.15	104.55	101.34
27	Q1	201	CYC	CAA-C2A-C3A	2.15	131.87	127.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A3	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	W4	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	o5	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	g8	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	A6	1002	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	a9	603	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	T8	302	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	U8	1003	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	X8	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	cz	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	dk	1001	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	dL	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	eC	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	fl	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
29	Y9	303	PVN	O19-C19-N4	-2.14	120.09	125.08
27	g1	201	CYC	CAA-C2A-C3A	2.14	131.87	127.88
26	j9	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	aA	202	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	lo	201	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	fl	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	hI	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	f2	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	q2	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	D3	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	i5	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	l8	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	b9	403	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	e9	303	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	N9	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	ac	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	ao	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	aF	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	aL	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	aY	406	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	cM	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	ez	1002	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	eS	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	gf	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	aU	202	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	kX	1001	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	E3	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	g3	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F4	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	q4	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	q5	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	s5	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	f6	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	s8	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	O8	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	Z8	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	S9	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	X9	401	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	aW	302	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	cB	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	du	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	ea	201	PEB	CMB-C2B-C1B	2.14	128.37	125.06
26	gq	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	z6	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	H9	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	cV	203	PEB	C2A-C3A-C4A	2.14	104.55	101.34
27	b1	1001	CYC	CAA-C2A-C3A	2.14	131.87	127.88
26	X4	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	R5	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	j5	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	j7	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	z7	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	K8	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aq	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	bX	402	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	db	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	dp	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	bG	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	cl	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	k2	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	X3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	A4	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	t4	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	j8	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	k8	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	c8	302	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aE	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aG	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	by	1002	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	bz	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cW	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	da	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	f6	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	dT	202	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	cC	1002	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	hE	1002	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	G2	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	s3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	E4	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	M6	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	D8	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	T9	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	cV	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	eJ	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	kU	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
27	O1	201	CYC	CAA-C2A-C3A	2.14	131.87	127.88
27	k1	201	CYC	CAA-C2A-C3A	2.14	131.87	127.88
26	E3	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	bw	201	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	eS	202	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	v2	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	B3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	C4	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	g4	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	X6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	F9	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aW	301	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	dK	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	eC	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	gk	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	gq	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	jN	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	a6	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	u6	202	PEB	C2A-C3A-C4A	2.14	104.55	101.34
26	R2	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	U6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	b6	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	h6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	w8	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	L8	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	L9	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	bH	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ct	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	gs	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	A7	201	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	E7	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	W2	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	E4	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	Y4	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	j4	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	j5	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	O6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	x6	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	J8	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aX	401	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	di	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	lv	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	bD	202	PEB	C3B-C4B-NB	-2.14	106.94	110.05
26	S9	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	m3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	Z5	303	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	I6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	J6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	T6	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	G7	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	v7	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	b9	402	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	d9	303	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	v8	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	M8	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	h9	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	x9	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aP	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	do	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	hT	204	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	iC	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	kR	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	m2	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	I2	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	K2	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	Y2	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	N3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	W3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	J4	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O4	1001	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	q4	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	E5	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	t5	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	i6	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	o6	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	v8	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aF	204	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	dN	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	ez	1003	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	lu	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	hK	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	hR	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	P2	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	s3	202	PEB	CHC-C1D-ND	-2.14	111.46	113.95
26	gu	201	PEB	C2A-C3A-C4A	2.14	104.54	101.34
26	Z3	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	n4	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	M5	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aw	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aH	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	aZ	302	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	bR	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	cI	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	cU	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	cW	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	de	201	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	do	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	dr	202	PEB	CMB-C2B-C1B	2.14	128.36	125.06
26	dz	401	PEB	CMB-C2B-C1B	2.14	128.36	125.06
27	d1	1001	CYC	CAA-C2A-C3A	2.14	131.86	127.88
26	w5	201	PEB	C2A-C3A-C4A	2.14	104.54	101.34
26	D5	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	v5	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	p6	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	C7	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	d9	301	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	z9	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	O9	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	aa	1001	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	bF	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	bZ	303	PEB	CMB-C2B-C1B	2.14	128.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cS	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	df	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	dG	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	eB	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	eO	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	fs	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	gc	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	iE	1001	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	kQ	1001	PEB	CMB-C2B-C1B	2.14	128.35	125.06
27	e1	201	CYC	CAA-C2A-C3A	2.14	131.86	127.88
26	hW	202	PEB	CHC-C1D-ND	-2.14	111.47	113.95
27	L1	201	CYC	CAA-C2A-C3A	2.14	131.86	127.88
27	a1	201	CYC	CAA-C2A-C3A	2.14	131.86	127.88
27	s1	201	CYC	CAA-C2A-C3A	2.14	131.86	127.88
26	ak	201	PEB	C2A-C3A-C4A	2.14	104.54	101.34
26	O2	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	Z2	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	34	1007	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	R6	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	u8	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	T7	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	aC	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	bt	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	dl	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	dw	402	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	ly	401	PEB	C2A-C3A-C4A	2.14	104.54	101.34
26	u2	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	S4	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	Q5	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	r5	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	y6	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	s7	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	e8	302	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	B8	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	H8	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	P8	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	Q8	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	aC	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	aM	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	bk	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	dt	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	eV	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	eY	402	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	gu	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	iD	1001	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	f6	202	PEB	CHC-C1D-ND	-2.14	111.47	113.95
26	M9	202	PEB	CHC-C1D-ND	-2.14	111.47	113.95
27	H1	201	CYC	C2B-C1B-NB	2.14	110.11	106.99
27	h1	201	CYC	C2B-C1B-NB	2.14	110.11	106.99
26	a3	1001	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	F6	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	bo	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	br	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	cw	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	dA	202	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	eR	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	lq	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
26	hW	201	PEB	CMB-C2B-C1B	2.14	128.35	125.06
29	A2	1004	PVN	C16-C17-C18	-2.14	105.64	107.87
29	a3	1004	PVN	C16-C17-C18	-2.14	105.64	107.87
27	w1	201	CYC	CAA-C2A-C3A	2.13	131.85	127.88
26	I9	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	u2	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	w2	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	B2	501	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	J4	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	l6	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	g7	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	M9	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	aK	1001	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	bi	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ci	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	S7	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	bE	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	Y3	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	V4	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	N5	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	A6	1001	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	F6	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	m6	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	x7	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	a9	602	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	z8	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	Q9	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aB	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	eH	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ga	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	am	1001	PEB	C2A-C3A-C4A	2.13	104.53	101.34
27	J1	201	CYC	C2B-C1B-NB	2.13	110.11	106.99
27	p1	201	CYC	C2B-C1B-NB	2.13	110.11	106.99
26	o4	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	v6	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	e9	301	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	D8	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	S8	401	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	y9	1002	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	aN	204	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	bO	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	cL	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	cR	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	dY	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	lt	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	fv	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	s4	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
29	d3	302	PVN	C12-C11-N3	-2.13	106.95	110.05
26	O3	1001	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	P4	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	t7	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	f9	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	g9	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	bc	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	bB	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	cV	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	dr	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ej	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	lb	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	fd	303	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ff	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	hI	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	cG	201	PEB	C2A-C3A-C4A	2.13	104.53	101.34
26	o8	201	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	c8	301	PEB	CHC-C1D-ND	-2.13	111.47	113.95
27	K1	201	CYC	CAA-C2A-C3A	2.13	131.85	127.88
26	F3	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	L5	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	q6	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	r6	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	s6	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	i7	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	b9	404	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	F8	1001	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ap	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	cC	1003	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	eh	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	gw	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	gz	301	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	hM	1001	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	hN	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	Z9	1001	PEB	C2A-C3A-C4A	2.13	104.53	101.34
26	M7	1003	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	bM	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	gz	302	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	U4	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	N8	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	f9	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	aJ	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	aR	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ck	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	cA	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	dt	202	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	ew	301	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	gb	1001	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	gt	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
26	gv	201	PEB	CMB-C2B-C1B	2.13	128.35	125.06
27	n1	201	CYC	CAA-C2A-C3A	2.13	131.85	127.88
26	o5	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	de	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	l2	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	T3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	I4	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	t4	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	l5	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	M6	1002	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	c6	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	l6	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	z6	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	A8	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	Z9	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	cp	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	cP	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dG	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dU	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eo	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	le	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	fw	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
27	S1	201	CYC	C2B-C1B-NB	2.13	110.11	106.99
27	j1	201	CYC	C2B-C1B-NB	2.13	110.11	106.99
26	x2	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	U3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	a3	1003	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	u4	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	u5	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	O6	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	Y6	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	k6	1002	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	W7	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	H9	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	au	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	aY	402	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bx	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	cO	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	ly	401	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	fq	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
27	S1	202	CYC	C2B-C1B-NB	2.13	110.11	106.99
26	f3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	y7	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	ay	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bt	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bP	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dC	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eW	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	fd	301	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	fo	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	gj	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	gn	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	jK	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	O9	202	PEB	CHC-C1D-ND	-2.13	111.47	113.95
26	m2	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	u4	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	i8	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k8	203	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	y6	203	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	h9	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	r9	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	D9	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	at	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	aS	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bd	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	cv	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eK	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
27	G1	1001	CYC	CAA-C2A-C3A	2.13	131.84	127.88
27	Z1	201	CYC	CAA-C2A-C3A	2.13	131.84	127.88
27	f1	201	CYC	CAA-C2A-C3A	2.13	131.84	127.88
26	s2	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	C2	301	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	c4	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	k4	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	U5	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	as	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	aD	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	cZ	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	du	203	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	li	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	gy	303	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	hO	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	o6	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bp	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dI	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eG	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	lc	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	fa	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dT	201	PEB	C2A-C3A-C4A	2.13	104.53	101.34
26	V2	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	z3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	D4	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	O4	1002	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	24	401	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	a4	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	C6	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	y6	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	q8	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	U8	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	m9	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	aU	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bz	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	cu	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dB	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dM	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eW	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	hA	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	n2	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	M3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	R3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	w3	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	K5	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	e5	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	H6	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bl	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	by	1001	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	ee	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	gi	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	hJ	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
27	V1	201	CYC	CAA-C2A-C3A	2.13	131.84	127.88
26	i3	202	PEB	CHC-C1D-ND	-2.13	111.48	113.95
26	H4	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	Y4	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	g5	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	P6	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	O7	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	a8	602	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	F8	1002	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	H8	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	bm	1002	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	cU	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dE	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	dS	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eD	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eK	202	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	eP	203	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	fe	201	PEB	CMB-C2B-C1B	2.13	128.34	125.06
26	M4	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	E6	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	e6	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	w8	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	V9	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	al	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	er	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	es	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	ly	403	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	lz	402	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	fb	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	ge	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	E3	202	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	a3	1002	PEB	CHC-C1D-ND	-2.12	111.48	113.95
29	bY	1004	PVN	C16-C15-C14	-2.12	122.89	128.08
29	A2	1004	PVN	C15-C16-C17	2.12	131.16	126.95
29	a3	1004	PVN	C15-C16-C17	2.12	131.16	126.95
26	H3	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	Q6	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	q6	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	Q7	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	bu	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	dn	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	ds	202	PEB	CMB-C2B-C1B	2.12	128.34	125.06
26	lp	201	PEB	CMB-C2B-C1B	2.12	128.34	125.06
27	t1	201	CYC	C2B-C1B-NB	2.12	110.10	106.99
26	bO	202	PEB	CHC-C1D-ND	-2.12	111.48	113.95
29	d9	304	PVN	C16-C17-C18	-2.12	105.66	107.87
26	J2	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	S4	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	b8	1003	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	aA	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	cX	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	hZ	402	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	bU	202	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	i2	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	e4	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	f4	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	h4	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	z4	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	W5	301	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	h5	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	K6	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	b8	1001	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	b8	1002	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	K8	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U8	1002	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dy	401	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dz	402	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dF	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dW	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	ef	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	ep	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	M2	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	Q2	1001	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	L3	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	l8	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	L6	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	a6	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	a9	601	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	ah	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dD	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dH	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	ln	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	lq	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	hL	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
27	Y1	201	CYC	C2B-C1B-NB	2.12	110.09	106.99
26	eM	1001	PEB	C2A-C3A-C4A	2.12	104.52	101.34
26	i2	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	v3	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	Y8	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	bh	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	cy	1001	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	cO	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	eq	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	ey	1002	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	fr	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	hT	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
29	Z5	304	PVN	O1-C1-N1	-2.12	122.79	125.93
26	bQ	202	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	g6	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	d7	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	aj	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	bg	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
27	W1	201	CYC	CAA-C2A-C3A	2.12	131.83	127.88
26	K7	202	PEB	CHC-C1D-ND	-2.12	111.48	113.95
26	G5	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	n7	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	i9	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	j9	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	x9	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	bx	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	bU	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	eO	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	hP	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	iB	1001	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	jO	1001	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	kT	1001	PEB	CMB-C2B-C1B	2.12	128.33	125.06
29	dx	405	PVN	C21-C2-C3	2.12	134.03	129.67
29	44	303	PVN	O1-C1-N1	-2.12	122.79	125.93
26	F5	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	x5	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	T6	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	h6	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	j9	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	t9	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	z9	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	aV	202	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dx	403	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	la	1002	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dQ	201	PEB	C2A-C3A-C4A	2.12	104.51	101.34
26	dk	1002	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	c9	302	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	P8	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	C9	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	dd	201	PEB	CMB-C2B-C1B	2.12	128.33	125.06
26	f5	201	PEB	CHC-C1D-ND	-2.12	111.49	113.95
26	w7	1002	PEB	CHC-C1D-ND	-2.12	111.49	113.95
26	I3	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	44	301	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	s6	202	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	v9	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	I9	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	ai	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	cX	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	y2	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	Z5	301	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	h8	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	fj	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	U4	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v4	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	s9	202	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	az	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	bs	1002	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	hY	401	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	X4	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	ag	201	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	aN	202	PEB	CMB-C2B-C1B	2.12	128.32	125.06
26	dW	202	PEB	CMB-C2B-C1B	2.12	128.32	125.06
27	c1	201	CYC	C2B-C1B-NB	2.12	110.08	106.99
27	v1	201	CYC	C2B-C1B-NB	2.12	110.08	106.99
26	aO	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	dp	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	eU	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	jL	1001	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	D7	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	m7	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	E9	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	z2	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	D2	302	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	b3	501	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	e3	1001	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	b4	1001	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	m6	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	lk	202	PEB	CHC-C1D-ND	-2.11	111.49	113.95
26	aX	402	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	cc	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	cE	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
29	b8	1004	PVN	C92-C91-C18	2.11	118.26	112.43
29	b9	405	PVN	C92-C91-C18	2.11	118.26	112.43
29	D2	303	PVN	C12-C11-N3	-2.11	106.98	110.05
26	b5	1001	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	W8	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	l9	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	bf	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	ep	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	ls	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	lz	401	PEB	CMB-C2B-C1B	2.11	128.32	125.06
27	a2	902	CYC	C2B-C1B-NB	2.11	110.08	106.99
27	b2	1001	CYC	C2B-C1B-NB	2.11	110.08	106.99
26	r3	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	p8	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	e7	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	A9	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	cK	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	dR	202	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	hF	201	PEB	CMB-C2B-C1B	2.11	128.32	125.06
26	M2	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	x6	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	M7	1002	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	cA	202	PEB	CHC-C1D-ND	-2.11	111.50	113.95
29	44	303	PVN	C10-C11-N3	-2.11	125.90	128.83
26	u7	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	a8	601	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	bw	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	dM	1002	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	ll	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	kW	1001	PEB	CMB-C2B-C1B	2.11	128.31	125.06
29	aY	403	PVN	C16-C15-C14	-2.11	122.92	128.08
26	a9	602	PEB	C2A-C3A-C4A	2.11	104.50	101.34
26	Z6	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	aM	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	cn	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	dV	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	V3	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	f8	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	t6	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	S6	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	R7	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	ch	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
29	ey	1004	PVN	C51-C52-C53	-2.11	107.85	113.76
26	u3	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	gg	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	L4	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	bm	1001	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	cx	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	eI	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	em	202	PEB	CMD-C2D-C3D	-2.11	127.09	130.06
26	cl	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	gm	1001	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	kS	1001	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	l3	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	S7	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	e7	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aU	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	go	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	eP	201	PEB	CHC-C1D-ND	-2.11	111.50	113.95
26	H4	201	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	z6	202	PEB	CMB-C2B-C1B	2.11	128.31	125.06
26	K9	1001	PEB	CMB-C2B-C1B	2.11	128.31	125.06
27	z1	201	CYC	C2B-C1B-NB	2.10	110.07	106.99
26	bj	201	PEB	CMB-C2B-C1B	2.10	128.31	125.06
26	bs	1001	PEB	CMB-C2B-C1B	2.10	128.31	125.06
26	bY	1001	PEB	CMB-C2B-C1B	2.10	128.31	125.06
26	cj	201	PEB	CMB-C2B-C1B	2.10	128.31	125.06
26	iF	1001	PEB	CMB-C2B-C1B	2.10	128.31	125.06
26	l5	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	k8	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	dC	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	gp	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	d7	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	d8	302	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	bB	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	kS	1002	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	j2	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	aK	1002	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	L2	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	X6	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
29	bZ	304	PVN	C15-C16-N4	-2.10	121.55	126.06
26	d6	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	f2	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	aj	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	dL	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	dN	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
29	aY	403	PVN	C92-C91-C18	2.10	118.22	112.43
26	V5	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	l9	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	bG	201	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	dH	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	gx	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	a7	202	PEB	CMB-C2B-C1B	2.10	128.30	125.06
26	o8	202	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	L7	201	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	lh	202	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	ga	202	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	kX	1002	PEB	CMB-C2B-C1B	2.10	128.29	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	ca	1001	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	dO	201	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	ak	201	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	F3	202	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	eZ	401	PEB	CMB-C2B-C1B	2.10	128.29	125.06
26	cv	202	PEB	CMD-C2D-C3D	-2.10	127.11	130.06
26	e4	202	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	B5	202	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	ar	201	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	ch	201	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	eU	201	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	bV	202	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	J3	201	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	fs	202	PEB	CMB-C2B-C1B	2.09	128.29	125.06
27	I1	201	CYC	C2A-C1A-NA	2.09	113.09	110.05
29	d9	304	PVN	C15-C16-C17	2.09	131.09	126.95
26	T2	202	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	ec	202	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	ek	1001	PEB	CMB-C2B-C1B	2.09	128.29	125.06
26	V2	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	E6	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	eq	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
27	X1	201	CYC	C2A-C1A-NA	2.09	113.09	110.05
26	D4	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	cq	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	di	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	kW	1002	PEB	CMB-C2B-C1B	2.09	128.28	125.06
29	Y5	1004	PVN	C41-C7-C8	2.09	128.88	124.94
26	N3	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	av	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	dT	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	z5	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	bQ	203	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	hB	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
29	bY	1004	PVN	C92-C91-C18	2.09	118.19	112.43
26	J5	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	dj	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	t3	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	e3	1002	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	em	202	PEB	CHC-C1D-ND	-2.09	111.52	113.95
26	cs	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	fu	201	PEB	CMB-C2B-C1B	2.09	128.28	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	v9	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	dQ	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	jM	1002	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	kQ	1002	PEB	CMB-C2B-C1B	2.09	128.28	125.06
27	V1	201	CYC	C2A-C1A-NA	2.09	113.08	110.05
27	n1	201	CYC	C2A-C1A-NA	2.09	113.08	110.05
26	w4	202	PEB	CMD-C2D-C3D	-2.09	127.12	130.06
26	cx	202	PEB	CMD-C2D-C3D	-2.09	127.12	130.06
26	p2	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	g4	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
26	n6	202	PEB	CMB-C2B-C1B	2.09	128.28	125.06
27	k1	201	CYC	C2A-C1A-NA	2.09	113.08	110.05
26	34	1001	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	N7	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	C8	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	af	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	cr	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	hL	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	X2	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	Z5	304	PVN	C10-C11-N3	-2.08	125.94	128.83
26	M7	1001	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	bE	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	bN	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	df	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	jI	1002	PEB	CMB-C2B-C1B	2.08	128.27	125.06
27	d1	1001	CYC	C2A-C1A-NA	2.08	113.08	110.05
26	g5	201	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	x7	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	er	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
27	R1	1001	CYC	C2A-C1A-NA	2.08	113.08	110.05
27	i1	1001	CYC	C2A-C1A-NA	2.08	113.08	110.05
26	R6	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	V7	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	lw	203	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	l4	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	D5	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	J9	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	dU	202	PEB	CMD-C2D-C3D	-2.08	127.13	130.06
26	j2	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	t5	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	Z7	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	ad	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	aD	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	cY	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	gn	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	L2	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	J5	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	S5	203	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	bH	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	ld	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	ln	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	hJ	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	h8	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
26	al	202	PEB	CMB-C2B-C1B	2.08	128.27	125.06
29	dw	404	PVN	C12-C11-N3	-2.08	107.03	110.05
26	F7	201	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	ar	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	cd	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	dT	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	eX	201	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	fc	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	fm	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	hS	202	PEB	CMD-C2D-C3D	-2.08	127.13	130.06
26	l2	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	A2	1003	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	Z2	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	v3	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	bP	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	cz	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	cE	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	dl	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	bO	202	PEB	CMD-C2D-C3D	-2.08	127.14	130.06
26	n3	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	v4	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	F5	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	v5	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	T7	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	ee	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	fy	201	PEB	CMB-C2B-C1B	2.08	128.26	125.06
29	hZ	403	PVN	C41-C7-C8	2.08	128.86	124.94
29	e8	303	PVN	C15-C16-C17	2.08	131.06	126.95
26	R3	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	j4	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
26	dh	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	U1	201	CYC	C2A-C1A-NA	2.08	113.07	110.05
27	d2	101	CYC	C2A-C1A-NA	2.08	113.07	110.05
26	fq	202	PEB	CMB-C2B-C1B	2.08	128.26	125.06
29	bZ	304	PVN	C51-C8-C7	-2.08	121.28	127.25
26	P2	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	u5	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	O7	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	n4	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
26	J6	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
29	D2	303	PVN	C61-C62-C63	-2.07	109.14	113.60
29	hY	404	PVN	C41-C7-C8	2.07	128.85	124.94
29	aZ	303	PVN	C51-C8-C7	-2.07	121.29	127.25
26	T3	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
26	az	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
26	fj	202	PEB	CMB-C2B-C1B	2.07	128.26	125.06
26	gz	302	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
27	G1	1001	CYC	C2A-C1A-NA	2.07	113.06	110.05
26	K3	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
27	b1	1001	CYC	C2A-C1A-NA	2.07	113.06	110.05
26	bJ	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	hR	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	l7	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	cb	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	fw	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	U5	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	bU	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	bL	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	ge	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	jL	1002	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	jN	1002	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	aq	202	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	gb	1002	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	B4	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	ei	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
27	y1	201	CYC	C2A-C1A-NA	2.07	113.06	110.05
26	t6	201	PEB	CMD-C2D-C3D	-2.07	127.14	130.06
26	ab	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	dX	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	hH	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
27	Z1	201	CYC	C2A-C1A-NA	2.07	113.06	110.05
26	O9	202	PEB	CMD-C2D-C3D	-2.07	127.15	130.06
29	e9	304	PVN	C16-C17-C18	-2.07	105.71	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P5	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	n5	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	aF	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	bF	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	cH	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	hT	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
27	q1	201	CYC	C2A-C1A-NA	2.07	113.06	110.05
26	cp	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	lf	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	lr	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	kR	1002	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	gy	302	PEB	CMD-C2D-C3D	-2.07	127.15	130.06
26	Z3	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	J7	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	an	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	eV	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
27	u1	1001	CYC	C2A-C1A-NA	2.07	113.06	110.05
26	H2	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	n8	201	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	ap	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	cL	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	eA	1002	PEB	CMD-C2D-C3D	-2.07	127.15	130.06
26	gj	202	PEB	CMD-C2D-C3D	-2.07	127.15	130.06
26	D3	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	L3	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	ff	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	fo	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	A1	301	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	B1	301	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	cJ	202	PEB	CMB-C2B-C1B	2.07	128.25	125.06
26	ea	203	PEB	CMB-C2B-C1B	2.07	128.25	125.06
29	d3	302	PVN	C61-C62-C63	-2.07	109.16	113.60
26	H3	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	W3	203	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	m5	1003	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	cF	201	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	I5	202	PEB	CMD-C2D-C3D	-2.06	127.15	130.06
26	p6	202	PEB	CMD-C2D-C3D	-2.06	127.15	130.06
27	O1	201	CYC	C2A-C1A-NA	2.06	113.05	110.05
27	g1	201	CYC	C2A-C1A-NA	2.06	113.05	110.05
26	X7	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	R9	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	lp	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	gd	201	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	hD	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	k7	1002	PEB	CMD-C2D-C3D	-2.06	127.15	130.06
26	hA	202	PEB	CMD-C2D-C3D	-2.06	127.15	130.06
26	gp	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	iD	1002	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	jJ	1002	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	jP	1002	PEB	CMB-C2B-C1B	2.06	128.24	125.06
27	K1	201	CYC	C1B-C2B-C3B	-2.06	105.72	107.87
26	j3	201	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	L5	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	eB	203	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	kU	1002	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	lw	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	et	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	eJ	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	lo	203	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	gt	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
29	d8	303	PVN	C15-C16-C17	2.06	131.03	126.95
27	n1	201	CYC	C1B-C2B-C3B	-2.06	105.72	107.87
26	U3	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	ld	201	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	lo	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	as	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	da	1002	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	ey	1001	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
27	G1	1001	CYC	CAC-C3C-C4C	-2.06	107.38	112.67
26	B3	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	p3	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	r5	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	co	201	PEB	CMB-C2B-C1B	2.06	128.24	125.06
27	o1	1001	CYC	C2A-C1A-NA	2.06	113.05	110.05
26	K7	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	dY	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	fg	201	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	iC	1002	PEB	CMB-C2B-C1B	2.06	128.24	125.06
27	K1	201	CYC	C2A-C1A-NA	2.06	113.05	110.05
26	cI	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	N7	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	R7	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
27	K1	201	CYC	CAC-C3C-C4C	-2.06	107.39	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t8	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	g7	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	r3	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
26	t7	202	PEB	CMB-C2B-C1B	2.06	128.24	125.06
27	b1	1001	CYC	CAC-C3C-C4C	-2.06	107.39	112.67
26	w5	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	dZ	1002	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	N5	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	p8	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	y7	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	B9	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
29	dw	404	PVN	C51-C52-C53	-2.06	107.99	113.76
26	z7	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	ax	201	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	dd	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
27	I1	201	CYC	CAC-C3C-C4C	-2.06	107.39	112.67
26	bC	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	lo	201	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
27	w1	201	CYC	C2A-C1A-NA	2.06	113.04	110.05
29	ez	1004	PVN	C52-C51-C8	-2.06	109.11	112.62
27	Q1	201	CYC	CAC-C3C-C4C	-2.06	107.39	112.67
26	p4	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	bT	201	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	i7	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	ct	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
29	34	1004	PVN	C41-C7-C8	2.06	128.82	124.94
26	cf	201	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	C3	1002	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	lt	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	fv	202	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	iF	1002	PEB	CMD-C2D-C3D	-2.06	127.16	130.06
26	h2	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	r7	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	F9	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	N9	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	P9	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	V9	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	cj	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
27	k1	201	CYC	CAC-C3C-C4C	-2.06	107.39	112.67
26	Z5	302	PEB	CMD-C2D-C3D	-2.06	127.17	130.06
26	z3	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06
26	cB	202	PEB	CMB-C2B-C1B	2.06	128.23	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A4	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	Q9	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	V3	202	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	H7	202	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	h7	201	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	s5	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	c8	301	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	cA	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	lc	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	hE	1002	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	li	203	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	G7	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	m7	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	gf	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	P3	202	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	h3	201	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	T9	202	PEB	CMB-C2B-C1B	2.05	128.23	125.06
26	ev	202	PEB	CMB-C2B-C1B	2.05	128.23	125.06
29	e9	304	PVN	C15-C16-C17	2.05	131.02	126.95
27	X1	201	CYC	CAC-C3C-C4C	-2.05	107.40	112.67
26	G5	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	fk	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	Y7	1003	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	f7	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	v7	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	hN	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	hV	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
27	d1	1001	CYC	C1B-C2B-C3B	-2.05	105.73	107.87
26	O5	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	gq	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	hM	1002	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	J3	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	n7	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	y8	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	eg	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	eL	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
27	f1	201	CYC	CAC-C3C-C4C	-2.05	107.40	112.67
27	u1	1001	CYC	C1B-C2B-C3B	-2.05	105.73	107.87
27	m1	201	CYC	CAC-C3C-C4C	-2.05	107.41	112.67
26	bI	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	cu	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	gg	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	jK	1002	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	jO	1002	PEB	CMB-C2B-C1B	2.05	128.22	125.06
27	P1	201	CYC	C1B-C2B-C3B	-2.05	105.73	107.87
26	R5	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	gi	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	gm	1002	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
27	o1	1001	CYC	CAC-C3C-C4C	-2.05	107.41	112.67
26	B6	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	c4	201	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	de	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	fn	1002	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
27	L1	201	CYC	C2A-C1A-NA	2.05	113.03	110.05
27	a1	201	CYC	C2A-C1A-NA	2.05	113.03	110.05
26	ll	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	V6	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	S3	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	j7	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
26	bA	202	PEB	CMD-C2D-C3D	-2.05	127.17	130.06
27	N1	201	CYC	CAC-C3C-C4C	-2.05	107.41	112.67
29	aZ	303	PVN	C15-C16-N4	-2.05	121.66	126.06
26	A5	203	PEB	CMB-C2B-C1B	2.05	128.22	125.06
27	s1	201	CYC	C2A-C1A-NA	2.05	113.03	110.05
26	Y7	1002	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	f7	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	lq	203	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	fh	1002	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
29	a3	1004	PVN	C71-C13-C12	2.05	131.68	126.12
28	bJ	203	PUB	CMA-C2A-C1A	2.05	126.21	121.39
26	s3	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	ev	201	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	iA	1002	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	iB	1002	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	el	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
29	dx	405	PVN	C5-C6-C7	2.05	133.83	130.34
27	P1	201	CYC	C2A-C1A-NA	2.05	113.03	110.05
27	w1	201	CYC	CAC-C3C-C4C	-2.05	107.42	112.67
26	R2	201	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	A3	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	C9	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	dJ	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	fe	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	x3	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	r4	201	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	L9	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	ah	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	bD	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	hP	202	PEB	CMB-C2B-C1B	2.05	128.22	125.06
26	iE	1002	PEB	CMB-C2B-C1B	2.05	128.22	125.06
27	a1	201	CYC	CAC-C3C-C4C	-2.05	107.42	112.67
26	A2	1001	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	n6	201	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	C7	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	P7	202	PEB	CMB-C2B-C1B	2.05	128.21	125.06
28	av	203	PUB	CMA-C2A-C1A	2.05	126.20	121.39
26	U2	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	m3	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	C5	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	q8	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	E9	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	I9	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
26	hW	202	PEB	CMD-C2D-C3D	-2.05	127.18	130.06
27	I1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
26	cA	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	hX	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
27	f1	201	CYC	C2A-C1A-NA	2.04	113.02	110.05
29	d3	302	PVN	C21-C2-C1	-2.04	116.59	121.39
26	N4	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
26	h4	201	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
26	cD	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
26	hQ	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
26	n2	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	gr	201	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	gv	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
27	Q1	201	CYC	C2A-C1A-NA	2.04	113.02	110.05
26	u7	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
26	gs	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
29	dw	404	PVN	C21-C2-C3	2.04	133.87	129.67
26	at	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	gk	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	kT	1002	PEB	CMB-C2B-C1B	2.04	128.21	125.06
27	P1	201	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
27	e1	201	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
26	hG	201	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	I3	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A5	202	PEB	CMD-C2D-C3D	-2.04	127.18	130.06
27	W1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
27	d1	1001	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
27	N1	201	CYC	C2A-C1A-NA	2.04	113.02	110.05
27	W1	201	CYC	C2A-C1A-NA	2.04	113.02	110.05
26	m5	1002	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	bG	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
27	U1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
27	d2	101	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
26	Q3	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	k3	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	bQ	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
27	L1	201	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
26	34	1002	PEB	CMB-C2B-C1B	2.04	128.21	125.06
27	U1	201	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
27	d2	101	CYC	CAC-C3C-C4C	-2.04	107.43	112.67
29	A2	1004	PVN	C71-C13-C12	2.04	131.66	126.12
26	lu	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	fr	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
27	q1	201	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
26	f3	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
26	H9	202	PEB	CMB-C2B-C1B	2.04	128.21	125.06
27	R1	1001	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
27	i1	1001	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
26	aw	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
27	y1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
27	W1	201	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
27	s1	201	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
26	s8	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	M9	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	ay	1002	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	cy	1002	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	dg	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	fx	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	D7	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
27	e1	201	CYC	C2A-C1A-NA	2.04	113.01	110.05
27	L1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
27	a1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
27	k1	201	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
26	eL	201	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	cl	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
27	m1	201	CYC	C2A-C1A-NA	2.04	113.01	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S5	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	o5	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	hU	201	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
27	O1	201	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
27	V1	201	CYC	CAC-C3C-C4C	-2.04	107.44	112.67
26	g3	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	E7	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	cC	1002	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	lm	1002	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	fg	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	hC	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	dU	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
26	U6	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	fb	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	eN	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
26	D9	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
26	en	202	PEB	CMB-C2B-C1B	2.04	128.20	125.06
26	c3	301	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	o8	201	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	dc	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	lg	201	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	ft	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	gc	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	hI	202	PEB	CMD-C2D-C3D	-2.04	127.19	130.06
26	E5	202	PEB	CMB-C2B-C1B	2.03	128.20	125.06
26	E2	1002	PEB	CMD-C2D-C3D	-2.03	127.19	130.06
26	hZ	401	PEB	CMD-C2D-C3D	-2.03	127.19	130.06
28	T7	203	PUB	CMA-C2A-C1A	2.03	126.18	121.39
27	y1	201	CYC	CAC-C3C-C4C	-2.03	107.45	112.67
26	c7	202	PEB	CMB-C2B-C1B	2.03	128.20	125.06
26	fi	202	PEB	CMB-C2B-C1B	2.03	128.20	125.06
26	cZ	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	e9	306	PUB	CMA-C2A-C1A	2.03	126.17	121.39
28	aY	405	PUB	CMA-C2A-C1A	2.03	126.17	121.39
26	I5	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	B7	201	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	Q5	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	c5	201	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	f6	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	Y9	301	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	bM	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	J3	203	PUB	CMA-C2A-C1A	2.03	126.17	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B7	202	PUB	CMA-C2A-C1A	2.03	126.17	121.39
29	D2	303	PVN	C21-C2-C1	-2.03	116.61	121.39
26	kV	1002	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	M3	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	C4	1002	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	Z9	1002	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	bK	1002	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	cG	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	ei	201	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	ls	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	fl	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
27	n1	201	CYC	CAC-C3C-C4C	-2.03	107.46	112.67
27	X1	201	CYC	C1B-C2B-C3B	-2.03	105.75	107.87
26	lj	201	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	f2	203	PUB	CMA-C2A-C1A	2.03	126.17	121.39
26	w4	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	G3	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	y5	1002	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	d6	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	db	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	hY	402	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	T8	304	PUB	CMA-C2A-C1A	2.03	126.17	121.39
27	m1	201	CYC	C1B-C2B-C3B	-2.03	105.75	107.87
26	K7	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
27	u1	1001	CYC	CAC-C3C-C4C	-2.03	107.46	112.67
26	O3	1002	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	o3	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	W7	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	aR	203	PUB	CMA-C2A-C1A	2.03	126.17	121.39
28	bZ	305	PUB	CMA-C2A-C1A	2.03	126.17	121.39
26	dJ	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
27	g1	201	CYC	CAC-C3C-C4C	-2.03	107.46	112.67
27	N1	201	CYC	C1B-C2B-C3B	-2.03	105.75	107.87
26	h5	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
27	Z1	201	CYC	CAC-C3C-C4C	-2.03	107.46	112.67
26	i3	203	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	f5	201	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	S7	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	h7	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	bS	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	F2	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	B5	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	J5	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	P5	202	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	ap	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
26	c4	201	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	fl	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
28	dR	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
27	f1	201	CYC	C1B-C2B-C3B	-2.03	105.75	107.87
26	u3	202	PEB	CMB-C2B-C1B	2.03	128.19	125.06
26	e3	1002	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	y3	202	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	et	201	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
26	eP	201	PEB	CMD-C2D-C3D	-2.03	127.20	130.06
28	34	1005	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	F7	202	PUB	CMA-C2A-C1A	2.03	126.16	121.39
27	Q1	201	CYC	C1B-C2B-C3B	-2.03	105.76	107.87
26	d3	301	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	w3	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	Q7	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	lg	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
28	V4	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	bY	1005	PUB	CMA-C2A-C1A	2.03	126.16	121.39
26	ao	202	PEB	CMB-C2B-C1B	2.03	128.18	125.06
26	i3	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	N6	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
28	x5	202	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	cs	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	eN	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
28	eX	202	PUB	CMA-C2A-C1A	2.03	126.16	121.39
26	c3	301	PEB	CMB-C2B-C1B	2.03	128.18	125.06
28	Z2	203	PUB	CMA-C2A-C1A	2.03	126.16	121.39
26	W3	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	Y3	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	cw	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
26	hF	202	PEB	CMD-C2D-C3D	-2.03	127.21	130.06
28	E8	203	PUB	CMA-C2A-C1A	2.02	126.16	121.39
28	bH	203	PUB	CMA-C2A-C1A	2.02	126.16	121.39
28	bL	203	PUB	CMA-C2A-C1A	2.02	126.16	121.39
28	ln	203	PUB	CMA-C2A-C1A	2.02	126.16	121.39
28	ff	203	PUB	CMA-C2A-C1A	2.02	126.16	121.39
28	fo	203	PUB	CMA-C2A-C1A	2.02	126.16	121.39
26	ec	201	PEB	CMD-C2D-C3D	-2.02	127.21	130.06
28	b9	407	PUB	CMA-C2A-C1A	2.02	126.15	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	gz	306	PUB	CMA-C2A-C1A	2.02	126.15	121.39
29	44	303	PVN	C92-C91-C18	2.02	118.01	112.43
26	gm	1002	PEB	CMB-C2B-C1B	2.02	128.18	125.06
28	d3	303	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	bo	202	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	P2	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	aJ	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
26	c5	201	PEB	CMB-C2B-C1B	2.02	128.18	125.06
29	Z5	304	PVN	C92-C91-C18	2.02	118.01	112.43
28	n4	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	dB	202	PUB	CMA-C2A-C1A	2.02	126.15	121.39
27	O1	201	CYC	C1B-C2B-C3B	-2.02	105.76	107.87
28	bR	202	PUB	CMA-C2A-C1A	2.02	126.15	121.39
26	e6	202	PEB	CMD-C2D-C3D	-2.02	127.21	130.06
26	bZ	302	PEB	CMD-C2D-C3D	-2.02	127.21	130.06
28	X4	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	l6	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	er	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	hH	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
26	M7	1003	PEB	CMB-C2B-C1B	2.02	128.18	125.06
26	cw	202	PEB	CMB-C2B-C1B	2.02	128.18	125.06
28	b8	1006	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	ge	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
26	A9	202	PEB	CMD-C2D-C3D	-2.02	127.21	130.06
26	go	202	PEB	CMD-C2D-C3D	-2.02	127.21	130.06
26	E9	202	PEB	CMB-C2B-C1B	2.02	128.18	125.06
28	U8	1005	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	az	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	c3	304	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	aT	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
28	hP	203	PUB	CMA-C2A-C1A	2.02	126.15	121.39
27	b1	1001	CYC	C1B-C2B-C3B	-2.02	105.76	107.87
26	d8	301	PEB	CMB-C2B-C1B	2.02	128.18	125.06
29	Z9	1004	PVN	C16-C15-C14	-2.02	123.14	128.08
28	R3	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	kV	1003	PUB	CMA-C2A-C1A	2.02	126.14	121.39
26	G6	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	o7	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	L7	202	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	G8	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	dw	405	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	iC	1003	PUB	CMA-C2A-C1A	2.02	126.14	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h5	202	PEB	CMB-C2B-C1B	2.02	128.17	125.06
26	o8	201	PEB	CMB-C2B-C1B	2.02	128.17	125.06
26	K5	1002	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	s7	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	hK	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	p3	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	ee	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	ly	406	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	lz	405	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	hL	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
27	R1	1001	CYC	C1B-C2B-C3B	-2.02	105.76	107.87
27	i1	1001	CYC	C1B-C2B-C3B	-2.02	105.76	107.87
28	h3	202	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	Y9	305	PUB	CMA-C2A-C1A	2.02	126.14	121.39
26	q5	202	PEB	CMB-C2B-C1B	2.02	128.17	125.06
26	s4	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	a6	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	u8	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	v9	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	F7	202	PUB	CBB-CAB-C3B	-2.02	109.18	112.62
26	H6	201	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	cK	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	le	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	gu	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	V2	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	V6	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	n7	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	eY	405	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	fs	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	gr	202	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	hZ	405	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	n3	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	c7	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	p9	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	eJ	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	gy	305	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	kX	1003	PUB	CMA-C2A-C1A	2.02	126.14	121.39
29	dw	404	PVN	O65-C63-C62	2.02	120.51	114.03
26	gs	202	PEB	CMB-C2B-C1B	2.02	128.17	125.06
26	N2	201	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	bn	202	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	cL	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	cN	202	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	eF	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
26	p5	201	PEB	CMB-C2B-C1B	2.02	128.17	125.06
28	A2	1006	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	R2	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	v4	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	A8	203	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	Z9	1005	PUB	CMA-C2A-C1A	2.02	126.14	121.39
26	E3	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	44	304	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	Z5	305	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	ey	1006	PUB	CMA-C2A-C1A	2.02	126.14	121.39
28	jK	1003	PUB	CMA-C2A-C1A	2.02	126.14	121.39
26	W3	202	PEB	CMB-C2B-C1B	2.02	128.17	125.06
26	q7	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	cm	1002	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	34	1006	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	V5	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	z5	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	J6	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	M8	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	R9	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	T9	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	ez	1005	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	eB	204	PUB	CMA-C2A-C1A	2.02	126.13	121.39
26	Z5	302	PEB	CMB-C2B-C1B	2.02	128.17	125.06
28	n2	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	V7	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	cE	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	dx	406	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	ep	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
26	q5	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
26	ao	202	PEB	CMD-C2D-C3D	-2.02	127.22	130.06
28	F3	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	Z6	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	a6	203	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	aZ	305	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	bY	1006	PUB	CMA-C2A-C1A	2.02	126.13	121.39
28	kQ	1003	PUB	CMA-C2A-C1A	2.02	126.13	121.39
26	A3	202	PEB	CMB-C2B-C1B	2.01	128.17	125.06
26	C3	1002	PEB	CMB-C2B-C1B	2.01	128.17	125.06
26	G6	202	PEB	CMB-C2B-C1B	2.01	128.17	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	dc	202	PEB	CMB-C2B-C1B	2.01	128.17	125.06
26	hU	201	PEB	CMB-C2B-C1B	2.01	128.17	125.06
26	hW	202	PEB	CMB-C2B-C1B	2.01	128.17	125.06
28	t3	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	p4	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	cH	202	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	lz	404	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	kW	1003	PUB	CMA-C2A-C1A	2.01	126.13	121.39
26	U7	202	PEB	CMD-C2D-C3D	-2.01	127.22	130.06
26	hO	202	PEB	CMD-C2D-C3D	-2.01	127.22	130.06
26	U3	202	PEB	CMB-C2B-C1B	2.01	128.17	125.06
26	I7	202	PEB	CMB-C2B-C1B	2.01	128.17	125.06
28	J2	202	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	j3	202	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	N4	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	N5	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	e8	304	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	fi	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
29	U8	1004	PVN	C16-C15-C14	-2.01	123.16	128.08
26	U9	202	PEB	CMD-C2D-C3D	-2.01	127.22	130.06
28	N2	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	V3	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	D5	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	cO	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	dh	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	dL	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	ld	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	fa	202	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	hN	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
26	eh	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	lw	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	D2	304	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	x6	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	z6	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	p7	202	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	aN	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
27	w1	201	CYC	C1B-C2B-C3B	-2.01	105.77	107.87
26	fz	301	PEB	CMD-C2D-C3D	-2.01	127.22	130.06
26	R2	201	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	T3	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	F6	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	p8	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	fc	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	Z5	306	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	c6	1004	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	cR	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	dj	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
28	dt	203	PUB	CMA-C2A-C1A	2.01	126.13	121.39
26	S2	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	K9	1002	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	eh	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	gh	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	N6	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	cx	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	fg	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	B9	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	bT	202	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	dV	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	jN	1003	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	bS	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	ey	1001	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	lh	201	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	fp	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
28	v3	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	dr	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	dT	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	en	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	lf	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	gi	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	R5	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	d8	304	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	n9	202	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	z9	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	eL	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	lv	202	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	iG	1002	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	bK	1002	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	bQ	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
29	dx	405	PVN	O65-C63-C62	2.01	120.49	114.03
26	u3	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	S9	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
28	h2	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	p2	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	N3	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	e8	305	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	dp	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	lh	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	ll	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	gv	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	iD	1003	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	iE	1003	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	lo	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	gb	1002	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	z2	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	L5	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	c9	305	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	bs	1004	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	ey	1005	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	bE	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
28	Q8	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	V9	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	cq	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	cY	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	et	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	gn	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	iF	1003	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	m5	1002	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	p7	201	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	de	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	C2	305	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	Y5	1006	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	r5	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	eY	404	PUB	CMA-C2A-C1A	2.01	126.12	121.39
27	G1	1001	CYC	C1B-C2B-C3B	-2.01	105.77	107.87
26	M9	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	Q9	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	bI	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	B3	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	C8	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	br	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	Y5	1002	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	M7	1003	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	bY	1002	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
28	D6	202	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	gg	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	U6	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Y5	1005	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	B6	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	N6	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	R6	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	aH	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	dN	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	eZ	403	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	lt	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
28	fm	203	PUB	CMA-C2A-C1A	2.01	126.12	121.39
26	E5	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	w7	1002	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	au	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	gw	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
28	H3	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	H4	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	di	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	lp	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	ly	405	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	hB	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	lw	201	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	fn	1002	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	gl	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
27	o1	1001	CYC	C1B-C2B-C3B	-2.01	105.78	107.87
27	q1	201	CYC	C1B-C2B-C3B	-2.01	105.78	107.87
26	a3	1002	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	A7	201	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
28	L6	202	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	H7	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	eZ	404	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	G5	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	fr	202	PEB	CMB-C2B-C1B	2.01	128.16	125.06
26	iB	1002	PEB	CMB-C2B-C1B	2.01	128.16	125.06
28	r2	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	L3	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	D4	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	t4	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	T5	202	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	b6	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	t6	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	Z7	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	D9	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	dF	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	ga	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	jJ	1003	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	jL	1003	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	jM	1003	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	r8	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
27	s1	201	CYC	C1B-C2B-C3B	-2.01	105.78	107.87
28	v2	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	l7	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	c8	305	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	F9	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	bD	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	o7	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
28	U8	1006	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	eR	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	fy	202	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	d8	301	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	G9	202	PEB	CMD-C2D-C3D	-2.01	127.23	130.06
26	s8	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
26	bG	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
26	fh	1002	PEB	CMB-C2B-C1B	2.01	128.15	125.06
26	hI	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
26	hS	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
28	f8	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	n8	202	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	fw	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	gx	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	hY	406	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	eY	401	PEB	CMD-C2D-C3D	-2.01	127.24	130.06
26	lh	201	PEB	CMD-C2D-C3D	-2.01	127.24	130.06
28	P4	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	T4	202	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	h8	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	P6	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	X7	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	y7	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	aY	404	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	cQ	202	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	dl	203	PUB	CMA-C2A-C1A	2.01	126.11	121.39
28	kS	1003	PUB	CMA-C2A-C1A	2.01	126.11	121.39
26	G3	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
26	V6	202	PEB	CMB-C2B-C1B	2.01	128.15	125.06
26	hZ	401	PEB	CMB-C2B-C1B	2.01	128.15	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	F4	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	T6	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	r6	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	D7	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	e9	305	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	Z9	1006	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	cP	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
27	V1	201	CYC	C1B-C2B-C3B	-2.00	105.78	107.87
26	H6	201	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	as	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	cv	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
28	f3	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	l3	202	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	z4	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	g8	202	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	y6	204	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	e7	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	O8	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	at	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	bP	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	cB	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	dx	407	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	dD	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	dP	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	p6	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	aZ	304	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	bp	202	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	dv	202	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	ei	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	lj	202	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	lx	201	PUB	CMA-C2A-C1A	2.00	126.11	121.39
26	d3	301	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	dZ	1002	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	hK	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
28	r3	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	B4	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	o8	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	a7	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	v7	203	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	cn	202	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	hZ	404	PUB	CMA-C2A-C1A	2.00	126.11	121.39
28	jI	1003	PUB	CMA-C2A-C1A	2.00	126.11	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A2	1004	PVN	C32-C31-C3	2.00	116.02	112.98
29	a3	1004	PVN	C32-C31-C3	2.00	116.02	112.98
26	o3	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	G7	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	eB	201	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	I7	202	PEB	CMD-C2D-C3D	-2.00	127.24	130.06
28	r4	202	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	x7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	cM	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	ec	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	eT	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
27	e1	201	CYC	C1B-C2B-C3B	-2.00	105.78	107.87
27	g1	201	CYC	C1B-C2B-C3B	-2.00	105.78	107.87
28	l2	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	P3	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	R4	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	d7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	c9	304	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	w8	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	aV	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	hT	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	jO	1003	PUB	CMA-C2A-C1A	2.00	126.10	121.39
26	Q3	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	aw	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	gc	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	gf	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
28	D2	305	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	D3	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	c3	305	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	fj	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	bD	203	PUB	CBB-CAB-C3B	-2.00	109.20	112.62
26	i7	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	lt	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
28	s7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	bq	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	cJ	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
26	lw	201	PEB	CMD-C2D-C3D	-2.00	127.24	130.06
26	gl	202	PEB	CMD-C2D-C3D	-2.00	127.24	130.06
28	bN	203	PUB	CBB-CAB-C3B	-2.00	109.20	112.62
28	N7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	aP	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	cp	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	dH	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	jP	1003	PUB	CMA-C2A-C1A	2.00	126.10	121.39
26	k3	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	C5	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
26	s7	202	PEB	CMB-C2B-C1B	2.00	128.15	125.06
28	bY	1005	PUB	CBB-CAB-C3B	-2.00	109.20	112.62
28	T2	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	X2	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	x3	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	R7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	r7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	L9	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	eH	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	hX	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
26	lq	203	PEB	CMB-C2B-C1B	2.00	128.15	125.06
28	A2	1005	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	d3	304	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	x4	202	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	H6	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	t7	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	I8	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	N9	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	gk	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	gt	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	hG	202	PUB	CMA-C2A-C1A	2.00	126.10	121.39
26	M5	202	PEB	CMD-C2D-C3D	-2.00	127.24	130.06
28	b8	1005	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	cz	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	cF	202	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	dn	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	hR	203	PUB	CMA-C2A-C1A	2.00	126.10	121.39
28	kT	1003	PUB	CMA-C2A-C1A	2.00	126.10	121.39
26	M3	202	PEB	CMB-C2B-C1B	2.00	128.14	125.06
26	s4	202	PEB	CMB-C2B-C1B	2.00	128.14	125.06
26	lk	202	PEB	CMB-C2B-C1B	2.00	128.14	125.06

All (36) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A2	1004	PVN	C4
29	C2	303	PVN	C4
29	D2	303	PVN	C4

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Mol	Chain	Res	Type	Atom
29	a3	1004	PVN	C4
29	c3	303	PVN	C4
29	d3	302	PVN	C4
29	34	1004	PVN	C4
29	44	303	PVN	C4
29	Y5	1004	PVN	C4
29	Z5	304	PVN	C4
29	b8	1004	PVN	C4
29	c8	303	PVN	C4
29	d8	303	PVN	C4
29	e8	303	PVN	C4
29	b9	405	PVN	C4
29	c9	303	PVN	C4
29	d9	304	PVN	C4
29	e9	304	PVN	C4
29	T8	303	PVN	C4
29	U8	1004	PVN	C4
29	Y9	303	PVN	C4
29	Z9	1004	PVN	C4
29	aY	403	PVN	C4
29	aZ	303	PVN	C4
29	bY	1004	PVN	C4
29	bZ	304	PVN	C4
29	dw	404	PVN	C4
29	dx	405	PVN	C4
29	ey	1004	PVN	C4
29	ez	1004	PVN	C4
29	eY	403	PVN	C4
29	eZ	402	PVN	C4
29	ly	404	PVN	C4
29	lz	403	PVN	C4
29	hY	404	PVN	C4
29	hZ	403	PVN	C4

All (16017) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A1	301	PEB	C1C-C2C-CAC-CBC
26	A1	301	PEB	C3C-C2C-CAC-CBC
26	A1	301	PEB	NB-C1B-CHA-C4A
26	A1	301	PEB	C2B-C1B-CHA-C4A
26	B1	301	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	B1	301	PEB	C3C-C2C-CAC-CBC
26	B1	301	PEB	NB-C1B-CHA-C4A
26	B1	301	PEB	C2B-C1B-CHA-C4A
26	e2	201	PEB	NA-C4A-CHA-C1B
26	e2	201	PEB	C3A-C4A-CHA-C1B
26	e2	201	PEB	NB-C1B-CHA-C4A
26	e2	201	PEB	C2B-C1B-CHA-C4A
26	e2	202	PEB	NA-C4A-CHA-C1B
26	e2	202	PEB	C3A-C4A-CHA-C1B
26	e2	202	PEB	NB-C1B-CHA-C4A
26	e2	202	PEB	C2B-C1B-CHA-C4A
26	f2	201	PEB	NA-C4A-CHA-C1B
26	f2	201	PEB	C3A-C4A-CHA-C1B
26	f2	201	PEB	NB-C1B-CHA-C4A
26	f2	201	PEB	C2B-C1B-CHA-C4A
26	f2	202	PEB	C1C-C2C-CAC-CBC
26	f2	202	PEB	C3C-C2C-CAC-CBC
26	f2	202	PEB	NB-C1B-CHA-C4A
26	f2	202	PEB	C2B-C1B-CHA-C4A
26	g2	201	PEB	NA-C4A-CHA-C1B
26	g2	201	PEB	C3A-C4A-CHA-C1B
26	g2	201	PEB	NB-C1B-CHA-C4A
26	g2	201	PEB	C2B-C1B-CHA-C4A
26	g2	202	PEB	NA-C4A-CHA-C1B
26	g2	202	PEB	C3A-C4A-CHA-C1B
26	g2	202	PEB	NB-C1B-CHA-C4A
26	g2	202	PEB	C2B-C1B-CHA-C4A
26	h2	201	PEB	NA-C4A-CHA-C1B
26	h2	201	PEB	C3A-C4A-CHA-C1B
26	h2	201	PEB	NB-C1B-CHA-C4A
26	h2	201	PEB	C2B-C1B-CHA-C4A
26	h2	202	PEB	C1C-C2C-CAC-CBC
26	h2	202	PEB	C3C-C2C-CAC-CBC
26	h2	202	PEB	NB-C1B-CHA-C4A
26	h2	202	PEB	C2B-C1B-CHA-C4A
26	i2	201	PEB	NA-C4A-CHA-C1B
26	i2	201	PEB	C3A-C4A-CHA-C1B
26	i2	201	PEB	NB-C1B-CHA-C4A
26	i2	201	PEB	C2B-C1B-CHA-C4A
26	i2	202	PEB	NA-C4A-CHA-C1B
26	i2	202	PEB	C3A-C4A-CHA-C1B
26	i2	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	i2	202	PEB	C2B-C1B-CHA-C4A
26	j2	201	PEB	NA-C4A-CHA-C1B
26	j2	201	PEB	C3A-C4A-CHA-C1B
26	j2	201	PEB	NB-C1B-CHA-C4A
26	j2	201	PEB	C2B-C1B-CHA-C4A
26	j2	202	PEB	C1C-C2C-CAC-CBC
26	j2	202	PEB	C3C-C2C-CAC-CBC
26	j2	202	PEB	NB-C1B-CHA-C4A
26	j2	202	PEB	C2B-C1B-CHA-C4A
26	k2	201	PEB	NA-C4A-CHA-C1B
26	k2	201	PEB	C3A-C4A-CHA-C1B
26	k2	201	PEB	NB-C1B-CHA-C4A
26	k2	201	PEB	C2B-C1B-CHA-C4A
26	k2	202	PEB	NA-C4A-CHA-C1B
26	k2	202	PEB	C3A-C4A-CHA-C1B
26	k2	202	PEB	NB-C1B-CHA-C4A
26	k2	202	PEB	C2B-C1B-CHA-C4A
26	l2	201	PEB	NA-C4A-CHA-C1B
26	l2	201	PEB	C3A-C4A-CHA-C1B
26	l2	201	PEB	NB-C1B-CHA-C4A
26	l2	201	PEB	C2B-C1B-CHA-C4A
26	l2	202	PEB	C1C-C2C-CAC-CBC
26	l2	202	PEB	C3C-C2C-CAC-CBC
26	l2	202	PEB	NB-C1B-CHA-C4A
26	l2	202	PEB	C2B-C1B-CHA-C4A
26	m2	201	PEB	NA-C4A-CHA-C1B
26	m2	201	PEB	C3A-C4A-CHA-C1B
26	m2	201	PEB	NB-C1B-CHA-C4A
26	m2	201	PEB	C2B-C1B-CHA-C4A
26	m2	202	PEB	NA-C4A-CHA-C1B
26	m2	202	PEB	C3A-C4A-CHA-C1B
26	m2	202	PEB	NB-C1B-CHA-C4A
26	m2	202	PEB	C2B-C1B-CHA-C4A
26	n2	201	PEB	NA-C4A-CHA-C1B
26	n2	201	PEB	C3A-C4A-CHA-C1B
26	n2	201	PEB	NB-C1B-CHA-C4A
26	n2	201	PEB	C2B-C1B-CHA-C4A
26	n2	202	PEB	C1C-C2C-CAC-CBC
26	n2	202	PEB	C3C-C2C-CAC-CBC
26	n2	202	PEB	NB-C1B-CHA-C4A
26	n2	202	PEB	C2B-C1B-CHA-C4A
26	o2	1001	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	o2	1001	PEB	C3A-C4A-CHA-C1B
26	o2	1001	PEB	NB-C1B-CHA-C4A
26	o2	1001	PEB	C2B-C1B-CHA-C4A
26	o2	1002	PEB	NA-C4A-CHA-C1B
26	o2	1002	PEB	C3A-C4A-CHA-C1B
26	o2	1002	PEB	NB-C1B-CHA-C4A
26	o2	1002	PEB	C2B-C1B-CHA-C4A
26	p2	201	PEB	NA-C4A-CHA-C1B
26	p2	201	PEB	C3A-C4A-CHA-C1B
26	p2	201	PEB	NB-C1B-CHA-C4A
26	p2	201	PEB	C2B-C1B-CHA-C4A
26	p2	202	PEB	C1C-C2C-CAC-CBC
26	p2	202	PEB	C3C-C2C-CAC-CBC
26	p2	202	PEB	NB-C1B-CHA-C4A
26	p2	202	PEB	C2B-C1B-CHA-C4A
26	q2	201	PEB	NA-C4A-CHA-C1B
26	q2	201	PEB	C3A-C4A-CHA-C1B
26	q2	201	PEB	NB-C1B-CHA-C4A
26	q2	201	PEB	C2B-C1B-CHA-C4A
26	q2	202	PEB	NA-C4A-CHA-C1B
26	q2	202	PEB	C3A-C4A-CHA-C1B
26	q2	202	PEB	NB-C1B-CHA-C4A
26	q2	202	PEB	C2B-C1B-CHA-C4A
26	r2	201	PEB	NA-C4A-CHA-C1B
26	r2	201	PEB	C3A-C4A-CHA-C1B
26	r2	201	PEB	NB-C1B-CHA-C4A
26	r2	201	PEB	C2B-C1B-CHA-C4A
26	r2	202	PEB	NA-C4A-CHA-C1B
26	r2	202	PEB	C3A-C4A-CHA-C1B
26	r2	202	PEB	NB-C1B-CHA-C4A
26	r2	202	PEB	C2B-C1B-CHA-C4A
26	s2	201	PEB	NA-C4A-CHA-C1B
26	s2	201	PEB	C3A-C4A-CHA-C1B
26	s2	201	PEB	NB-C1B-CHA-C4A
26	s2	201	PEB	C2B-C1B-CHA-C4A
26	s2	202	PEB	NA-C4A-CHA-C1B
26	s2	202	PEB	C3A-C4A-CHA-C1B
26	s2	202	PEB	NB-C1B-CHA-C4A
26	s2	202	PEB	C2B-C1B-CHA-C4A
26	t2	201	PEB	NA-C4A-CHA-C1B
26	t2	201	PEB	C3A-C4A-CHA-C1B
26	t2	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	t2	201	PEB	C2B-C1B-CHA-C4A
26	t2	202	PEB	NA-C4A-CHA-C1B
26	t2	202	PEB	C3A-C4A-CHA-C1B
26	t2	202	PEB	NB-C1B-CHA-C4A
26	t2	202	PEB	C2B-C1B-CHA-C4A
26	u2	201	PEB	NA-C4A-CHA-C1B
26	u2	201	PEB	C3A-C4A-CHA-C1B
26	u2	201	PEB	NB-C1B-CHA-C4A
26	u2	201	PEB	C2B-C1B-CHA-C4A
26	u2	202	PEB	NA-C4A-CHA-C1B
26	u2	202	PEB	C3A-C4A-CHA-C1B
26	u2	202	PEB	NB-C1B-CHA-C4A
26	u2	202	PEB	C2B-C1B-CHA-C4A
26	v2	201	PEB	NA-C4A-CHA-C1B
26	v2	201	PEB	C3A-C4A-CHA-C1B
26	v2	201	PEB	NB-C1B-CHA-C4A
26	v2	201	PEB	C2B-C1B-CHA-C4A
26	v2	202	PEB	NA-C4A-CHA-C1B
26	v2	202	PEB	C3A-C4A-CHA-C1B
26	v2	202	PEB	NB-C1B-CHA-C4A
26	v2	202	PEB	C2B-C1B-CHA-C4A
26	w2	201	PEB	NA-C4A-CHA-C1B
26	w2	201	PEB	C3A-C4A-CHA-C1B
26	w2	201	PEB	NB-C1B-CHA-C4A
26	w2	201	PEB	C2B-C1B-CHA-C4A
26	w2	202	PEB	NA-C4A-CHA-C1B
26	w2	202	PEB	C3A-C4A-CHA-C1B
26	w2	202	PEB	NB-C1B-CHA-C4A
26	w2	202	PEB	C2B-C1B-CHA-C4A
26	w2	203	PEB	NA-C4A-CHA-C1B
26	w2	203	PEB	C3A-C4A-CHA-C1B
26	w2	203	PEB	NB-C1B-CHA-C4A
26	w2	203	PEB	C2B-C1B-CHA-C4A
26	x2	201	PEB	NA-C4A-CHA-C1B
26	x2	201	PEB	C3A-C4A-CHA-C1B
26	x2	201	PEB	NB-C1B-CHA-C4A
26	x2	201	PEB	C2B-C1B-CHA-C4A
26	y2	201	PEB	NA-C4A-CHA-C1B
26	y2	201	PEB	C3A-C4A-CHA-C1B
26	y2	201	PEB	NB-C1B-CHA-C4A
26	y2	201	PEB	C2B-C1B-CHA-C4A
26	y2	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	y2	202	PEB	C3A-C4A-CHA-C1B
26	y2	202	PEB	NB-C1B-CHA-C4A
26	y2	202	PEB	C2B-C1B-CHA-C4A
26	z2	201	PEB	NA-C4A-CHA-C1B
26	z2	201	PEB	C3A-C4A-CHA-C1B
26	z2	201	PEB	NB-C1B-CHA-C4A
26	z2	201	PEB	C2B-C1B-CHA-C4A
26	z2	202	PEB	NA-C4A-CHA-C1B
26	z2	202	PEB	C3A-C4A-CHA-C1B
26	z2	202	PEB	NB-C1B-CHA-C4A
26	z2	202	PEB	C2B-C1B-CHA-C4A
26	A2	1001	PEB	NB-C1B-CHA-C4A
26	A2	1001	PEB	C2B-C1B-CHA-C4A
26	A2	1002	PEB	NA-C4A-CHA-C1B
26	A2	1002	PEB	C3A-C4A-CHA-C1B
26	A2	1002	PEB	NB-C1B-CHA-C4A
26	A2	1002	PEB	C2B-C1B-CHA-C4A
26	A2	1003	PEB	C1C-C2C-CAC-CBC
26	A2	1003	PEB	C3C-C2C-CAC-CBC
26	A2	1003	PEB	NB-C1B-CHA-C4A
26	A2	1003	PEB	C2B-C1B-CHA-C4A
26	B2	501	PEB	NA-C4A-CHA-C1B
26	B2	501	PEB	C3A-C4A-CHA-C1B
26	B2	501	PEB	NB-C1B-CHA-C4A
26	B2	501	PEB	C2B-C1B-CHA-C4A
26	B2	502	PEB	NA-C4A-CHA-C1B
26	B2	502	PEB	C3A-C4A-CHA-C1B
26	B2	502	PEB	NB-C1B-CHA-C4A
26	B2	502	PEB	C2B-C1B-CHA-C4A
26	C2	301	PEB	NA-C4A-CHA-C1B
26	C2	301	PEB	C3A-C4A-CHA-C1B
26	C2	301	PEB	NB-C1B-CHA-C4A
26	C2	301	PEB	C2B-C1B-CHA-C4A
26	C2	302	PEB	NA-C4A-CHA-C1B
26	C2	302	PEB	C3A-C4A-CHA-C1B
26	C2	302	PEB	NB-C1B-CHA-C4A
26	C2	302	PEB	C2B-C1B-CHA-C4A
26	D2	301	PEB	NA-C4A-CHA-C1B
26	D2	301	PEB	C3A-C4A-CHA-C1B
26	D2	301	PEB	NB-C1B-CHA-C4A
26	D2	301	PEB	C2B-C1B-CHA-C4A
26	D2	302	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	D2	302	PEB	C3A-C4A-CHA-C1B
26	D2	302	PEB	NB-C1B-CHA-C4A
26	D2	302	PEB	C2B-C1B-CHA-C4A
26	E2	1001	PEB	NA-C4A-CHA-C1B
26	E2	1001	PEB	C3A-C4A-CHA-C1B
26	E2	1001	PEB	NB-C1B-CHA-C4A
26	E2	1001	PEB	C2B-C1B-CHA-C4A
26	E2	1002	PEB	NB-C1B-CHA-C4A
26	E2	1002	PEB	C2B-C1B-CHA-C4A
26	F2	201	PEB	NA-C4A-CHA-C1B
26	F2	201	PEB	C3A-C4A-CHA-C1B
26	F2	201	PEB	NB-C1B-CHA-C4A
26	F2	201	PEB	C2B-C1B-CHA-C4A
26	F2	202	PEB	NA-C4A-CHA-C1B
26	F2	202	PEB	C3A-C4A-CHA-C1B
26	F2	202	PEB	NB-C1B-CHA-C4A
26	F2	202	PEB	C2B-C1B-CHA-C4A
26	G2	201	PEB	NA-C4A-CHA-C1B
26	G2	201	PEB	C3A-C4A-CHA-C1B
26	G2	201	PEB	NB-C1B-CHA-C4A
26	G2	201	PEB	C2B-C1B-CHA-C4A
26	G2	202	PEB	NA-C4A-CHA-C1B
26	G2	202	PEB	C3A-C4A-CHA-C1B
26	G2	202	PEB	NB-C1B-CHA-C4A
26	G2	202	PEB	C2B-C1B-CHA-C4A
26	H2	201	PEB	C1C-C2C-CAC-CBC
26	H2	201	PEB	C3C-C2C-CAC-CBC
26	H2	201	PEB	NB-C1B-CHA-C4A
26	H2	201	PEB	C2B-C1B-CHA-C4A
26	I2	201	PEB	NA-C4A-CHA-C1B
26	I2	201	PEB	C3A-C4A-CHA-C1B
26	I2	201	PEB	NB-C1B-CHA-C4A
26	I2	201	PEB	C2B-C1B-CHA-C4A
26	I2	202	PEB	NA-C4A-CHA-C1B
26	I2	202	PEB	C3A-C4A-CHA-C1B
26	I2	202	PEB	NB-C1B-CHA-C4A
26	I2	202	PEB	C2B-C1B-CHA-C4A
26	J2	201	PEB	NA-C4A-CHA-C1B
26	J2	201	PEB	C3A-C4A-CHA-C1B
26	J2	201	PEB	NB-C1B-CHA-C4A
26	J2	201	PEB	C2B-C1B-CHA-C4A
26	K2	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	K2	201	PEB	C3A-C4A-CHA-C1B
26	K2	201	PEB	NB-C1B-CHA-C4A
26	K2	201	PEB	C2B-C1B-CHA-C4A
26	K2	202	PEB	NA-C4A-CHA-C1B
26	K2	202	PEB	C3A-C4A-CHA-C1B
26	K2	202	PEB	NB-C1B-CHA-C4A
26	K2	202	PEB	C2B-C1B-CHA-C4A
26	L2	201	PEB	NA-C4A-CHA-C1B
26	L2	201	PEB	C3A-C4A-CHA-C1B
26	L2	201	PEB	NB-C1B-CHA-C4A
26	L2	201	PEB	C2B-C1B-CHA-C4A
26	L2	202	PEB	C1C-C2C-CAC-CBC
26	L2	202	PEB	C3C-C2C-CAC-CBC
26	L2	202	PEB	NB-C1B-CHA-C4A
26	L2	202	PEB	C2B-C1B-CHA-C4A
26	M2	201	PEB	NA-C4A-CHA-C1B
26	M2	201	PEB	C3A-C4A-CHA-C1B
26	M2	201	PEB	NB-C1B-CHA-C4A
26	M2	201	PEB	C2B-C1B-CHA-C4A
26	M2	202	PEB	NA-C4A-CHA-C1B
26	M2	202	PEB	C3A-C4A-CHA-C1B
26	M2	202	PEB	NB-C1B-CHA-C4A
26	M2	202	PEB	C2B-C1B-CHA-C4A
26	N2	201	PEB	NB-C1B-CHA-C4A
26	N2	201	PEB	C2B-C1B-CHA-C4A
26	N2	202	PEB	NA-C4A-CHA-C1B
26	N2	202	PEB	C3A-C4A-CHA-C1B
26	N2	202	PEB	NB-C1B-CHA-C4A
26	N2	202	PEB	C2B-C1B-CHA-C4A
26	O2	201	PEB	NA-C4A-CHA-C1B
26	O2	201	PEB	C3A-C4A-CHA-C1B
26	O2	201	PEB	NB-C1B-CHA-C4A
26	O2	201	PEB	C2B-C1B-CHA-C4A
26	O2	202	PEB	NA-C4A-CHA-C1B
26	O2	202	PEB	C3A-C4A-CHA-C1B
26	O2	202	PEB	NB-C1B-CHA-C4A
26	O2	202	PEB	C2B-C1B-CHA-C4A
26	P2	201	PEB	NA-C4A-CHA-C1B
26	P2	201	PEB	C3A-C4A-CHA-C1B
26	P2	201	PEB	NB-C1B-CHA-C4A
26	P2	201	PEB	C2B-C1B-CHA-C4A
26	P2	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	P2	202	PEB	C2B-C1B-CHA-C4A
26	Q2	1001	PEB	NA-C4A-CHA-C1B
26	Q2	1001	PEB	C3A-C4A-CHA-C1B
26	Q2	1001	PEB	NB-C1B-CHA-C4A
26	Q2	1001	PEB	C2B-C1B-CHA-C4A
26	R2	201	PEB	NB-C1B-CHA-C4A
26	R2	201	PEB	C2B-C1B-CHA-C4A
26	R2	202	PEB	NA-C4A-CHA-C1B
26	R2	202	PEB	C3A-C4A-CHA-C1B
26	R2	202	PEB	NB-C1B-CHA-C4A
26	R2	202	PEB	C2B-C1B-CHA-C4A
26	S2	201	PEB	NA-C4A-CHA-C1B
26	S2	201	PEB	C3A-C4A-CHA-C1B
26	S2	201	PEB	NB-C1B-CHA-C4A
26	S2	201	PEB	C2B-C1B-CHA-C4A
26	S2	202	PEB	NB-C1B-CHA-C4A
26	S2	202	PEB	C2B-C1B-CHA-C4A
26	T2	201	PEB	NA-C4A-CHA-C1B
26	T2	201	PEB	C3A-C4A-CHA-C1B
26	T2	201	PEB	NB-C1B-CHA-C4A
26	T2	201	PEB	C2B-C1B-CHA-C4A
26	T2	202	PEB	C1C-C2C-CAC-CBC
26	T2	202	PEB	C3C-C2C-CAC-CBC
26	T2	202	PEB	NB-C1B-CHA-C4A
26	T2	202	PEB	C2B-C1B-CHA-C4A
26	U2	201	PEB	NA-C4A-CHA-C1B
26	U2	201	PEB	C3A-C4A-CHA-C1B
26	U2	201	PEB	NB-C1B-CHA-C4A
26	U2	201	PEB	C2B-C1B-CHA-C4A
26	U2	202	PEB	NB-C1B-CHA-C4A
26	U2	202	PEB	C2B-C1B-CHA-C4A
26	V2	201	PEB	NA-C4A-CHA-C1B
26	V2	201	PEB	C3A-C4A-CHA-C1B
26	V2	201	PEB	NB-C1B-CHA-C4A
26	V2	201	PEB	C2B-C1B-CHA-C4A
26	V2	202	PEB	C1C-C2C-CAC-CBC
26	V2	202	PEB	C3C-C2C-CAC-CBC
26	V2	202	PEB	NB-C1B-CHA-C4A
26	V2	202	PEB	C2B-C1B-CHA-C4A
26	W2	201	PEB	NA-C4A-CHA-C1B
26	W2	201	PEB	C3A-C4A-CHA-C1B
26	W2	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	W2	201	PEB	C2B-C1B-CHA-C4A
26	W2	202	PEB	NA-C4A-CHA-C1B
26	W2	202	PEB	C3A-C4A-CHA-C1B
26	W2	202	PEB	NB-C1B-CHA-C4A
26	W2	202	PEB	C2B-C1B-CHA-C4A
26	X2	201	PEB	NA-C4A-CHA-C1B
26	X2	201	PEB	C3A-C4A-CHA-C1B
26	X2	201	PEB	NB-C1B-CHA-C4A
26	X2	201	PEB	C2B-C1B-CHA-C4A
26	X2	202	PEB	C1C-C2C-CAC-CBC
26	X2	202	PEB	C3C-C2C-CAC-CBC
26	X2	202	PEB	NB-C1B-CHA-C4A
26	X2	202	PEB	C2B-C1B-CHA-C4A
26	Y2	201	PEB	NA-C4A-CHA-C1B
26	Y2	201	PEB	C3A-C4A-CHA-C1B
26	Y2	201	PEB	NB-C1B-CHA-C4A
26	Y2	201	PEB	C2B-C1B-CHA-C4A
26	Y2	202	PEB	NA-C4A-CHA-C1B
26	Y2	202	PEB	C3A-C4A-CHA-C1B
26	Y2	202	PEB	NB-C1B-CHA-C4A
26	Y2	202	PEB	C2B-C1B-CHA-C4A
26	Z2	201	PEB	NA-C4A-CHA-C1B
26	Z2	201	PEB	C3A-C4A-CHA-C1B
26	Z2	201	PEB	NB-C1B-CHA-C4A
26	Z2	201	PEB	C2B-C1B-CHA-C4A
26	Z2	202	PEB	C1C-C2C-CAC-CBC
26	Z2	202	PEB	C3C-C2C-CAC-CBC
26	Z2	202	PEB	NB-C1B-CHA-C4A
26	Z2	202	PEB	C2B-C1B-CHA-C4A
26	A3	201	PEB	NA-C4A-CHA-C1B
26	A3	201	PEB	C3A-C4A-CHA-C1B
26	A3	201	PEB	NB-C1B-CHA-C4A
26	A3	201	PEB	C2B-C1B-CHA-C4A
26	A3	202	PEB	NB-C1B-CHA-C4A
26	A3	202	PEB	C2B-C1B-CHA-C4A
26	B3	201	PEB	NA-C4A-CHA-C1B
26	B3	201	PEB	C3A-C4A-CHA-C1B
26	B3	201	PEB	NB-C1B-CHA-C4A
26	B3	201	PEB	C2B-C1B-CHA-C4A
26	B3	202	PEB	C1C-C2C-CAC-CBC
26	B3	202	PEB	C3C-C2C-CAC-CBC
26	B3	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	B3	202	PEB	C2B-C1B-CHA-C4A
26	C3	1001	PEB	NA-C4A-CHA-C1B
26	C3	1001	PEB	C3A-C4A-CHA-C1B
26	C3	1001	PEB	NB-C1B-CHA-C4A
26	C3	1001	PEB	C2B-C1B-CHA-C4A
26	C3	1002	PEB	NB-C1B-CHA-C4A
26	C3	1002	PEB	C2B-C1B-CHA-C4A
26	D3	201	PEB	NA-C4A-CHA-C1B
26	D3	201	PEB	C3A-C4A-CHA-C1B
26	D3	201	PEB	NB-C1B-CHA-C4A
26	D3	201	PEB	C2B-C1B-CHA-C4A
26	D3	202	PEB	C1C-C2C-CAC-CBC
26	D3	202	PEB	C3C-C2C-CAC-CBC
26	D3	202	PEB	NB-C1B-CHA-C4A
26	D3	202	PEB	C2B-C1B-CHA-C4A
26	E3	201	PEB	NA-C4A-CHA-C1B
26	E3	201	PEB	C3A-C4A-CHA-C1B
26	E3	201	PEB	NB-C1B-CHA-C4A
26	E3	201	PEB	C2B-C1B-CHA-C4A
26	E3	202	PEB	NB-C1B-CHA-C4A
26	E3	202	PEB	C2B-C1B-CHA-C4A
26	F3	201	PEB	NA-C4A-CHA-C1B
26	F3	201	PEB	C3A-C4A-CHA-C1B
26	F3	201	PEB	NB-C1B-CHA-C4A
26	F3	201	PEB	C2B-C1B-CHA-C4A
26	F3	202	PEB	C1C-C2C-CAC-CBC
26	F3	202	PEB	C3C-C2C-CAC-CBC
26	F3	202	PEB	NB-C1B-CHA-C4A
26	F3	202	PEB	C2B-C1B-CHA-C4A
26	G3	201	PEB	NA-C4A-CHA-C1B
26	G3	201	PEB	C3A-C4A-CHA-C1B
26	G3	201	PEB	NB-C1B-CHA-C4A
26	G3	201	PEB	C2B-C1B-CHA-C4A
26	G3	202	PEB	NB-C1B-CHA-C4A
26	G3	202	PEB	C2B-C1B-CHA-C4A
26	H3	201	PEB	NA-C4A-CHA-C1B
26	H3	201	PEB	C3A-C4A-CHA-C1B
26	H3	201	PEB	NB-C1B-CHA-C4A
26	H3	201	PEB	C2B-C1B-CHA-C4A
26	H3	202	PEB	C1C-C2C-CAC-CBC
26	H3	202	PEB	C3C-C2C-CAC-CBC
26	H3	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	H3	202	PEB	C2B-C1B-CHA-C4A
26	I3	201	PEB	NA-C4A-CHA-C1B
26	I3	201	PEB	C3A-C4A-CHA-C1B
26	I3	201	PEB	NB-C1B-CHA-C4A
26	I3	201	PEB	C2B-C1B-CHA-C4A
26	I3	202	PEB	NB-C1B-CHA-C4A
26	I3	202	PEB	C2B-C1B-CHA-C4A
26	J3	201	PEB	NA-C4A-CHA-C1B
26	J3	201	PEB	C3A-C4A-CHA-C1B
26	J3	201	PEB	NB-C1B-CHA-C4A
26	J3	201	PEB	C2B-C1B-CHA-C4A
26	J3	202	PEB	C1C-C2C-CAC-CBC
26	J3	202	PEB	C3C-C2C-CAC-CBC
26	J3	202	PEB	NB-C1B-CHA-C4A
26	J3	202	PEB	C2B-C1B-CHA-C4A
26	K3	201	PEB	NA-C4A-CHA-C1B
26	K3	201	PEB	C3A-C4A-CHA-C1B
26	K3	201	PEB	NB-C1B-CHA-C4A
26	K3	201	PEB	C2B-C1B-CHA-C4A
26	K3	202	PEB	NB-C1B-CHA-C4A
26	K3	202	PEB	C2B-C1B-CHA-C4A
26	L3	201	PEB	NA-C4A-CHA-C1B
26	L3	201	PEB	C3A-C4A-CHA-C1B
26	L3	201	PEB	NB-C1B-CHA-C4A
26	L3	201	PEB	C2B-C1B-CHA-C4A
26	L3	202	PEB	C1C-C2C-CAC-CBC
26	L3	202	PEB	C3C-C2C-CAC-CBC
26	L3	202	PEB	NB-C1B-CHA-C4A
26	L3	202	PEB	C2B-C1B-CHA-C4A
26	M3	201	PEB	NA-C4A-CHA-C1B
26	M3	201	PEB	C3A-C4A-CHA-C1B
26	M3	201	PEB	NB-C1B-CHA-C4A
26	M3	201	PEB	C2B-C1B-CHA-C4A
26	M3	202	PEB	NB-C1B-CHA-C4A
26	M3	202	PEB	C2B-C1B-CHA-C4A
26	N3	201	PEB	NA-C4A-CHA-C1B
26	N3	201	PEB	C3A-C4A-CHA-C1B
26	N3	201	PEB	NB-C1B-CHA-C4A
26	N3	201	PEB	C2B-C1B-CHA-C4A
26	N3	202	PEB	C1C-C2C-CAC-CBC
26	N3	202	PEB	C3C-C2C-CAC-CBC
26	N3	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	N3	202	PEB	C2B-C1B-CHA-C4A
26	O3	1001	PEB	NA-C4A-CHA-C1B
26	O3	1001	PEB	C3A-C4A-CHA-C1B
26	O3	1001	PEB	NB-C1B-CHA-C4A
26	O3	1001	PEB	C2B-C1B-CHA-C4A
26	O3	1002	PEB	NB-C1B-CHA-C4A
26	O3	1002	PEB	C2B-C1B-CHA-C4A
26	P3	201	PEB	NA-C4A-CHA-C1B
26	P3	201	PEB	C3A-C4A-CHA-C1B
26	P3	201	PEB	NB-C1B-CHA-C4A
26	P3	201	PEB	C2B-C1B-CHA-C4A
26	P3	202	PEB	C1C-C2C-CAC-CBC
26	P3	202	PEB	C3C-C2C-CAC-CBC
26	P3	202	PEB	NB-C1B-CHA-C4A
26	P3	202	PEB	C2B-C1B-CHA-C4A
26	Q3	201	PEB	NA-C4A-CHA-C1B
26	Q3	201	PEB	C3A-C4A-CHA-C1B
26	Q3	201	PEB	NB-C1B-CHA-C4A
26	Q3	201	PEB	C2B-C1B-CHA-C4A
26	Q3	202	PEB	NB-C1B-CHA-C4A
26	Q3	202	PEB	C2B-C1B-CHA-C4A
26	R3	201	PEB	NA-C4A-CHA-C1B
26	R3	201	PEB	C3A-C4A-CHA-C1B
26	R3	201	PEB	NB-C1B-CHA-C4A
26	R3	201	PEB	C2B-C1B-CHA-C4A
26	R3	202	PEB	C1C-C2C-CAC-CBC
26	R3	202	PEB	C3C-C2C-CAC-CBC
26	R3	202	PEB	NB-C1B-CHA-C4A
26	R3	202	PEB	C2B-C1B-CHA-C4A
26	S3	201	PEB	NA-C4A-CHA-C1B
26	S3	201	PEB	C3A-C4A-CHA-C1B
26	S3	201	PEB	NB-C1B-CHA-C4A
26	S3	201	PEB	C2B-C1B-CHA-C4A
26	S3	202	PEB	NB-C1B-CHA-C4A
26	S3	202	PEB	C2B-C1B-CHA-C4A
26	S3	203	PEB	NA-C4A-CHA-C1B
26	S3	203	PEB	C3A-C4A-CHA-C1B
26	S3	203	PEB	NB-C1B-CHA-C4A
26	S3	203	PEB	C2B-C1B-CHA-C4A
26	T3	201	PEB	NA-C4A-CHA-C1B
26	T3	201	PEB	C3A-C4A-CHA-C1B
26	T3	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	T3	201	PEB	C2B-C1B-CHA-C4A
26	T3	202	PEB	C1C-C2C-CAC-CBC
26	T3	202	PEB	C3C-C2C-CAC-CBC
26	T3	202	PEB	NB-C1B-CHA-C4A
26	T3	202	PEB	C2B-C1B-CHA-C4A
26	U3	201	PEB	NA-C4A-CHA-C1B
26	U3	201	PEB	C3A-C4A-CHA-C1B
26	U3	201	PEB	NB-C1B-CHA-C4A
26	U3	201	PEB	C2B-C1B-CHA-C4A
26	U3	202	PEB	NB-C1B-CHA-C4A
26	U3	202	PEB	C2B-C1B-CHA-C4A
26	V3	201	PEB	NA-C4A-CHA-C1B
26	V3	201	PEB	C3A-C4A-CHA-C1B
26	V3	201	PEB	NB-C1B-CHA-C4A
26	V3	201	PEB	C2B-C1B-CHA-C4A
26	V3	202	PEB	C1C-C2C-CAC-CBC
26	V3	202	PEB	C3C-C2C-CAC-CBC
26	V3	202	PEB	NB-C1B-CHA-C4A
26	V3	202	PEB	C2B-C1B-CHA-C4A
26	W3	201	PEB	NA-C4A-CHA-C1B
26	W3	201	PEB	C3A-C4A-CHA-C1B
26	W3	201	PEB	NB-C1B-CHA-C4A
26	W3	201	PEB	C2B-C1B-CHA-C4A
26	W3	202	PEB	NB-C1B-CHA-C4A
26	W3	202	PEB	C2B-C1B-CHA-C4A
26	W3	203	PEB	C1C-C2C-CAC-CBC
26	W3	203	PEB	C3C-C2C-CAC-CBC
26	W3	203	PEB	NB-C1B-CHA-C4A
26	W3	203	PEB	C2B-C1B-CHA-C4A
26	X3	201	PEB	NA-C4A-CHA-C1B
26	X3	201	PEB	C3A-C4A-CHA-C1B
26	X3	201	PEB	NB-C1B-CHA-C4A
26	X3	201	PEB	C2B-C1B-CHA-C4A
26	Y3	201	PEB	NA-C4A-CHA-C1B
26	Y3	201	PEB	C3A-C4A-CHA-C1B
26	Y3	201	PEB	NB-C1B-CHA-C4A
26	Y3	201	PEB	C2B-C1B-CHA-C4A
26	Y3	202	PEB	NB-C1B-CHA-C4A
26	Y3	202	PEB	C2B-C1B-CHA-C4A
26	Z3	201	PEB	NA-C4A-CHA-C1B
26	Z3	201	PEB	C3A-C4A-CHA-C1B
26	Z3	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	Z3	201	PEB	C2B-C1B-CHA-C4A
26	Z3	202	PEB	C1C-C2C-CAC-CBC
26	Z3	202	PEB	C3C-C2C-CAC-CBC
26	Z3	202	PEB	NB-C1B-CHA-C4A
26	Z3	202	PEB	C2B-C1B-CHA-C4A
26	a3	1001	PEB	NA-C4A-CHA-C1B
26	a3	1001	PEB	C3A-C4A-CHA-C1B
26	a3	1001	PEB	NB-C1B-CHA-C4A
26	a3	1001	PEB	C2B-C1B-CHA-C4A
26	a3	1002	PEB	NB-C1B-CHA-C4A
26	a3	1002	PEB	C2B-C1B-CHA-C4A
26	a3	1003	PEB	NA-C4A-CHA-C1B
26	a3	1003	PEB	C3A-C4A-CHA-C1B
26	a3	1003	PEB	NB-C1B-CHA-C4A
26	a3	1003	PEB	C2B-C1B-CHA-C4A
26	b3	501	PEB	NA-C4A-CHA-C1B
26	b3	501	PEB	C3A-C4A-CHA-C1B
26	b3	501	PEB	NB-C1B-CHA-C4A
26	b3	501	PEB	C2B-C1B-CHA-C4A
26	b3	502	PEB	NA-C4A-CHA-C1B
26	b3	502	PEB	C3A-C4A-CHA-C1B
26	b3	502	PEB	NB-C1B-CHA-C4A
26	b3	502	PEB	C2B-C1B-CHA-C4A
26	c3	301	PEB	NB-C1B-CHA-C4A
26	c3	301	PEB	C2B-C1B-CHA-C4A
26	c3	302	PEB	NA-C4A-CHA-C1B
26	c3	302	PEB	C3A-C4A-CHA-C1B
26	c3	302	PEB	NB-C1B-CHA-C4A
26	c3	302	PEB	C2B-C1B-CHA-C4A
26	d3	301	PEB	NB-C1B-CHA-C4A
26	d3	301	PEB	C2B-C1B-CHA-C4A
26	e3	1001	PEB	NA-C4A-CHA-C1B
26	e3	1001	PEB	C3A-C4A-CHA-C1B
26	e3	1001	PEB	NB-C1B-CHA-C4A
26	e3	1001	PEB	C2B-C1B-CHA-C4A
26	e3	1002	PEB	NB-C1B-CHA-C4A
26	e3	1002	PEB	C2B-C1B-CHA-C4A
26	f3	201	PEB	NA-C4A-CHA-C1B
26	f3	201	PEB	C3A-C4A-CHA-C1B
26	f3	201	PEB	NB-C1B-CHA-C4A
26	f3	201	PEB	C2B-C1B-CHA-C4A
26	f3	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	f3	202	PEB	C3C-C2C-CAC-CBC
26	f3	202	PEB	NB-C1B-CHA-C4A
26	f3	202	PEB	C2B-C1B-CHA-C4A
26	g3	201	PEB	NA-C4A-CHA-C1B
26	g3	201	PEB	C3A-C4A-CHA-C1B
26	g3	201	PEB	NB-C1B-CHA-C4A
26	g3	201	PEB	C2B-C1B-CHA-C4A
26	g3	202	PEB	NB-C1B-CHA-C4A
26	g3	202	PEB	C2B-C1B-CHA-C4A
26	h3	201	PEB	C1C-C2C-CAC-CBC
26	h3	201	PEB	C3C-C2C-CAC-CBC
26	h3	201	PEB	NB-C1B-CHA-C4A
26	h3	201	PEB	C2B-C1B-CHA-C4A
26	i3	201	PEB	NA-C4A-CHA-C1B
26	i3	201	PEB	C3A-C4A-CHA-C1B
26	i3	201	PEB	NB-C1B-CHA-C4A
26	i3	201	PEB	C2B-C1B-CHA-C4A
26	i3	202	PEB	NB-C1B-CHA-C4A
26	i3	202	PEB	C2B-C1B-CHA-C4A
26	i3	203	PEB	C1C-C2C-CAC-CBC
26	i3	203	PEB	C3C-C2C-CAC-CBC
26	i3	203	PEB	NB-C1B-CHA-C4A
26	i3	203	PEB	C2B-C1B-CHA-C4A
26	j3	201	PEB	C1C-C2C-CAC-CBC
26	j3	201	PEB	C3C-C2C-CAC-CBC
26	j3	201	PEB	NB-C1B-CHA-C4A
26	j3	201	PEB	C2B-C1B-CHA-C4A
26	k3	201	PEB	NA-C4A-CHA-C1B
26	k3	201	PEB	C3A-C4A-CHA-C1B
26	k3	201	PEB	NB-C1B-CHA-C4A
26	k3	201	PEB	C2B-C1B-CHA-C4A
26	k3	202	PEB	NB-C1B-CHA-C4A
26	k3	202	PEB	C2B-C1B-CHA-C4A
26	l3	201	PEB	NA-C4A-CHA-C1B
26	l3	201	PEB	C3A-C4A-CHA-C1B
26	l3	201	PEB	NB-C1B-CHA-C4A
26	l3	201	PEB	C2B-C1B-CHA-C4A
26	m3	201	PEB	NA-C4A-CHA-C1B
26	m3	201	PEB	C3A-C4A-CHA-C1B
26	m3	201	PEB	NB-C1B-CHA-C4A
26	m3	201	PEB	C2B-C1B-CHA-C4A
26	m3	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	m3	202	PEB	C2B-C1B-CHA-C4A
26	n3	201	PEB	NA-C4A-CHA-C1B
26	n3	201	PEB	C3A-C4A-CHA-C1B
26	n3	201	PEB	NB-C1B-CHA-C4A
26	n3	201	PEB	C2B-C1B-CHA-C4A
26	n3	202	PEB	C1C-C2C-CAC-CBC
26	n3	202	PEB	C3C-C2C-CAC-CBC
26	n3	202	PEB	NB-C1B-CHA-C4A
26	n3	202	PEB	C2B-C1B-CHA-C4A
26	o3	201	PEB	NA-C4A-CHA-C1B
26	o3	201	PEB	C3A-C4A-CHA-C1B
26	o3	201	PEB	NB-C1B-CHA-C4A
26	o3	201	PEB	C2B-C1B-CHA-C4A
26	o3	202	PEB	NB-C1B-CHA-C4A
26	o3	202	PEB	C2B-C1B-CHA-C4A
26	p3	201	PEB	NA-C4A-CHA-C1B
26	p3	201	PEB	C3A-C4A-CHA-C1B
26	p3	201	PEB	NB-C1B-CHA-C4A
26	p3	201	PEB	C2B-C1B-CHA-C4A
26	p3	202	PEB	C1C-C2C-CAC-CBC
26	p3	202	PEB	C3C-C2C-CAC-CBC
26	p3	202	PEB	NB-C1B-CHA-C4A
26	p3	202	PEB	C2B-C1B-CHA-C4A
26	q3	1001	PEB	NA-C4A-CHA-C1B
26	q3	1001	PEB	C3A-C4A-CHA-C1B
26	q3	1001	PEB	NB-C1B-CHA-C4A
26	q3	1001	PEB	C2B-C1B-CHA-C4A
26	r3	201	PEB	NA-C4A-CHA-C1B
26	r3	201	PEB	C3A-C4A-CHA-C1B
26	r3	201	PEB	NB-C1B-CHA-C4A
26	r3	201	PEB	C2B-C1B-CHA-C4A
26	r3	202	PEB	C1C-C2C-CAC-CBC
26	r3	202	PEB	C3C-C2C-CAC-CBC
26	r3	202	PEB	NB-C1B-CHA-C4A
26	r3	202	PEB	C2B-C1B-CHA-C4A
26	s3	201	PEB	NA-C4A-CHA-C1B
26	s3	201	PEB	C3A-C4A-CHA-C1B
26	s3	201	PEB	NB-C1B-CHA-C4A
26	s3	201	PEB	C2B-C1B-CHA-C4A
26	s3	202	PEB	NB-C1B-CHA-C4A
26	s3	202	PEB	C2B-C1B-CHA-C4A
26	t3	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	t3	201	PEB	C3A-C4A-CHA-C1B
26	t3	201	PEB	NB-C1B-CHA-C4A
26	t3	201	PEB	C2B-C1B-CHA-C4A
26	t3	202	PEB	C1C-C2C-CAC-CBC
26	t3	202	PEB	C3C-C2C-CAC-CBC
26	t3	202	PEB	NB-C1B-CHA-C4A
26	t3	202	PEB	C2B-C1B-CHA-C4A
26	u3	201	PEB	NA-C4A-CHA-C1B
26	u3	201	PEB	C3A-C4A-CHA-C1B
26	u3	201	PEB	NB-C1B-CHA-C4A
26	u3	201	PEB	C2B-C1B-CHA-C4A
26	u3	202	PEB	NB-C1B-CHA-C4A
26	u3	202	PEB	C2B-C1B-CHA-C4A
26	v3	201	PEB	NA-C4A-CHA-C1B
26	v3	201	PEB	C3A-C4A-CHA-C1B
26	v3	201	PEB	NB-C1B-CHA-C4A
26	v3	201	PEB	C2B-C1B-CHA-C4A
26	v3	202	PEB	C1C-C2C-CAC-CBC
26	v3	202	PEB	C3C-C2C-CAC-CBC
26	v3	202	PEB	NB-C1B-CHA-C4A
26	v3	202	PEB	C2B-C1B-CHA-C4A
26	w3	201	PEB	NA-C4A-CHA-C1B
26	w3	201	PEB	C3A-C4A-CHA-C1B
26	w3	201	PEB	NB-C1B-CHA-C4A
26	w3	201	PEB	C2B-C1B-CHA-C4A
26	w3	202	PEB	NB-C1B-CHA-C4A
26	w3	202	PEB	C2B-C1B-CHA-C4A
26	x3	201	PEB	NA-C4A-CHA-C1B
26	x3	201	PEB	C3A-C4A-CHA-C1B
26	x3	201	PEB	NB-C1B-CHA-C4A
26	x3	201	PEB	C2B-C1B-CHA-C4A
26	x3	202	PEB	C1C-C2C-CAC-CBC
26	x3	202	PEB	C3C-C2C-CAC-CBC
26	x3	202	PEB	NB-C1B-CHA-C4A
26	x3	202	PEB	C2B-C1B-CHA-C4A
26	y3	201	PEB	NA-C4A-CHA-C1B
26	y3	201	PEB	C3A-C4A-CHA-C1B
26	y3	201	PEB	NB-C1B-CHA-C4A
26	y3	201	PEB	C2B-C1B-CHA-C4A
26	y3	202	PEB	NB-C1B-CHA-C4A
26	y3	202	PEB	C2B-C1B-CHA-C4A
26	z3	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	z3	201	PEB	C3A-C4A-CHA-C1B
26	z3	201	PEB	NB-C1B-CHA-C4A
26	z3	201	PEB	C2B-C1B-CHA-C4A
26	z3	202	PEB	C1C-C2C-CAC-CBC
26	z3	202	PEB	C3C-C2C-CAC-CBC
26	z3	202	PEB	NB-C1B-CHA-C4A
26	z3	202	PEB	C2B-C1B-CHA-C4A
26	A4	201	PEB	NA-C4A-CHA-C1B
26	A4	201	PEB	C3A-C4A-CHA-C1B
26	A4	201	PEB	NB-C1B-CHA-C4A
26	A4	201	PEB	C2B-C1B-CHA-C4A
26	A4	202	PEB	NB-C1B-CHA-C4A
26	A4	202	PEB	C2B-C1B-CHA-C4A
26	B4	201	PEB	NA-C4A-CHA-C1B
26	B4	201	PEB	C3A-C4A-CHA-C1B
26	B4	201	PEB	NB-C1B-CHA-C4A
26	B4	201	PEB	C2B-C1B-CHA-C4A
26	B4	202	PEB	C1C-C2C-CAC-CBC
26	B4	202	PEB	C3C-C2C-CAC-CBC
26	B4	202	PEB	NB-C1B-CHA-C4A
26	B4	202	PEB	C2B-C1B-CHA-C4A
26	C4	1001	PEB	NA-C4A-CHA-C1B
26	C4	1001	PEB	C3A-C4A-CHA-C1B
26	C4	1001	PEB	NB-C1B-CHA-C4A
26	C4	1001	PEB	C2B-C1B-CHA-C4A
26	C4	1002	PEB	NB-C1B-CHA-C4A
26	C4	1002	PEB	C2B-C1B-CHA-C4A
26	D4	201	PEB	NA-C4A-CHA-C1B
26	D4	201	PEB	C3A-C4A-CHA-C1B
26	D4	201	PEB	NB-C1B-CHA-C4A
26	D4	201	PEB	C2B-C1B-CHA-C4A
26	D4	202	PEB	C1C-C2C-CAC-CBC
26	D4	202	PEB	C3C-C2C-CAC-CBC
26	D4	202	PEB	NB-C1B-CHA-C4A
26	D4	202	PEB	C2B-C1B-CHA-C4A
26	E4	201	PEB	NA-C4A-CHA-C1B
26	E4	201	PEB	C3A-C4A-CHA-C1B
26	E4	201	PEB	NB-C1B-CHA-C4A
26	E4	201	PEB	C2B-C1B-CHA-C4A
26	E4	202	PEB	NA-C4A-CHA-C1B
26	E4	202	PEB	C3A-C4A-CHA-C1B
26	E4	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	E4	202	PEB	C2B-C1B-CHA-C4A
26	F4	201	PEB	NA-C4A-CHA-C1B
26	F4	201	PEB	C3A-C4A-CHA-C1B
26	F4	201	PEB	NB-C1B-CHA-C4A
26	F4	201	PEB	C2B-C1B-CHA-C4A
26	F4	202	PEB	NA-C4A-CHA-C1B
26	F4	202	PEB	C3A-C4A-CHA-C1B
26	F4	202	PEB	NB-C1B-CHA-C4A
26	F4	202	PEB	C2B-C1B-CHA-C4A
26	G4	201	PEB	NA-C4A-CHA-C1B
26	G4	201	PEB	C3A-C4A-CHA-C1B
26	G4	201	PEB	NB-C1B-CHA-C4A
26	G4	201	PEB	C2B-C1B-CHA-C4A
26	G4	202	PEB	NA-C4A-CHA-C1B
26	G4	202	PEB	C3A-C4A-CHA-C1B
26	G4	202	PEB	NB-C1B-CHA-C4A
26	G4	202	PEB	C2B-C1B-CHA-C4A
26	H4	201	PEB	NA-C4A-CHA-C1B
26	H4	201	PEB	C3A-C4A-CHA-C1B
26	H4	201	PEB	NB-C1B-CHA-C4A
26	H4	201	PEB	C2B-C1B-CHA-C4A
26	H4	202	PEB	NA-C4A-CHA-C1B
26	H4	202	PEB	C3A-C4A-CHA-C1B
26	H4	202	PEB	NB-C1B-CHA-C4A
26	H4	202	PEB	C2B-C1B-CHA-C4A
26	I4	201	PEB	NA-C4A-CHA-C1B
26	I4	201	PEB	C3A-C4A-CHA-C1B
26	I4	201	PEB	NB-C1B-CHA-C4A
26	I4	201	PEB	C2B-C1B-CHA-C4A
26	I4	202	PEB	NA-C4A-CHA-C1B
26	I4	202	PEB	C3A-C4A-CHA-C1B
26	I4	202	PEB	NB-C1B-CHA-C4A
26	I4	202	PEB	C2B-C1B-CHA-C4A
26	J4	201	PEB	NA-C4A-CHA-C1B
26	J4	201	PEB	C3A-C4A-CHA-C1B
26	J4	201	PEB	NB-C1B-CHA-C4A
26	J4	201	PEB	C2B-C1B-CHA-C4A
26	J4	202	PEB	NA-C4A-CHA-C1B
26	J4	202	PEB	C3A-C4A-CHA-C1B
26	J4	202	PEB	NB-C1B-CHA-C4A
26	J4	202	PEB	C2B-C1B-CHA-C4A
26	K4	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	K4	201	PEB	C3A-C4A-CHA-C1B
26	K4	201	PEB	NB-C1B-CHA-C4A
26	K4	201	PEB	C2B-C1B-CHA-C4A
26	K4	202	PEB	NA-C4A-CHA-C1B
26	K4	202	PEB	C3A-C4A-CHA-C1B
26	K4	202	PEB	NB-C1B-CHA-C4A
26	K4	202	PEB	C2B-C1B-CHA-C4A
26	L4	201	PEB	NA-C4A-CHA-C1B
26	L4	201	PEB	C3A-C4A-CHA-C1B
26	L4	201	PEB	NB-C1B-CHA-C4A
26	L4	201	PEB	C2B-C1B-CHA-C4A
26	L4	202	PEB	NA-C4A-CHA-C1B
26	L4	202	PEB	C3A-C4A-CHA-C1B
26	L4	202	PEB	NB-C1B-CHA-C4A
26	L4	202	PEB	C2B-C1B-CHA-C4A
26	M4	201	PEB	NA-C4A-CHA-C1B
26	M4	201	PEB	C3A-C4A-CHA-C1B
26	M4	201	PEB	NB-C1B-CHA-C4A
26	M4	201	PEB	C2B-C1B-CHA-C4A
26	M4	202	PEB	NA-C4A-CHA-C1B
26	M4	202	PEB	C3A-C4A-CHA-C1B
26	M4	202	PEB	NB-C1B-CHA-C4A
26	M4	202	PEB	C2B-C1B-CHA-C4A
26	N4	201	PEB	NA-C4A-CHA-C1B
26	N4	201	PEB	C3A-C4A-CHA-C1B
26	N4	201	PEB	NB-C1B-CHA-C4A
26	N4	201	PEB	C2B-C1B-CHA-C4A
26	N4	202	PEB	NB-C1B-CHA-C4A
26	N4	202	PEB	C2B-C1B-CHA-C4A
26	O4	1001	PEB	NA-C4A-CHA-C1B
26	O4	1001	PEB	C3A-C4A-CHA-C1B
26	O4	1001	PEB	NB-C1B-CHA-C4A
26	O4	1001	PEB	C2B-C1B-CHA-C4A
26	O4	1002	PEB	NA-C4A-CHA-C1B
26	O4	1002	PEB	C3A-C4A-CHA-C1B
26	O4	1002	PEB	NB-C1B-CHA-C4A
26	O4	1002	PEB	C2B-C1B-CHA-C4A
26	P4	201	PEB	NA-C4A-CHA-C1B
26	P4	201	PEB	C3A-C4A-CHA-C1B
26	P4	201	PEB	NB-C1B-CHA-C4A
26	P4	201	PEB	C2B-C1B-CHA-C4A
26	P4	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	P4	202	PEB	C3A-C4A-CHA-C1B
26	P4	202	PEB	NB-C1B-CHA-C4A
26	P4	202	PEB	C2B-C1B-CHA-C4A
26	Q4	201	PEB	NA-C4A-CHA-C1B
26	Q4	201	PEB	C3A-C4A-CHA-C1B
26	Q4	201	PEB	NB-C1B-CHA-C4A
26	Q4	201	PEB	C2B-C1B-CHA-C4A
26	Q4	202	PEB	NA-C4A-CHA-C1B
26	Q4	202	PEB	C3A-C4A-CHA-C1B
26	Q4	202	PEB	NB-C1B-CHA-C4A
26	Q4	202	PEB	C2B-C1B-CHA-C4A
26	Q4	203	PEB	NA-C4A-CHA-C1B
26	Q4	203	PEB	C3A-C4A-CHA-C1B
26	Q4	203	PEB	NB-C1B-CHA-C4A
26	Q4	203	PEB	C2B-C1B-CHA-C4A
26	R4	201	PEB	NA-C4A-CHA-C1B
26	R4	201	PEB	C3A-C4A-CHA-C1B
26	R4	201	PEB	NB-C1B-CHA-C4A
26	R4	201	PEB	C2B-C1B-CHA-C4A
26	R4	202	PEB	NA-C4A-CHA-C1B
26	R4	202	PEB	C3A-C4A-CHA-C1B
26	R4	202	PEB	NB-C1B-CHA-C4A
26	R4	202	PEB	C2B-C1B-CHA-C4A
26	S4	201	PEB	NA-C4A-CHA-C1B
26	S4	201	PEB	C3A-C4A-CHA-C1B
26	S4	201	PEB	NB-C1B-CHA-C4A
26	S4	201	PEB	C2B-C1B-CHA-C4A
26	S4	202	PEB	NA-C4A-CHA-C1B
26	S4	202	PEB	C3A-C4A-CHA-C1B
26	S4	202	PEB	NB-C1B-CHA-C4A
26	S4	202	PEB	C2B-C1B-CHA-C4A
26	T4	201	PEB	NA-C4A-CHA-C1B
26	T4	201	PEB	C3A-C4A-CHA-C1B
26	T4	201	PEB	NB-C1B-CHA-C4A
26	T4	201	PEB	C2B-C1B-CHA-C4A
26	U4	201	PEB	NA-C4A-CHA-C1B
26	U4	201	PEB	C3A-C4A-CHA-C1B
26	U4	201	PEB	NB-C1B-CHA-C4A
26	U4	201	PEB	C2B-C1B-CHA-C4A
26	U4	202	PEB	NA-C4A-CHA-C1B
26	U4	202	PEB	C3A-C4A-CHA-C1B
26	U4	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	U4	202	PEB	C2B-C1B-CHA-C4A
26	V4	201	PEB	NA-C4A-CHA-C1B
26	V4	201	PEB	C3A-C4A-CHA-C1B
26	V4	201	PEB	NB-C1B-CHA-C4A
26	V4	201	PEB	C2B-C1B-CHA-C4A
26	V4	202	PEB	NA-C4A-CHA-C1B
26	V4	202	PEB	C3A-C4A-CHA-C1B
26	V4	202	PEB	NB-C1B-CHA-C4A
26	V4	202	PEB	C2B-C1B-CHA-C4A
26	W4	201	PEB	NA-C4A-CHA-C1B
26	W4	201	PEB	C3A-C4A-CHA-C1B
26	W4	201	PEB	NB-C1B-CHA-C4A
26	W4	201	PEB	C2B-C1B-CHA-C4A
26	W4	202	PEB	NA-C4A-CHA-C1B
26	W4	202	PEB	C3A-C4A-CHA-C1B
26	W4	202	PEB	NB-C1B-CHA-C4A
26	W4	202	PEB	C2B-C1B-CHA-C4A
26	X4	201	PEB	NA-C4A-CHA-C1B
26	X4	201	PEB	C3A-C4A-CHA-C1B
26	X4	201	PEB	NB-C1B-CHA-C4A
26	X4	201	PEB	C2B-C1B-CHA-C4A
26	X4	202	PEB	NA-C4A-CHA-C1B
26	X4	202	PEB	C3A-C4A-CHA-C1B
26	X4	202	PEB	NB-C1B-CHA-C4A
26	X4	202	PEB	C2B-C1B-CHA-C4A
26	Y4	201	PEB	NA-C4A-CHA-C1B
26	Y4	201	PEB	C3A-C4A-CHA-C1B
26	Y4	201	PEB	NB-C1B-CHA-C4A
26	Y4	201	PEB	C2B-C1B-CHA-C4A
26	Y4	202	PEB	NA-C4A-CHA-C1B
26	Y4	202	PEB	C3A-C4A-CHA-C1B
26	Y4	202	PEB	NB-C1B-CHA-C4A
26	Y4	202	PEB	C2B-C1B-CHA-C4A
26	Z4	201	PEB	NA-C4A-CHA-C1B
26	Z4	201	PEB	C3A-C4A-CHA-C1B
26	Z4	201	PEB	NB-C1B-CHA-C4A
26	Z4	201	PEB	C2B-C1B-CHA-C4A
26	Z4	202	PEB	NA-C4A-CHA-C1B
26	Z4	202	PEB	C3A-C4A-CHA-C1B
26	Z4	202	PEB	NB-C1B-CHA-C4A
26	Z4	202	PEB	C2B-C1B-CHA-C4A
26	24	401	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	24	401	PEB	C3A-C4A-CHA-C1B
26	24	401	PEB	NB-C1B-CHA-C4A
26	24	401	PEB	C2B-C1B-CHA-C4A
26	34	1001	PEB	C1C-C2C-CAC-CBC
26	34	1001	PEB	C3C-C2C-CAC-CBC
26	34	1001	PEB	NB-C1B-CHA-C4A
26	34	1001	PEB	C2B-C1B-CHA-C4A
26	34	1002	PEB	C1C-C2C-CAC-CBC
26	34	1002	PEB	C3C-C2C-CAC-CBC
26	34	1002	PEB	NB-C1B-CHA-C4A
26	34	1002	PEB	C2B-C1B-CHA-C4A
26	34	1003	PEB	NA-C4A-CHA-C1B
26	34	1003	PEB	C3A-C4A-CHA-C1B
26	34	1003	PEB	NB-C1B-CHA-C4A
26	34	1003	PEB	C2B-C1B-CHA-C4A
26	34	1007	PEB	NA-C4A-CHA-C1B
26	34	1007	PEB	C3A-C4A-CHA-C1B
26	34	1007	PEB	NB-C1B-CHA-C4A
26	34	1007	PEB	C2B-C1B-CHA-C4A
26	44	301	PEB	NA-C4A-CHA-C1B
26	44	301	PEB	C3A-C4A-CHA-C1B
26	44	301	PEB	NB-C1B-CHA-C4A
26	44	301	PEB	C2B-C1B-CHA-C4A
26	44	302	PEB	NA-C4A-CHA-C1B
26	44	302	PEB	C3A-C4A-CHA-C1B
26	44	302	PEB	NB-C1B-CHA-C4A
26	44	302	PEB	C2B-C1B-CHA-C4A
26	a4	201	PEB	NA-C4A-CHA-C1B
26	a4	201	PEB	C3A-C4A-CHA-C1B
26	a4	201	PEB	NB-C1B-CHA-C4A
26	a4	201	PEB	C2B-C1B-CHA-C4A
26	b4	1001	PEB	NA-C4A-CHA-C1B
26	b4	1001	PEB	C3A-C4A-CHA-C1B
26	b4	1001	PEB	NB-C1B-CHA-C4A
26	b4	1001	PEB	C2B-C1B-CHA-C4A
26	c4	201	PEB	NB-C1B-CHA-C4A
26	c4	201	PEB	C2B-C1B-CHA-C4A
26	c4	202	PEB	NA-C4A-CHA-C1B
26	c4	202	PEB	C3A-C4A-CHA-C1B
26	c4	202	PEB	NB-C1B-CHA-C4A
26	c4	202	PEB	C2B-C1B-CHA-C4A
26	d4	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	d4	201	PEB	C3A-C4A-CHA-C1B
26	d4	201	PEB	NB-C1B-CHA-C4A
26	d4	201	PEB	C2B-C1B-CHA-C4A
26	e4	201	PEB	NA-C4A-CHA-C1B
26	e4	201	PEB	C3A-C4A-CHA-C1B
26	e4	201	PEB	NB-C1B-CHA-C4A
26	e4	201	PEB	C2B-C1B-CHA-C4A
26	e4	202	PEB	C1C-C2C-CAC-CBC
26	e4	202	PEB	C3C-C2C-CAC-CBC
26	e4	202	PEB	NB-C1B-CHA-C4A
26	e4	202	PEB	C2B-C1B-CHA-C4A
26	f4	201	PEB	NA-C4A-CHA-C1B
26	f4	201	PEB	C3A-C4A-CHA-C1B
26	f4	201	PEB	NB-C1B-CHA-C4A
26	f4	201	PEB	C2B-C1B-CHA-C4A
26	g4	201	PEB	NA-C4A-CHA-C1B
26	g4	201	PEB	C3A-C4A-CHA-C1B
26	g4	201	PEB	NB-C1B-CHA-C4A
26	g4	201	PEB	C2B-C1B-CHA-C4A
26	g4	202	PEB	C1C-C2C-CAC-CBC
26	g4	202	PEB	C3C-C2C-CAC-CBC
26	g4	202	PEB	NB-C1B-CHA-C4A
26	g4	202	PEB	C2B-C1B-CHA-C4A
26	h4	201	PEB	NB-C1B-CHA-C4A
26	h4	201	PEB	C2B-C1B-CHA-C4A
26	h4	202	PEB	NA-C4A-CHA-C1B
26	h4	202	PEB	C3A-C4A-CHA-C1B
26	h4	202	PEB	NB-C1B-CHA-C4A
26	h4	202	PEB	C2B-C1B-CHA-C4A
26	i4	201	PEB	NA-C4A-CHA-C1B
26	i4	201	PEB	C3A-C4A-CHA-C1B
26	i4	201	PEB	NB-C1B-CHA-C4A
26	i4	201	PEB	C2B-C1B-CHA-C4A
26	j4	201	PEB	NA-C4A-CHA-C1B
26	j4	201	PEB	C3A-C4A-CHA-C1B
26	j4	201	PEB	NB-C1B-CHA-C4A
26	j4	201	PEB	C2B-C1B-CHA-C4A
26	j4	202	PEB	C1C-C2C-CAC-CBC
26	j4	202	PEB	C3C-C2C-CAC-CBC
26	j4	202	PEB	NB-C1B-CHA-C4A
26	j4	202	PEB	C2B-C1B-CHA-C4A
26	k4	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	k4	201	PEB	C3A-C4A-CHA-C1B
26	k4	201	PEB	NB-C1B-CHA-C4A
26	k4	201	PEB	C2B-C1B-CHA-C4A
26	l4	201	PEB	NA-C4A-CHA-C1B
26	l4	201	PEB	C3A-C4A-CHA-C1B
26	l4	201	PEB	NB-C1B-CHA-C4A
26	l4	201	PEB	C2B-C1B-CHA-C4A
26	l4	202	PEB	C1C-C2C-CAC-CBC
26	l4	202	PEB	C3C-C2C-CAC-CBC
26	l4	202	PEB	NB-C1B-CHA-C4A
26	l4	202	PEB	C2B-C1B-CHA-C4A
26	m4	1001	PEB	NA-C4A-CHA-C1B
26	m4	1001	PEB	C3A-C4A-CHA-C1B
26	m4	1001	PEB	NB-C1B-CHA-C4A
26	m4	1001	PEB	C2B-C1B-CHA-C4A
26	n4	201	PEB	NA-C4A-CHA-C1B
26	n4	201	PEB	C3A-C4A-CHA-C1B
26	n4	201	PEB	NB-C1B-CHA-C4A
26	n4	201	PEB	C2B-C1B-CHA-C4A
26	n4	202	PEB	C1C-C2C-CAC-CBC
26	n4	202	PEB	C3C-C2C-CAC-CBC
26	n4	202	PEB	NB-C1B-CHA-C4A
26	n4	202	PEB	C2B-C1B-CHA-C4A
26	o4	201	PEB	NA-C4A-CHA-C1B
26	o4	201	PEB	C3A-C4A-CHA-C1B
26	o4	201	PEB	NB-C1B-CHA-C4A
26	o4	201	PEB	C2B-C1B-CHA-C4A
26	o4	202	PEB	NA-C4A-CHA-C1B
26	o4	202	PEB	C3A-C4A-CHA-C1B
26	o4	202	PEB	NB-C1B-CHA-C4A
26	o4	202	PEB	C2B-C1B-CHA-C4A
26	p4	201	PEB	NA-C4A-CHA-C1B
26	p4	201	PEB	C3A-C4A-CHA-C1B
26	p4	201	PEB	NB-C1B-CHA-C4A
26	p4	201	PEB	C2B-C1B-CHA-C4A
26	p4	202	PEB	C1C-C2C-CAC-CBC
26	p4	202	PEB	C3C-C2C-CAC-CBC
26	p4	202	PEB	NB-C1B-CHA-C4A
26	p4	202	PEB	C2B-C1B-CHA-C4A
26	q4	201	PEB	NA-C4A-CHA-C1B
26	q4	201	PEB	C3A-C4A-CHA-C1B
26	q4	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	q4	201	PEB	C2B-C1B-CHA-C4A
26	q4	202	PEB	NA-C4A-CHA-C1B
26	q4	202	PEB	C3A-C4A-CHA-C1B
26	q4	202	PEB	NB-C1B-CHA-C4A
26	q4	202	PEB	C2B-C1B-CHA-C4A
26	r4	201	PEB	C1C-C2C-CAC-CBC
26	r4	201	PEB	C3C-C2C-CAC-CBC
26	r4	201	PEB	NB-C1B-CHA-C4A
26	r4	201	PEB	C2B-C1B-CHA-C4A
26	s4	201	PEB	NA-C4A-CHA-C1B
26	s4	201	PEB	C3A-C4A-CHA-C1B
26	s4	201	PEB	NB-C1B-CHA-C4A
26	s4	201	PEB	C2B-C1B-CHA-C4A
26	s4	202	PEB	NB-C1B-CHA-C4A
26	s4	202	PEB	C2B-C1B-CHA-C4A
26	t4	201	PEB	NA-C4A-CHA-C1B
26	t4	201	PEB	C3A-C4A-CHA-C1B
26	t4	201	PEB	NB-C1B-CHA-C4A
26	t4	201	PEB	C2B-C1B-CHA-C4A
26	t4	202	PEB	NA-C4A-CHA-C1B
26	t4	202	PEB	C3A-C4A-CHA-C1B
26	t4	202	PEB	NB-C1B-CHA-C4A
26	t4	202	PEB	C2B-C1B-CHA-C4A
26	u4	201	PEB	NA-C4A-CHA-C1B
26	u4	201	PEB	C3A-C4A-CHA-C1B
26	u4	201	PEB	NB-C1B-CHA-C4A
26	u4	201	PEB	C2B-C1B-CHA-C4A
26	u4	202	PEB	NA-C4A-CHA-C1B
26	u4	202	PEB	C3A-C4A-CHA-C1B
26	u4	202	PEB	NB-C1B-CHA-C4A
26	u4	202	PEB	C2B-C1B-CHA-C4A
26	v4	201	PEB	NA-C4A-CHA-C1B
26	v4	201	PEB	C3A-C4A-CHA-C1B
26	v4	201	PEB	NB-C1B-CHA-C4A
26	v4	201	PEB	C2B-C1B-CHA-C4A
26	v4	202	PEB	C1C-C2C-CAC-CBC
26	v4	202	PEB	C3C-C2C-CAC-CBC
26	v4	202	PEB	NB-C1B-CHA-C4A
26	v4	202	PEB	C2B-C1B-CHA-C4A
26	w4	201	PEB	NA-C4A-CHA-C1B
26	w4	201	PEB	C3A-C4A-CHA-C1B
26	w4	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	w4	201	PEB	C2B-C1B-CHA-C4A
26	w4	202	PEB	NB-C1B-CHA-C4A
26	w4	202	PEB	C2B-C1B-CHA-C4A
26	x4	201	PEB	NA-C4A-CHA-C1B
26	x4	201	PEB	C3A-C4A-CHA-C1B
26	x4	201	PEB	NB-C1B-CHA-C4A
26	x4	201	PEB	C2B-C1B-CHA-C4A
26	y4	1001	PEB	NA-C4A-CHA-C1B
26	y4	1001	PEB	C3A-C4A-CHA-C1B
26	y4	1001	PEB	NB-C1B-CHA-C4A
26	y4	1001	PEB	C2B-C1B-CHA-C4A
26	y4	1002	PEB	NA-C4A-CHA-C1B
26	y4	1002	PEB	C3A-C4A-CHA-C1B
26	y4	1002	PEB	NB-C1B-CHA-C4A
26	y4	1002	PEB	C2B-C1B-CHA-C4A
26	z4	201	PEB	NA-C4A-CHA-C1B
26	z4	201	PEB	C3A-C4A-CHA-C1B
26	z4	201	PEB	NB-C1B-CHA-C4A
26	z4	201	PEB	C2B-C1B-CHA-C4A
26	z4	202	PEB	NA-C4A-CHA-C1B
26	z4	202	PEB	C3A-C4A-CHA-C1B
26	z4	202	PEB	NB-C1B-CHA-C4A
26	z4	202	PEB	C2B-C1B-CHA-C4A
26	A5	201	PEB	NA-C4A-CHA-C1B
26	A5	201	PEB	C3A-C4A-CHA-C1B
26	A5	201	PEB	NB-C1B-CHA-C4A
26	A5	201	PEB	C2B-C1B-CHA-C4A
26	A5	202	PEB	NB-C1B-CHA-C4A
26	A5	202	PEB	C2B-C1B-CHA-C4A
26	A5	203	PEB	C1C-C2C-CAC-CBC
26	A5	203	PEB	C3C-C2C-CAC-CBC
26	A5	203	PEB	NB-C1B-CHA-C4A
26	A5	203	PEB	C2B-C1B-CHA-C4A
26	B5	201	PEB	NA-C4A-CHA-C1B
26	B5	201	PEB	C3A-C4A-CHA-C1B
26	B5	201	PEB	NB-C1B-CHA-C4A
26	B5	201	PEB	C2B-C1B-CHA-C4A
26	B5	202	PEB	C1C-C2C-CAC-CBC
26	B5	202	PEB	C3C-C2C-CAC-CBC
26	B5	202	PEB	NB-C1B-CHA-C4A
26	B5	202	PEB	C2B-C1B-CHA-C4A
26	C5	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	C5	201	PEB	C3A-C4A-CHA-C1B
26	C5	201	PEB	NB-C1B-CHA-C4A
26	C5	201	PEB	C2B-C1B-CHA-C4A
26	C5	202	PEB	NB-C1B-CHA-C4A
26	C5	202	PEB	C2B-C1B-CHA-C4A
26	D5	201	PEB	NA-C4A-CHA-C1B
26	D5	201	PEB	C3A-C4A-CHA-C1B
26	D5	201	PEB	NB-C1B-CHA-C4A
26	D5	201	PEB	C2B-C1B-CHA-C4A
26	D5	202	PEB	C1C-C2C-CAC-CBC
26	D5	202	PEB	C3C-C2C-CAC-CBC
26	D5	202	PEB	NB-C1B-CHA-C4A
26	D5	202	PEB	C2B-C1B-CHA-C4A
26	E5	201	PEB	NA-C4A-CHA-C1B
26	E5	201	PEB	C3A-C4A-CHA-C1B
26	E5	201	PEB	NB-C1B-CHA-C4A
26	E5	201	PEB	C2B-C1B-CHA-C4A
26	E5	202	PEB	NB-C1B-CHA-C4A
26	E5	202	PEB	C2B-C1B-CHA-C4A
26	F5	201	PEB	NA-C4A-CHA-C1B
26	F5	201	PEB	C3A-C4A-CHA-C1B
26	F5	201	PEB	NB-C1B-CHA-C4A
26	F5	201	PEB	C2B-C1B-CHA-C4A
26	F5	202	PEB	C1C-C2C-CAC-CBC
26	F5	202	PEB	C3C-C2C-CAC-CBC
26	F5	202	PEB	NB-C1B-CHA-C4A
26	F5	202	PEB	C2B-C1B-CHA-C4A
26	G5	201	PEB	NA-C4A-CHA-C1B
26	G5	201	PEB	C3A-C4A-CHA-C1B
26	G5	201	PEB	NB-C1B-CHA-C4A
26	G5	201	PEB	C2B-C1B-CHA-C4A
26	G5	202	PEB	NB-C1B-CHA-C4A
26	G5	202	PEB	C2B-C1B-CHA-C4A
26	H5	201	PEB	NA-C4A-CHA-C1B
26	H5	201	PEB	C3A-C4A-CHA-C1B
26	H5	201	PEB	NB-C1B-CHA-C4A
26	H5	201	PEB	C2B-C1B-CHA-C4A
26	I5	201	PEB	NA-C4A-CHA-C1B
26	I5	201	PEB	C3A-C4A-CHA-C1B
26	I5	201	PEB	NB-C1B-CHA-C4A
26	I5	201	PEB	C2B-C1B-CHA-C4A
26	I5	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	I5	202	PEB	C2B-C1B-CHA-C4A
26	J5	201	PEB	NA-C4A-CHA-C1B
26	J5	201	PEB	C3A-C4A-CHA-C1B
26	J5	201	PEB	NB-C1B-CHA-C4A
26	J5	201	PEB	C2B-C1B-CHA-C4A
26	J5	202	PEB	C1C-C2C-CAC-CBC
26	J5	202	PEB	C3C-C2C-CAC-CBC
26	J5	202	PEB	NB-C1B-CHA-C4A
26	J5	202	PEB	C2B-C1B-CHA-C4A
26	K5	1001	PEB	NA-C4A-CHA-C1B
26	K5	1001	PEB	C3A-C4A-CHA-C1B
26	K5	1001	PEB	NB-C1B-CHA-C4A
26	K5	1001	PEB	C2B-C1B-CHA-C4A
26	K5	1002	PEB	NB-C1B-CHA-C4A
26	K5	1002	PEB	C2B-C1B-CHA-C4A
26	L5	201	PEB	NA-C4A-CHA-C1B
26	L5	201	PEB	C3A-C4A-CHA-C1B
26	L5	201	PEB	NB-C1B-CHA-C4A
26	L5	201	PEB	C2B-C1B-CHA-C4A
26	L5	202	PEB	C1C-C2C-CAC-CBC
26	L5	202	PEB	C3C-C2C-CAC-CBC
26	L5	202	PEB	NB-C1B-CHA-C4A
26	L5	202	PEB	C2B-C1B-CHA-C4A
26	M5	201	PEB	NA-C4A-CHA-C1B
26	M5	201	PEB	C3A-C4A-CHA-C1B
26	M5	201	PEB	NB-C1B-CHA-C4A
26	M5	201	PEB	C2B-C1B-CHA-C4A
26	M5	202	PEB	NB-C1B-CHA-C4A
26	M5	202	PEB	C2B-C1B-CHA-C4A
26	N5	201	PEB	NA-C4A-CHA-C1B
26	N5	201	PEB	C3A-C4A-CHA-C1B
26	N5	201	PEB	NB-C1B-CHA-C4A
26	N5	201	PEB	C2B-C1B-CHA-C4A
26	N5	202	PEB	C1C-C2C-CAC-CBC
26	N5	202	PEB	C3C-C2C-CAC-CBC
26	N5	202	PEB	NB-C1B-CHA-C4A
26	N5	202	PEB	C2B-C1B-CHA-C4A
26	O5	201	PEB	NA-C4A-CHA-C1B
26	O5	201	PEB	C3A-C4A-CHA-C1B
26	O5	201	PEB	NB-C1B-CHA-C4A
26	O5	201	PEB	C2B-C1B-CHA-C4A
26	O5	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	O5	202	PEB	C2B-C1B-CHA-C4A
26	P5	201	PEB	C1C-C2C-CAC-CBC
26	P5	201	PEB	C3C-C2C-CAC-CBC
26	P5	201	PEB	NB-C1B-CHA-C4A
26	P5	201	PEB	C2B-C1B-CHA-C4A
26	Q5	201	PEB	NA-C4A-CHA-C1B
26	Q5	201	PEB	C3A-C4A-CHA-C1B
26	Q5	201	PEB	NB-C1B-CHA-C4A
26	Q5	201	PEB	C2B-C1B-CHA-C4A
26	Q5	202	PEB	NB-C1B-CHA-C4A
26	Q5	202	PEB	C2B-C1B-CHA-C4A
26	R5	201	PEB	NA-C4A-CHA-C1B
26	R5	201	PEB	C3A-C4A-CHA-C1B
26	R5	201	PEB	NB-C1B-CHA-C4A
26	R5	201	PEB	C2B-C1B-CHA-C4A
26	R5	202	PEB	C1C-C2C-CAC-CBC
26	R5	202	PEB	C3C-C2C-CAC-CBC
26	R5	202	PEB	NB-C1B-CHA-C4A
26	R5	202	PEB	C2B-C1B-CHA-C4A
26	S5	201	PEB	NA-C4A-CHA-C1B
26	S5	201	PEB	C3A-C4A-CHA-C1B
26	S5	201	PEB	NB-C1B-CHA-C4A
26	S5	201	PEB	C2B-C1B-CHA-C4A
26	S5	202	PEB	NB-C1B-CHA-C4A
26	S5	202	PEB	C2B-C1B-CHA-C4A
26	S5	203	PEB	C1C-C2C-CAC-CBC
26	S5	203	PEB	C3C-C2C-CAC-CBC
26	S5	203	PEB	NB-C1B-CHA-C4A
26	S5	203	PEB	C2B-C1B-CHA-C4A
26	T5	201	PEB	NA-C4A-CHA-C1B
26	T5	201	PEB	C3A-C4A-CHA-C1B
26	T5	201	PEB	NB-C1B-CHA-C4A
26	T5	201	PEB	C2B-C1B-CHA-C4A
26	U5	201	PEB	NA-C4A-CHA-C1B
26	U5	201	PEB	C3A-C4A-CHA-C1B
26	U5	201	PEB	NB-C1B-CHA-C4A
26	U5	201	PEB	C2B-C1B-CHA-C4A
26	U5	202	PEB	NB-C1B-CHA-C4A
26	U5	202	PEB	C2B-C1B-CHA-C4A
26	V5	201	PEB	NA-C4A-CHA-C1B
26	V5	201	PEB	C3A-C4A-CHA-C1B
26	V5	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	V5	201	PEB	C2B-C1B-CHA-C4A
26	V5	202	PEB	C1C-C2C-CAC-CBC
26	V5	202	PEB	C3C-C2C-CAC-CBC
26	V5	202	PEB	NB-C1B-CHA-C4A
26	V5	202	PEB	C2B-C1B-CHA-C4A
26	W5	301	PEB	NA-C4A-CHA-C1B
26	W5	301	PEB	C3A-C4A-CHA-C1B
26	W5	301	PEB	NB-C1B-CHA-C4A
26	W5	301	PEB	C2B-C1B-CHA-C4A
26	X5	401	PEB	NA-C4A-CHA-C1B
26	X5	401	PEB	C3A-C4A-CHA-C1B
26	X5	401	PEB	NB-C1B-CHA-C4A
26	X5	401	PEB	C2B-C1B-CHA-C4A
26	Y5	1001	PEB	NA-C4A-CHA-C1B
26	Y5	1001	PEB	C3A-C4A-CHA-C1B
26	Y5	1001	PEB	NB-C1B-CHA-C4A
26	Y5	1001	PEB	C2B-C1B-CHA-C4A
26	Y5	1002	PEB	NB-C1B-CHA-C4A
26	Y5	1002	PEB	C2B-C1B-CHA-C4A
26	Y5	1003	PEB	NA-C4A-CHA-C1B
26	Y5	1003	PEB	C3A-C4A-CHA-C1B
26	Y5	1003	PEB	NB-C1B-CHA-C4A
26	Y5	1003	PEB	C2B-C1B-CHA-C4A
26	Z5	301	PEB	NA-C4A-CHA-C1B
26	Z5	301	PEB	C3A-C4A-CHA-C1B
26	Z5	301	PEB	NB-C1B-CHA-C4A
26	Z5	301	PEB	C2B-C1B-CHA-C4A
26	Z5	302	PEB	NB-C1B-CHA-C4A
26	Z5	302	PEB	C2B-C1B-CHA-C4A
26	Z5	303	PEB	NA-C4A-CHA-C1B
26	Z5	303	PEB	C3A-C4A-CHA-C1B
26	Z5	303	PEB	NB-C1B-CHA-C4A
26	Z5	303	PEB	C2B-C1B-CHA-C4A
26	a5	201	PEB	NA-C4A-CHA-C1B
26	a5	201	PEB	C3A-C4A-CHA-C1B
26	a5	201	PEB	NB-C1B-CHA-C4A
26	a5	201	PEB	C2B-C1B-CHA-C4A
26	b5	1001	PEB	NA-C4A-CHA-C1B
26	b5	1001	PEB	C3A-C4A-CHA-C1B
26	b5	1001	PEB	NB-C1B-CHA-C4A
26	b5	1001	PEB	C2B-C1B-CHA-C4A
26	c5	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	c5	201	PEB	C2B-C1B-CHA-C4A
26	c5	202	PEB	NA-C4A-CHA-C1B
26	c5	202	PEB	C3A-C4A-CHA-C1B
26	c5	202	PEB	NB-C1B-CHA-C4A
26	c5	202	PEB	C2B-C1B-CHA-C4A
26	d5	201	PEB	NA-C4A-CHA-C1B
26	d5	201	PEB	C3A-C4A-CHA-C1B
26	d5	201	PEB	NB-C1B-CHA-C4A
26	d5	201	PEB	C2B-C1B-CHA-C4A
26	e5	201	PEB	NA-C4A-CHA-C1B
26	e5	201	PEB	C3A-C4A-CHA-C1B
26	e5	201	PEB	NB-C1B-CHA-C4A
26	e5	201	PEB	C2B-C1B-CHA-C4A
26	f5	201	PEB	NB-C1B-CHA-C4A
26	f5	201	PEB	C2B-C1B-CHA-C4A
26	g5	201	PEB	NA-C4A-CHA-C1B
26	g5	201	PEB	C3A-C4A-CHA-C1B
26	g5	201	PEB	NB-C1B-CHA-C4A
26	g5	201	PEB	C2B-C1B-CHA-C4A
26	g5	202	PEB	C1C-C2C-CAC-CBC
26	g5	202	PEB	C3C-C2C-CAC-CBC
26	g5	202	PEB	NB-C1B-CHA-C4A
26	g5	202	PEB	C2B-C1B-CHA-C4A
26	h5	201	PEB	NA-C4A-CHA-C1B
26	h5	201	PEB	C3A-C4A-CHA-C1B
26	h5	201	PEB	NB-C1B-CHA-C4A
26	h5	201	PEB	C2B-C1B-CHA-C4A
26	h5	202	PEB	NB-C1B-CHA-C4A
26	h5	202	PEB	C2B-C1B-CHA-C4A
26	i5	201	PEB	NA-C4A-CHA-C1B
26	i5	201	PEB	C3A-C4A-CHA-C1B
26	i5	201	PEB	NB-C1B-CHA-C4A
26	i5	201	PEB	C2B-C1B-CHA-C4A
26	j5	201	PEB	NA-C4A-CHA-C1B
26	j5	201	PEB	C3A-C4A-CHA-C1B
26	j5	201	PEB	NB-C1B-CHA-C4A
26	j5	201	PEB	C2B-C1B-CHA-C4A
26	j5	202	PEB	NA-C4A-CHA-C1B
26	j5	202	PEB	C3A-C4A-CHA-C1B
26	j5	202	PEB	NB-C1B-CHA-C4A
26	j5	202	PEB	C2B-C1B-CHA-C4A
26	k5	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	k5	201	PEB	C3A-C4A-CHA-C1B
26	k5	201	PEB	NB-C1B-CHA-C4A
26	k5	201	PEB	C2B-C1B-CHA-C4A
26	l5	201	PEB	NA-C4A-CHA-C1B
26	l5	201	PEB	C3A-C4A-CHA-C1B
26	l5	201	PEB	NB-C1B-CHA-C4A
26	l5	201	PEB	C2B-C1B-CHA-C4A
26	l5	202	PEB	NA-C4A-CHA-C1B
26	l5	202	PEB	C3A-C4A-CHA-C1B
26	l5	202	PEB	NB-C1B-CHA-C4A
26	l5	202	PEB	C2B-C1B-CHA-C4A
26	m5	1001	PEB	NA-C4A-CHA-C1B
26	m5	1001	PEB	C3A-C4A-CHA-C1B
26	m5	1001	PEB	NB-C1B-CHA-C4A
26	m5	1001	PEB	C2B-C1B-CHA-C4A
26	m5	1002	PEB	NB-C1B-CHA-C4A
26	m5	1002	PEB	C2B-C1B-CHA-C4A
26	m5	1003	PEB	C1C-C2C-CAC-CBC
26	m5	1003	PEB	C3C-C2C-CAC-CBC
26	m5	1003	PEB	NB-C1B-CHA-C4A
26	m5	1003	PEB	C2B-C1B-CHA-C4A
26	n5	201	PEB	NA-C4A-CHA-C1B
26	n5	201	PEB	C3A-C4A-CHA-C1B
26	n5	201	PEB	NB-C1B-CHA-C4A
26	n5	201	PEB	C2B-C1B-CHA-C4A
26	n5	202	PEB	C1C-C2C-CAC-CBC
26	n5	202	PEB	C3C-C2C-CAC-CBC
26	n5	202	PEB	NB-C1B-CHA-C4A
26	n5	202	PEB	C2B-C1B-CHA-C4A
26	o5	201	PEB	NA-C4A-CHA-C1B
26	o5	201	PEB	C3A-C4A-CHA-C1B
26	o5	201	PEB	NB-C1B-CHA-C4A
26	o5	201	PEB	C2B-C1B-CHA-C4A
26	o5	202	PEB	NB-C1B-CHA-C4A
26	o5	202	PEB	C2B-C1B-CHA-C4A
26	p5	201	PEB	C1C-C2C-CAC-CBC
26	p5	201	PEB	C3C-C2C-CAC-CBC
26	p5	201	PEB	NB-C1B-CHA-C4A
26	p5	201	PEB	C2B-C1B-CHA-C4A
26	q5	201	PEB	NA-C4A-CHA-C1B
26	q5	201	PEB	C3A-C4A-CHA-C1B
26	q5	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	q5	201	PEB	C2B-C1B-CHA-C4A
26	q5	202	PEB	NB-C1B-CHA-C4A
26	q5	202	PEB	C2B-C1B-CHA-C4A
26	r5	201	PEB	NA-C4A-CHA-C1B
26	r5	201	PEB	C3A-C4A-CHA-C1B
26	r5	201	PEB	NB-C1B-CHA-C4A
26	r5	201	PEB	C2B-C1B-CHA-C4A
26	r5	202	PEB	C1C-C2C-CAC-CBC
26	r5	202	PEB	C3C-C2C-CAC-CBC
26	r5	202	PEB	NB-C1B-CHA-C4A
26	r5	202	PEB	C2B-C1B-CHA-C4A
26	s5	201	PEB	NA-C4A-CHA-C1B
26	s5	201	PEB	C3A-C4A-CHA-C1B
26	s5	201	PEB	NB-C1B-CHA-C4A
26	s5	201	PEB	C2B-C1B-CHA-C4A
26	s5	202	PEB	NB-C1B-CHA-C4A
26	s5	202	PEB	C2B-C1B-CHA-C4A
26	t5	201	PEB	NA-C4A-CHA-C1B
26	t5	201	PEB	C3A-C4A-CHA-C1B
26	t5	201	PEB	NB-C1B-CHA-C4A
26	t5	201	PEB	C2B-C1B-CHA-C4A
26	t5	202	PEB	C1C-C2C-CAC-CBC
26	t5	202	PEB	C3C-C2C-CAC-CBC
26	t5	202	PEB	NB-C1B-CHA-C4A
26	t5	202	PEB	C2B-C1B-CHA-C4A
26	u5	201	PEB	NA-C4A-CHA-C1B
26	u5	201	PEB	C3A-C4A-CHA-C1B
26	u5	201	PEB	NB-C1B-CHA-C4A
26	u5	201	PEB	C2B-C1B-CHA-C4A
26	u5	202	PEB	NB-C1B-CHA-C4A
26	u5	202	PEB	C2B-C1B-CHA-C4A
26	v5	201	PEB	NA-C4A-CHA-C1B
26	v5	201	PEB	C3A-C4A-CHA-C1B
26	v5	201	PEB	NB-C1B-CHA-C4A
26	v5	201	PEB	C2B-C1B-CHA-C4A
26	v5	202	PEB	C1C-C2C-CAC-CBC
26	v5	202	PEB	C3C-C2C-CAC-CBC
26	v5	202	PEB	NB-C1B-CHA-C4A
26	v5	202	PEB	C2B-C1B-CHA-C4A
26	w5	201	PEB	NA-C4A-CHA-C1B
26	w5	201	PEB	C3A-C4A-CHA-C1B
26	w5	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	w5	201	PEB	C2B-C1B-CHA-C4A
26	w5	202	PEB	NB-C1B-CHA-C4A
26	w5	202	PEB	C2B-C1B-CHA-C4A
26	x5	201	PEB	NA-C4A-CHA-C1B
26	x5	201	PEB	C3A-C4A-CHA-C1B
26	x5	201	PEB	NB-C1B-CHA-C4A
26	x5	201	PEB	C2B-C1B-CHA-C4A
26	y5	1001	PEB	NA-C4A-CHA-C1B
26	y5	1001	PEB	C3A-C4A-CHA-C1B
26	y5	1001	PEB	NB-C1B-CHA-C4A
26	y5	1001	PEB	C2B-C1B-CHA-C4A
26	y5	1002	PEB	NB-C1B-CHA-C4A
26	y5	1002	PEB	C2B-C1B-CHA-C4A
26	z5	201	PEB	NA-C4A-CHA-C1B
26	z5	201	PEB	C3A-C4A-CHA-C1B
26	z5	201	PEB	NB-C1B-CHA-C4A
26	z5	201	PEB	C2B-C1B-CHA-C4A
26	z5	202	PEB	C1C-C2C-CAC-CBC
26	z5	202	PEB	C3C-C2C-CAC-CBC
26	z5	202	PEB	NB-C1B-CHA-C4A
26	z5	202	PEB	C2B-C1B-CHA-C4A
26	f8	201	PEB	NA-C4A-CHA-C1B
26	f8	201	PEB	C3A-C4A-CHA-C1B
26	f8	201	PEB	NB-C1B-CHA-C4A
26	f8	201	PEB	C2B-C1B-CHA-C4A
26	f8	202	PEB	NA-C4A-CHA-C1B
26	f8	202	PEB	C3A-C4A-CHA-C1B
26	f8	202	PEB	NB-C1B-CHA-C4A
26	f8	202	PEB	C2B-C1B-CHA-C4A
26	g8	201	PEB	NA-C4A-CHA-C1B
26	g8	201	PEB	C3A-C4A-CHA-C1B
26	g8	201	PEB	NB-C1B-CHA-C4A
26	g8	201	PEB	C2B-C1B-CHA-C4A
26	h8	201	PEB	NA-C4A-CHA-C1B
26	h8	201	PEB	C3A-C4A-CHA-C1B
26	h8	201	PEB	NB-C1B-CHA-C4A
26	h8	201	PEB	C2B-C1B-CHA-C4A
26	h8	202	PEB	C1C-C2C-CAC-CBC
26	h8	202	PEB	C3C-C2C-CAC-CBC
26	h8	202	PEB	NB-C1B-CHA-C4A
26	h8	202	PEB	C2B-C1B-CHA-C4A
26	i8	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	i8	201	PEB	C3A-C4A-CHA-C1B
26	i8	201	PEB	NB-C1B-CHA-C4A
26	i8	201	PEB	C2B-C1B-CHA-C4A
26	j8	201	PEB	NA-C4A-CHA-C1B
26	j8	201	PEB	C3A-C4A-CHA-C1B
26	j8	201	PEB	NB-C1B-CHA-C4A
26	j8	201	PEB	C2B-C1B-CHA-C4A
26	j8	202	PEB	NA-C4A-CHA-C1B
26	j8	202	PEB	C3A-C4A-CHA-C1B
26	j8	202	PEB	NB-C1B-CHA-C4A
26	j8	202	PEB	C2B-C1B-CHA-C4A
26	k8	201	PEB	NA-C4A-CHA-C1B
26	k8	201	PEB	C3A-C4A-CHA-C1B
26	k8	201	PEB	NB-C1B-CHA-C4A
26	k8	201	PEB	C2B-C1B-CHA-C4A
26	k8	202	PEB	NA-C4A-CHA-C1B
26	k8	202	PEB	C3A-C4A-CHA-C1B
26	k8	202	PEB	NB-C1B-CHA-C4A
26	k8	202	PEB	C2B-C1B-CHA-C4A
26	k8	203	PEB	NA-C4A-CHA-C1B
26	k8	203	PEB	C3A-C4A-CHA-C1B
26	k8	203	PEB	NB-C1B-CHA-C4A
26	k8	203	PEB	C2B-C1B-CHA-C4A
26	l8	201	PEB	NA-C4A-CHA-C1B
26	l8	201	PEB	C3A-C4A-CHA-C1B
26	l8	201	PEB	NB-C1B-CHA-C4A
26	l8	201	PEB	C2B-C1B-CHA-C4A
26	l8	202	PEB	NA-C4A-CHA-C1B
26	l8	202	PEB	C3A-C4A-CHA-C1B
26	l8	202	PEB	NB-C1B-CHA-C4A
26	l8	202	PEB	C2B-C1B-CHA-C4A
26	m8	201	PEB	NA-C4A-CHA-C1B
26	m8	201	PEB	C3A-C4A-CHA-C1B
26	m8	201	PEB	NB-C1B-CHA-C4A
26	m8	201	PEB	C2B-C1B-CHA-C4A
26	m8	202	PEB	NA-C4A-CHA-C1B
26	m8	202	PEB	C3A-C4A-CHA-C1B
26	m8	202	PEB	NB-C1B-CHA-C4A
26	m8	202	PEB	C2B-C1B-CHA-C4A
26	A6	1001	PEB	NA-C4A-CHA-C1B
26	A6	1001	PEB	C3A-C4A-CHA-C1B
26	A6	1001	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	A6	1001	PEB	C2B-C1B-CHA-C4A
26	A6	1002	PEB	NA-C4A-CHA-C1B
26	A6	1002	PEB	C3A-C4A-CHA-C1B
26	A6	1002	PEB	NB-C1B-CHA-C4A
26	A6	1002	PEB	C2B-C1B-CHA-C4A
26	B6	201	PEB	NA-C4A-CHA-C1B
26	B6	201	PEB	C3A-C4A-CHA-C1B
26	B6	201	PEB	NB-C1B-CHA-C4A
26	B6	201	PEB	C2B-C1B-CHA-C4A
26	B6	202	PEB	C1C-C2C-CAC-CBC
26	B6	202	PEB	C3C-C2C-CAC-CBC
26	B6	202	PEB	NB-C1B-CHA-C4A
26	B6	202	PEB	C2B-C1B-CHA-C4A
26	C6	201	PEB	NA-C4A-CHA-C1B
26	C6	201	PEB	C3A-C4A-CHA-C1B
26	C6	201	PEB	NB-C1B-CHA-C4A
26	C6	201	PEB	C2B-C1B-CHA-C4A
26	C6	202	PEB	NA-C4A-CHA-C1B
26	C6	202	PEB	C3A-C4A-CHA-C1B
26	C6	202	PEB	NB-C1B-CHA-C4A
26	C6	202	PEB	C2B-C1B-CHA-C4A
26	D6	201	PEB	NA-C4A-CHA-C1B
26	D6	201	PEB	C3A-C4A-CHA-C1B
26	D6	201	PEB	NB-C1B-CHA-C4A
26	D6	201	PEB	C2B-C1B-CHA-C4A
26	E6	201	PEB	NA-C4A-CHA-C1B
26	E6	201	PEB	C3A-C4A-CHA-C1B
26	E6	201	PEB	NB-C1B-CHA-C4A
26	E6	201	PEB	C2B-C1B-CHA-C4A
26	E6	202	PEB	NA-C4A-CHA-C1B
26	E6	202	PEB	C3A-C4A-CHA-C1B
26	E6	202	PEB	NB-C1B-CHA-C4A
26	E6	202	PEB	C2B-C1B-CHA-C4A
26	F6	201	PEB	NA-C4A-CHA-C1B
26	F6	201	PEB	C3A-C4A-CHA-C1B
26	F6	201	PEB	NB-C1B-CHA-C4A
26	F6	201	PEB	C2B-C1B-CHA-C4A
26	F6	202	PEB	NA-C4A-CHA-C1B
26	F6	202	PEB	C3A-C4A-CHA-C1B
26	F6	202	PEB	NB-C1B-CHA-C4A
26	F6	202	PEB	C2B-C1B-CHA-C4A
26	G6	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	G6	201	PEB	C3A-C4A-CHA-C1B
26	G6	201	PEB	NB-C1B-CHA-C4A
26	G6	201	PEB	C2B-C1B-CHA-C4A
26	G6	202	PEB	NB-C1B-CHA-C4A
26	G6	202	PEB	C2B-C1B-CHA-C4A
26	H6	201	PEB	NB-C1B-CHA-C4A
26	H6	201	PEB	C2B-C1B-CHA-C4A
26	H6	202	PEB	NA-C4A-CHA-C1B
26	H6	202	PEB	C3A-C4A-CHA-C1B
26	H6	202	PEB	NB-C1B-CHA-C4A
26	H6	202	PEB	C2B-C1B-CHA-C4A
26	I6	201	PEB	NA-C4A-CHA-C1B
26	I6	201	PEB	C3A-C4A-CHA-C1B
26	I6	201	PEB	NB-C1B-CHA-C4A
26	I6	201	PEB	C2B-C1B-CHA-C4A
26	I6	202	PEB	NA-C4A-CHA-C1B
26	I6	202	PEB	C3A-C4A-CHA-C1B
26	I6	202	PEB	NB-C1B-CHA-C4A
26	I6	202	PEB	C2B-C1B-CHA-C4A
26	J6	201	PEB	NA-C4A-CHA-C1B
26	J6	201	PEB	C3A-C4A-CHA-C1B
26	J6	201	PEB	NB-C1B-CHA-C4A
26	J6	201	PEB	C2B-C1B-CHA-C4A
26	J6	202	PEB	C1C-C2C-CAC-CBC
26	J6	202	PEB	C3C-C2C-CAC-CBC
26	J6	202	PEB	NB-C1B-CHA-C4A
26	J6	202	PEB	C2B-C1B-CHA-C4A
26	K6	201	PEB	NA-C4A-CHA-C1B
26	K6	201	PEB	C3A-C4A-CHA-C1B
26	K6	201	PEB	NB-C1B-CHA-C4A
26	K6	201	PEB	C2B-C1B-CHA-C4A
26	K6	202	PEB	NA-C4A-CHA-C1B
26	K6	202	PEB	C3A-C4A-CHA-C1B
26	K6	202	PEB	NB-C1B-CHA-C4A
26	K6	202	PEB	C2B-C1B-CHA-C4A
26	L6	201	PEB	NA-C4A-CHA-C1B
26	L6	201	PEB	C3A-C4A-CHA-C1B
26	L6	201	PEB	NB-C1B-CHA-C4A
26	L6	201	PEB	C2B-C1B-CHA-C4A
26	M6	1001	PEB	NA-C4A-CHA-C1B
26	M6	1001	PEB	C3A-C4A-CHA-C1B
26	M6	1001	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	M6	1001	PEB	C2B-C1B-CHA-C4A
26	M6	1002	PEB	NA-C4A-CHA-C1B
26	M6	1002	PEB	C3A-C4A-CHA-C1B
26	M6	1002	PEB	NB-C1B-CHA-C4A
26	M6	1002	PEB	C2B-C1B-CHA-C4A
26	N6	201	PEB	NA-C4A-CHA-C1B
26	N6	201	PEB	C3A-C4A-CHA-C1B
26	N6	201	PEB	NB-C1B-CHA-C4A
26	N6	201	PEB	C2B-C1B-CHA-C4A
26	N6	202	PEB	NB-C1B-CHA-C4A
26	N6	202	PEB	C2B-C1B-CHA-C4A
26	O6	201	PEB	NA-C4A-CHA-C1B
26	O6	201	PEB	C3A-C4A-CHA-C1B
26	O6	201	PEB	NB-C1B-CHA-C4A
26	O6	201	PEB	C2B-C1B-CHA-C4A
26	O6	202	PEB	NA-C4A-CHA-C1B
26	O6	202	PEB	C3A-C4A-CHA-C1B
26	O6	202	PEB	NB-C1B-CHA-C4A
26	O6	202	PEB	C2B-C1B-CHA-C4A
26	P6	201	PEB	NA-C4A-CHA-C1B
26	P6	201	PEB	C3A-C4A-CHA-C1B
26	P6	201	PEB	NB-C1B-CHA-C4A
26	P6	201	PEB	C2B-C1B-CHA-C4A
26	P6	202	PEB	NA-C4A-CHA-C1B
26	P6	202	PEB	C3A-C4A-CHA-C1B
26	P6	202	PEB	NB-C1B-CHA-C4A
26	P6	202	PEB	C2B-C1B-CHA-C4A
26	Q6	201	PEB	NA-C4A-CHA-C1B
26	Q6	201	PEB	C3A-C4A-CHA-C1B
26	Q6	201	PEB	NB-C1B-CHA-C4A
26	Q6	201	PEB	C2B-C1B-CHA-C4A
26	Q6	202	PEB	NA-C4A-CHA-C1B
26	Q6	202	PEB	C3A-C4A-CHA-C1B
26	Q6	202	PEB	NB-C1B-CHA-C4A
26	Q6	202	PEB	C2B-C1B-CHA-C4A
26	R6	201	PEB	NA-C4A-CHA-C1B
26	R6	201	PEB	C3A-C4A-CHA-C1B
26	R6	201	PEB	NB-C1B-CHA-C4A
26	R6	201	PEB	C2B-C1B-CHA-C4A
26	R6	202	PEB	C1C-C2C-CAC-CBC
26	R6	202	PEB	C3C-C2C-CAC-CBC
26	R6	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	R6	202	PEB	C2B-C1B-CHA-C4A
26	S6	201	PEB	NA-C4A-CHA-C1B
26	S6	201	PEB	C3A-C4A-CHA-C1B
26	S6	201	PEB	NB-C1B-CHA-C4A
26	S6	201	PEB	C2B-C1B-CHA-C4A
26	S6	202	PEB	NA-C4A-CHA-C1B
26	S6	202	PEB	C3A-C4A-CHA-C1B
26	S6	202	PEB	NB-C1B-CHA-C4A
26	S6	202	PEB	C2B-C1B-CHA-C4A
26	T6	201	PEB	NA-C4A-CHA-C1B
26	T6	201	PEB	C3A-C4A-CHA-C1B
26	T6	201	PEB	NB-C1B-CHA-C4A
26	T6	201	PEB	C2B-C1B-CHA-C4A
26	T6	202	PEB	NA-C4A-CHA-C1B
26	T6	202	PEB	C3A-C4A-CHA-C1B
26	T6	202	PEB	NB-C1B-CHA-C4A
26	T6	202	PEB	C2B-C1B-CHA-C4A
26	U6	201	PEB	NA-C4A-CHA-C1B
26	U6	201	PEB	C3A-C4A-CHA-C1B
26	U6	201	PEB	NB-C1B-CHA-C4A
26	U6	201	PEB	C2B-C1B-CHA-C4A
26	U6	202	PEB	NB-C1B-CHA-C4A
26	U6	202	PEB	C2B-C1B-CHA-C4A
26	V6	201	PEB	NA-C4A-CHA-C1B
26	V6	201	PEB	C3A-C4A-CHA-C1B
26	V6	201	PEB	NB-C1B-CHA-C4A
26	V6	201	PEB	C2B-C1B-CHA-C4A
26	V6	202	PEB	NB-C1B-CHA-C4A
26	V6	202	PEB	C2B-C1B-CHA-C4A
26	W6	201	PEB	NA-C4A-CHA-C1B
26	W6	201	PEB	C3A-C4A-CHA-C1B
26	W6	201	PEB	NB-C1B-CHA-C4A
26	W6	201	PEB	C2B-C1B-CHA-C4A
26	W6	202	PEB	NA-C4A-CHA-C1B
26	W6	202	PEB	C3A-C4A-CHA-C1B
26	W6	202	PEB	NB-C1B-CHA-C4A
26	W6	202	PEB	C2B-C1B-CHA-C4A
26	X6	201	PEB	NA-C4A-CHA-C1B
26	X6	201	PEB	C3A-C4A-CHA-C1B
26	X6	201	PEB	NB-C1B-CHA-C4A
26	X6	201	PEB	C2B-C1B-CHA-C4A
26	X6	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	X6	202	PEB	C3C-C2C-CAC-CBC
26	X6	202	PEB	NB-C1B-CHA-C4A
26	X6	202	PEB	C2B-C1B-CHA-C4A
26	Y6	201	PEB	NA-C4A-CHA-C1B
26	Y6	201	PEB	C3A-C4A-CHA-C1B
26	Y6	201	PEB	NB-C1B-CHA-C4A
26	Y6	201	PEB	C2B-C1B-CHA-C4A
26	Z6	201	PEB	NA-C4A-CHA-C1B
26	Z6	201	PEB	C3A-C4A-CHA-C1B
26	Z6	201	PEB	NB-C1B-CHA-C4A
26	Z6	201	PEB	C2B-C1B-CHA-C4A
26	Z6	202	PEB	NA-C4A-CHA-C1B
26	Z6	202	PEB	C3A-C4A-CHA-C1B
26	Z6	202	PEB	NB-C1B-CHA-C4A
26	Z6	202	PEB	C2B-C1B-CHA-C4A
26	a6	201	PEB	NA-C4A-CHA-C1B
26	a6	201	PEB	C3A-C4A-CHA-C1B
26	a6	201	PEB	NB-C1B-CHA-C4A
26	a6	201	PEB	C2B-C1B-CHA-C4A
26	a6	202	PEB	NB-C1B-CHA-C4A
26	a6	202	PEB	C2B-C1B-CHA-C4A
26	b6	201	PEB	NA-C4A-CHA-C1B
26	b6	201	PEB	C3A-C4A-CHA-C1B
26	b6	201	PEB	NB-C1B-CHA-C4A
26	b6	201	PEB	C2B-C1B-CHA-C4A
26	b6	202	PEB	NA-C4A-CHA-C1B
26	b6	202	PEB	C3A-C4A-CHA-C1B
26	b6	202	PEB	NB-C1B-CHA-C4A
26	b6	202	PEB	C2B-C1B-CHA-C4A
26	c6	1001	PEB	NA-C4A-CHA-C1B
26	c6	1001	PEB	C3A-C4A-CHA-C1B
26	c6	1001	PEB	NB-C1B-CHA-C4A
26	c6	1001	PEB	C2B-C1B-CHA-C4A
26	c6	1002	PEB	NA-C4A-CHA-C1B
26	c6	1002	PEB	C3A-C4A-CHA-C1B
26	c6	1002	PEB	NB-C1B-CHA-C4A
26	c6	1002	PEB	C2B-C1B-CHA-C4A
26	c6	1003	PEB	NA-C4A-CHA-C1B
26	c6	1003	PEB	C3A-C4A-CHA-C1B
26	c6	1003	PEB	NB-C1B-CHA-C4A
26	c6	1003	PEB	C2B-C1B-CHA-C4A
26	d6	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	d6	201	PEB	C3A-C4A-CHA-C1B
26	d6	201	PEB	NB-C1B-CHA-C4A
26	d6	201	PEB	C2B-C1B-CHA-C4A
26	d6	202	PEB	NB-C1B-CHA-C4A
26	d6	202	PEB	C2B-C1B-CHA-C4A
26	e6	201	PEB	NA-C4A-CHA-C1B
26	e6	201	PEB	C3A-C4A-CHA-C1B
26	e6	201	PEB	NB-C1B-CHA-C4A
26	e6	201	PEB	C2B-C1B-CHA-C4A
26	e6	202	PEB	NB-C1B-CHA-C4A
26	e6	202	PEB	C2B-C1B-CHA-C4A
26	f6	201	PEB	NA-C4A-CHA-C1B
26	f6	201	PEB	C3A-C4A-CHA-C1B
26	f6	201	PEB	NB-C1B-CHA-C4A
26	f6	201	PEB	C2B-C1B-CHA-C4A
26	f6	202	PEB	NB-C1B-CHA-C4A
26	f6	202	PEB	C2B-C1B-CHA-C4A
26	g6	201	PEB	NA-C4A-CHA-C1B
26	g6	201	PEB	C3A-C4A-CHA-C1B
26	g6	201	PEB	NB-C1B-CHA-C4A
26	g6	201	PEB	C2B-C1B-CHA-C4A
26	g6	202	PEB	NA-C4A-CHA-C1B
26	g6	202	PEB	C3A-C4A-CHA-C1B
26	g6	202	PEB	NB-C1B-CHA-C4A
26	g6	202	PEB	C2B-C1B-CHA-C4A
26	h6	201	PEB	NA-C4A-CHA-C1B
26	h6	201	PEB	C3A-C4A-CHA-C1B
26	h6	201	PEB	NB-C1B-CHA-C4A
26	h6	201	PEB	C2B-C1B-CHA-C4A
26	h6	202	PEB	NA-C4A-CHA-C1B
26	h6	202	PEB	C3A-C4A-CHA-C1B
26	h6	202	PEB	NB-C1B-CHA-C4A
26	h6	202	PEB	C2B-C1B-CHA-C4A
26	i6	201	PEB	NA-C4A-CHA-C1B
26	i6	201	PEB	C3A-C4A-CHA-C1B
26	i6	201	PEB	NB-C1B-CHA-C4A
26	i6	201	PEB	C2B-C1B-CHA-C4A
26	i6	202	PEB	NA-C4A-CHA-C1B
26	i6	202	PEB	C3A-C4A-CHA-C1B
26	i6	202	PEB	NB-C1B-CHA-C4A
26	i6	202	PEB	C2B-C1B-CHA-C4A
26	j6	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	j6	201	PEB	C3A-C4A-CHA-C1B
26	j6	201	PEB	NB-C1B-CHA-C4A
26	j6	201	PEB	C2B-C1B-CHA-C4A
26	j6	202	PEB	NA-C4A-CHA-C1B
26	j6	202	PEB	C3A-C4A-CHA-C1B
26	j6	202	PEB	NB-C1B-CHA-C4A
26	j6	202	PEB	C2B-C1B-CHA-C4A
26	k6	1001	PEB	NA-C4A-CHA-C1B
26	k6	1001	PEB	C3A-C4A-CHA-C1B
26	k6	1001	PEB	NB-C1B-CHA-C4A
26	k6	1001	PEB	C2B-C1B-CHA-C4A
26	k6	1002	PEB	NA-C4A-CHA-C1B
26	k6	1002	PEB	C3A-C4A-CHA-C1B
26	k6	1002	PEB	NB-C1B-CHA-C4A
26	k6	1002	PEB	C2B-C1B-CHA-C4A
26	l6	201	PEB	NA-C4A-CHA-C1B
26	l6	201	PEB	C3A-C4A-CHA-C1B
26	l6	201	PEB	NB-C1B-CHA-C4A
26	l6	201	PEB	C2B-C1B-CHA-C4A
26	l6	202	PEB	NA-C4A-CHA-C1B
26	l6	202	PEB	C3A-C4A-CHA-C1B
26	l6	202	PEB	NB-C1B-CHA-C4A
26	l6	202	PEB	C2B-C1B-CHA-C4A
26	m6	201	PEB	NA-C4A-CHA-C1B
26	m6	201	PEB	C3A-C4A-CHA-C1B
26	m6	201	PEB	NB-C1B-CHA-C4A
26	m6	201	PEB	C2B-C1B-CHA-C4A
26	m6	202	PEB	NA-C4A-CHA-C1B
26	m6	202	PEB	C3A-C4A-CHA-C1B
26	m6	202	PEB	NB-C1B-CHA-C4A
26	m6	202	PEB	C2B-C1B-CHA-C4A
26	n6	201	PEB	NB-C1B-CHA-C4A
26	n6	201	PEB	C2B-C1B-CHA-C4A
26	n6	202	PEB	C1C-C2C-CAC-CBC
26	n6	202	PEB	C3C-C2C-CAC-CBC
26	n6	202	PEB	NB-C1B-CHA-C4A
26	n6	202	PEB	C2B-C1B-CHA-C4A
26	o6	201	PEB	NA-C4A-CHA-C1B
26	o6	201	PEB	C3A-C4A-CHA-C1B
26	o6	201	PEB	NB-C1B-CHA-C4A
26	o6	201	PEB	C2B-C1B-CHA-C4A
26	o6	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	o6	202	PEB	C3A-C4A-CHA-C1B
26	o6	202	PEB	NB-C1B-CHA-C4A
26	o6	202	PEB	C2B-C1B-CHA-C4A
26	p6	201	PEB	NA-C4A-CHA-C1B
26	p6	201	PEB	C3A-C4A-CHA-C1B
26	p6	201	PEB	NB-C1B-CHA-C4A
26	p6	201	PEB	C2B-C1B-CHA-C4A
26	p6	202	PEB	NB-C1B-CHA-C4A
26	p6	202	PEB	C2B-C1B-CHA-C4A
26	q6	201	PEB	NA-C4A-CHA-C1B
26	q6	201	PEB	C3A-C4A-CHA-C1B
26	q6	201	PEB	NB-C1B-CHA-C4A
26	q6	201	PEB	C2B-C1B-CHA-C4A
26	q6	202	PEB	NA-C4A-CHA-C1B
26	q6	202	PEB	C3A-C4A-CHA-C1B
26	q6	202	PEB	NB-C1B-CHA-C4A
26	q6	202	PEB	C2B-C1B-CHA-C4A
26	r6	201	PEB	NA-C4A-CHA-C1B
26	r6	201	PEB	C3A-C4A-CHA-C1B
26	r6	201	PEB	NB-C1B-CHA-C4A
26	r6	201	PEB	C2B-C1B-CHA-C4A
26	r6	202	PEB	NA-C4A-CHA-C1B
26	r6	202	PEB	C3A-C4A-CHA-C1B
26	r6	202	PEB	NB-C1B-CHA-C4A
26	r6	202	PEB	C2B-C1B-CHA-C4A
26	s6	201	PEB	NA-C4A-CHA-C1B
26	s6	201	PEB	C3A-C4A-CHA-C1B
26	s6	201	PEB	NB-C1B-CHA-C4A
26	s6	201	PEB	C2B-C1B-CHA-C4A
26	s6	202	PEB	NA-C4A-CHA-C1B
26	s6	202	PEB	C3A-C4A-CHA-C1B
26	s6	202	PEB	NB-C1B-CHA-C4A
26	s6	202	PEB	C2B-C1B-CHA-C4A
26	t6	201	PEB	NB-C1B-CHA-C4A
26	t6	201	PEB	C2B-C1B-CHA-C4A
26	t6	202	PEB	NA-C4A-CHA-C1B
26	t6	202	PEB	C3A-C4A-CHA-C1B
26	t6	202	PEB	NB-C1B-CHA-C4A
26	t6	202	PEB	C2B-C1B-CHA-C4A
26	u6	201	PEB	NA-C4A-CHA-C1B
26	u6	201	PEB	C3A-C4A-CHA-C1B
26	u6	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	u6	201	PEB	C2B-C1B-CHA-C4A
26	u6	202	PEB	NA-C4A-CHA-C1B
26	u6	202	PEB	C3A-C4A-CHA-C1B
26	u6	202	PEB	NB-C1B-CHA-C4A
26	u6	202	PEB	C2B-C1B-CHA-C4A
26	v6	201	PEB	NA-C4A-CHA-C1B
26	v6	201	PEB	C3A-C4A-CHA-C1B
26	v6	201	PEB	NB-C1B-CHA-C4A
26	v6	201	PEB	C2B-C1B-CHA-C4A
26	v6	202	PEB	NA-C4A-CHA-C1B
26	v6	202	PEB	C3A-C4A-CHA-C1B
26	v6	202	PEB	NB-C1B-CHA-C4A
26	v6	202	PEB	C2B-C1B-CHA-C4A
26	w6	1001	PEB	NA-C4A-CHA-C1B
26	w6	1001	PEB	C3A-C4A-CHA-C1B
26	w6	1001	PEB	NB-C1B-CHA-C4A
26	w6	1001	PEB	C2B-C1B-CHA-C4A
26	w6	1002	PEB	NA-C4A-CHA-C1B
26	w6	1002	PEB	C3A-C4A-CHA-C1B
26	w6	1002	PEB	NB-C1B-CHA-C4A
26	w6	1002	PEB	C2B-C1B-CHA-C4A
26	x6	201	PEB	NA-C4A-CHA-C1B
26	x6	201	PEB	C3A-C4A-CHA-C1B
26	x6	201	PEB	NB-C1B-CHA-C4A
26	x6	201	PEB	C2B-C1B-CHA-C4A
26	x6	202	PEB	NA-C4A-CHA-C1B
26	x6	202	PEB	C3A-C4A-CHA-C1B
26	x6	202	PEB	NB-C1B-CHA-C4A
26	x6	202	PEB	C2B-C1B-CHA-C4A
26	y6	201	PEB	NA-C4A-CHA-C1B
26	y6	201	PEB	C3A-C4A-CHA-C1B
26	y6	201	PEB	NB-C1B-CHA-C4A
26	y6	201	PEB	C2B-C1B-CHA-C4A
26	y6	202	PEB	NA-C4A-CHA-C1B
26	y6	202	PEB	C3A-C4A-CHA-C1B
26	y6	202	PEB	NB-C1B-CHA-C4A
26	y6	202	PEB	C2B-C1B-CHA-C4A
26	y6	203	PEB	NA-C4A-CHA-C1B
26	y6	203	PEB	C3A-C4A-CHA-C1B
26	y6	203	PEB	NB-C1B-CHA-C4A
26	y6	203	PEB	C2B-C1B-CHA-C4A
26	z6	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	z6	201	PEB	C3A-C4A-CHA-C1B
26	z6	201	PEB	NB-C1B-CHA-C4A
26	z6	201	PEB	C2B-C1B-CHA-C4A
26	z6	202	PEB	NA-C4A-CHA-C1B
26	z6	202	PEB	C3A-C4A-CHA-C1B
26	z6	202	PEB	NB-C1B-CHA-C4A
26	z6	202	PEB	C2B-C1B-CHA-C4A
26	n8	201	PEB	C1C-C2C-CAC-CBC
26	n8	201	PEB	C3C-C2C-CAC-CBC
26	n8	201	PEB	NB-C1B-CHA-C4A
26	n8	201	PEB	C2B-C1B-CHA-C4A
26	o8	201	PEB	NB-C1B-CHA-C4A
26	o8	201	PEB	C2B-C1B-CHA-C4A
26	o8	202	PEB	NA-C4A-CHA-C1B
26	o8	202	PEB	C3A-C4A-CHA-C1B
26	o8	202	PEB	NB-C1B-CHA-C4A
26	o8	202	PEB	C2B-C1B-CHA-C4A
26	p8	201	PEB	NA-C4A-CHA-C1B
26	p8	201	PEB	C3A-C4A-CHA-C1B
26	p8	201	PEB	NB-C1B-CHA-C4A
26	p8	201	PEB	C2B-C1B-CHA-C4A
26	p8	202	PEB	C1C-C2C-CAC-CBC
26	p8	202	PEB	C3C-C2C-CAC-CBC
26	p8	202	PEB	NB-C1B-CHA-C4A
26	p8	202	PEB	C2B-C1B-CHA-C4A
26	q8	201	PEB	NA-C4A-CHA-C1B
26	q8	201	PEB	C3A-C4A-CHA-C1B
26	q8	201	PEB	NB-C1B-CHA-C4A
26	q8	201	PEB	C2B-C1B-CHA-C4A
26	q8	202	PEB	NB-C1B-CHA-C4A
26	q8	202	PEB	C2B-C1B-CHA-C4A
26	r8	201	PEB	NA-C4A-CHA-C1B
26	r8	201	PEB	C3A-C4A-CHA-C1B
26	r8	201	PEB	NB-C1B-CHA-C4A
26	r8	201	PEB	C2B-C1B-CHA-C4A
26	r8	202	PEB	NB-C1B-CHA-C4A
26	r8	202	PEB	C2B-C1B-CHA-C4A
26	s8	201	PEB	NA-C4A-CHA-C1B
26	s8	201	PEB	C3A-C4A-CHA-C1B
26	s8	201	PEB	NB-C1B-CHA-C4A
26	s8	201	PEB	C2B-C1B-CHA-C4A
26	s8	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	s8	202	PEB	C2B-C1B-CHA-C4A
26	t8	201	PEB	NA-C4A-CHA-C1B
26	t8	201	PEB	C3A-C4A-CHA-C1B
26	t8	201	PEB	NB-C1B-CHA-C4A
26	t8	201	PEB	C2B-C1B-CHA-C4A
26	t8	202	PEB	NB-C1B-CHA-C4A
26	t8	202	PEB	C2B-C1B-CHA-C4A
26	u8	201	PEB	NA-C4A-CHA-C1B
26	u8	201	PEB	C3A-C4A-CHA-C1B
26	u8	201	PEB	NB-C1B-CHA-C4A
26	u8	201	PEB	C2B-C1B-CHA-C4A
26	u8	202	PEB	NB-C1B-CHA-C4A
26	u8	202	PEB	C2B-C1B-CHA-C4A
26	A7	201	PEB	NB-C1B-CHA-C4A
26	A7	201	PEB	C2B-C1B-CHA-C4A
26	B7	201	PEB	C1C-C2C-CAC-CBC
26	B7	201	PEB	C3C-C2C-CAC-CBC
26	B7	201	PEB	NB-C1B-CHA-C4A
26	B7	201	PEB	C2B-C1B-CHA-C4A
26	C7	201	PEB	NA-C4A-CHA-C1B
26	C7	201	PEB	C3A-C4A-CHA-C1B
26	C7	201	PEB	NB-C1B-CHA-C4A
26	C7	201	PEB	C2B-C1B-CHA-C4A
26	C7	202	PEB	NB-C1B-CHA-C4A
26	C7	202	PEB	C2B-C1B-CHA-C4A
26	D7	201	PEB	NA-C4A-CHA-C1B
26	D7	201	PEB	C3A-C4A-CHA-C1B
26	D7	201	PEB	NB-C1B-CHA-C4A
26	D7	201	PEB	C2B-C1B-CHA-C4A
26	D7	202	PEB	C1C-C2C-CAC-CBC
26	D7	202	PEB	C3C-C2C-CAC-CBC
26	D7	202	PEB	NB-C1B-CHA-C4A
26	D7	202	PEB	C2B-C1B-CHA-C4A
26	E7	201	PEB	NA-C4A-CHA-C1B
26	E7	201	PEB	C3A-C4A-CHA-C1B
26	E7	201	PEB	NB-C1B-CHA-C4A
26	E7	201	PEB	C2B-C1B-CHA-C4A
26	E7	202	PEB	NB-C1B-CHA-C4A
26	E7	202	PEB	C2B-C1B-CHA-C4A
26	F7	201	PEB	C1C-C2C-CAC-CBC
26	F7	201	PEB	C3C-C2C-CAC-CBC
26	F7	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	F7	201	PEB	C2B-C1B-CHA-C4A
26	G7	201	PEB	NA-C4A-CHA-C1B
26	G7	201	PEB	C3A-C4A-CHA-C1B
26	G7	201	PEB	NB-C1B-CHA-C4A
26	G7	201	PEB	C2B-C1B-CHA-C4A
26	G7	202	PEB	NB-C1B-CHA-C4A
26	G7	202	PEB	C2B-C1B-CHA-C4A
26	H7	201	PEB	NA-C4A-CHA-C1B
26	H7	201	PEB	C3A-C4A-CHA-C1B
26	H7	201	PEB	NB-C1B-CHA-C4A
26	H7	201	PEB	C2B-C1B-CHA-C4A
26	H7	202	PEB	C1C-C2C-CAC-CBC
26	H7	202	PEB	C3C-C2C-CAC-CBC
26	H7	202	PEB	NB-C1B-CHA-C4A
26	H7	202	PEB	C2B-C1B-CHA-C4A
26	I7	201	PEB	NA-C4A-CHA-C1B
26	I7	201	PEB	C3A-C4A-CHA-C1B
26	I7	201	PEB	NB-C1B-CHA-C4A
26	I7	201	PEB	C2B-C1B-CHA-C4A
26	I7	202	PEB	NB-C1B-CHA-C4A
26	I7	202	PEB	C2B-C1B-CHA-C4A
26	J7	201	PEB	C1C-C2C-CAC-CBC
26	J7	201	PEB	C3C-C2C-CAC-CBC
26	J7	201	PEB	NB-C1B-CHA-C4A
26	J7	201	PEB	C2B-C1B-CHA-C4A
26	K7	201	PEB	NA-C4A-CHA-C1B
26	K7	201	PEB	C3A-C4A-CHA-C1B
26	K7	201	PEB	NB-C1B-CHA-C4A
26	K7	201	PEB	C2B-C1B-CHA-C4A
26	K7	202	PEB	NB-C1B-CHA-C4A
26	K7	202	PEB	C2B-C1B-CHA-C4A
26	L7	201	PEB	C1C-C2C-CAC-CBC
26	L7	201	PEB	C3C-C2C-CAC-CBC
26	L7	201	PEB	NB-C1B-CHA-C4A
26	L7	201	PEB	C2B-C1B-CHA-C4A
26	M7	1001	PEB	NA-C4A-CHA-C1B
26	M7	1001	PEB	C3A-C4A-CHA-C1B
26	M7	1001	PEB	NB-C1B-CHA-C4A
26	M7	1001	PEB	C2B-C1B-CHA-C4A
26	M7	1002	PEB	NA-C4A-CHA-C1B
26	M7	1002	PEB	C3A-C4A-CHA-C1B
26	M7	1002	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	M7	1002	PEB	C2B-C1B-CHA-C4A
26	M7	1003	PEB	NB-C1B-CHA-C4A
26	M7	1003	PEB	C2B-C1B-CHA-C4A
26	N7	201	PEB	NA-C4A-CHA-C1B
26	N7	201	PEB	C3A-C4A-CHA-C1B
26	N7	201	PEB	NB-C1B-CHA-C4A
26	N7	201	PEB	C2B-C1B-CHA-C4A
26	N7	202	PEB	C1C-C2C-CAC-CBC
26	N7	202	PEB	C3C-C2C-CAC-CBC
26	N7	202	PEB	NB-C1B-CHA-C4A
26	N7	202	PEB	C2B-C1B-CHA-C4A
26	O7	201	PEB	NA-C4A-CHA-C1B
26	O7	201	PEB	C3A-C4A-CHA-C1B
26	O7	201	PEB	NB-C1B-CHA-C4A
26	O7	201	PEB	C2B-C1B-CHA-C4A
26	O7	202	PEB	NB-C1B-CHA-C4A
26	O7	202	PEB	C2B-C1B-CHA-C4A
26	P7	201	PEB	NA-C4A-CHA-C1B
26	P7	201	PEB	C3A-C4A-CHA-C1B
26	P7	201	PEB	NB-C1B-CHA-C4A
26	P7	201	PEB	C2B-C1B-CHA-C4A
26	P7	202	PEB	C1C-C2C-CAC-CBC
26	P7	202	PEB	C3C-C2C-CAC-CBC
26	P7	202	PEB	NB-C1B-CHA-C4A
26	P7	202	PEB	C2B-C1B-CHA-C4A
26	Q7	201	PEB	NA-C4A-CHA-C1B
26	Q7	201	PEB	C3A-C4A-CHA-C1B
26	Q7	201	PEB	NB-C1B-CHA-C4A
26	Q7	201	PEB	C2B-C1B-CHA-C4A
26	Q7	202	PEB	NB-C1B-CHA-C4A
26	Q7	202	PEB	C2B-C1B-CHA-C4A
26	R7	201	PEB	NA-C4A-CHA-C1B
26	R7	201	PEB	C3A-C4A-CHA-C1B
26	R7	201	PEB	NB-C1B-CHA-C4A
26	R7	201	PEB	C2B-C1B-CHA-C4A
26	R7	202	PEB	C1C-C2C-CAC-CBC
26	R7	202	PEB	C3C-C2C-CAC-CBC
26	R7	202	PEB	NB-C1B-CHA-C4A
26	R7	202	PEB	C2B-C1B-CHA-C4A
26	S7	201	PEB	NA-C4A-CHA-C1B
26	S7	201	PEB	C3A-C4A-CHA-C1B
26	S7	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	S7	201	PEB	C2B-C1B-CHA-C4A
26	S7	202	PEB	NB-C1B-CHA-C4A
26	S7	202	PEB	C2B-C1B-CHA-C4A
26	T7	201	PEB	NA-C4A-CHA-C1B
26	T7	201	PEB	C3A-C4A-CHA-C1B
26	T7	201	PEB	NB-C1B-CHA-C4A
26	T7	201	PEB	C2B-C1B-CHA-C4A
26	T7	202	PEB	C1C-C2C-CAC-CBC
26	T7	202	PEB	C3C-C2C-CAC-CBC
26	T7	202	PEB	NB-C1B-CHA-C4A
26	T7	202	PEB	C2B-C1B-CHA-C4A
26	U7	201	PEB	NA-C4A-CHA-C1B
26	U7	201	PEB	C3A-C4A-CHA-C1B
26	U7	201	PEB	NB-C1B-CHA-C4A
26	U7	201	PEB	C2B-C1B-CHA-C4A
26	U7	202	PEB	NB-C1B-CHA-C4A
26	U7	202	PEB	C2B-C1B-CHA-C4A
26	V7	201	PEB	NA-C4A-CHA-C1B
26	V7	201	PEB	C3A-C4A-CHA-C1B
26	V7	201	PEB	NB-C1B-CHA-C4A
26	V7	201	PEB	C2B-C1B-CHA-C4A
26	V7	202	PEB	C1C-C2C-CAC-CBC
26	V7	202	PEB	C3C-C2C-CAC-CBC
26	V7	202	PEB	NB-C1B-CHA-C4A
26	V7	202	PEB	C2B-C1B-CHA-C4A
26	W7	201	PEB	NA-C4A-CHA-C1B
26	W7	201	PEB	C3A-C4A-CHA-C1B
26	W7	201	PEB	NB-C1B-CHA-C4A
26	W7	201	PEB	C2B-C1B-CHA-C4A
26	W7	202	PEB	NB-C1B-CHA-C4A
26	W7	202	PEB	C2B-C1B-CHA-C4A
26	X7	201	PEB	NA-C4A-CHA-C1B
26	X7	201	PEB	C3A-C4A-CHA-C1B
26	X7	201	PEB	NB-C1B-CHA-C4A
26	X7	201	PEB	C2B-C1B-CHA-C4A
26	X7	202	PEB	C1C-C2C-CAC-CBC
26	X7	202	PEB	C3C-C2C-CAC-CBC
26	X7	202	PEB	NB-C1B-CHA-C4A
26	X7	202	PEB	C2B-C1B-CHA-C4A
26	Y7	1001	PEB	NA-C4A-CHA-C1B
26	Y7	1001	PEB	C3A-C4A-CHA-C1B
26	Y7	1001	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	Y7	1001	PEB	C2B-C1B-CHA-C4A
26	Y7	1002	PEB	NB-C1B-CHA-C4A
26	Y7	1002	PEB	C2B-C1B-CHA-C4A
26	Y7	1003	PEB	C1C-C2C-CAC-CBC
26	Y7	1003	PEB	C3C-C2C-CAC-CBC
26	Y7	1003	PEB	NB-C1B-CHA-C4A
26	Y7	1003	PEB	C2B-C1B-CHA-C4A
26	Z7	201	PEB	NA-C4A-CHA-C1B
26	Z7	201	PEB	C3A-C4A-CHA-C1B
26	Z7	201	PEB	NB-C1B-CHA-C4A
26	Z7	201	PEB	C2B-C1B-CHA-C4A
26	Z7	202	PEB	C1C-C2C-CAC-CBC
26	Z7	202	PEB	C3C-C2C-CAC-CBC
26	Z7	202	PEB	NB-C1B-CHA-C4A
26	Z7	202	PEB	C2B-C1B-CHA-C4A
26	a7	201	PEB	NA-C4A-CHA-C1B
26	a7	201	PEB	C3A-C4A-CHA-C1B
26	a7	201	PEB	NB-C1B-CHA-C4A
26	a7	201	PEB	C2B-C1B-CHA-C4A
26	a7	202	PEB	C1C-C2C-CAC-CBC
26	a7	202	PEB	C3C-C2C-CAC-CBC
26	a7	202	PEB	NB-C1B-CHA-C4A
26	a7	202	PEB	C2B-C1B-CHA-C4A
26	b7	201	PEB	NA-C4A-CHA-C1B
26	b7	201	PEB	C3A-C4A-CHA-C1B
26	b7	201	PEB	NB-C1B-CHA-C4A
26	b7	201	PEB	C2B-C1B-CHA-C4A
26	c7	201	PEB	NA-C4A-CHA-C1B
26	c7	201	PEB	C3A-C4A-CHA-C1B
26	c7	201	PEB	NB-C1B-CHA-C4A
26	c7	201	PEB	C2B-C1B-CHA-C4A
26	c7	202	PEB	C1C-C2C-CAC-CBC
26	c7	202	PEB	C3C-C2C-CAC-CBC
26	c7	202	PEB	NB-C1B-CHA-C4A
26	c7	202	PEB	C2B-C1B-CHA-C4A
26	d7	201	PEB	NA-C4A-CHA-C1B
26	d7	201	PEB	C3A-C4A-CHA-C1B
26	d7	201	PEB	NB-C1B-CHA-C4A
26	d7	201	PEB	C2B-C1B-CHA-C4A
26	d7	202	PEB	C1C-C2C-CAC-CBC
26	d7	202	PEB	C3C-C2C-CAC-CBC
26	d7	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	d7	202	PEB	C2B-C1B-CHA-C4A
26	e7	201	PEB	NA-C4A-CHA-C1B
26	e7	201	PEB	C3A-C4A-CHA-C1B
26	e7	201	PEB	NB-C1B-CHA-C4A
26	e7	201	PEB	C2B-C1B-CHA-C4A
26	e7	202	PEB	C1C-C2C-CAC-CBC
26	e7	202	PEB	C3C-C2C-CAC-CBC
26	e7	202	PEB	NB-C1B-CHA-C4A
26	e7	202	PEB	C2B-C1B-CHA-C4A
26	f7	201	PEB	NA-C4A-CHA-C1B
26	f7	201	PEB	C3A-C4A-CHA-C1B
26	f7	201	PEB	NB-C1B-CHA-C4A
26	f7	201	PEB	C2B-C1B-CHA-C4A
26	f7	202	PEB	NB-C1B-CHA-C4A
26	f7	202	PEB	C2B-C1B-CHA-C4A
26	g7	201	PEB	NA-C4A-CHA-C1B
26	g7	201	PEB	C3A-C4A-CHA-C1B
26	g7	201	PEB	NB-C1B-CHA-C4A
26	g7	201	PEB	C2B-C1B-CHA-C4A
26	g7	202	PEB	NB-C1B-CHA-C4A
26	g7	202	PEB	C2B-C1B-CHA-C4A
26	h7	201	PEB	NA-C4A-CHA-C1B
26	h7	201	PEB	C3A-C4A-CHA-C1B
26	h7	201	PEB	NB-C1B-CHA-C4A
26	h7	201	PEB	C2B-C1B-CHA-C4A
26	h7	202	PEB	NB-C1B-CHA-C4A
26	h7	202	PEB	C2B-C1B-CHA-C4A
26	i7	201	PEB	NA-C4A-CHA-C1B
26	i7	201	PEB	C3A-C4A-CHA-C1B
26	i7	201	PEB	NB-C1B-CHA-C4A
26	i7	201	PEB	C2B-C1B-CHA-C4A
26	i7	202	PEB	NB-C1B-CHA-C4A
26	i7	202	PEB	C2B-C1B-CHA-C4A
26	j7	201	PEB	NA-C4A-CHA-C1B
26	j7	201	PEB	C3A-C4A-CHA-C1B
26	j7	201	PEB	NB-C1B-CHA-C4A
26	j7	201	PEB	C2B-C1B-CHA-C4A
26	j7	202	PEB	NB-C1B-CHA-C4A
26	j7	202	PEB	C2B-C1B-CHA-C4A
26	k7	1001	PEB	NA-C4A-CHA-C1B
26	k7	1001	PEB	C3A-C4A-CHA-C1B
26	k7	1001	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	k7	1001	PEB	C2B-C1B-CHA-C4A
26	k7	1002	PEB	NB-C1B-CHA-C4A
26	k7	1002	PEB	C2B-C1B-CHA-C4A
26	l7	201	PEB	NA-C4A-CHA-C1B
26	l7	201	PEB	C3A-C4A-CHA-C1B
26	l7	201	PEB	NB-C1B-CHA-C4A
26	l7	201	PEB	C2B-C1B-CHA-C4A
26	l7	202	PEB	C1C-C2C-CAC-CBC
26	l7	202	PEB	C3C-C2C-CAC-CBC
26	l7	202	PEB	NB-C1B-CHA-C4A
26	l7	202	PEB	C2B-C1B-CHA-C4A
26	m7	201	PEB	NA-C4A-CHA-C1B
26	m7	201	PEB	C3A-C4A-CHA-C1B
26	m7	201	PEB	NB-C1B-CHA-C4A
26	m7	201	PEB	C2B-C1B-CHA-C4A
26	m7	202	PEB	NB-C1B-CHA-C4A
26	m7	202	PEB	C2B-C1B-CHA-C4A
26	n7	201	PEB	NA-C4A-CHA-C1B
26	n7	201	PEB	C3A-C4A-CHA-C1B
26	n7	201	PEB	NB-C1B-CHA-C4A
26	n7	201	PEB	C2B-C1B-CHA-C4A
26	n7	202	PEB	C1C-C2C-CAC-CBC
26	n7	202	PEB	C3C-C2C-CAC-CBC
26	n7	202	PEB	NB-C1B-CHA-C4A
26	n7	202	PEB	C2B-C1B-CHA-C4A
26	o7	201	PEB	NA-C4A-CHA-C1B
26	o7	201	PEB	C3A-C4A-CHA-C1B
26	o7	201	PEB	NB-C1B-CHA-C4A
26	o7	201	PEB	C2B-C1B-CHA-C4A
26	o7	202	PEB	NB-C1B-CHA-C4A
26	o7	202	PEB	C2B-C1B-CHA-C4A
26	p7	201	PEB	C1C-C2C-CAC-CBC
26	p7	201	PEB	C3C-C2C-CAC-CBC
26	p7	201	PEB	NB-C1B-CHA-C4A
26	p7	201	PEB	C2B-C1B-CHA-C4A
26	q7	201	PEB	NA-C4A-CHA-C1B
26	q7	201	PEB	C3A-C4A-CHA-C1B
26	q7	201	PEB	NB-C1B-CHA-C4A
26	q7	201	PEB	C2B-C1B-CHA-C4A
26	q7	202	PEB	NB-C1B-CHA-C4A
26	q7	202	PEB	C2B-C1B-CHA-C4A
26	r7	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	r7	201	PEB	C3A-C4A-CHA-C1B
26	r7	201	PEB	NB-C1B-CHA-C4A
26	r7	201	PEB	C2B-C1B-CHA-C4A
26	r7	202	PEB	C1C-C2C-CAC-CBC
26	r7	202	PEB	C3C-C2C-CAC-CBC
26	r7	202	PEB	NB-C1B-CHA-C4A
26	r7	202	PEB	C2B-C1B-CHA-C4A
26	s7	201	PEB	NA-C4A-CHA-C1B
26	s7	201	PEB	C3A-C4A-CHA-C1B
26	s7	201	PEB	NB-C1B-CHA-C4A
26	s7	201	PEB	C2B-C1B-CHA-C4A
26	s7	202	PEB	NB-C1B-CHA-C4A
26	s7	202	PEB	C2B-C1B-CHA-C4A
26	t7	201	PEB	NA-C4A-CHA-C1B
26	t7	201	PEB	C3A-C4A-CHA-C1B
26	t7	201	PEB	NB-C1B-CHA-C4A
26	t7	201	PEB	C2B-C1B-CHA-C4A
26	t7	202	PEB	C1C-C2C-CAC-CBC
26	t7	202	PEB	C3C-C2C-CAC-CBC
26	t7	202	PEB	NB-C1B-CHA-C4A
26	t7	202	PEB	C2B-C1B-CHA-C4A
26	u7	201	PEB	NA-C4A-CHA-C1B
26	u7	201	PEB	C3A-C4A-CHA-C1B
26	u7	201	PEB	NB-C1B-CHA-C4A
26	u7	201	PEB	C2B-C1B-CHA-C4A
26	u7	202	PEB	NB-C1B-CHA-C4A
26	u7	202	PEB	C2B-C1B-CHA-C4A
26	v7	201	PEB	NA-C4A-CHA-C1B
26	v7	201	PEB	C3A-C4A-CHA-C1B
26	v7	201	PEB	NB-C1B-CHA-C4A
26	v7	201	PEB	C2B-C1B-CHA-C4A
26	v7	202	PEB	C1C-C2C-CAC-CBC
26	v7	202	PEB	C3C-C2C-CAC-CBC
26	v7	202	PEB	NB-C1B-CHA-C4A
26	v7	202	PEB	C2B-C1B-CHA-C4A
26	w7	1001	PEB	NA-C4A-CHA-C1B
26	w7	1001	PEB	C3A-C4A-CHA-C1B
26	w7	1001	PEB	NB-C1B-CHA-C4A
26	w7	1001	PEB	C2B-C1B-CHA-C4A
26	w7	1002	PEB	NB-C1B-CHA-C4A
26	w7	1002	PEB	C2B-C1B-CHA-C4A
26	x7	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	x7	201	PEB	C3A-C4A-CHA-C1B
26	x7	201	PEB	NB-C1B-CHA-C4A
26	x7	201	PEB	C2B-C1B-CHA-C4A
26	x7	202	PEB	C1C-C2C-CAC-CBC
26	x7	202	PEB	C3C-C2C-CAC-CBC
26	x7	202	PEB	NB-C1B-CHA-C4A
26	x7	202	PEB	C2B-C1B-CHA-C4A
26	y7	201	PEB	NA-C4A-CHA-C1B
26	y7	201	PEB	C3A-C4A-CHA-C1B
26	y7	201	PEB	NB-C1B-CHA-C4A
26	y7	201	PEB	C2B-C1B-CHA-C4A
26	y7	202	PEB	C1C-C2C-CAC-CBC
26	y7	202	PEB	C3C-C2C-CAC-CBC
26	y7	202	PEB	NB-C1B-CHA-C4A
26	y7	202	PEB	C2B-C1B-CHA-C4A
26	z7	201	PEB	NA-C4A-CHA-C1B
26	z7	201	PEB	C3A-C4A-CHA-C1B
26	z7	201	PEB	NB-C1B-CHA-C4A
26	z7	201	PEB	C2B-C1B-CHA-C4A
26	z7	202	PEB	C1C-C2C-CAC-CBC
26	z7	202	PEB	C3C-C2C-CAC-CBC
26	z7	202	PEB	NB-C1B-CHA-C4A
26	z7	202	PEB	C2B-C1B-CHA-C4A
26	a8	601	PEB	NA-C4A-CHA-C1B
26	a8	601	PEB	C3A-C4A-CHA-C1B
26	a8	601	PEB	NB-C1B-CHA-C4A
26	a8	601	PEB	C2B-C1B-CHA-C4A
26	a8	602	PEB	NA-C4A-CHA-C1B
26	a8	602	PEB	C3A-C4A-CHA-C1B
26	a8	602	PEB	NB-C1B-CHA-C4A
26	a8	602	PEB	C2B-C1B-CHA-C4A
26	b8	1001	PEB	NA-C4A-CHA-C1B
26	b8	1001	PEB	C3A-C4A-CHA-C1B
26	b8	1001	PEB	NB-C1B-CHA-C4A
26	b8	1001	PEB	C2B-C1B-CHA-C4A
26	b8	1002	PEB	NA-C4A-CHA-C1B
26	b8	1002	PEB	C3A-C4A-CHA-C1B
26	b8	1002	PEB	NB-C1B-CHA-C4A
26	b8	1002	PEB	C2B-C1B-CHA-C4A
26	b8	1003	PEB	NA-C4A-CHA-C1B
26	b8	1003	PEB	C3A-C4A-CHA-C1B
26	b8	1003	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	b8	1003	PEB	C2B-C1B-CHA-C4A
26	c8	301	PEB	NB-C1B-CHA-C4A
26	c8	301	PEB	C2B-C1B-CHA-C4A
26	c8	302	PEB	NA-C4A-CHA-C1B
26	c8	302	PEB	C3A-C4A-CHA-C1B
26	c8	302	PEB	NB-C1B-CHA-C4A
26	c8	302	PEB	C2B-C1B-CHA-C4A
26	d8	301	PEB	NB-C1B-CHA-C4A
26	d8	301	PEB	C2B-C1B-CHA-C4A
26	d8	302	PEB	NA-C4A-CHA-C1B
26	d8	302	PEB	C3A-C4A-CHA-C1B
26	d8	302	PEB	NB-C1B-CHA-C4A
26	d8	302	PEB	C2B-C1B-CHA-C4A
26	e8	301	PEB	NA-C4A-CHA-C1B
26	e8	301	PEB	C3A-C4A-CHA-C1B
26	e8	301	PEB	NB-C1B-CHA-C4A
26	e8	301	PEB	C2B-C1B-CHA-C4A
26	e8	302	PEB	NA-C4A-CHA-C1B
26	e8	302	PEB	C3A-C4A-CHA-C1B
26	e8	302	PEB	NB-C1B-CHA-C4A
26	e8	302	PEB	C2B-C1B-CHA-C4A
26	a9	601	PEB	NA-C4A-CHA-C1B
26	a9	601	PEB	C3A-C4A-CHA-C1B
26	a9	601	PEB	NB-C1B-CHA-C4A
26	a9	601	PEB	C2B-C1B-CHA-C4A
26	a9	602	PEB	NA-C4A-CHA-C1B
26	a9	602	PEB	C3A-C4A-CHA-C1B
26	a9	602	PEB	NB-C1B-CHA-C4A
26	a9	602	PEB	C2B-C1B-CHA-C4A
26	a9	603	PEB	NA-C4A-CHA-C1B
26	a9	603	PEB	C3A-C4A-CHA-C1B
26	a9	603	PEB	NB-C1B-CHA-C4A
26	a9	603	PEB	C2B-C1B-CHA-C4A
26	b9	401	PEB	NA-C4A-CHA-C1B
26	b9	401	PEB	C3A-C4A-CHA-C1B
26	b9	401	PEB	NB-C1B-CHA-C4A
26	b9	401	PEB	C2B-C1B-CHA-C4A
26	b9	402	PEB	NA-C4A-CHA-C1B
26	b9	402	PEB	C3A-C4A-CHA-C1B
26	b9	402	PEB	NB-C1B-CHA-C4A
26	b9	402	PEB	C2B-C1B-CHA-C4A
26	b9	403	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	b9	403	PEB	C3A-C4A-CHA-C1B
26	b9	403	PEB	NB-C1B-CHA-C4A
26	b9	403	PEB	C2B-C1B-CHA-C4A
26	b9	404	PEB	NA-C4A-CHA-C1B
26	b9	404	PEB	C3A-C4A-CHA-C1B
26	b9	404	PEB	NB-C1B-CHA-C4A
26	b9	404	PEB	C2B-C1B-CHA-C4A
26	c9	301	PEB	NA-C4A-CHA-C1B
26	c9	301	PEB	C3A-C4A-CHA-C1B
26	c9	301	PEB	NB-C1B-CHA-C4A
26	c9	301	PEB	C2B-C1B-CHA-C4A
26	c9	302	PEB	NA-C4A-CHA-C1B
26	c9	302	PEB	C3A-C4A-CHA-C1B
26	c9	302	PEB	NB-C1B-CHA-C4A
26	c9	302	PEB	C2B-C1B-CHA-C4A
26	d9	301	PEB	NA-C4A-CHA-C1B
26	d9	301	PEB	C3A-C4A-CHA-C1B
26	d9	301	PEB	NB-C1B-CHA-C4A
26	d9	301	PEB	C2B-C1B-CHA-C4A
26	d9	302	PEB	NA-C4A-CHA-C1B
26	d9	302	PEB	C3A-C4A-CHA-C1B
26	d9	302	PEB	NB-C1B-CHA-C4A
26	d9	302	PEB	C2B-C1B-CHA-C4A
26	d9	303	PEB	NA-C4A-CHA-C1B
26	d9	303	PEB	C3A-C4A-CHA-C1B
26	d9	303	PEB	NB-C1B-CHA-C4A
26	d9	303	PEB	C2B-C1B-CHA-C4A
26	e9	301	PEB	NA-C4A-CHA-C1B
26	e9	301	PEB	C3A-C4A-CHA-C1B
26	e9	301	PEB	NB-C1B-CHA-C4A
26	e9	301	PEB	C2B-C1B-CHA-C4A
26	e9	302	PEB	NA-C4A-CHA-C1B
26	e9	302	PEB	C3A-C4A-CHA-C1B
26	e9	302	PEB	NB-C1B-CHA-C4A
26	e9	302	PEB	C2B-C1B-CHA-C4A
26	e9	303	PEB	NA-C4A-CHA-C1B
26	e9	303	PEB	C3A-C4A-CHA-C1B
26	e9	303	PEB	NB-C1B-CHA-C4A
26	e9	303	PEB	C2B-C1B-CHA-C4A
26	v8	201	PEB	NA-C4A-CHA-C1B
26	v8	201	PEB	C3A-C4A-CHA-C1B
26	v8	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	v8	201	PEB	C2B-C1B-CHA-C4A
26	v8	202	PEB	NA-C4A-CHA-C1B
26	v8	202	PEB	C3A-C4A-CHA-C1B
26	v8	202	PEB	NB-C1B-CHA-C4A
26	v8	202	PEB	C2B-C1B-CHA-C4A
26	w8	201	PEB	NA-C4A-CHA-C1B
26	w8	201	PEB	C3A-C4A-CHA-C1B
26	w8	201	PEB	NB-C1B-CHA-C4A
26	w8	201	PEB	C2B-C1B-CHA-C4A
26	w8	202	PEB	NA-C4A-CHA-C1B
26	w8	202	PEB	C3A-C4A-CHA-C1B
26	w8	202	PEB	NB-C1B-CHA-C4A
26	w8	202	PEB	C2B-C1B-CHA-C4A
26	x8	201	PEB	NA-C4A-CHA-C1B
26	x8	201	PEB	C3A-C4A-CHA-C1B
26	x8	201	PEB	NB-C1B-CHA-C4A
26	x8	201	PEB	C2B-C1B-CHA-C4A
26	x8	202	PEB	NA-C4A-CHA-C1B
26	x8	202	PEB	C3A-C4A-CHA-C1B
26	x8	202	PEB	NB-C1B-CHA-C4A
26	x8	202	PEB	C2B-C1B-CHA-C4A
26	y8	201	PEB	NA-C4A-CHA-C1B
26	y8	201	PEB	C3A-C4A-CHA-C1B
26	y8	201	PEB	NB-C1B-CHA-C4A
26	y8	201	PEB	C2B-C1B-CHA-C4A
26	y8	202	PEB	C1C-C2C-CAC-CBC
26	y8	202	PEB	C3C-C2C-CAC-CBC
26	y8	202	PEB	NB-C1B-CHA-C4A
26	y8	202	PEB	C2B-C1B-CHA-C4A
26	z8	201	PEB	NA-C4A-CHA-C1B
26	z8	201	PEB	C3A-C4A-CHA-C1B
26	z8	201	PEB	NB-C1B-CHA-C4A
26	z8	201	PEB	C2B-C1B-CHA-C4A
26	z8	202	PEB	NA-C4A-CHA-C1B
26	z8	202	PEB	C3A-C4A-CHA-C1B
26	z8	202	PEB	NB-C1B-CHA-C4A
26	z8	202	PEB	C2B-C1B-CHA-C4A
26	A8	201	PEB	NA-C4A-CHA-C1B
26	A8	201	PEB	C3A-C4A-CHA-C1B
26	A8	201	PEB	NB-C1B-CHA-C4A
26	A8	201	PEB	C2B-C1B-CHA-C4A
26	A8	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	A8	202	PEB	C3A-C4A-CHA-C1B
26	A8	202	PEB	NB-C1B-CHA-C4A
26	A8	202	PEB	C2B-C1B-CHA-C4A
26	B8	201	PEB	NA-C4A-CHA-C1B
26	B8	201	PEB	C3A-C4A-CHA-C1B
26	B8	201	PEB	NB-C1B-CHA-C4A
26	B8	201	PEB	C2B-C1B-CHA-C4A
26	B8	202	PEB	NA-C4A-CHA-C1B
26	B8	202	PEB	C3A-C4A-CHA-C1B
26	B8	202	PEB	NB-C1B-CHA-C4A
26	B8	202	PEB	C2B-C1B-CHA-C4A
26	C8	201	PEB	NA-C4A-CHA-C1B
26	C8	201	PEB	C3A-C4A-CHA-C1B
26	C8	201	PEB	NB-C1B-CHA-C4A
26	C8	201	PEB	C2B-C1B-CHA-C4A
26	C8	202	PEB	C1C-C2C-CAC-CBC
26	C8	202	PEB	C3C-C2C-CAC-CBC
26	C8	202	PEB	NB-C1B-CHA-C4A
26	C8	202	PEB	C2B-C1B-CHA-C4A
26	D8	201	PEB	NA-C4A-CHA-C1B
26	D8	201	PEB	C3A-C4A-CHA-C1B
26	D8	201	PEB	NB-C1B-CHA-C4A
26	D8	201	PEB	C2B-C1B-CHA-C4A
26	D8	202	PEB	NA-C4A-CHA-C1B
26	D8	202	PEB	C3A-C4A-CHA-C1B
26	D8	202	PEB	NB-C1B-CHA-C4A
26	D8	202	PEB	C2B-C1B-CHA-C4A
26	E8	201	PEB	NA-C4A-CHA-C1B
26	E8	201	PEB	C3A-C4A-CHA-C1B
26	E8	201	PEB	NB-C1B-CHA-C4A
26	E8	201	PEB	C2B-C1B-CHA-C4A
26	E8	202	PEB	NA-C4A-CHA-C1B
26	E8	202	PEB	C3A-C4A-CHA-C1B
26	E8	202	PEB	NB-C1B-CHA-C4A
26	E8	202	PEB	C2B-C1B-CHA-C4A
26	F8	1001	PEB	NA-C4A-CHA-C1B
26	F8	1001	PEB	C3A-C4A-CHA-C1B
26	F8	1001	PEB	NB-C1B-CHA-C4A
26	F8	1001	PEB	C2B-C1B-CHA-C4A
26	F8	1002	PEB	NA-C4A-CHA-C1B
26	F8	1002	PEB	C3A-C4A-CHA-C1B
26	F8	1002	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	F8	1002	PEB	C2B-C1B-CHA-C4A
26	G8	201	PEB	NA-C4A-CHA-C1B
26	G8	201	PEB	C3A-C4A-CHA-C1B
26	G8	201	PEB	NB-C1B-CHA-C4A
26	G8	201	PEB	C2B-C1B-CHA-C4A
26	G8	202	PEB	NA-C4A-CHA-C1B
26	G8	202	PEB	C3A-C4A-CHA-C1B
26	G8	202	PEB	NB-C1B-CHA-C4A
26	G8	202	PEB	C2B-C1B-CHA-C4A
26	H8	201	PEB	NA-C4A-CHA-C1B
26	H8	201	PEB	C3A-C4A-CHA-C1B
26	H8	201	PEB	NB-C1B-CHA-C4A
26	H8	201	PEB	C2B-C1B-CHA-C4A
26	H8	202	PEB	NA-C4A-CHA-C1B
26	H8	202	PEB	C3A-C4A-CHA-C1B
26	H8	202	PEB	NB-C1B-CHA-C4A
26	H8	202	PEB	C2B-C1B-CHA-C4A
26	I8	201	PEB	NA-C4A-CHA-C1B
26	I8	201	PEB	C3A-C4A-CHA-C1B
26	I8	201	PEB	NB-C1B-CHA-C4A
26	I8	201	PEB	C2B-C1B-CHA-C4A
26	I8	202	PEB	NA-C4A-CHA-C1B
26	I8	202	PEB	C3A-C4A-CHA-C1B
26	I8	202	PEB	NB-C1B-CHA-C4A
26	I8	202	PEB	C2B-C1B-CHA-C4A
26	J8	201	PEB	NA-C4A-CHA-C1B
26	J8	201	PEB	C3A-C4A-CHA-C1B
26	J8	201	PEB	NB-C1B-CHA-C4A
26	J8	201	PEB	C2B-C1B-CHA-C4A
26	J8	202	PEB	NA-C4A-CHA-C1B
26	J8	202	PEB	C3A-C4A-CHA-C1B
26	J8	202	PEB	NB-C1B-CHA-C4A
26	J8	202	PEB	C2B-C1B-CHA-C4A
26	K8	201	PEB	NA-C4A-CHA-C1B
26	K8	201	PEB	C3A-C4A-CHA-C1B
26	K8	201	PEB	NB-C1B-CHA-C4A
26	K8	201	PEB	C2B-C1B-CHA-C4A
26	K8	202	PEB	NA-C4A-CHA-C1B
26	K8	202	PEB	C3A-C4A-CHA-C1B
26	K8	202	PEB	NB-C1B-CHA-C4A
26	K8	202	PEB	C2B-C1B-CHA-C4A
26	L8	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	L8	201	PEB	C3A-C4A-CHA-C1B
26	L8	201	PEB	NB-C1B-CHA-C4A
26	L8	201	PEB	C2B-C1B-CHA-C4A
26	L8	202	PEB	NA-C4A-CHA-C1B
26	L8	202	PEB	C3A-C4A-CHA-C1B
26	L8	202	PEB	NB-C1B-CHA-C4A
26	L8	202	PEB	C2B-C1B-CHA-C4A
26	M8	201	PEB	NA-C4A-CHA-C1B
26	M8	201	PEB	C3A-C4A-CHA-C1B
26	M8	201	PEB	NB-C1B-CHA-C4A
26	M8	201	PEB	C2B-C1B-CHA-C4A
26	M8	202	PEB	NA-C4A-CHA-C1B
26	M8	202	PEB	C3A-C4A-CHA-C1B
26	M8	202	PEB	NB-C1B-CHA-C4A
26	M8	202	PEB	C2B-C1B-CHA-C4A
26	N8	201	PEB	NA-C4A-CHA-C1B
26	N8	201	PEB	C3A-C4A-CHA-C1B
26	N8	201	PEB	NB-C1B-CHA-C4A
26	N8	201	PEB	C2B-C1B-CHA-C4A
26	N8	202	PEB	NA-C4A-CHA-C1B
26	N8	202	PEB	C3A-C4A-CHA-C1B
26	N8	202	PEB	NB-C1B-CHA-C4A
26	N8	202	PEB	C2B-C1B-CHA-C4A
26	O8	201	PEB	NA-C4A-CHA-C1B
26	O8	201	PEB	C3A-C4A-CHA-C1B
26	O8	201	PEB	NB-C1B-CHA-C4A
26	O8	201	PEB	C2B-C1B-CHA-C4A
26	O8	202	PEB	NA-C4A-CHA-C1B
26	O8	202	PEB	C3A-C4A-CHA-C1B
26	O8	202	PEB	NB-C1B-CHA-C4A
26	O8	202	PEB	C2B-C1B-CHA-C4A
26	P8	201	PEB	NA-C4A-CHA-C1B
26	P8	201	PEB	C3A-C4A-CHA-C1B
26	P8	201	PEB	NB-C1B-CHA-C4A
26	P8	201	PEB	C2B-C1B-CHA-C4A
26	P8	202	PEB	NA-C4A-CHA-C1B
26	P8	202	PEB	C3A-C4A-CHA-C1B
26	P8	202	PEB	NB-C1B-CHA-C4A
26	P8	202	PEB	C2B-C1B-CHA-C4A
26	Q8	201	PEB	NA-C4A-CHA-C1B
26	Q8	201	PEB	C3A-C4A-CHA-C1B
26	Q8	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	Q8	201	PEB	C2B-C1B-CHA-C4A
26	Q8	202	PEB	NA-C4A-CHA-C1B
26	Q8	202	PEB	C3A-C4A-CHA-C1B
26	Q8	202	PEB	NB-C1B-CHA-C4A
26	Q8	202	PEB	C2B-C1B-CHA-C4A
26	S8	401	PEB	NA-C4A-CHA-C1B
26	S8	401	PEB	C3A-C4A-CHA-C1B
26	S8	401	PEB	NB-C1B-CHA-C4A
26	S8	401	PEB	C2B-C1B-CHA-C4A
26	T8	301	PEB	NA-C4A-CHA-C1B
26	T8	301	PEB	C3A-C4A-CHA-C1B
26	T8	301	PEB	NB-C1B-CHA-C4A
26	T8	301	PEB	C2B-C1B-CHA-C4A
26	T8	302	PEB	NA-C4A-CHA-C1B
26	T8	302	PEB	C3A-C4A-CHA-C1B
26	T8	302	PEB	NB-C1B-CHA-C4A
26	T8	302	PEB	C2B-C1B-CHA-C4A
26	U8	1001	PEB	NA-C4A-CHA-C1B
26	U8	1001	PEB	C3A-C4A-CHA-C1B
26	U8	1001	PEB	NB-C1B-CHA-C4A
26	U8	1001	PEB	C2B-C1B-CHA-C4A
26	U8	1002	PEB	NA-C4A-CHA-C1B
26	U8	1002	PEB	C3A-C4A-CHA-C1B
26	U8	1002	PEB	NB-C1B-CHA-C4A
26	U8	1002	PEB	C2B-C1B-CHA-C4A
26	U8	1003	PEB	NA-C4A-CHA-C1B
26	U8	1003	PEB	C3A-C4A-CHA-C1B
26	U8	1003	PEB	NB-C1B-CHA-C4A
26	U8	1003	PEB	C2B-C1B-CHA-C4A
26	V8	1001	PEB	NA-C4A-CHA-C1B
26	V8	1001	PEB	C3A-C4A-CHA-C1B
26	V8	1001	PEB	NB-C1B-CHA-C4A
26	V8	1001	PEB	C2B-C1B-CHA-C4A
26	W8	201	PEB	NA-C4A-CHA-C1B
26	W8	201	PEB	C3A-C4A-CHA-C1B
26	W8	201	PEB	NB-C1B-CHA-C4A
26	W8	201	PEB	C2B-C1B-CHA-C4A
26	W8	202	PEB	NA-C4A-CHA-C1B
26	W8	202	PEB	C3A-C4A-CHA-C1B
26	W8	202	PEB	NB-C1B-CHA-C4A
26	W8	202	PEB	C2B-C1B-CHA-C4A
26	X8	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	X8	201	PEB	C3A-C4A-CHA-C1B
26	X8	201	PEB	NB-C1B-CHA-C4A
26	X8	201	PEB	C2B-C1B-CHA-C4A
26	Y8	201	PEB	NA-C4A-CHA-C1B
26	Y8	201	PEB	C3A-C4A-CHA-C1B
26	Y8	201	PEB	NB-C1B-CHA-C4A
26	Y8	201	PEB	C2B-C1B-CHA-C4A
26	Y8	202	PEB	NA-C4A-CHA-C1B
26	Y8	202	PEB	C3A-C4A-CHA-C1B
26	Y8	202	PEB	NB-C1B-CHA-C4A
26	Y8	202	PEB	C2B-C1B-CHA-C4A
26	Z8	201	PEB	NA-C4A-CHA-C1B
26	Z8	201	PEB	C3A-C4A-CHA-C1B
26	Z8	201	PEB	NB-C1B-CHA-C4A
26	Z8	201	PEB	C2B-C1B-CHA-C4A
26	f9	201	PEB	NA-C4A-CHA-C1B
26	f9	201	PEB	C3A-C4A-CHA-C1B
26	f9	201	PEB	NB-C1B-CHA-C4A
26	f9	201	PEB	C2B-C1B-CHA-C4A
26	f9	202	PEB	NA-C4A-CHA-C1B
26	f9	202	PEB	C3A-C4A-CHA-C1B
26	f9	202	PEB	NB-C1B-CHA-C4A
26	f9	202	PEB	C2B-C1B-CHA-C4A
26	g9	201	PEB	NA-C4A-CHA-C1B
26	g9	201	PEB	C3A-C4A-CHA-C1B
26	g9	201	PEB	NB-C1B-CHA-C4A
26	g9	201	PEB	C2B-C1B-CHA-C4A
26	h9	201	PEB	NA-C4A-CHA-C1B
26	h9	201	PEB	C3A-C4A-CHA-C1B
26	h9	201	PEB	NB-C1B-CHA-C4A
26	h9	201	PEB	C2B-C1B-CHA-C4A
26	h9	202	PEB	NA-C4A-CHA-C1B
26	h9	202	PEB	C3A-C4A-CHA-C1B
26	h9	202	PEB	NB-C1B-CHA-C4A
26	h9	202	PEB	C2B-C1B-CHA-C4A
26	i9	201	PEB	NA-C4A-CHA-C1B
26	i9	201	PEB	C3A-C4A-CHA-C1B
26	i9	201	PEB	NB-C1B-CHA-C4A
26	i9	201	PEB	C2B-C1B-CHA-C4A
26	j9	201	PEB	NA-C4A-CHA-C1B
26	j9	201	PEB	C3A-C4A-CHA-C1B
26	j9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	j9	201	PEB	C2B-C1B-CHA-C4A
26	j9	202	PEB	NA-C4A-CHA-C1B
26	j9	202	PEB	C3A-C4A-CHA-C1B
26	j9	202	PEB	NB-C1B-CHA-C4A
26	j9	202	PEB	C2B-C1B-CHA-C4A
26	k9	201	PEB	NA-C4A-CHA-C1B
26	k9	201	PEB	C3A-C4A-CHA-C1B
26	k9	201	PEB	NB-C1B-CHA-C4A
26	k9	201	PEB	C2B-C1B-CHA-C4A
26	l9	201	PEB	NA-C4A-CHA-C1B
26	l9	201	PEB	C3A-C4A-CHA-C1B
26	l9	201	PEB	NB-C1B-CHA-C4A
26	l9	201	PEB	C2B-C1B-CHA-C4A
26	l9	202	PEB	NA-C4A-CHA-C1B
26	l9	202	PEB	C3A-C4A-CHA-C1B
26	l9	202	PEB	NB-C1B-CHA-C4A
26	l9	202	PEB	C2B-C1B-CHA-C4A
26	m9	1001	PEB	NA-C4A-CHA-C1B
26	m9	1001	PEB	C3A-C4A-CHA-C1B
26	m9	1001	PEB	NB-C1B-CHA-C4A
26	m9	1001	PEB	C2B-C1B-CHA-C4A
26	n9	201	PEB	NA-C4A-CHA-C1B
26	n9	201	PEB	C3A-C4A-CHA-C1B
26	n9	201	PEB	NB-C1B-CHA-C4A
26	n9	201	PEB	C2B-C1B-CHA-C4A
26	o9	201	PEB	NA-C4A-CHA-C1B
26	o9	201	PEB	C3A-C4A-CHA-C1B
26	o9	201	PEB	NB-C1B-CHA-C4A
26	o9	201	PEB	C2B-C1B-CHA-C4A
26	p9	201	PEB	NA-C4A-CHA-C1B
26	p9	201	PEB	C3A-C4A-CHA-C1B
26	p9	201	PEB	NB-C1B-CHA-C4A
26	p9	201	PEB	C2B-C1B-CHA-C4A
26	p9	202	PEB	NA-C4A-CHA-C1B
26	p9	202	PEB	C3A-C4A-CHA-C1B
26	p9	202	PEB	NB-C1B-CHA-C4A
26	p9	202	PEB	C2B-C1B-CHA-C4A
26	q9	201	PEB	NA-C4A-CHA-C1B
26	q9	201	PEB	C3A-C4A-CHA-C1B
26	q9	201	PEB	NB-C1B-CHA-C4A
26	q9	201	PEB	C2B-C1B-CHA-C4A
26	q9	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	q9	202	PEB	C3A-C4A-CHA-C1B
26	q9	202	PEB	NB-C1B-CHA-C4A
26	q9	202	PEB	C2B-C1B-CHA-C4A
26	r9	201	PEB	NA-C4A-CHA-C1B
26	r9	201	PEB	C3A-C4A-CHA-C1B
26	r9	201	PEB	NB-C1B-CHA-C4A
26	r9	201	PEB	C2B-C1B-CHA-C4A
26	r9	202	PEB	NA-C4A-CHA-C1B
26	r9	202	PEB	C3A-C4A-CHA-C1B
26	r9	202	PEB	NB-C1B-CHA-C4A
26	r9	202	PEB	C2B-C1B-CHA-C4A
26	s9	201	PEB	NA-C4A-CHA-C1B
26	s9	201	PEB	C3A-C4A-CHA-C1B
26	s9	201	PEB	NB-C1B-CHA-C4A
26	s9	201	PEB	C2B-C1B-CHA-C4A
26	s9	202	PEB	NA-C4A-CHA-C1B
26	s9	202	PEB	C3A-C4A-CHA-C1B
26	s9	202	PEB	NB-C1B-CHA-C4A
26	s9	202	PEB	C2B-C1B-CHA-C4A
26	t9	201	PEB	NA-C4A-CHA-C1B
26	t9	201	PEB	C3A-C4A-CHA-C1B
26	t9	201	PEB	NB-C1B-CHA-C4A
26	t9	201	PEB	C2B-C1B-CHA-C4A
26	t9	202	PEB	NA-C4A-CHA-C1B
26	t9	202	PEB	C3A-C4A-CHA-C1B
26	t9	202	PEB	NB-C1B-CHA-C4A
26	t9	202	PEB	C2B-C1B-CHA-C4A
26	u9	201	PEB	NA-C4A-CHA-C1B
26	u9	201	PEB	C3A-C4A-CHA-C1B
26	u9	201	PEB	NB-C1B-CHA-C4A
26	u9	201	PEB	C2B-C1B-CHA-C4A
26	u9	202	PEB	NA-C4A-CHA-C1B
26	u9	202	PEB	C3A-C4A-CHA-C1B
26	u9	202	PEB	NB-C1B-CHA-C4A
26	u9	202	PEB	C2B-C1B-CHA-C4A
26	v9	201	PEB	NA-C4A-CHA-C1B
26	v9	201	PEB	C3A-C4A-CHA-C1B
26	v9	201	PEB	NB-C1B-CHA-C4A
26	v9	201	PEB	C2B-C1B-CHA-C4A
26	v9	202	PEB	C1C-C2C-CAC-CBC
26	v9	202	PEB	C3C-C2C-CAC-CBC
26	v9	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	v9	202	PEB	C2B-C1B-CHA-C4A
26	w9	201	PEB	NA-C4A-CHA-C1B
26	w9	201	PEB	C3A-C4A-CHA-C1B
26	w9	201	PEB	NB-C1B-CHA-C4A
26	w9	201	PEB	C2B-C1B-CHA-C4A
26	w9	202	PEB	NA-C4A-CHA-C1B
26	w9	202	PEB	C3A-C4A-CHA-C1B
26	w9	202	PEB	NB-C1B-CHA-C4A
26	w9	202	PEB	C2B-C1B-CHA-C4A
26	x9	201	PEB	NA-C4A-CHA-C1B
26	x9	201	PEB	C3A-C4A-CHA-C1B
26	x9	201	PEB	NB-C1B-CHA-C4A
26	x9	201	PEB	C2B-C1B-CHA-C4A
26	x9	202	PEB	NA-C4A-CHA-C1B
26	x9	202	PEB	C3A-C4A-CHA-C1B
26	x9	202	PEB	NB-C1B-CHA-C4A
26	x9	202	PEB	C2B-C1B-CHA-C4A
26	y9	1001	PEB	NA-C4A-CHA-C1B
26	y9	1001	PEB	C3A-C4A-CHA-C1B
26	y9	1001	PEB	NB-C1B-CHA-C4A
26	y9	1001	PEB	C2B-C1B-CHA-C4A
26	y9	1002	PEB	NA-C4A-CHA-C1B
26	y9	1002	PEB	C3A-C4A-CHA-C1B
26	y9	1002	PEB	NB-C1B-CHA-C4A
26	y9	1002	PEB	C2B-C1B-CHA-C4A
26	z9	201	PEB	NA-C4A-CHA-C1B
26	z9	201	PEB	C3A-C4A-CHA-C1B
26	z9	201	PEB	NB-C1B-CHA-C4A
26	z9	201	PEB	C2B-C1B-CHA-C4A
26	z9	202	PEB	NA-C4A-CHA-C1B
26	z9	202	PEB	C3A-C4A-CHA-C1B
26	z9	202	PEB	NB-C1B-CHA-C4A
26	z9	202	PEB	C2B-C1B-CHA-C4A
26	A9	201	PEB	NA-C4A-CHA-C1B
26	A9	201	PEB	C3A-C4A-CHA-C1B
26	A9	201	PEB	NB-C1B-CHA-C4A
26	A9	201	PEB	C2B-C1B-CHA-C4A
26	A9	202	PEB	NB-C1B-CHA-C4A
26	A9	202	PEB	C2B-C1B-CHA-C4A
26	B9	201	PEB	NA-C4A-CHA-C1B
26	B9	201	PEB	C3A-C4A-CHA-C1B
26	B9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	B9	201	PEB	C2B-C1B-CHA-C4A
26	B9	202	PEB	C1C-C2C-CAC-CBC
26	B9	202	PEB	C3C-C2C-CAC-CBC
26	B9	202	PEB	NB-C1B-CHA-C4A
26	B9	202	PEB	C2B-C1B-CHA-C4A
26	C9	201	PEB	NA-C4A-CHA-C1B
26	C9	201	PEB	C3A-C4A-CHA-C1B
26	C9	201	PEB	NB-C1B-CHA-C4A
26	C9	201	PEB	C2B-C1B-CHA-C4A
26	C9	202	PEB	NB-C1B-CHA-C4A
26	C9	202	PEB	C2B-C1B-CHA-C4A
26	D9	201	PEB	NA-C4A-CHA-C1B
26	D9	201	PEB	C3A-C4A-CHA-C1B
26	D9	201	PEB	NB-C1B-CHA-C4A
26	D9	201	PEB	C2B-C1B-CHA-C4A
26	D9	202	PEB	C1C-C2C-CAC-CBC
26	D9	202	PEB	C3C-C2C-CAC-CBC
26	D9	202	PEB	NB-C1B-CHA-C4A
26	D9	202	PEB	C2B-C1B-CHA-C4A
26	E9	201	PEB	NA-C4A-CHA-C1B
26	E9	201	PEB	C3A-C4A-CHA-C1B
26	E9	201	PEB	NB-C1B-CHA-C4A
26	E9	201	PEB	C2B-C1B-CHA-C4A
26	E9	202	PEB	NB-C1B-CHA-C4A
26	E9	202	PEB	C2B-C1B-CHA-C4A
26	F9	201	PEB	NA-C4A-CHA-C1B
26	F9	201	PEB	C3A-C4A-CHA-C1B
26	F9	201	PEB	NB-C1B-CHA-C4A
26	F9	201	PEB	C2B-C1B-CHA-C4A
26	F9	202	PEB	C1C-C2C-CAC-CBC
26	F9	202	PEB	C3C-C2C-CAC-CBC
26	F9	202	PEB	NB-C1B-CHA-C4A
26	F9	202	PEB	C2B-C1B-CHA-C4A
26	G9	201	PEB	NA-C4A-CHA-C1B
26	G9	201	PEB	C3A-C4A-CHA-C1B
26	G9	201	PEB	NB-C1B-CHA-C4A
26	G9	201	PEB	C2B-C1B-CHA-C4A
26	G9	202	PEB	NB-C1B-CHA-C4A
26	G9	202	PEB	C2B-C1B-CHA-C4A
26	H9	201	PEB	NA-C4A-CHA-C1B
26	H9	201	PEB	C3A-C4A-CHA-C1B
26	H9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	H9	201	PEB	C2B-C1B-CHA-C4A
26	H9	202	PEB	C1C-C2C-CAC-CBC
26	H9	202	PEB	C3C-C2C-CAC-CBC
26	H9	202	PEB	NB-C1B-CHA-C4A
26	H9	202	PEB	C2B-C1B-CHA-C4A
26	I9	201	PEB	NA-C4A-CHA-C1B
26	I9	201	PEB	C3A-C4A-CHA-C1B
26	I9	201	PEB	NB-C1B-CHA-C4A
26	I9	201	PEB	C2B-C1B-CHA-C4A
26	I9	202	PEB	NB-C1B-CHA-C4A
26	I9	202	PEB	C2B-C1B-CHA-C4A
26	J9	201	PEB	NA-C4A-CHA-C1B
26	J9	201	PEB	C3A-C4A-CHA-C1B
26	J9	201	PEB	NB-C1B-CHA-C4A
26	J9	201	PEB	C2B-C1B-CHA-C4A
26	J9	202	PEB	C1C-C2C-CAC-CBC
26	J9	202	PEB	C3C-C2C-CAC-CBC
26	J9	202	PEB	NB-C1B-CHA-C4A
26	J9	202	PEB	C2B-C1B-CHA-C4A
26	K9	1001	PEB	NA-C4A-CHA-C1B
26	K9	1001	PEB	C3A-C4A-CHA-C1B
26	K9	1001	PEB	NB-C1B-CHA-C4A
26	K9	1001	PEB	C2B-C1B-CHA-C4A
26	K9	1002	PEB	NB-C1B-CHA-C4A
26	K9	1002	PEB	C2B-C1B-CHA-C4A
26	L9	201	PEB	NA-C4A-CHA-C1B
26	L9	201	PEB	C3A-C4A-CHA-C1B
26	L9	201	PEB	NB-C1B-CHA-C4A
26	L9	201	PEB	C2B-C1B-CHA-C4A
26	L9	202	PEB	C1C-C2C-CAC-CBC
26	L9	202	PEB	C3C-C2C-CAC-CBC
26	L9	202	PEB	NB-C1B-CHA-C4A
26	L9	202	PEB	C2B-C1B-CHA-C4A
26	M9	201	PEB	NA-C4A-CHA-C1B
26	M9	201	PEB	C3A-C4A-CHA-C1B
26	M9	201	PEB	NB-C1B-CHA-C4A
26	M9	201	PEB	C2B-C1B-CHA-C4A
26	M9	202	PEB	NB-C1B-CHA-C4A
26	M9	202	PEB	C2B-C1B-CHA-C4A
26	N9	201	PEB	NA-C4A-CHA-C1B
26	N9	201	PEB	C3A-C4A-CHA-C1B
26	N9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	N9	201	PEB	C2B-C1B-CHA-C4A
26	N9	202	PEB	C1C-C2C-CAC-CBC
26	N9	202	PEB	C3C-C2C-CAC-CBC
26	N9	202	PEB	NB-C1B-CHA-C4A
26	N9	202	PEB	C2B-C1B-CHA-C4A
26	O9	201	PEB	NA-C4A-CHA-C1B
26	O9	201	PEB	C3A-C4A-CHA-C1B
26	O9	201	PEB	NB-C1B-CHA-C4A
26	O9	201	PEB	C2B-C1B-CHA-C4A
26	O9	202	PEB	NB-C1B-CHA-C4A
26	O9	202	PEB	C2B-C1B-CHA-C4A
26	P9	201	PEB	NA-C4A-CHA-C1B
26	P9	201	PEB	C3A-C4A-CHA-C1B
26	P9	201	PEB	NB-C1B-CHA-C4A
26	P9	201	PEB	C2B-C1B-CHA-C4A
26	P9	202	PEB	C1C-C2C-CAC-CBC
26	P9	202	PEB	C3C-C2C-CAC-CBC
26	P9	202	PEB	NB-C1B-CHA-C4A
26	P9	202	PEB	C2B-C1B-CHA-C4A
26	Q9	201	PEB	NA-C4A-CHA-C1B
26	Q9	201	PEB	C3A-C4A-CHA-C1B
26	Q9	201	PEB	NB-C1B-CHA-C4A
26	Q9	201	PEB	C2B-C1B-CHA-C4A
26	Q9	202	PEB	NB-C1B-CHA-C4A
26	Q9	202	PEB	C2B-C1B-CHA-C4A
26	R9	201	PEB	NA-C4A-CHA-C1B
26	R9	201	PEB	C3A-C4A-CHA-C1B
26	R9	201	PEB	NB-C1B-CHA-C4A
26	R9	201	PEB	C2B-C1B-CHA-C4A
26	R9	202	PEB	C1C-C2C-CAC-CBC
26	R9	202	PEB	C3C-C2C-CAC-CBC
26	R9	202	PEB	NB-C1B-CHA-C4A
26	R9	202	PEB	C2B-C1B-CHA-C4A
26	S9	201	PEB	NA-C4A-CHA-C1B
26	S9	201	PEB	C3A-C4A-CHA-C1B
26	S9	201	PEB	NB-C1B-CHA-C4A
26	S9	201	PEB	C2B-C1B-CHA-C4A
26	S9	202	PEB	NB-C1B-CHA-C4A
26	S9	202	PEB	C2B-C1B-CHA-C4A
26	T9	201	PEB	NA-C4A-CHA-C1B
26	T9	201	PEB	C3A-C4A-CHA-C1B
26	T9	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	T9	201	PEB	C2B-C1B-CHA-C4A
26	T9	202	PEB	C1C-C2C-CAC-CBC
26	T9	202	PEB	C3C-C2C-CAC-CBC
26	T9	202	PEB	NB-C1B-CHA-C4A
26	T9	202	PEB	C2B-C1B-CHA-C4A
26	U9	201	PEB	NA-C4A-CHA-C1B
26	U9	201	PEB	C3A-C4A-CHA-C1B
26	U9	201	PEB	NB-C1B-CHA-C4A
26	U9	201	PEB	C2B-C1B-CHA-C4A
26	U9	202	PEB	NB-C1B-CHA-C4A
26	U9	202	PEB	C2B-C1B-CHA-C4A
26	V9	201	PEB	NA-C4A-CHA-C1B
26	V9	201	PEB	C3A-C4A-CHA-C1B
26	V9	201	PEB	NB-C1B-CHA-C4A
26	V9	201	PEB	C2B-C1B-CHA-C4A
26	V9	202	PEB	C1C-C2C-CAC-CBC
26	V9	202	PEB	C3C-C2C-CAC-CBC
26	V9	202	PEB	NB-C1B-CHA-C4A
26	V9	202	PEB	C2B-C1B-CHA-C4A
26	X9	401	PEB	NA-C4A-CHA-C1B
26	X9	401	PEB	C3A-C4A-CHA-C1B
26	X9	401	PEB	NB-C1B-CHA-C4A
26	X9	401	PEB	C2B-C1B-CHA-C4A
26	Y9	301	PEB	NB-C1B-CHA-C4A
26	Y9	301	PEB	C2B-C1B-CHA-C4A
26	Y9	302	PEB	NA-C4A-CHA-C1B
26	Y9	302	PEB	C3A-C4A-CHA-C1B
26	Y9	302	PEB	NB-C1B-CHA-C4A
26	Y9	302	PEB	C2B-C1B-CHA-C4A
26	Z9	1001	PEB	NA-C4A-CHA-C1B
26	Z9	1001	PEB	C3A-C4A-CHA-C1B
26	Z9	1001	PEB	NB-C1B-CHA-C4A
26	Z9	1001	PEB	C2B-C1B-CHA-C4A
26	Z9	1002	PEB	NB-C1B-CHA-C4A
26	Z9	1002	PEB	C2B-C1B-CHA-C4A
26	Z9	1003	PEB	NA-C4A-CHA-C1B
26	Z9	1003	PEB	C3A-C4A-CHA-C1B
26	Z9	1003	PEB	NB-C1B-CHA-C4A
26	Z9	1003	PEB	C2B-C1B-CHA-C4A
26	Z9	1007	PEB	NA-C4A-CHA-C1B
26	Z9	1007	PEB	C3A-C4A-CHA-C1B
26	Z9	1007	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	Z9	1007	PEB	C2B-C1B-CHA-C4A
26	aa	1001	PEB	NA-C4A-CHA-C1B
26	aa	1001	PEB	C3A-C4A-CHA-C1B
26	aa	1001	PEB	NB-C1B-CHA-C4A
26	aa	1001	PEB	C2B-C1B-CHA-C4A
26	ab	201	PEB	NA-C4A-CHA-C1B
26	ab	201	PEB	C3A-C4A-CHA-C1B
26	ab	201	PEB	NB-C1B-CHA-C4A
26	ab	201	PEB	C2B-C1B-CHA-C4A
26	ab	202	PEB	C1C-C2C-CAC-CBC
26	ab	202	PEB	C3C-C2C-CAC-CBC
26	ab	202	PEB	NB-C1B-CHA-C4A
26	ab	202	PEB	C2B-C1B-CHA-C4A
26	ac	201	PEB	NA-C4A-CHA-C1B
26	ac	201	PEB	C3A-C4A-CHA-C1B
26	ac	201	PEB	NB-C1B-CHA-C4A
26	ac	201	PEB	C2B-C1B-CHA-C4A
26	ad	201	PEB	NA-C4A-CHA-C1B
26	ad	201	PEB	C3A-C4A-CHA-C1B
26	ad	201	PEB	NB-C1B-CHA-C4A
26	ad	201	PEB	C2B-C1B-CHA-C4A
26	ad	202	PEB	C1C-C2C-CAC-CBC
26	ad	202	PEB	C3C-C2C-CAC-CBC
26	ad	202	PEB	NB-C1B-CHA-C4A
26	ad	202	PEB	C2B-C1B-CHA-C4A
26	ae	201	PEB	NA-C4A-CHA-C1B
26	ae	201	PEB	C3A-C4A-CHA-C1B
26	ae	201	PEB	NB-C1B-CHA-C4A
26	ae	201	PEB	C2B-C1B-CHA-C4A
26	af	201	PEB	NA-C4A-CHA-C1B
26	af	201	PEB	C3A-C4A-CHA-C1B
26	af	201	PEB	NB-C1B-CHA-C4A
26	af	201	PEB	C2B-C1B-CHA-C4A
26	af	202	PEB	C1C-C2C-CAC-CBC
26	af	202	PEB	C3C-C2C-CAC-CBC
26	af	202	PEB	NB-C1B-CHA-C4A
26	af	202	PEB	C2B-C1B-CHA-C4A
26	ag	201	PEB	NA-C4A-CHA-C1B
26	ag	201	PEB	C3A-C4A-CHA-C1B
26	ag	201	PEB	NB-C1B-CHA-C4A
26	ag	201	PEB	C2B-C1B-CHA-C4A
26	ah	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	ah	201	PEB	C3A-C4A-CHA-C1B
26	ah	201	PEB	NB-C1B-CHA-C4A
26	ah	201	PEB	C2B-C1B-CHA-C4A
26	ah	202	PEB	C1C-C2C-CAC-CBC
26	ah	202	PEB	C3C-C2C-CAC-CBC
26	ah	202	PEB	NB-C1B-CHA-C4A
26	ah	202	PEB	C2B-C1B-CHA-C4A
26	ai	201	PEB	NA-C4A-CHA-C1B
26	ai	201	PEB	C3A-C4A-CHA-C1B
26	ai	201	PEB	NB-C1B-CHA-C4A
26	ai	201	PEB	C2B-C1B-CHA-C4A
26	aj	201	PEB	NA-C4A-CHA-C1B
26	aj	201	PEB	C3A-C4A-CHA-C1B
26	aj	201	PEB	NB-C1B-CHA-C4A
26	aj	201	PEB	C2B-C1B-CHA-C4A
26	aj	202	PEB	C1C-C2C-CAC-CBC
26	aj	202	PEB	C3C-C2C-CAC-CBC
26	aj	202	PEB	NB-C1B-CHA-C4A
26	aj	202	PEB	C2B-C1B-CHA-C4A
26	ak	201	PEB	NA-C4A-CHA-C1B
26	ak	201	PEB	C3A-C4A-CHA-C1B
26	ak	201	PEB	NB-C1B-CHA-C4A
26	ak	201	PEB	C2B-C1B-CHA-C4A
26	al	201	PEB	NA-C4A-CHA-C1B
26	al	201	PEB	C3A-C4A-CHA-C1B
26	al	201	PEB	NB-C1B-CHA-C4A
26	al	201	PEB	C2B-C1B-CHA-C4A
26	al	202	PEB	C1C-C2C-CAC-CBC
26	al	202	PEB	C3C-C2C-CAC-CBC
26	al	202	PEB	NB-C1B-CHA-C4A
26	al	202	PEB	C2B-C1B-CHA-C4A
26	am	1001	PEB	NA-C4A-CHA-C1B
26	am	1001	PEB	C3A-C4A-CHA-C1B
26	am	1001	PEB	NB-C1B-CHA-C4A
26	am	1001	PEB	C2B-C1B-CHA-C4A
26	an	201	PEB	C1C-C2C-CAC-CBC
26	an	201	PEB	C3C-C2C-CAC-CBC
26	an	201	PEB	NB-C1B-CHA-C4A
26	an	201	PEB	C2B-C1B-CHA-C4A
26	ao	201	PEB	NA-C4A-CHA-C1B
26	ao	201	PEB	C3A-C4A-CHA-C1B
26	ao	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	ao	201	PEB	C2B-C1B-CHA-C4A
26	ao	202	PEB	NB-C1B-CHA-C4A
26	ao	202	PEB	C2B-C1B-CHA-C4A
26	ap	201	PEB	NA-C4A-CHA-C1B
26	ap	201	PEB	C3A-C4A-CHA-C1B
26	ap	201	PEB	NB-C1B-CHA-C4A
26	ap	201	PEB	C2B-C1B-CHA-C4A
26	ap	202	PEB	C1C-C2C-CAC-CBC
26	ap	202	PEB	C3C-C2C-CAC-CBC
26	ap	202	PEB	NB-C1B-CHA-C4A
26	ap	202	PEB	C2B-C1B-CHA-C4A
26	aq	201	PEB	NA-C4A-CHA-C1B
26	aq	201	PEB	C3A-C4A-CHA-C1B
26	aq	201	PEB	NB-C1B-CHA-C4A
26	aq	201	PEB	C2B-C1B-CHA-C4A
26	aq	202	PEB	NB-C1B-CHA-C4A
26	aq	202	PEB	C2B-C1B-CHA-C4A
26	ar	201	PEB	NA-C4A-CHA-C1B
26	ar	201	PEB	C3A-C4A-CHA-C1B
26	ar	201	PEB	NB-C1B-CHA-C4A
26	ar	201	PEB	C2B-C1B-CHA-C4A
26	ar	202	PEB	C1C-C2C-CAC-CBC
26	ar	202	PEB	C3C-C2C-CAC-CBC
26	ar	202	PEB	NB-C1B-CHA-C4A
26	ar	202	PEB	C2B-C1B-CHA-C4A
26	as	201	PEB	NA-C4A-CHA-C1B
26	as	201	PEB	C3A-C4A-CHA-C1B
26	as	201	PEB	NB-C1B-CHA-C4A
26	as	201	PEB	C2B-C1B-CHA-C4A
26	as	202	PEB	NB-C1B-CHA-C4A
26	as	202	PEB	C2B-C1B-CHA-C4A
26	at	201	PEB	NA-C4A-CHA-C1B
26	at	201	PEB	C3A-C4A-CHA-C1B
26	at	201	PEB	NB-C1B-CHA-C4A
26	at	201	PEB	C2B-C1B-CHA-C4A
26	at	202	PEB	C1C-C2C-CAC-CBC
26	at	202	PEB	C3C-C2C-CAC-CBC
26	at	202	PEB	NB-C1B-CHA-C4A
26	at	202	PEB	C2B-C1B-CHA-C4A
26	au	201	PEB	NA-C4A-CHA-C1B
26	au	201	PEB	C3A-C4A-CHA-C1B
26	au	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	au	201	PEB	C2B-C1B-CHA-C4A
26	au	202	PEB	NB-C1B-CHA-C4A
26	au	202	PEB	C2B-C1B-CHA-C4A
26	av	201	PEB	NA-C4A-CHA-C1B
26	av	201	PEB	C3A-C4A-CHA-C1B
26	av	201	PEB	NB-C1B-CHA-C4A
26	av	201	PEB	C2B-C1B-CHA-C4A
26	av	202	PEB	C1C-C2C-CAC-CBC
26	av	202	PEB	C3C-C2C-CAC-CBC
26	av	202	PEB	NB-C1B-CHA-C4A
26	av	202	PEB	C2B-C1B-CHA-C4A
26	aw	201	PEB	NA-C4A-CHA-C1B
26	aw	201	PEB	C3A-C4A-CHA-C1B
26	aw	201	PEB	NB-C1B-CHA-C4A
26	aw	201	PEB	C2B-C1B-CHA-C4A
26	aw	202	PEB	NB-C1B-CHA-C4A
26	aw	202	PEB	C2B-C1B-CHA-C4A
26	ax	201	PEB	C1C-C2C-CAC-CBC
26	ax	201	PEB	C3C-C2C-CAC-CBC
26	ax	201	PEB	NB-C1B-CHA-C4A
26	ax	201	PEB	C2B-C1B-CHA-C4A
26	ay	1001	PEB	NA-C4A-CHA-C1B
26	ay	1001	PEB	C3A-C4A-CHA-C1B
26	ay	1001	PEB	NB-C1B-CHA-C4A
26	ay	1001	PEB	C2B-C1B-CHA-C4A
26	ay	1002	PEB	NB-C1B-CHA-C4A
26	ay	1002	PEB	C2B-C1B-CHA-C4A
26	az	201	PEB	NA-C4A-CHA-C1B
26	az	201	PEB	C3A-C4A-CHA-C1B
26	az	201	PEB	NB-C1B-CHA-C4A
26	az	201	PEB	C2B-C1B-CHA-C4A
26	az	202	PEB	C1C-C2C-CAC-CBC
26	az	202	PEB	C3C-C2C-CAC-CBC
26	az	202	PEB	NB-C1B-CHA-C4A
26	az	202	PEB	C2B-C1B-CHA-C4A
26	aA	201	PEB	NA-C4A-CHA-C1B
26	aA	201	PEB	C3A-C4A-CHA-C1B
26	aA	201	PEB	NB-C1B-CHA-C4A
26	aA	201	PEB	C2B-C1B-CHA-C4A
26	aA	202	PEB	NA-C4A-CHA-C1B
26	aA	202	PEB	C3A-C4A-CHA-C1B
26	aA	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	aA	202	PEB	C2B-C1B-CHA-C4A
26	aB	201	PEB	NA-C4A-CHA-C1B
26	aB	201	PEB	C3A-C4A-CHA-C1B
26	aB	201	PEB	NB-C1B-CHA-C4A
26	aB	201	PEB	C2B-C1B-CHA-C4A
26	aB	202	PEB	NA-C4A-CHA-C1B
26	aB	202	PEB	C3A-C4A-CHA-C1B
26	aB	202	PEB	NB-C1B-CHA-C4A
26	aB	202	PEB	C2B-C1B-CHA-C4A
26	aC	201	PEB	NA-C4A-CHA-C1B
26	aC	201	PEB	C3A-C4A-CHA-C1B
26	aC	201	PEB	NB-C1B-CHA-C4A
26	aC	201	PEB	C2B-C1B-CHA-C4A
26	aC	202	PEB	NA-C4A-CHA-C1B
26	aC	202	PEB	C3A-C4A-CHA-C1B
26	aC	202	PEB	NB-C1B-CHA-C4A
26	aC	202	PEB	C2B-C1B-CHA-C4A
26	aD	201	PEB	NA-C4A-CHA-C1B
26	aD	201	PEB	C3A-C4A-CHA-C1B
26	aD	201	PEB	NB-C1B-CHA-C4A
26	aD	201	PEB	C2B-C1B-CHA-C4A
26	aD	202	PEB	C1C-C2C-CAC-CBC
26	aD	202	PEB	C3C-C2C-CAC-CBC
26	aD	202	PEB	NB-C1B-CHA-C4A
26	aD	202	PEB	C2B-C1B-CHA-C4A
26	aE	201	PEB	NA-C4A-CHA-C1B
26	aE	201	PEB	C3A-C4A-CHA-C1B
26	aE	201	PEB	NB-C1B-CHA-C4A
26	aE	201	PEB	C2B-C1B-CHA-C4A
26	aE	202	PEB	NA-C4A-CHA-C1B
26	aE	202	PEB	C3A-C4A-CHA-C1B
26	aE	202	PEB	NB-C1B-CHA-C4A
26	aE	202	PEB	C2B-C1B-CHA-C4A
26	aF	201	PEB	NA-C4A-CHA-C1B
26	aF	201	PEB	C3A-C4A-CHA-C1B
26	aF	201	PEB	NB-C1B-CHA-C4A
26	aF	201	PEB	C2B-C1B-CHA-C4A
26	aF	202	PEB	C1C-C2C-CAC-CBC
26	aF	202	PEB	C3C-C2C-CAC-CBC
26	aF	202	PEB	NB-C1B-CHA-C4A
26	aF	202	PEB	C2B-C1B-CHA-C4A
26	aF	204	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	aF	204	PEB	C3A-C4A-CHA-C1B
26	aF	204	PEB	NB-C1B-CHA-C4A
26	aF	204	PEB	C2B-C1B-CHA-C4A
26	aG	201	PEB	NA-C4A-CHA-C1B
26	aG	201	PEB	C3A-C4A-CHA-C1B
26	aG	201	PEB	NB-C1B-CHA-C4A
26	aG	201	PEB	C2B-C1B-CHA-C4A
26	aH	201	PEB	NA-C4A-CHA-C1B
26	aH	201	PEB	C3A-C4A-CHA-C1B
26	aH	201	PEB	NB-C1B-CHA-C4A
26	aH	201	PEB	C2B-C1B-CHA-C4A
26	aH	202	PEB	NA-C4A-CHA-C1B
26	aH	202	PEB	C3A-C4A-CHA-C1B
26	aH	202	PEB	NB-C1B-CHA-C4A
26	aH	202	PEB	C2B-C1B-CHA-C4A
26	aI	201	PEB	NA-C4A-CHA-C1B
26	aI	201	PEB	C3A-C4A-CHA-C1B
26	aI	201	PEB	NB-C1B-CHA-C4A
26	aI	201	PEB	C2B-C1B-CHA-C4A
26	aI	202	PEB	NA-C4A-CHA-C1B
26	aI	202	PEB	C3A-C4A-CHA-C1B
26	aI	202	PEB	NB-C1B-CHA-C4A
26	aI	202	PEB	C2B-C1B-CHA-C4A
26	aJ	201	PEB	NA-C4A-CHA-C1B
26	aJ	201	PEB	C3A-C4A-CHA-C1B
26	aJ	201	PEB	NB-C1B-CHA-C4A
26	aJ	201	PEB	C2B-C1B-CHA-C4A
26	aJ	202	PEB	NA-C4A-CHA-C1B
26	aJ	202	PEB	C3A-C4A-CHA-C1B
26	aJ	202	PEB	NB-C1B-CHA-C4A
26	aJ	202	PEB	C2B-C1B-CHA-C4A
26	aK	1001	PEB	NA-C4A-CHA-C1B
26	aK	1001	PEB	C3A-C4A-CHA-C1B
26	aK	1001	PEB	NB-C1B-CHA-C4A
26	aK	1001	PEB	C2B-C1B-CHA-C4A
26	aK	1002	PEB	NA-C4A-CHA-C1B
26	aK	1002	PEB	C3A-C4A-CHA-C1B
26	aK	1002	PEB	NB-C1B-CHA-C4A
26	aK	1002	PEB	C2B-C1B-CHA-C4A
26	aL	201	PEB	NA-C4A-CHA-C1B
26	aL	201	PEB	C3A-C4A-CHA-C1B
26	aL	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	aL	201	PEB	C2B-C1B-CHA-C4A
26	aL	202	PEB	NA-C4A-CHA-C1B
26	aL	202	PEB	C3A-C4A-CHA-C1B
26	aL	202	PEB	NB-C1B-CHA-C4A
26	aL	202	PEB	C2B-C1B-CHA-C4A
26	aM	201	PEB	NA-C4A-CHA-C1B
26	aM	201	PEB	C3A-C4A-CHA-C1B
26	aM	201	PEB	NB-C1B-CHA-C4A
26	aM	201	PEB	C2B-C1B-CHA-C4A
26	aM	202	PEB	NA-C4A-CHA-C1B
26	aM	202	PEB	C3A-C4A-CHA-C1B
26	aM	202	PEB	NB-C1B-CHA-C4A
26	aM	202	PEB	C2B-C1B-CHA-C4A
26	aN	201	PEB	NA-C4A-CHA-C1B
26	aN	201	PEB	C3A-C4A-CHA-C1B
26	aN	201	PEB	NB-C1B-CHA-C4A
26	aN	201	PEB	C2B-C1B-CHA-C4A
26	aN	202	PEB	NA-C4A-CHA-C1B
26	aN	202	PEB	C3A-C4A-CHA-C1B
26	aN	202	PEB	NB-C1B-CHA-C4A
26	aN	202	PEB	C2B-C1B-CHA-C4A
26	aN	204	PEB	NA-C4A-CHA-C1B
26	aN	204	PEB	C3A-C4A-CHA-C1B
26	aN	204	PEB	NB-C1B-CHA-C4A
26	aN	204	PEB	C2B-C1B-CHA-C4A
26	aO	201	PEB	NA-C4A-CHA-C1B
26	aO	201	PEB	C3A-C4A-CHA-C1B
26	aO	201	PEB	NB-C1B-CHA-C4A
26	aO	201	PEB	C2B-C1B-CHA-C4A
26	aP	201	PEB	NA-C4A-CHA-C1B
26	aP	201	PEB	C3A-C4A-CHA-C1B
26	aP	201	PEB	NB-C1B-CHA-C4A
26	aP	201	PEB	C2B-C1B-CHA-C4A
26	aP	202	PEB	NA-C4A-CHA-C1B
26	aP	202	PEB	C3A-C4A-CHA-C1B
26	aP	202	PEB	NB-C1B-CHA-C4A
26	aP	202	PEB	C2B-C1B-CHA-C4A
26	aQ	201	PEB	NA-C4A-CHA-C1B
26	aQ	201	PEB	C3A-C4A-CHA-C1B
26	aQ	201	PEB	NB-C1B-CHA-C4A
26	aQ	201	PEB	C2B-C1B-CHA-C4A
26	aQ	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	aQ	202	PEB	C3A-C4A-CHA-C1B
26	aQ	202	PEB	NB-C1B-CHA-C4A
26	aQ	202	PEB	C2B-C1B-CHA-C4A
26	aR	201	PEB	NA-C4A-CHA-C1B
26	aR	201	PEB	C3A-C4A-CHA-C1B
26	aR	201	PEB	NB-C1B-CHA-C4A
26	aR	201	PEB	C2B-C1B-CHA-C4A
26	aR	202	PEB	NA-C4A-CHA-C1B
26	aR	202	PEB	C3A-C4A-CHA-C1B
26	aR	202	PEB	NB-C1B-CHA-C4A
26	aR	202	PEB	C2B-C1B-CHA-C4A
26	aS	201	PEB	NA-C4A-CHA-C1B
26	aS	201	PEB	C3A-C4A-CHA-C1B
26	aS	201	PEB	NB-C1B-CHA-C4A
26	aS	201	PEB	C2B-C1B-CHA-C4A
26	aS	202	PEB	NA-C4A-CHA-C1B
26	aS	202	PEB	C3A-C4A-CHA-C1B
26	aS	202	PEB	NB-C1B-CHA-C4A
26	aS	202	PEB	C2B-C1B-CHA-C4A
26	aT	201	PEB	NA-C4A-CHA-C1B
26	aT	201	PEB	C3A-C4A-CHA-C1B
26	aT	201	PEB	NB-C1B-CHA-C4A
26	aT	201	PEB	C2B-C1B-CHA-C4A
26	aT	202	PEB	NA-C4A-CHA-C1B
26	aT	202	PEB	C3A-C4A-CHA-C1B
26	aT	202	PEB	NB-C1B-CHA-C4A
26	aT	202	PEB	C2B-C1B-CHA-C4A
26	aU	201	PEB	NA-C4A-CHA-C1B
26	aU	201	PEB	C3A-C4A-CHA-C1B
26	aU	201	PEB	NB-C1B-CHA-C4A
26	aU	201	PEB	C2B-C1B-CHA-C4A
26	aU	202	PEB	NA-C4A-CHA-C1B
26	aU	202	PEB	C3A-C4A-CHA-C1B
26	aU	202	PEB	NB-C1B-CHA-C4A
26	aU	202	PEB	C2B-C1B-CHA-C4A
26	aV	201	PEB	NA-C4A-CHA-C1B
26	aV	201	PEB	C3A-C4A-CHA-C1B
26	aV	201	PEB	NB-C1B-CHA-C4A
26	aV	201	PEB	C2B-C1B-CHA-C4A
26	aV	202	PEB	NA-C4A-CHA-C1B
26	aV	202	PEB	C3A-C4A-CHA-C1B
26	aV	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	aV	202	PEB	C2B-C1B-CHA-C4A
26	aW	301	PEB	NA-C4A-CHA-C1B
26	aW	301	PEB	C3A-C4A-CHA-C1B
26	aW	301	PEB	NB-C1B-CHA-C4A
26	aW	301	PEB	C2B-C1B-CHA-C4A
26	aW	302	PEB	NA-C4A-CHA-C1B
26	aW	302	PEB	C3A-C4A-CHA-C1B
26	aW	302	PEB	NB-C1B-CHA-C4A
26	aW	302	PEB	C2B-C1B-CHA-C4A
26	aX	401	PEB	NA-C4A-CHA-C1B
26	aX	401	PEB	C3A-C4A-CHA-C1B
26	aX	401	PEB	NB-C1B-CHA-C4A
26	aX	401	PEB	C2B-C1B-CHA-C4A
26	aX	402	PEB	NA-C4A-CHA-C1B
26	aX	402	PEB	C3A-C4A-CHA-C1B
26	aX	402	PEB	NB-C1B-CHA-C4A
26	aX	402	PEB	C2B-C1B-CHA-C4A
26	aY	401	PEB	NA-C4A-CHA-C1B
26	aY	401	PEB	C3A-C4A-CHA-C1B
26	aY	401	PEB	NB-C1B-CHA-C4A
26	aY	401	PEB	C2B-C1B-CHA-C4A
26	aY	402	PEB	NA-C4A-CHA-C1B
26	aY	402	PEB	C3A-C4A-CHA-C1B
26	aY	402	PEB	NB-C1B-CHA-C4A
26	aY	402	PEB	C2B-C1B-CHA-C4A
26	aY	406	PEB	NA-C4A-CHA-C1B
26	aY	406	PEB	C3A-C4A-CHA-C1B
26	aY	406	PEB	NB-C1B-CHA-C4A
26	aY	406	PEB	C2B-C1B-CHA-C4A
26	aZ	301	PEB	NA-C4A-CHA-C1B
26	aZ	301	PEB	C3A-C4A-CHA-C1B
26	aZ	301	PEB	NB-C1B-CHA-C4A
26	aZ	301	PEB	C2B-C1B-CHA-C4A
26	aZ	302	PEB	NA-C4A-CHA-C1B
26	aZ	302	PEB	C3A-C4A-CHA-C1B
26	aZ	302	PEB	NB-C1B-CHA-C4A
26	aZ	302	PEB	C2B-C1B-CHA-C4A
26	ba	1001	PEB	NA-C4A-CHA-C1B
26	ba	1001	PEB	C3A-C4A-CHA-C1B
26	ba	1001	PEB	NB-C1B-CHA-C4A
26	ba	1001	PEB	C2B-C1B-CHA-C4A
26	bb	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	bb	201	PEB	C3A-C4A-CHA-C1B
26	bb	201	PEB	NB-C1B-CHA-C4A
26	bb	201	PEB	C2B-C1B-CHA-C4A
26	bc	201	PEB	NA-C4A-CHA-C1B
26	bc	201	PEB	C3A-C4A-CHA-C1B
26	bc	201	PEB	NB-C1B-CHA-C4A
26	bc	201	PEB	C2B-C1B-CHA-C4A
26	bd	201	PEB	NA-C4A-CHA-C1B
26	bd	201	PEB	C3A-C4A-CHA-C1B
26	bd	201	PEB	NB-C1B-CHA-C4A
26	bd	201	PEB	C2B-C1B-CHA-C4A
26	bd	202	PEB	NA-C4A-CHA-C1B
26	bd	202	PEB	C3A-C4A-CHA-C1B
26	bd	202	PEB	NB-C1B-CHA-C4A
26	bd	202	PEB	C2B-C1B-CHA-C4A
26	be	201	PEB	NA-C4A-CHA-C1B
26	be	201	PEB	C3A-C4A-CHA-C1B
26	be	201	PEB	NB-C1B-CHA-C4A
26	be	201	PEB	C2B-C1B-CHA-C4A
26	bf	201	PEB	NA-C4A-CHA-C1B
26	bf	201	PEB	C3A-C4A-CHA-C1B
26	bf	201	PEB	NB-C1B-CHA-C4A
26	bf	201	PEB	C2B-C1B-CHA-C4A
26	bg	201	PEB	NA-C4A-CHA-C1B
26	bg	201	PEB	C3A-C4A-CHA-C1B
26	bg	201	PEB	NB-C1B-CHA-C4A
26	bg	201	PEB	C2B-C1B-CHA-C4A
26	bh	201	PEB	NA-C4A-CHA-C1B
26	bh	201	PEB	C3A-C4A-CHA-C1B
26	bh	201	PEB	NB-C1B-CHA-C4A
26	bh	201	PEB	C2B-C1B-CHA-C4A
26	bh	202	PEB	NA-C4A-CHA-C1B
26	bh	202	PEB	C3A-C4A-CHA-C1B
26	bh	202	PEB	NB-C1B-CHA-C4A
26	bh	202	PEB	C2B-C1B-CHA-C4A
26	bi	201	PEB	NA-C4A-CHA-C1B
26	bi	201	PEB	C3A-C4A-CHA-C1B
26	bi	201	PEB	NB-C1B-CHA-C4A
26	bi	201	PEB	C2B-C1B-CHA-C4A
26	bj	201	PEB	NA-C4A-CHA-C1B
26	bj	201	PEB	C3A-C4A-CHA-C1B
26	bj	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bj	201	PEB	C2B-C1B-CHA-C4A
26	bj	202	PEB	NA-C4A-CHA-C1B
26	bj	202	PEB	C3A-C4A-CHA-C1B
26	bj	202	PEB	NB-C1B-CHA-C4A
26	bj	202	PEB	C2B-C1B-CHA-C4A
26	bk	201	PEB	NA-C4A-CHA-C1B
26	bk	201	PEB	C3A-C4A-CHA-C1B
26	bk	201	PEB	NB-C1B-CHA-C4A
26	bk	201	PEB	C2B-C1B-CHA-C4A
26	bl	201	PEB	NA-C4A-CHA-C1B
26	bl	201	PEB	C3A-C4A-CHA-C1B
26	bl	201	PEB	NB-C1B-CHA-C4A
26	bl	201	PEB	C2B-C1B-CHA-C4A
26	bl	202	PEB	NA-C4A-CHA-C1B
26	bl	202	PEB	C3A-C4A-CHA-C1B
26	bl	202	PEB	NB-C1B-CHA-C4A
26	bl	202	PEB	C2B-C1B-CHA-C4A
26	bm	1001	PEB	NA-C4A-CHA-C1B
26	bm	1001	PEB	C3A-C4A-CHA-C1B
26	bm	1001	PEB	NB-C1B-CHA-C4A
26	bm	1001	PEB	C2B-C1B-CHA-C4A
26	bm	1002	PEB	NA-C4A-CHA-C1B
26	bm	1002	PEB	C3A-C4A-CHA-C1B
26	bm	1002	PEB	NB-C1B-CHA-C4A
26	bm	1002	PEB	C2B-C1B-CHA-C4A
26	bn	201	PEB	NA-C4A-CHA-C1B
26	bn	201	PEB	C3A-C4A-CHA-C1B
26	bn	201	PEB	NB-C1B-CHA-C4A
26	bn	201	PEB	C2B-C1B-CHA-C4A
26	bo	201	PEB	NA-C4A-CHA-C1B
26	bo	201	PEB	C3A-C4A-CHA-C1B
26	bo	201	PEB	NB-C1B-CHA-C4A
26	bo	201	PEB	C2B-C1B-CHA-C4A
26	bp	201	PEB	NA-C4A-CHA-C1B
26	bp	201	PEB	C3A-C4A-CHA-C1B
26	bp	201	PEB	NB-C1B-CHA-C4A
26	bp	201	PEB	C2B-C1B-CHA-C4A
26	bq	201	PEB	NA-C4A-CHA-C1B
26	bq	201	PEB	C3A-C4A-CHA-C1B
26	bq	201	PEB	NB-C1B-CHA-C4A
26	bq	201	PEB	C2B-C1B-CHA-C4A
26	bq	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	bq	202	PEB	C3A-C4A-CHA-C1B
26	bq	202	PEB	NB-C1B-CHA-C4A
26	bq	202	PEB	C2B-C1B-CHA-C4A
26	br	201	PEB	NA-C4A-CHA-C1B
26	br	201	PEB	C3A-C4A-CHA-C1B
26	br	201	PEB	NB-C1B-CHA-C4A
26	br	201	PEB	C2B-C1B-CHA-C4A
26	br	202	PEB	NA-C4A-CHA-C1B
26	br	202	PEB	C3A-C4A-CHA-C1B
26	br	202	PEB	NB-C1B-CHA-C4A
26	br	202	PEB	C2B-C1B-CHA-C4A
26	bs	1001	PEB	NA-C4A-CHA-C1B
26	bs	1001	PEB	C3A-C4A-CHA-C1B
26	bs	1001	PEB	NB-C1B-CHA-C4A
26	bs	1001	PEB	C2B-C1B-CHA-C4A
26	bs	1002	PEB	NA-C4A-CHA-C1B
26	bs	1002	PEB	C3A-C4A-CHA-C1B
26	bs	1002	PEB	NB-C1B-CHA-C4A
26	bs	1002	PEB	C2B-C1B-CHA-C4A
26	bs	1003	PEB	NA-C4A-CHA-C1B
26	bs	1003	PEB	C3A-C4A-CHA-C1B
26	bs	1003	PEB	NB-C1B-CHA-C4A
26	bs	1003	PEB	C2B-C1B-CHA-C4A
26	bt	201	PEB	NA-C4A-CHA-C1B
26	bt	201	PEB	C3A-C4A-CHA-C1B
26	bt	201	PEB	NB-C1B-CHA-C4A
26	bt	201	PEB	C2B-C1B-CHA-C4A
26	bt	202	PEB	NA-C4A-CHA-C1B
26	bt	202	PEB	C3A-C4A-CHA-C1B
26	bt	202	PEB	NB-C1B-CHA-C4A
26	bt	202	PEB	C2B-C1B-CHA-C4A
26	bu	201	PEB	NA-C4A-CHA-C1B
26	bu	201	PEB	C3A-C4A-CHA-C1B
26	bu	201	PEB	NB-C1B-CHA-C4A
26	bu	201	PEB	C2B-C1B-CHA-C4A
26	bu	202	PEB	NA-C4A-CHA-C1B
26	bu	202	PEB	C3A-C4A-CHA-C1B
26	bu	202	PEB	NB-C1B-CHA-C4A
26	bu	202	PEB	C2B-C1B-CHA-C4A
26	bv	201	PEB	NA-C4A-CHA-C1B
26	bv	201	PEB	C3A-C4A-CHA-C1B
26	bv	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bv	201	PEB	C2B-C1B-CHA-C4A
26	bv	202	PEB	NA-C4A-CHA-C1B
26	bv	202	PEB	C3A-C4A-CHA-C1B
26	bv	202	PEB	NB-C1B-CHA-C4A
26	bv	202	PEB	C2B-C1B-CHA-C4A
26	bw	201	PEB	NA-C4A-CHA-C1B
26	bw	201	PEB	C3A-C4A-CHA-C1B
26	bw	201	PEB	NB-C1B-CHA-C4A
26	bw	201	PEB	C2B-C1B-CHA-C4A
26	bw	202	PEB	NA-C4A-CHA-C1B
26	bw	202	PEB	C3A-C4A-CHA-C1B
26	bw	202	PEB	NB-C1B-CHA-C4A
26	bw	202	PEB	C2B-C1B-CHA-C4A
26	bx	201	PEB	NA-C4A-CHA-C1B
26	bx	201	PEB	C3A-C4A-CHA-C1B
26	bx	201	PEB	NB-C1B-CHA-C4A
26	bx	201	PEB	C2B-C1B-CHA-C4A
26	bx	202	PEB	NA-C4A-CHA-C1B
26	bx	202	PEB	C3A-C4A-CHA-C1B
26	bx	202	PEB	NB-C1B-CHA-C4A
26	bx	202	PEB	C2B-C1B-CHA-C4A
26	by	1001	PEB	NA-C4A-CHA-C1B
26	by	1001	PEB	C3A-C4A-CHA-C1B
26	by	1001	PEB	NB-C1B-CHA-C4A
26	by	1001	PEB	C2B-C1B-CHA-C4A
26	by	1002	PEB	NA-C4A-CHA-C1B
26	by	1002	PEB	C3A-C4A-CHA-C1B
26	by	1002	PEB	NB-C1B-CHA-C4A
26	by	1002	PEB	C2B-C1B-CHA-C4A
26	bz	201	PEB	NA-C4A-CHA-C1B
26	bz	201	PEB	C3A-C4A-CHA-C1B
26	bz	201	PEB	NB-C1B-CHA-C4A
26	bz	201	PEB	C2B-C1B-CHA-C4A
26	bz	202	PEB	NA-C4A-CHA-C1B
26	bz	202	PEB	C3A-C4A-CHA-C1B
26	bz	202	PEB	NB-C1B-CHA-C4A
26	bz	202	PEB	C2B-C1B-CHA-C4A
26	bA	201	PEB	NA-C4A-CHA-C1B
26	bA	201	PEB	C3A-C4A-CHA-C1B
26	bA	201	PEB	NB-C1B-CHA-C4A
26	bA	201	PEB	C2B-C1B-CHA-C4A
26	bA	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bA	202	PEB	C2B-C1B-CHA-C4A
26	bB	201	PEB	NA-C4A-CHA-C1B
26	bB	201	PEB	C3A-C4A-CHA-C1B
26	bB	201	PEB	NB-C1B-CHA-C4A
26	bB	201	PEB	C2B-C1B-CHA-C4A
26	bB	202	PEB	C1C-C2C-CAC-CBC
26	bB	202	PEB	C3C-C2C-CAC-CBC
26	bB	202	PEB	NB-C1B-CHA-C4A
26	bB	202	PEB	C2B-C1B-CHA-C4A
26	bC	201	PEB	NA-C4A-CHA-C1B
26	bC	201	PEB	C3A-C4A-CHA-C1B
26	bC	201	PEB	NB-C1B-CHA-C4A
26	bC	201	PEB	C2B-C1B-CHA-C4A
26	bC	202	PEB	NB-C1B-CHA-C4A
26	bC	202	PEB	C2B-C1B-CHA-C4A
26	bD	201	PEB	NA-C4A-CHA-C1B
26	bD	201	PEB	C3A-C4A-CHA-C1B
26	bD	201	PEB	NB-C1B-CHA-C4A
26	bD	201	PEB	C2B-C1B-CHA-C4A
26	bD	202	PEB	C1C-C2C-CAC-CBC
26	bD	202	PEB	C3C-C2C-CAC-CBC
26	bD	202	PEB	NB-C1B-CHA-C4A
26	bD	202	PEB	C2B-C1B-CHA-C4A
26	bE	201	PEB	NA-C4A-CHA-C1B
26	bE	201	PEB	C3A-C4A-CHA-C1B
26	bE	201	PEB	NB-C1B-CHA-C4A
26	bE	201	PEB	C2B-C1B-CHA-C4A
26	bE	202	PEB	NB-C1B-CHA-C4A
26	bE	202	PEB	C2B-C1B-CHA-C4A
26	bF	201	PEB	NA-C4A-CHA-C1B
26	bF	201	PEB	C3A-C4A-CHA-C1B
26	bF	201	PEB	NB-C1B-CHA-C4A
26	bF	201	PEB	C2B-C1B-CHA-C4A
26	bF	202	PEB	C1C-C2C-CAC-CBC
26	bF	202	PEB	C3C-C2C-CAC-CBC
26	bF	202	PEB	NB-C1B-CHA-C4A
26	bF	202	PEB	C2B-C1B-CHA-C4A
26	bG	201	PEB	NA-C4A-CHA-C1B
26	bG	201	PEB	C3A-C4A-CHA-C1B
26	bG	201	PEB	NB-C1B-CHA-C4A
26	bG	201	PEB	C2B-C1B-CHA-C4A
26	bG	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bG	202	PEB	C2B-C1B-CHA-C4A
26	bH	201	PEB	NA-C4A-CHA-C1B
26	bH	201	PEB	C3A-C4A-CHA-C1B
26	bH	201	PEB	NB-C1B-CHA-C4A
26	bH	201	PEB	C2B-C1B-CHA-C4A
26	bH	202	PEB	C1C-C2C-CAC-CBC
26	bH	202	PEB	C3C-C2C-CAC-CBC
26	bH	202	PEB	NB-C1B-CHA-C4A
26	bH	202	PEB	C2B-C1B-CHA-C4A
26	bI	201	PEB	NA-C4A-CHA-C1B
26	bI	201	PEB	C3A-C4A-CHA-C1B
26	bI	201	PEB	NB-C1B-CHA-C4A
26	bI	201	PEB	C2B-C1B-CHA-C4A
26	bI	202	PEB	NB-C1B-CHA-C4A
26	bI	202	PEB	C2B-C1B-CHA-C4A
26	bJ	201	PEB	NA-C4A-CHA-C1B
26	bJ	201	PEB	C3A-C4A-CHA-C1B
26	bJ	201	PEB	NB-C1B-CHA-C4A
26	bJ	201	PEB	C2B-C1B-CHA-C4A
26	bJ	202	PEB	C1C-C2C-CAC-CBC
26	bJ	202	PEB	C3C-C2C-CAC-CBC
26	bJ	202	PEB	NB-C1B-CHA-C4A
26	bJ	202	PEB	C2B-C1B-CHA-C4A
26	bK	1001	PEB	NA-C4A-CHA-C1B
26	bK	1001	PEB	C3A-C4A-CHA-C1B
26	bK	1001	PEB	NB-C1B-CHA-C4A
26	bK	1001	PEB	C2B-C1B-CHA-C4A
26	bK	1002	PEB	NB-C1B-CHA-C4A
26	bK	1002	PEB	C2B-C1B-CHA-C4A
26	bL	201	PEB	NA-C4A-CHA-C1B
26	bL	201	PEB	C3A-C4A-CHA-C1B
26	bL	201	PEB	NB-C1B-CHA-C4A
26	bL	201	PEB	C2B-C1B-CHA-C4A
26	bL	202	PEB	C1C-C2C-CAC-CBC
26	bL	202	PEB	C3C-C2C-CAC-CBC
26	bL	202	PEB	NB-C1B-CHA-C4A
26	bL	202	PEB	C2B-C1B-CHA-C4A
26	bM	201	PEB	NA-C4A-CHA-C1B
26	bM	201	PEB	C3A-C4A-CHA-C1B
26	bM	201	PEB	NB-C1B-CHA-C4A
26	bM	201	PEB	C2B-C1B-CHA-C4A
26	bM	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bM	202	PEB	C2B-C1B-CHA-C4A
26	bN	201	PEB	NA-C4A-CHA-C1B
26	bN	201	PEB	C3A-C4A-CHA-C1B
26	bN	201	PEB	NB-C1B-CHA-C4A
26	bN	201	PEB	C2B-C1B-CHA-C4A
26	bN	202	PEB	C1C-C2C-CAC-CBC
26	bN	202	PEB	C3C-C2C-CAC-CBC
26	bN	202	PEB	NB-C1B-CHA-C4A
26	bN	202	PEB	C2B-C1B-CHA-C4A
26	bO	201	PEB	NA-C4A-CHA-C1B
26	bO	201	PEB	C3A-C4A-CHA-C1B
26	bO	201	PEB	NB-C1B-CHA-C4A
26	bO	201	PEB	C2B-C1B-CHA-C4A
26	bO	202	PEB	NB-C1B-CHA-C4A
26	bO	202	PEB	C2B-C1B-CHA-C4A
26	bP	201	PEB	NA-C4A-CHA-C1B
26	bP	201	PEB	C3A-C4A-CHA-C1B
26	bP	201	PEB	NB-C1B-CHA-C4A
26	bP	201	PEB	C2B-C1B-CHA-C4A
26	bP	202	PEB	C1C-C2C-CAC-CBC
26	bP	202	PEB	C3C-C2C-CAC-CBC
26	bP	202	PEB	NB-C1B-CHA-C4A
26	bP	202	PEB	C2B-C1B-CHA-C4A
26	bQ	201	PEB	NA-C4A-CHA-C1B
26	bQ	201	PEB	C3A-C4A-CHA-C1B
26	bQ	201	PEB	NB-C1B-CHA-C4A
26	bQ	201	PEB	C2B-C1B-CHA-C4A
26	bQ	202	PEB	NB-C1B-CHA-C4A
26	bQ	202	PEB	C2B-C1B-CHA-C4A
26	bQ	203	PEB	C1C-C2C-CAC-CBC
26	bQ	203	PEB	C3C-C2C-CAC-CBC
26	bQ	203	PEB	NB-C1B-CHA-C4A
26	bQ	203	PEB	C2B-C1B-CHA-C4A
26	bR	201	PEB	NA-C4A-CHA-C1B
26	bR	201	PEB	C3A-C4A-CHA-C1B
26	bR	201	PEB	NB-C1B-CHA-C4A
26	bR	201	PEB	C2B-C1B-CHA-C4A
26	bS	201	PEB	NA-C4A-CHA-C1B
26	bS	201	PEB	C3A-C4A-CHA-C1B
26	bS	201	PEB	NB-C1B-CHA-C4A
26	bS	201	PEB	C2B-C1B-CHA-C4A
26	bS	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	bS	202	PEB	C2B-C1B-CHA-C4A
26	bT	201	PEB	C1C-C2C-CAC-CBC
26	bT	201	PEB	C3C-C2C-CAC-CBC
26	bT	201	PEB	NB-C1B-CHA-C4A
26	bT	201	PEB	C2B-C1B-CHA-C4A
26	bU	201	PEB	NA-C4A-CHA-C1B
26	bU	201	PEB	C3A-C4A-CHA-C1B
26	bU	201	PEB	NB-C1B-CHA-C4A
26	bU	201	PEB	C2B-C1B-CHA-C4A
26	bU	202	PEB	NB-C1B-CHA-C4A
26	bU	202	PEB	C2B-C1B-CHA-C4A
26	bV	201	PEB	NA-C4A-CHA-C1B
26	bV	201	PEB	C3A-C4A-CHA-C1B
26	bV	201	PEB	NB-C1B-CHA-C4A
26	bV	201	PEB	C2B-C1B-CHA-C4A
26	bV	202	PEB	C1C-C2C-CAC-CBC
26	bV	202	PEB	C3C-C2C-CAC-CBC
26	bV	202	PEB	NB-C1B-CHA-C4A
26	bV	202	PEB	C2B-C1B-CHA-C4A
26	bW	301	PEB	NA-C4A-CHA-C1B
26	bW	301	PEB	C3A-C4A-CHA-C1B
26	bW	301	PEB	NB-C1B-CHA-C4A
26	bW	301	PEB	C2B-C1B-CHA-C4A
26	bX	401	PEB	NA-C4A-CHA-C1B
26	bX	401	PEB	C3A-C4A-CHA-C1B
26	bX	401	PEB	NB-C1B-CHA-C4A
26	bX	401	PEB	C2B-C1B-CHA-C4A
26	bX	402	PEB	NA-C4A-CHA-C1B
26	bX	402	PEB	C3A-C4A-CHA-C1B
26	bX	402	PEB	NB-C1B-CHA-C4A
26	bX	402	PEB	C2B-C1B-CHA-C4A
26	bY	1001	PEB	NA-C4A-CHA-C1B
26	bY	1001	PEB	C3A-C4A-CHA-C1B
26	bY	1001	PEB	NB-C1B-CHA-C4A
26	bY	1001	PEB	C2B-C1B-CHA-C4A
26	bY	1002	PEB	NB-C1B-CHA-C4A
26	bY	1002	PEB	C2B-C1B-CHA-C4A
26	bY	1003	PEB	NA-C4A-CHA-C1B
26	bY	1003	PEB	C3A-C4A-CHA-C1B
26	bY	1003	PEB	NB-C1B-CHA-C4A
26	bY	1003	PEB	C2B-C1B-CHA-C4A
26	bZ	301	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	bZ	301	PEB	C3A-C4A-CHA-C1B
26	bZ	301	PEB	NB-C1B-CHA-C4A
26	bZ	301	PEB	C2B-C1B-CHA-C4A
26	bZ	302	PEB	NB-C1B-CHA-C4A
26	bZ	302	PEB	C2B-C1B-CHA-C4A
26	bZ	303	PEB	NA-C4A-CHA-C1B
26	bZ	303	PEB	C3A-C4A-CHA-C1B
26	bZ	303	PEB	NB-C1B-CHA-C4A
26	bZ	303	PEB	C2B-C1B-CHA-C4A
26	ca	1001	PEB	NA-C4A-CHA-C1B
26	ca	1001	PEB	C3A-C4A-CHA-C1B
26	ca	1001	PEB	NB-C1B-CHA-C4A
26	ca	1001	PEB	C2B-C1B-CHA-C4A
26	cb	201	PEB	NA-C4A-CHA-C1B
26	cb	201	PEB	C3A-C4A-CHA-C1B
26	cb	201	PEB	NB-C1B-CHA-C4A
26	cb	201	PEB	C2B-C1B-CHA-C4A
26	cb	202	PEB	C1C-C2C-CAC-CBC
26	cb	202	PEB	C3C-C2C-CAC-CBC
26	cb	202	PEB	NB-C1B-CHA-C4A
26	cb	202	PEB	C2B-C1B-CHA-C4A
26	cc	201	PEB	NA-C4A-CHA-C1B
26	cc	201	PEB	C3A-C4A-CHA-C1B
26	cc	201	PEB	NB-C1B-CHA-C4A
26	cc	201	PEB	C2B-C1B-CHA-C4A
26	cd	201	PEB	NA-C4A-CHA-C1B
26	cd	201	PEB	C3A-C4A-CHA-C1B
26	cd	201	PEB	NB-C1B-CHA-C4A
26	cd	201	PEB	C2B-C1B-CHA-C4A
26	cd	202	PEB	C1C-C2C-CAC-CBC
26	cd	202	PEB	C3C-C2C-CAC-CBC
26	cd	202	PEB	NB-C1B-CHA-C4A
26	cd	202	PEB	C2B-C1B-CHA-C4A
26	ce	201	PEB	NA-C4A-CHA-C1B
26	ce	201	PEB	C3A-C4A-CHA-C1B
26	ce	201	PEB	NB-C1B-CHA-C4A
26	ce	201	PEB	C2B-C1B-CHA-C4A
26	cf	201	PEB	C1C-C2C-CAC-CBC
26	cf	201	PEB	C3C-C2C-CAC-CBC
26	cf	201	PEB	NB-C1B-CHA-C4A
26	cf	201	PEB	C2B-C1B-CHA-C4A
26	cg	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cg	201	PEB	C3A-C4A-CHA-C1B
26	cg	201	PEB	NB-C1B-CHA-C4A
26	cg	201	PEB	C2B-C1B-CHA-C4A
26	ch	201	PEB	NA-C4A-CHA-C1B
26	ch	201	PEB	C3A-C4A-CHA-C1B
26	ch	201	PEB	NB-C1B-CHA-C4A
26	ch	201	PEB	C2B-C1B-CHA-C4A
26	ch	202	PEB	C1C-C2C-CAC-CBC
26	ch	202	PEB	C3C-C2C-CAC-CBC
26	ch	202	PEB	NB-C1B-CHA-C4A
26	ch	202	PEB	C2B-C1B-CHA-C4A
26	ci	201	PEB	NA-C4A-CHA-C1B
26	ci	201	PEB	C3A-C4A-CHA-C1B
26	ci	201	PEB	NB-C1B-CHA-C4A
26	ci	201	PEB	C2B-C1B-CHA-C4A
26	cj	201	PEB	NA-C4A-CHA-C1B
26	cj	201	PEB	C3A-C4A-CHA-C1B
26	cj	201	PEB	NB-C1B-CHA-C4A
26	cj	201	PEB	C2B-C1B-CHA-C4A
26	cj	202	PEB	C1C-C2C-CAC-CBC
26	cj	202	PEB	C3C-C2C-CAC-CBC
26	cj	202	PEB	NB-C1B-CHA-C4A
26	cj	202	PEB	C2B-C1B-CHA-C4A
26	ck	201	PEB	NA-C4A-CHA-C1B
26	ck	201	PEB	C3A-C4A-CHA-C1B
26	ck	201	PEB	NB-C1B-CHA-C4A
26	ck	201	PEB	C2B-C1B-CHA-C4A
26	cl	201	PEB	NA-C4A-CHA-C1B
26	cl	201	PEB	C3A-C4A-CHA-C1B
26	cl	201	PEB	NB-C1B-CHA-C4A
26	cl	201	PEB	C2B-C1B-CHA-C4A
26	cl	202	PEB	C1C-C2C-CAC-CBC
26	cl	202	PEB	C3C-C2C-CAC-CBC
26	cl	202	PEB	NB-C1B-CHA-C4A
26	cl	202	PEB	C2B-C1B-CHA-C4A
26	cm	1001	PEB	NA-C4A-CHA-C1B
26	cm	1001	PEB	C3A-C4A-CHA-C1B
26	cm	1001	PEB	NB-C1B-CHA-C4A
26	cm	1001	PEB	C2B-C1B-CHA-C4A
26	cm	1002	PEB	NB-C1B-CHA-C4A
26	cm	1002	PEB	C2B-C1B-CHA-C4A
26	cn	201	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	cn	201	PEB	C3C-C2C-CAC-CBC
26	cn	201	PEB	NB-C1B-CHA-C4A
26	cn	201	PEB	C2B-C1B-CHA-C4A
26	co	201	PEB	C1C-C2C-CAC-CBC
26	co	201	PEB	C3C-C2C-CAC-CBC
26	co	201	PEB	NB-C1B-CHA-C4A
26	co	201	PEB	C2B-C1B-CHA-C4A
26	cp	201	PEB	NA-C4A-CHA-C1B
26	cp	201	PEB	C3A-C4A-CHA-C1B
26	cp	201	PEB	NB-C1B-CHA-C4A
26	cp	201	PEB	C2B-C1B-CHA-C4A
26	cp	202	PEB	C1C-C2C-CAC-CBC
26	cp	202	PEB	C3C-C2C-CAC-CBC
26	cp	202	PEB	NB-C1B-CHA-C4A
26	cp	202	PEB	C2B-C1B-CHA-C4A
26	cq	201	PEB	NA-C4A-CHA-C1B
26	cq	201	PEB	C3A-C4A-CHA-C1B
26	cq	201	PEB	NB-C1B-CHA-C4A
26	cq	201	PEB	C2B-C1B-CHA-C4A
26	cq	202	PEB	C1C-C2C-CAC-CBC
26	cq	202	PEB	C3C-C2C-CAC-CBC
26	cq	202	PEB	NB-C1B-CHA-C4A
26	cq	202	PEB	C2B-C1B-CHA-C4A
26	cr	201	PEB	NA-C4A-CHA-C1B
26	cr	201	PEB	C3A-C4A-CHA-C1B
26	cr	201	PEB	NB-C1B-CHA-C4A
26	cr	201	PEB	C2B-C1B-CHA-C4A
26	cr	202	PEB	C1C-C2C-CAC-CBC
26	cr	202	PEB	C3C-C2C-CAC-CBC
26	cr	202	PEB	NB-C1B-CHA-C4A
26	cr	202	PEB	C2B-C1B-CHA-C4A
26	cs	201	PEB	NA-C4A-CHA-C1B
26	cs	201	PEB	C3A-C4A-CHA-C1B
26	cs	201	PEB	NB-C1B-CHA-C4A
26	cs	201	PEB	C2B-C1B-CHA-C4A
26	cs	202	PEB	C1C-C2C-CAC-CBC
26	cs	202	PEB	C3C-C2C-CAC-CBC
26	cs	202	PEB	NB-C1B-CHA-C4A
26	cs	202	PEB	C2B-C1B-CHA-C4A
26	ct	201	PEB	NA-C4A-CHA-C1B
26	ct	201	PEB	C3A-C4A-CHA-C1B
26	ct	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	ct	201	PEB	C2B-C1B-CHA-C4A
26	ct	202	PEB	NB-C1B-CHA-C4A
26	ct	202	PEB	C2B-C1B-CHA-C4A
26	cu	201	PEB	NA-C4A-CHA-C1B
26	cu	201	PEB	C3A-C4A-CHA-C1B
26	cu	201	PEB	NB-C1B-CHA-C4A
26	cu	201	PEB	C2B-C1B-CHA-C4A
26	cu	202	PEB	NB-C1B-CHA-C4A
26	cu	202	PEB	C2B-C1B-CHA-C4A
26	cv	201	PEB	NA-C4A-CHA-C1B
26	cv	201	PEB	C3A-C4A-CHA-C1B
26	cv	201	PEB	NB-C1B-CHA-C4A
26	cv	201	PEB	C2B-C1B-CHA-C4A
26	cv	202	PEB	NB-C1B-CHA-C4A
26	cv	202	PEB	C2B-C1B-CHA-C4A
26	cw	201	PEB	NA-C4A-CHA-C1B
26	cw	201	PEB	C3A-C4A-CHA-C1B
26	cw	201	PEB	NB-C1B-CHA-C4A
26	cw	201	PEB	C2B-C1B-CHA-C4A
26	cw	202	PEB	NB-C1B-CHA-C4A
26	cw	202	PEB	C2B-C1B-CHA-C4A
26	cx	201	PEB	NA-C4A-CHA-C1B
26	cx	201	PEB	C3A-C4A-CHA-C1B
26	cx	201	PEB	NB-C1B-CHA-C4A
26	cx	201	PEB	C2B-C1B-CHA-C4A
26	cx	202	PEB	NB-C1B-CHA-C4A
26	cx	202	PEB	C2B-C1B-CHA-C4A
26	cy	1001	PEB	NA-C4A-CHA-C1B
26	cy	1001	PEB	C3A-C4A-CHA-C1B
26	cy	1001	PEB	NB-C1B-CHA-C4A
26	cy	1001	PEB	C2B-C1B-CHA-C4A
26	cy	1002	PEB	NB-C1B-CHA-C4A
26	cy	1002	PEB	C2B-C1B-CHA-C4A
26	cz	201	PEB	NA-C4A-CHA-C1B
26	cz	201	PEB	C3A-C4A-CHA-C1B
26	cz	201	PEB	NB-C1B-CHA-C4A
26	cz	201	PEB	C2B-C1B-CHA-C4A
26	cz	202	PEB	C1C-C2C-CAC-CBC
26	cz	202	PEB	C3C-C2C-CAC-CBC
26	cz	202	PEB	NB-C1B-CHA-C4A
26	cz	202	PEB	C2B-C1B-CHA-C4A
26	cA	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cA	201	PEB	C3A-C4A-CHA-C1B
26	cA	201	PEB	NB-C1B-CHA-C4A
26	cA	201	PEB	C2B-C1B-CHA-C4A
26	cA	202	PEB	NB-C1B-CHA-C4A
26	cA	202	PEB	C2B-C1B-CHA-C4A
26	cB	201	PEB	NA-C4A-CHA-C1B
26	cB	201	PEB	C3A-C4A-CHA-C1B
26	cB	201	PEB	NB-C1B-CHA-C4A
26	cB	201	PEB	C2B-C1B-CHA-C4A
26	cB	202	PEB	C1C-C2C-CAC-CBC
26	cB	202	PEB	C3C-C2C-CAC-CBC
26	cB	202	PEB	NB-C1B-CHA-C4A
26	cB	202	PEB	C2B-C1B-CHA-C4A
26	cC	1001	PEB	NA-C4A-CHA-C1B
26	cC	1001	PEB	C3A-C4A-CHA-C1B
26	cC	1001	PEB	NB-C1B-CHA-C4A
26	cC	1001	PEB	C2B-C1B-CHA-C4A
26	cC	1002	PEB	NB-C1B-CHA-C4A
26	cC	1002	PEB	C2B-C1B-CHA-C4A
26	cC	1003	PEB	NA-C4A-CHA-C1B
26	cC	1003	PEB	C3A-C4A-CHA-C1B
26	cC	1003	PEB	NB-C1B-CHA-C4A
26	cC	1003	PEB	C2B-C1B-CHA-C4A
26	cD	201	PEB	NA-C4A-CHA-C1B
26	cD	201	PEB	C3A-C4A-CHA-C1B
26	cD	201	PEB	NB-C1B-CHA-C4A
26	cD	201	PEB	C2B-C1B-CHA-C4A
26	cD	202	PEB	NB-C1B-CHA-C4A
26	cD	202	PEB	C2B-C1B-CHA-C4A
26	cE	201	PEB	NA-C4A-CHA-C1B
26	cE	201	PEB	C3A-C4A-CHA-C1B
26	cE	201	PEB	NB-C1B-CHA-C4A
26	cE	201	PEB	C2B-C1B-CHA-C4A
26	cE	202	PEB	C1C-C2C-CAC-CBC
26	cE	202	PEB	C3C-C2C-CAC-CBC
26	cE	202	PEB	NB-C1B-CHA-C4A
26	cE	202	PEB	C2B-C1B-CHA-C4A
26	cF	201	PEB	C1C-C2C-CAC-CBC
26	cF	201	PEB	C3C-C2C-CAC-CBC
26	cF	201	PEB	NB-C1B-CHA-C4A
26	cF	201	PEB	C2B-C1B-CHA-C4A
26	cG	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cG	201	PEB	C3A-C4A-CHA-C1B
26	cG	201	PEB	NB-C1B-CHA-C4A
26	cG	201	PEB	C2B-C1B-CHA-C4A
26	cG	202	PEB	NB-C1B-CHA-C4A
26	cG	202	PEB	C2B-C1B-CHA-C4A
26	cH	201	PEB	C1C-C2C-CAC-CBC
26	cH	201	PEB	C3C-C2C-CAC-CBC
26	cH	201	PEB	NB-C1B-CHA-C4A
26	cH	201	PEB	C2B-C1B-CHA-C4A
26	cI	201	PEB	NA-C4A-CHA-C1B
26	cI	201	PEB	C3A-C4A-CHA-C1B
26	cI	201	PEB	NB-C1B-CHA-C4A
26	cI	201	PEB	C2B-C1B-CHA-C4A
26	cI	202	PEB	NB-C1B-CHA-C4A
26	cI	202	PEB	C2B-C1B-CHA-C4A
26	cJ	201	PEB	NA-C4A-CHA-C1B
26	cJ	201	PEB	C3A-C4A-CHA-C1B
26	cJ	201	PEB	NB-C1B-CHA-C4A
26	cJ	201	PEB	C2B-C1B-CHA-C4A
26	cJ	202	PEB	C1C-C2C-CAC-CBC
26	cJ	202	PEB	C3C-C2C-CAC-CBC
26	cJ	202	PEB	NB-C1B-CHA-C4A
26	cJ	202	PEB	C2B-C1B-CHA-C4A
26	cK	201	PEB	NA-C4A-CHA-C1B
26	cK	201	PEB	C3A-C4A-CHA-C1B
26	cK	201	PEB	NB-C1B-CHA-C4A
26	cK	201	PEB	C2B-C1B-CHA-C4A
26	cK	202	PEB	NB-C1B-CHA-C4A
26	cK	202	PEB	C2B-C1B-CHA-C4A
26	cL	201	PEB	NA-C4A-CHA-C1B
26	cL	201	PEB	C3A-C4A-CHA-C1B
26	cL	201	PEB	NB-C1B-CHA-C4A
26	cL	201	PEB	C2B-C1B-CHA-C4A
26	cL	202	PEB	C1C-C2C-CAC-CBC
26	cL	202	PEB	C3C-C2C-CAC-CBC
26	cL	202	PEB	NB-C1B-CHA-C4A
26	cL	202	PEB	C2B-C1B-CHA-C4A
26	cM	201	PEB	NA-C4A-CHA-C1B
26	cM	201	PEB	C3A-C4A-CHA-C1B
26	cM	201	PEB	NB-C1B-CHA-C4A
26	cM	201	PEB	C2B-C1B-CHA-C4A
26	cM	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cM	202	PEB	C3A-C4A-CHA-C1B
26	cM	202	PEB	NB-C1B-CHA-C4A
26	cM	202	PEB	C2B-C1B-CHA-C4A
26	cN	201	PEB	NA-C4A-CHA-C1B
26	cN	201	PEB	C3A-C4A-CHA-C1B
26	cN	201	PEB	NB-C1B-CHA-C4A
26	cN	201	PEB	C2B-C1B-CHA-C4A
26	cO	201	PEB	NA-C4A-CHA-C1B
26	cO	201	PEB	C3A-C4A-CHA-C1B
26	cO	201	PEB	NB-C1B-CHA-C4A
26	cO	201	PEB	C2B-C1B-CHA-C4A
26	cO	202	PEB	NA-C4A-CHA-C1B
26	cO	202	PEB	C3A-C4A-CHA-C1B
26	cO	202	PEB	NB-C1B-CHA-C4A
26	cO	202	PEB	C2B-C1B-CHA-C4A
26	cP	201	PEB	NA-C4A-CHA-C1B
26	cP	201	PEB	C3A-C4A-CHA-C1B
26	cP	201	PEB	NB-C1B-CHA-C4A
26	cP	201	PEB	C2B-C1B-CHA-C4A
26	cP	202	PEB	NA-C4A-CHA-C1B
26	cP	202	PEB	C3A-C4A-CHA-C1B
26	cP	202	PEB	NB-C1B-CHA-C4A
26	cP	202	PEB	C2B-C1B-CHA-C4A
26	cQ	201	PEB	NA-C4A-CHA-C1B
26	cQ	201	PEB	C3A-C4A-CHA-C1B
26	cQ	201	PEB	NB-C1B-CHA-C4A
26	cQ	201	PEB	C2B-C1B-CHA-C4A
26	cR	201	PEB	NA-C4A-CHA-C1B
26	cR	201	PEB	C3A-C4A-CHA-C1B
26	cR	201	PEB	NB-C1B-CHA-C4A
26	cR	201	PEB	C2B-C1B-CHA-C4A
26	cR	202	PEB	NA-C4A-CHA-C1B
26	cR	202	PEB	C3A-C4A-CHA-C1B
26	cR	202	PEB	NB-C1B-CHA-C4A
26	cR	202	PEB	C2B-C1B-CHA-C4A
26	cS	201	PEB	NA-C4A-CHA-C1B
26	cS	201	PEB	C3A-C4A-CHA-C1B
26	cS	201	PEB	NB-C1B-CHA-C4A
26	cS	201	PEB	C2B-C1B-CHA-C4A
26	cS	202	PEB	NA-C4A-CHA-C1B
26	cS	202	PEB	C3A-C4A-CHA-C1B
26	cS	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	cS	202	PEB	C2B-C1B-CHA-C4A
26	cT	1001	PEB	NA-C4A-CHA-C1B
26	cT	1001	PEB	C3A-C4A-CHA-C1B
26	cT	1001	PEB	NB-C1B-CHA-C4A
26	cT	1001	PEB	C2B-C1B-CHA-C4A
26	cT	1002	PEB	NA-C4A-CHA-C1B
26	cT	1002	PEB	C3A-C4A-CHA-C1B
26	cT	1002	PEB	NB-C1B-CHA-C4A
26	cT	1002	PEB	C2B-C1B-CHA-C4A
26	cU	201	PEB	NA-C4A-CHA-C1B
26	cU	201	PEB	C3A-C4A-CHA-C1B
26	cU	201	PEB	NB-C1B-CHA-C4A
26	cU	201	PEB	C2B-C1B-CHA-C4A
26	cU	202	PEB	NA-C4A-CHA-C1B
26	cU	202	PEB	C3A-C4A-CHA-C1B
26	cU	202	PEB	NB-C1B-CHA-C4A
26	cU	202	PEB	C2B-C1B-CHA-C4A
26	cV	201	PEB	NA-C4A-CHA-C1B
26	cV	201	PEB	C3A-C4A-CHA-C1B
26	cV	201	PEB	NB-C1B-CHA-C4A
26	cV	201	PEB	C2B-C1B-CHA-C4A
26	cV	202	PEB	NA-C4A-CHA-C1B
26	cV	202	PEB	C3A-C4A-CHA-C1B
26	cV	202	PEB	NB-C1B-CHA-C4A
26	cV	202	PEB	C2B-C1B-CHA-C4A
26	cV	203	PEB	NA-C4A-CHA-C1B
26	cV	203	PEB	C3A-C4A-CHA-C1B
26	cV	203	PEB	NB-C1B-CHA-C4A
26	cV	203	PEB	C2B-C1B-CHA-C4A
26	cW	201	PEB	NA-C4A-CHA-C1B
26	cW	201	PEB	C3A-C4A-CHA-C1B
26	cW	201	PEB	NB-C1B-CHA-C4A
26	cW	201	PEB	C2B-C1B-CHA-C4A
26	cW	202	PEB	NA-C4A-CHA-C1B
26	cW	202	PEB	C3A-C4A-CHA-C1B
26	cW	202	PEB	NB-C1B-CHA-C4A
26	cW	202	PEB	C2B-C1B-CHA-C4A
26	cX	201	PEB	NA-C4A-CHA-C1B
26	cX	201	PEB	C3A-C4A-CHA-C1B
26	cX	201	PEB	NB-C1B-CHA-C4A
26	cX	201	PEB	C2B-C1B-CHA-C4A
26	cX	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cX	202	PEB	C3A-C4A-CHA-C1B
26	cX	202	PEB	NB-C1B-CHA-C4A
26	cX	202	PEB	C2B-C1B-CHA-C4A
26	cY	201	PEB	NA-C4A-CHA-C1B
26	cY	201	PEB	C3A-C4A-CHA-C1B
26	cY	201	PEB	NB-C1B-CHA-C4A
26	cY	201	PEB	C2B-C1B-CHA-C4A
26	cY	202	PEB	C1C-C2C-CAC-CBC
26	cY	202	PEB	C3C-C2C-CAC-CBC
26	cY	202	PEB	NB-C1B-CHA-C4A
26	cY	202	PEB	C2B-C1B-CHA-C4A
26	cZ	201	PEB	NA-C4A-CHA-C1B
26	cZ	201	PEB	C3A-C4A-CHA-C1B
26	cZ	201	PEB	NB-C1B-CHA-C4A
26	cZ	201	PEB	C2B-C1B-CHA-C4A
26	cZ	202	PEB	NB-C1B-CHA-C4A
26	cZ	202	PEB	C2B-C1B-CHA-C4A
26	da	1001	PEB	NA-C4A-CHA-C1B
26	da	1001	PEB	C3A-C4A-CHA-C1B
26	da	1001	PEB	NB-C1B-CHA-C4A
26	da	1001	PEB	C2B-C1B-CHA-C4A
26	da	1002	PEB	NB-C1B-CHA-C4A
26	da	1002	PEB	C2B-C1B-CHA-C4A
26	db	201	PEB	NA-C4A-CHA-C1B
26	db	201	PEB	C3A-C4A-CHA-C1B
26	db	201	PEB	NB-C1B-CHA-C4A
26	db	201	PEB	C2B-C1B-CHA-C4A
26	db	202	PEB	NB-C1B-CHA-C4A
26	db	202	PEB	C2B-C1B-CHA-C4A
26	dc	201	PEB	NA-C4A-CHA-C1B
26	dc	201	PEB	C3A-C4A-CHA-C1B
26	dc	201	PEB	NB-C1B-CHA-C4A
26	dc	201	PEB	C2B-C1B-CHA-C4A
26	dc	202	PEB	NB-C1B-CHA-C4A
26	dc	202	PEB	C2B-C1B-CHA-C4A
26	dc	203	PEB	NA-C4A-CHA-C1B
26	dc	203	PEB	C3A-C4A-CHA-C1B
26	dc	203	PEB	NB-C1B-CHA-C4A
26	dc	203	PEB	C2B-C1B-CHA-C4A
26	dd	201	PEB	NA-C4A-CHA-C1B
26	dd	201	PEB	C3A-C4A-CHA-C1B
26	dd	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dd	201	PEB	C2B-C1B-CHA-C4A
26	dd	202	PEB	C1C-C2C-CAC-CBC
26	dd	202	PEB	C3C-C2C-CAC-CBC
26	dd	202	PEB	NB-C1B-CHA-C4A
26	dd	202	PEB	C2B-C1B-CHA-C4A
26	de	201	PEB	NA-C4A-CHA-C1B
26	de	201	PEB	C3A-C4A-CHA-C1B
26	de	201	PEB	NB-C1B-CHA-C4A
26	de	201	PEB	C2B-C1B-CHA-C4A
26	de	202	PEB	NB-C1B-CHA-C4A
26	de	202	PEB	C2B-C1B-CHA-C4A
26	df	201	PEB	NA-C4A-CHA-C1B
26	df	201	PEB	C3A-C4A-CHA-C1B
26	df	201	PEB	NB-C1B-CHA-C4A
26	df	201	PEB	C2B-C1B-CHA-C4A
26	df	202	PEB	C1C-C2C-CAC-CBC
26	df	202	PEB	C3C-C2C-CAC-CBC
26	df	202	PEB	NB-C1B-CHA-C4A
26	df	202	PEB	C2B-C1B-CHA-C4A
26	dg	201	PEB	NA-C4A-CHA-C1B
26	dg	201	PEB	C3A-C4A-CHA-C1B
26	dg	201	PEB	NB-C1B-CHA-C4A
26	dg	201	PEB	C2B-C1B-CHA-C4A
26	dg	202	PEB	NB-C1B-CHA-C4A
26	dg	202	PEB	C2B-C1B-CHA-C4A
26	dh	201	PEB	NA-C4A-CHA-C1B
26	dh	201	PEB	C3A-C4A-CHA-C1B
26	dh	201	PEB	NB-C1B-CHA-C4A
26	dh	201	PEB	C2B-C1B-CHA-C4A
26	dh	202	PEB	C1C-C2C-CAC-CBC
26	dh	202	PEB	C3C-C2C-CAC-CBC
26	dh	202	PEB	NB-C1B-CHA-C4A
26	dh	202	PEB	C2B-C1B-CHA-C4A
26	di	201	PEB	NA-C4A-CHA-C1B
26	di	201	PEB	C3A-C4A-CHA-C1B
26	di	201	PEB	NB-C1B-CHA-C4A
26	di	201	PEB	C2B-C1B-CHA-C4A
26	di	202	PEB	C1C-C2C-CAC-CBC
26	di	202	PEB	C3C-C2C-CAC-CBC
26	di	202	PEB	NB-C1B-CHA-C4A
26	di	202	PEB	C2B-C1B-CHA-C4A
26	dj	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	dj	201	PEB	C3A-C4A-CHA-C1B
26	dj	201	PEB	NB-C1B-CHA-C4A
26	dj	201	PEB	C2B-C1B-CHA-C4A
26	dj	202	PEB	C1C-C2C-CAC-CBC
26	dj	202	PEB	C3C-C2C-CAC-CBC
26	dj	202	PEB	NB-C1B-CHA-C4A
26	dj	202	PEB	C2B-C1B-CHA-C4A
26	dk	1001	PEB	NA-C4A-CHA-C1B
26	dk	1001	PEB	C3A-C4A-CHA-C1B
26	dk	1001	PEB	NB-C1B-CHA-C4A
26	dk	1001	PEB	C2B-C1B-CHA-C4A
26	dk	1002	PEB	NA-C4A-CHA-C1B
26	dk	1002	PEB	C3A-C4A-CHA-C1B
26	dk	1002	PEB	NB-C1B-CHA-C4A
26	dk	1002	PEB	C2B-C1B-CHA-C4A
26	dl	201	PEB	NA-C4A-CHA-C1B
26	dl	201	PEB	C3A-C4A-CHA-C1B
26	dl	201	PEB	NB-C1B-CHA-C4A
26	dl	201	PEB	C2B-C1B-CHA-C4A
26	dl	202	PEB	C1C-C2C-CAC-CBC
26	dl	202	PEB	C3C-C2C-CAC-CBC
26	dl	202	PEB	NB-C1B-CHA-C4A
26	dl	202	PEB	C2B-C1B-CHA-C4A
26	dm	201	PEB	NA-C4A-CHA-C1B
26	dm	201	PEB	C3A-C4A-CHA-C1B
26	dm	201	PEB	NB-C1B-CHA-C4A
26	dm	201	PEB	C2B-C1B-CHA-C4A
26	dm	202	PEB	NA-C4A-CHA-C1B
26	dm	202	PEB	C3A-C4A-CHA-C1B
26	dm	202	PEB	NB-C1B-CHA-C4A
26	dm	202	PEB	C2B-C1B-CHA-C4A
26	dn	201	PEB	NA-C4A-CHA-C1B
26	dn	201	PEB	C3A-C4A-CHA-C1B
26	dn	201	PEB	NB-C1B-CHA-C4A
26	dn	201	PEB	C2B-C1B-CHA-C4A
26	dn	202	PEB	NA-C4A-CHA-C1B
26	dn	202	PEB	C3A-C4A-CHA-C1B
26	dn	202	PEB	NB-C1B-CHA-C4A
26	dn	202	PEB	C2B-C1B-CHA-C4A
26	do	201	PEB	NA-C4A-CHA-C1B
26	do	201	PEB	C3A-C4A-CHA-C1B
26	do	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	do	201	PEB	C2B-C1B-CHA-C4A
26	do	202	PEB	NA-C4A-CHA-C1B
26	do	202	PEB	C3A-C4A-CHA-C1B
26	do	202	PEB	NB-C1B-CHA-C4A
26	do	202	PEB	C2B-C1B-CHA-C4A
26	dp	201	PEB	NA-C4A-CHA-C1B
26	dp	201	PEB	C3A-C4A-CHA-C1B
26	dp	201	PEB	NB-C1B-CHA-C4A
26	dp	201	PEB	C2B-C1B-CHA-C4A
26	dp	202	PEB	NA-C4A-CHA-C1B
26	dp	202	PEB	C3A-C4A-CHA-C1B
26	dp	202	PEB	NB-C1B-CHA-C4A
26	dp	202	PEB	C2B-C1B-CHA-C4A
26	dq	201	PEB	NA-C4A-CHA-C1B
26	dq	201	PEB	C3A-C4A-CHA-C1B
26	dq	201	PEB	NB-C1B-CHA-C4A
26	dq	201	PEB	C2B-C1B-CHA-C4A
26	dq	202	PEB	NA-C4A-CHA-C1B
26	dq	202	PEB	C3A-C4A-CHA-C1B
26	dq	202	PEB	NB-C1B-CHA-C4A
26	dq	202	PEB	C2B-C1B-CHA-C4A
26	dr	201	PEB	NA-C4A-CHA-C1B
26	dr	201	PEB	C3A-C4A-CHA-C1B
26	dr	201	PEB	NB-C1B-CHA-C4A
26	dr	201	PEB	C2B-C1B-CHA-C4A
26	dr	202	PEB	NA-C4A-CHA-C1B
26	dr	202	PEB	C3A-C4A-CHA-C1B
26	dr	202	PEB	NB-C1B-CHA-C4A
26	dr	202	PEB	C2B-C1B-CHA-C4A
26	ds	201	PEB	NA-C4A-CHA-C1B
26	ds	201	PEB	C3A-C4A-CHA-C1B
26	ds	201	PEB	NB-C1B-CHA-C4A
26	ds	201	PEB	C2B-C1B-CHA-C4A
26	ds	202	PEB	NA-C4A-CHA-C1B
26	ds	202	PEB	C3A-C4A-CHA-C1B
26	ds	202	PEB	NB-C1B-CHA-C4A
26	ds	202	PEB	C2B-C1B-CHA-C4A
26	dt	201	PEB	NA-C4A-CHA-C1B
26	dt	201	PEB	C3A-C4A-CHA-C1B
26	dt	201	PEB	NB-C1B-CHA-C4A
26	dt	201	PEB	C2B-C1B-CHA-C4A
26	dt	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	dt	202	PEB	C3A-C4A-CHA-C1B
26	dt	202	PEB	NB-C1B-CHA-C4A
26	dt	202	PEB	C2B-C1B-CHA-C4A
26	du	201	PEB	NA-C4A-CHA-C1B
26	du	201	PEB	C3A-C4A-CHA-C1B
26	du	201	PEB	NB-C1B-CHA-C4A
26	du	201	PEB	C2B-C1B-CHA-C4A
26	du	202	PEB	NA-C4A-CHA-C1B
26	du	202	PEB	C3A-C4A-CHA-C1B
26	du	202	PEB	NB-C1B-CHA-C4A
26	du	202	PEB	C2B-C1B-CHA-C4A
26	du	203	PEB	NA-C4A-CHA-C1B
26	du	203	PEB	C3A-C4A-CHA-C1B
26	du	203	PEB	NB-C1B-CHA-C4A
26	du	203	PEB	C2B-C1B-CHA-C4A
26	dv	201	PEB	NA-C4A-CHA-C1B
26	dv	201	PEB	C3A-C4A-CHA-C1B
26	dv	201	PEB	NB-C1B-CHA-C4A
26	dv	201	PEB	C2B-C1B-CHA-C4A
26	dw	401	PEB	NA-C4A-CHA-C1B
26	dw	401	PEB	C3A-C4A-CHA-C1B
26	dw	401	PEB	NB-C1B-CHA-C4A
26	dw	401	PEB	C2B-C1B-CHA-C4A
26	dw	402	PEB	NA-C4A-CHA-C1B
26	dw	402	PEB	C3A-C4A-CHA-C1B
26	dw	402	PEB	NB-C1B-CHA-C4A
26	dw	402	PEB	C2B-C1B-CHA-C4A
26	dw	403	PEB	NA-C4A-CHA-C1B
26	dw	403	PEB	C3A-C4A-CHA-C1B
26	dw	403	PEB	NB-C1B-CHA-C4A
26	dw	403	PEB	C2B-C1B-CHA-C4A
26	dx	401	PEB	NA-C4A-CHA-C1B
26	dx	401	PEB	C3A-C4A-CHA-C1B
26	dx	401	PEB	NB-C1B-CHA-C4A
26	dx	401	PEB	C2B-C1B-CHA-C4A
26	dx	402	PEB	NA-C4A-CHA-C1B
26	dx	402	PEB	C3A-C4A-CHA-C1B
26	dx	402	PEB	NB-C1B-CHA-C4A
26	dx	402	PEB	C2B-C1B-CHA-C4A
26	dx	403	PEB	NA-C4A-CHA-C1B
26	dx	403	PEB	C3A-C4A-CHA-C1B
26	dx	403	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dx	403	PEB	C2B-C1B-CHA-C4A
26	dx	404	PEB	NA-C4A-CHA-C1B
26	dx	404	PEB	C3A-C4A-CHA-C1B
26	dx	404	PEB	NB-C1B-CHA-C4A
26	dx	404	PEB	C2B-C1B-CHA-C4A
26	dy	401	PEB	NA-C4A-CHA-C1B
26	dy	401	PEB	C3A-C4A-CHA-C1B
26	dy	401	PEB	NB-C1B-CHA-C4A
26	dy	401	PEB	C2B-C1B-CHA-C4A
26	dz	401	PEB	NA-C4A-CHA-C1B
26	dz	401	PEB	C3A-C4A-CHA-C1B
26	dz	401	PEB	NB-C1B-CHA-C4A
26	dz	401	PEB	C2B-C1B-CHA-C4A
26	dz	402	PEB	NA-C4A-CHA-C1B
26	dz	402	PEB	C3A-C4A-CHA-C1B
26	dz	402	PEB	NB-C1B-CHA-C4A
26	dz	402	PEB	C2B-C1B-CHA-C4A
26	dA	201	PEB	NA-C4A-CHA-C1B
26	dA	201	PEB	C3A-C4A-CHA-C1B
26	dA	201	PEB	NB-C1B-CHA-C4A
26	dA	201	PEB	C2B-C1B-CHA-C4A
26	dA	202	PEB	NA-C4A-CHA-C1B
26	dA	202	PEB	C3A-C4A-CHA-C1B
26	dA	202	PEB	NB-C1B-CHA-C4A
26	dA	202	PEB	C2B-C1B-CHA-C4A
26	dB	201	PEB	NA-C4A-CHA-C1B
26	dB	201	PEB	C3A-C4A-CHA-C1B
26	dB	201	PEB	NB-C1B-CHA-C4A
26	dB	201	PEB	C2B-C1B-CHA-C4A
26	dC	201	PEB	NA-C4A-CHA-C1B
26	dC	201	PEB	C3A-C4A-CHA-C1B
26	dC	201	PEB	NB-C1B-CHA-C4A
26	dC	201	PEB	C2B-C1B-CHA-C4A
26	dC	202	PEB	NA-C4A-CHA-C1B
26	dC	202	PEB	C3A-C4A-CHA-C1B
26	dC	202	PEB	NB-C1B-CHA-C4A
26	dC	202	PEB	C2B-C1B-CHA-C4A
26	dD	201	PEB	NA-C4A-CHA-C1B
26	dD	201	PEB	C3A-C4A-CHA-C1B
26	dD	201	PEB	NB-C1B-CHA-C4A
26	dD	201	PEB	C2B-C1B-CHA-C4A
26	dD	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	dD	202	PEB	C3A-C4A-CHA-C1B
26	dD	202	PEB	NB-C1B-CHA-C4A
26	dD	202	PEB	C2B-C1B-CHA-C4A
26	dE	201	PEB	NA-C4A-CHA-C1B
26	dE	201	PEB	C3A-C4A-CHA-C1B
26	dE	201	PEB	NB-C1B-CHA-C4A
26	dE	201	PEB	C2B-C1B-CHA-C4A
26	dF	201	PEB	NA-C4A-CHA-C1B
26	dF	201	PEB	C3A-C4A-CHA-C1B
26	dF	201	PEB	NB-C1B-CHA-C4A
26	dF	201	PEB	C2B-C1B-CHA-C4A
26	dF	202	PEB	NA-C4A-CHA-C1B
26	dF	202	PEB	C3A-C4A-CHA-C1B
26	dF	202	PEB	NB-C1B-CHA-C4A
26	dF	202	PEB	C2B-C1B-CHA-C4A
26	dG	201	PEB	NA-C4A-CHA-C1B
26	dG	201	PEB	C3A-C4A-CHA-C1B
26	dG	201	PEB	NB-C1B-CHA-C4A
26	dG	201	PEB	C2B-C1B-CHA-C4A
26	dG	202	PEB	NA-C4A-CHA-C1B
26	dG	202	PEB	C3A-C4A-CHA-C1B
26	dG	202	PEB	NB-C1B-CHA-C4A
26	dG	202	PEB	C2B-C1B-CHA-C4A
26	dH	201	PEB	NA-C4A-CHA-C1B
26	dH	201	PEB	C3A-C4A-CHA-C1B
26	dH	201	PEB	NB-C1B-CHA-C4A
26	dH	201	PEB	C2B-C1B-CHA-C4A
26	dH	202	PEB	NA-C4A-CHA-C1B
26	dH	202	PEB	C3A-C4A-CHA-C1B
26	dH	202	PEB	NB-C1B-CHA-C4A
26	dH	202	PEB	C2B-C1B-CHA-C4A
26	dI	1001	PEB	NA-C4A-CHA-C1B
26	dI	1001	PEB	C3A-C4A-CHA-C1B
26	dI	1001	PEB	NB-C1B-CHA-C4A
26	dI	1001	PEB	C2B-C1B-CHA-C4A
26	dI	1002	PEB	NA-C4A-CHA-C1B
26	dI	1002	PEB	C3A-C4A-CHA-C1B
26	dI	1002	PEB	NB-C1B-CHA-C4A
26	dI	1002	PEB	C2B-C1B-CHA-C4A
26	dJ	201	PEB	NA-C4A-CHA-C1B
26	dJ	201	PEB	C3A-C4A-CHA-C1B
26	dJ	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dJ	201	PEB	C2B-C1B-CHA-C4A
26	dJ	202	PEB	NB-C1B-CHA-C4A
26	dJ	202	PEB	C2B-C1B-CHA-C4A
26	dK	201	PEB	NA-C4A-CHA-C1B
26	dK	201	PEB	C3A-C4A-CHA-C1B
26	dK	201	PEB	NB-C1B-CHA-C4A
26	dK	201	PEB	C2B-C1B-CHA-C4A
26	dK	202	PEB	NA-C4A-CHA-C1B
26	dK	202	PEB	C3A-C4A-CHA-C1B
26	dK	202	PEB	NB-C1B-CHA-C4A
26	dK	202	PEB	C2B-C1B-CHA-C4A
26	dL	201	PEB	NA-C4A-CHA-C1B
26	dL	201	PEB	C3A-C4A-CHA-C1B
26	dL	201	PEB	NB-C1B-CHA-C4A
26	dL	201	PEB	C2B-C1B-CHA-C4A
26	dL	202	PEB	C1C-C2C-CAC-CBC
26	dL	202	PEB	C3C-C2C-CAC-CBC
26	dL	202	PEB	NB-C1B-CHA-C4A
26	dL	202	PEB	C2B-C1B-CHA-C4A
26	dM	1001	PEB	NA-C4A-CHA-C1B
26	dM	1001	PEB	C3A-C4A-CHA-C1B
26	dM	1001	PEB	NB-C1B-CHA-C4A
26	dM	1001	PEB	C2B-C1B-CHA-C4A
26	dM	1002	PEB	NA-C4A-CHA-C1B
26	dM	1002	PEB	C3A-C4A-CHA-C1B
26	dM	1002	PEB	NB-C1B-CHA-C4A
26	dM	1002	PEB	C2B-C1B-CHA-C4A
26	dN	201	PEB	NA-C4A-CHA-C1B
26	dN	201	PEB	C3A-C4A-CHA-C1B
26	dN	201	PEB	NB-C1B-CHA-C4A
26	dN	201	PEB	C2B-C1B-CHA-C4A
26	dN	202	PEB	NA-C4A-CHA-C1B
26	dN	202	PEB	C3A-C4A-CHA-C1B
26	dN	202	PEB	NB-C1B-CHA-C4A
26	dN	202	PEB	C2B-C1B-CHA-C4A
26	dO	201	PEB	NA-C4A-CHA-C1B
26	dO	201	PEB	C3A-C4A-CHA-C1B
26	dO	201	PEB	NB-C1B-CHA-C4A
26	dO	201	PEB	C2B-C1B-CHA-C4A
26	dO	202	PEB	NA-C4A-CHA-C1B
26	dO	202	PEB	C3A-C4A-CHA-C1B
26	dO	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dO	202	PEB	C2B-C1B-CHA-C4A
26	dP	201	PEB	NA-C4A-CHA-C1B
26	dP	201	PEB	C3A-C4A-CHA-C1B
26	dP	201	PEB	NB-C1B-CHA-C4A
26	dP	201	PEB	C2B-C1B-CHA-C4A
26	dP	202	PEB	NA-C4A-CHA-C1B
26	dP	202	PEB	C3A-C4A-CHA-C1B
26	dP	202	PEB	NB-C1B-CHA-C4A
26	dP	202	PEB	C2B-C1B-CHA-C4A
26	dQ	201	PEB	NA-C4A-CHA-C1B
26	dQ	201	PEB	C3A-C4A-CHA-C1B
26	dQ	201	PEB	NB-C1B-CHA-C4A
26	dQ	201	PEB	C2B-C1B-CHA-C4A
26	dQ	202	PEB	NA-C4A-CHA-C1B
26	dQ	202	PEB	C3A-C4A-CHA-C1B
26	dQ	202	PEB	NB-C1B-CHA-C4A
26	dQ	202	PEB	C2B-C1B-CHA-C4A
26	dR	201	PEB	NA-C4A-CHA-C1B
26	dR	201	PEB	C3A-C4A-CHA-C1B
26	dR	201	PEB	NB-C1B-CHA-C4A
26	dR	201	PEB	C2B-C1B-CHA-C4A
26	dR	202	PEB	NA-C4A-CHA-C1B
26	dR	202	PEB	C3A-C4A-CHA-C1B
26	dR	202	PEB	NB-C1B-CHA-C4A
26	dR	202	PEB	C2B-C1B-CHA-C4A
26	dS	201	PEB	NA-C4A-CHA-C1B
26	dS	201	PEB	C3A-C4A-CHA-C1B
26	dS	201	PEB	NB-C1B-CHA-C4A
26	dS	201	PEB	C2B-C1B-CHA-C4A
26	dT	201	PEB	NA-C4A-CHA-C1B
26	dT	201	PEB	C3A-C4A-CHA-C1B
26	dT	201	PEB	NB-C1B-CHA-C4A
26	dT	201	PEB	C2B-C1B-CHA-C4A
26	dT	202	PEB	NA-C4A-CHA-C1B
26	dT	202	PEB	C3A-C4A-CHA-C1B
26	dT	202	PEB	NB-C1B-CHA-C4A
26	dT	202	PEB	C2B-C1B-CHA-C4A
26	dU	201	PEB	NA-C4A-CHA-C1B
26	dU	201	PEB	C3A-C4A-CHA-C1B
26	dU	201	PEB	NB-C1B-CHA-C4A
26	dU	201	PEB	C2B-C1B-CHA-C4A
26	dU	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	dU	202	PEB	C2B-C1B-CHA-C4A
26	dV	201	PEB	NA-C4A-CHA-C1B
26	dV	201	PEB	C3A-C4A-CHA-C1B
26	dV	201	PEB	NB-C1B-CHA-C4A
26	dV	201	PEB	C2B-C1B-CHA-C4A
26	dV	202	PEB	C1C-C2C-CAC-CBC
26	dV	202	PEB	C3C-C2C-CAC-CBC
26	dV	202	PEB	NB-C1B-CHA-C4A
26	dV	202	PEB	C2B-C1B-CHA-C4A
26	dW	201	PEB	NA-C4A-CHA-C1B
26	dW	201	PEB	C3A-C4A-CHA-C1B
26	dW	201	PEB	NB-C1B-CHA-C4A
26	dW	201	PEB	C2B-C1B-CHA-C4A
26	dW	202	PEB	NA-C4A-CHA-C1B
26	dW	202	PEB	C3A-C4A-CHA-C1B
26	dW	202	PEB	NB-C1B-CHA-C4A
26	dW	202	PEB	C2B-C1B-CHA-C4A
26	dX	201	PEB	NA-C4A-CHA-C1B
26	dX	201	PEB	C3A-C4A-CHA-C1B
26	dX	201	PEB	NB-C1B-CHA-C4A
26	dX	201	PEB	C2B-C1B-CHA-C4A
26	dX	202	PEB	NA-C4A-CHA-C1B
26	dX	202	PEB	C3A-C4A-CHA-C1B
26	dX	202	PEB	NB-C1B-CHA-C4A
26	dX	202	PEB	C2B-C1B-CHA-C4A
26	dY	201	PEB	NA-C4A-CHA-C1B
26	dY	201	PEB	C3A-C4A-CHA-C1B
26	dY	201	PEB	NB-C1B-CHA-C4A
26	dY	201	PEB	C2B-C1B-CHA-C4A
26	dY	202	PEB	C1C-C2C-CAC-CBC
26	dY	202	PEB	C3C-C2C-CAC-CBC
26	dY	202	PEB	NB-C1B-CHA-C4A
26	dY	202	PEB	C2B-C1B-CHA-C4A
26	dZ	1001	PEB	NA-C4A-CHA-C1B
26	dZ	1001	PEB	C3A-C4A-CHA-C1B
26	dZ	1001	PEB	NB-C1B-CHA-C4A
26	dZ	1001	PEB	C2B-C1B-CHA-C4A
26	dZ	1002	PEB	NB-C1B-CHA-C4A
26	dZ	1002	PEB	C2B-C1B-CHA-C4A
26	ea	201	PEB	NA-C4A-CHA-C1B
26	ea	201	PEB	C3A-C4A-CHA-C1B
26	ea	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	ea	201	PEB	C2B-C1B-CHA-C4A
26	ea	202	PEB	NA-C4A-CHA-C1B
26	ea	202	PEB	C3A-C4A-CHA-C1B
26	ea	202	PEB	NB-C1B-CHA-C4A
26	ea	202	PEB	C2B-C1B-CHA-C4A
26	ea	203	PEB	C1C-C2C-CAC-CBC
26	ea	203	PEB	C3C-C2C-CAC-CBC
26	ea	203	PEB	NB-C1B-CHA-C4A
26	ea	203	PEB	C2B-C1B-CHA-C4A
26	eb	201	PEB	NA-C4A-CHA-C1B
26	eb	201	PEB	C3A-C4A-CHA-C1B
26	eb	201	PEB	NB-C1B-CHA-C4A
26	eb	201	PEB	C2B-C1B-CHA-C4A
26	ec	201	PEB	NB-C1B-CHA-C4A
26	ec	201	PEB	C2B-C1B-CHA-C4A
26	ec	202	PEB	C1C-C2C-CAC-CBC
26	ec	202	PEB	C3C-C2C-CAC-CBC
26	ec	202	PEB	NB-C1B-CHA-C4A
26	ec	202	PEB	C2B-C1B-CHA-C4A
26	ed	201	PEB	NA-C4A-CHA-C1B
26	ed	201	PEB	C3A-C4A-CHA-C1B
26	ed	201	PEB	NB-C1B-CHA-C4A
26	ed	201	PEB	C2B-C1B-CHA-C4A
26	ed	202	PEB	NA-C4A-CHA-C1B
26	ed	202	PEB	C3A-C4A-CHA-C1B
26	ed	202	PEB	NB-C1B-CHA-C4A
26	ed	202	PEB	C2B-C1B-CHA-C4A
26	ee	201	PEB	NA-C4A-CHA-C1B
26	ee	201	PEB	C3A-C4A-CHA-C1B
26	ee	201	PEB	NB-C1B-CHA-C4A
26	ee	201	PEB	C2B-C1B-CHA-C4A
26	ee	202	PEB	C1C-C2C-CAC-CBC
26	ee	202	PEB	C3C-C2C-CAC-CBC
26	ee	202	PEB	NB-C1B-CHA-C4A
26	ee	202	PEB	C2B-C1B-CHA-C4A
26	ef	201	PEB	NA-C4A-CHA-C1B
26	ef	201	PEB	C3A-C4A-CHA-C1B
26	ef	201	PEB	NB-C1B-CHA-C4A
26	ef	201	PEB	C2B-C1B-CHA-C4A
26	ef	202	PEB	NB-C1B-CHA-C4A
26	ef	202	PEB	C2B-C1B-CHA-C4A
26	eg	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	eg	201	PEB	C3A-C4A-CHA-C1B
26	eg	201	PEB	NB-C1B-CHA-C4A
26	eg	201	PEB	C2B-C1B-CHA-C4A
26	eg	202	PEB	C1C-C2C-CAC-CBC
26	eg	202	PEB	C3C-C2C-CAC-CBC
26	eg	202	PEB	NB-C1B-CHA-C4A
26	eg	202	PEB	C2B-C1B-CHA-C4A
26	eh	201	PEB	NA-C4A-CHA-C1B
26	eh	201	PEB	C3A-C4A-CHA-C1B
26	eh	201	PEB	NB-C1B-CHA-C4A
26	eh	201	PEB	C2B-C1B-CHA-C4A
26	eh	202	PEB	NB-C1B-CHA-C4A
26	eh	202	PEB	C2B-C1B-CHA-C4A
26	ei	201	PEB	NB-C1B-CHA-C4A
26	ei	201	PEB	C2B-C1B-CHA-C4A
26	ei	202	PEB	C1C-C2C-CAC-CBC
26	ei	202	PEB	C3C-C2C-CAC-CBC
26	ei	202	PEB	NB-C1B-CHA-C4A
26	ei	202	PEB	C2B-C1B-CHA-C4A
26	ej	201	PEB	NA-C4A-CHA-C1B
26	ej	201	PEB	C3A-C4A-CHA-C1B
26	ej	201	PEB	NB-C1B-CHA-C4A
26	ej	201	PEB	C2B-C1B-CHA-C4A
26	ej	202	PEB	NA-C4A-CHA-C1B
26	ej	202	PEB	C3A-C4A-CHA-C1B
26	ej	202	PEB	NB-C1B-CHA-C4A
26	ej	202	PEB	C2B-C1B-CHA-C4A
26	ek	1001	PEB	NA-C4A-CHA-C1B
26	ek	1001	PEB	C3A-C4A-CHA-C1B
26	ek	1001	PEB	NB-C1B-CHA-C4A
26	ek	1001	PEB	C2B-C1B-CHA-C4A
26	ek	1002	PEB	NB-C1B-CHA-C4A
26	ek	1002	PEB	C2B-C1B-CHA-C4A
26	el	201	PEB	NA-C4A-CHA-C1B
26	el	201	PEB	C3A-C4A-CHA-C1B
26	el	201	PEB	NB-C1B-CHA-C4A
26	el	201	PEB	C2B-C1B-CHA-C4A
26	el	202	PEB	C1C-C2C-CAC-CBC
26	el	202	PEB	C3C-C2C-CAC-CBC
26	el	202	PEB	NB-C1B-CHA-C4A
26	el	202	PEB	C2B-C1B-CHA-C4A
26	em	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	em	201	PEB	C3A-C4A-CHA-C1B
26	em	201	PEB	NB-C1B-CHA-C4A
26	em	201	PEB	C2B-C1B-CHA-C4A
26	em	202	PEB	NB-C1B-CHA-C4A
26	em	202	PEB	C2B-C1B-CHA-C4A
26	en	201	PEB	NA-C4A-CHA-C1B
26	en	201	PEB	C3A-C4A-CHA-C1B
26	en	201	PEB	NB-C1B-CHA-C4A
26	en	201	PEB	C2B-C1B-CHA-C4A
26	en	202	PEB	C1C-C2C-CAC-CBC
26	en	202	PEB	C3C-C2C-CAC-CBC
26	en	202	PEB	NB-C1B-CHA-C4A
26	en	202	PEB	C2B-C1B-CHA-C4A
26	eo	201	PEB	NA-C4A-CHA-C1B
26	eo	201	PEB	C3A-C4A-CHA-C1B
26	eo	201	PEB	NB-C1B-CHA-C4A
26	eo	201	PEB	C2B-C1B-CHA-C4A
26	eo	202	PEB	NA-C4A-CHA-C1B
26	eo	202	PEB	C3A-C4A-CHA-C1B
26	eo	202	PEB	NB-C1B-CHA-C4A
26	eo	202	PEB	C2B-C1B-CHA-C4A
26	ep	201	PEB	NA-C4A-CHA-C1B
26	ep	201	PEB	C3A-C4A-CHA-C1B
26	ep	201	PEB	NB-C1B-CHA-C4A
26	ep	201	PEB	C2B-C1B-CHA-C4A
26	ep	202	PEB	C1C-C2C-CAC-CBC
26	ep	202	PEB	C3C-C2C-CAC-CBC
26	ep	202	PEB	NB-C1B-CHA-C4A
26	ep	202	PEB	C2B-C1B-CHA-C4A
26	eq	201	PEB	NA-C4A-CHA-C1B
26	eq	201	PEB	C3A-C4A-CHA-C1B
26	eq	201	PEB	NB-C1B-CHA-C4A
26	eq	201	PEB	C2B-C1B-CHA-C4A
26	eq	202	PEB	NA-C4A-CHA-C1B
26	eq	202	PEB	C3A-C4A-CHA-C1B
26	eq	202	PEB	NB-C1B-CHA-C4A
26	eq	202	PEB	C2B-C1B-CHA-C4A
26	er	201	PEB	NA-C4A-CHA-C1B
26	er	201	PEB	C3A-C4A-CHA-C1B
26	er	201	PEB	NB-C1B-CHA-C4A
26	er	201	PEB	C2B-C1B-CHA-C4A
26	er	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	er	202	PEB	C3C-C2C-CAC-CBC
26	er	202	PEB	NB-C1B-CHA-C4A
26	er	202	PEB	C2B-C1B-CHA-C4A
26	es	201	PEB	NA-C4A-CHA-C1B
26	es	201	PEB	C3A-C4A-CHA-C1B
26	es	201	PEB	NB-C1B-CHA-C4A
26	es	201	PEB	C2B-C1B-CHA-C4A
26	es	202	PEB	NA-C4A-CHA-C1B
26	es	202	PEB	C3A-C4A-CHA-C1B
26	es	202	PEB	NB-C1B-CHA-C4A
26	es	202	PEB	C2B-C1B-CHA-C4A
26	et	201	PEB	NB-C1B-CHA-C4A
26	et	201	PEB	C2B-C1B-CHA-C4A
26	et	202	PEB	C1C-C2C-CAC-CBC
26	et	202	PEB	C3C-C2C-CAC-CBC
26	et	202	PEB	NB-C1B-CHA-C4A
26	et	202	PEB	C2B-C1B-CHA-C4A
26	eu	201	PEB	NA-C4A-CHA-C1B
26	eu	201	PEB	C3A-C4A-CHA-C1B
26	eu	201	PEB	NB-C1B-CHA-C4A
26	eu	201	PEB	C2B-C1B-CHA-C4A
26	eu	202	PEB	NB-C1B-CHA-C4A
26	eu	202	PEB	C2B-C1B-CHA-C4A
26	ev	201	PEB	NB-C1B-CHA-C4A
26	ev	201	PEB	C2B-C1B-CHA-C4A
26	ev	202	PEB	C1C-C2C-CAC-CBC
26	ev	202	PEB	C3C-C2C-CAC-CBC
26	ev	202	PEB	NB-C1B-CHA-C4A
26	ev	202	PEB	C2B-C1B-CHA-C4A
26	ew	301	PEB	NA-C4A-CHA-C1B
26	ew	301	PEB	C3A-C4A-CHA-C1B
26	ew	301	PEB	NB-C1B-CHA-C4A
26	ew	301	PEB	C2B-C1B-CHA-C4A
26	ey	1001	PEB	NB-C1B-CHA-C4A
26	ey	1001	PEB	C2B-C1B-CHA-C4A
26	ey	1002	PEB	NA-C4A-CHA-C1B
26	ey	1002	PEB	C3A-C4A-CHA-C1B
26	ey	1002	PEB	NB-C1B-CHA-C4A
26	ey	1002	PEB	C2B-C1B-CHA-C4A
26	ey	1003	PEB	NA-C4A-CHA-C1B
26	ey	1003	PEB	C3A-C4A-CHA-C1B
26	ey	1003	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	ey	1003	PEB	C2B-C1B-CHA-C4A
26	ez	1001	PEB	NA-C4A-CHA-C1B
26	ez	1001	PEB	C3A-C4A-CHA-C1B
26	ez	1001	PEB	NB-C1B-CHA-C4A
26	ez	1001	PEB	C2B-C1B-CHA-C4A
26	ez	1002	PEB	NA-C4A-CHA-C1B
26	ez	1002	PEB	C3A-C4A-CHA-C1B
26	ez	1002	PEB	NB-C1B-CHA-C4A
26	ez	1002	PEB	C2B-C1B-CHA-C4A
26	ez	1003	PEB	NA-C4A-CHA-C1B
26	ez	1003	PEB	C3A-C4A-CHA-C1B
26	ez	1003	PEB	NB-C1B-CHA-C4A
26	ez	1003	PEB	C2B-C1B-CHA-C4A
26	eA	1001	PEB	NA-C4A-CHA-C1B
26	eA	1001	PEB	C3A-C4A-CHA-C1B
26	eA	1001	PEB	NB-C1B-CHA-C4A
26	eA	1001	PEB	C2B-C1B-CHA-C4A
26	eA	1002	PEB	NB-C1B-CHA-C4A
26	eA	1002	PEB	C2B-C1B-CHA-C4A
26	eB	201	PEB	NB-C1B-CHA-C4A
26	eB	201	PEB	C2B-C1B-CHA-C4A
26	eB	202	PEB	NA-C4A-CHA-C1B
26	eB	202	PEB	C3A-C4A-CHA-C1B
26	eB	202	PEB	NB-C1B-CHA-C4A
26	eB	202	PEB	C2B-C1B-CHA-C4A
26	eB	203	PEB	C1C-C2C-CAC-CBC
26	eB	203	PEB	C3C-C2C-CAC-CBC
26	eB	203	PEB	NB-C1B-CHA-C4A
26	eB	203	PEB	C2B-C1B-CHA-C4A
26	eC	201	PEB	NA-C4A-CHA-C1B
26	eC	201	PEB	C3A-C4A-CHA-C1B
26	eC	201	PEB	NB-C1B-CHA-C4A
26	eC	201	PEB	C2B-C1B-CHA-C4A
26	eC	202	PEB	NA-C4A-CHA-C1B
26	eC	202	PEB	C3A-C4A-CHA-C1B
26	eC	202	PEB	NB-C1B-CHA-C4A
26	eC	202	PEB	C2B-C1B-CHA-C4A
26	eD	201	PEB	NA-C4A-CHA-C1B
26	eD	201	PEB	C3A-C4A-CHA-C1B
26	eD	201	PEB	NB-C1B-CHA-C4A
26	eD	201	PEB	C2B-C1B-CHA-C4A
26	eD	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	eD	202	PEB	C3A-C4A-CHA-C1B
26	eD	202	PEB	NB-C1B-CHA-C4A
26	eD	202	PEB	C2B-C1B-CHA-C4A
26	eE	201	PEB	NA-C4A-CHA-C1B
26	eE	201	PEB	C3A-C4A-CHA-C1B
26	eE	201	PEB	NB-C1B-CHA-C4A
26	eE	201	PEB	C2B-C1B-CHA-C4A
26	eE	202	PEB	NA-C4A-CHA-C1B
26	eE	202	PEB	C3A-C4A-CHA-C1B
26	eE	202	PEB	NB-C1B-CHA-C4A
26	eE	202	PEB	C2B-C1B-CHA-C4A
26	eF	201	PEB	NA-C4A-CHA-C1B
26	eF	201	PEB	C3A-C4A-CHA-C1B
26	eF	201	PEB	NB-C1B-CHA-C4A
26	eF	201	PEB	C2B-C1B-CHA-C4A
26	eF	202	PEB	NA-C4A-CHA-C1B
26	eF	202	PEB	C3A-C4A-CHA-C1B
26	eF	202	PEB	NB-C1B-CHA-C4A
26	eF	202	PEB	C2B-C1B-CHA-C4A
26	eG	201	PEB	NA-C4A-CHA-C1B
26	eG	201	PEB	C3A-C4A-CHA-C1B
26	eG	201	PEB	NB-C1B-CHA-C4A
26	eG	201	PEB	C2B-C1B-CHA-C4A
26	eG	202	PEB	NA-C4A-CHA-C1B
26	eG	202	PEB	C3A-C4A-CHA-C1B
26	eG	202	PEB	NB-C1B-CHA-C4A
26	eG	202	PEB	C2B-C1B-CHA-C4A
26	eH	201	PEB	NA-C4A-CHA-C1B
26	eH	201	PEB	C3A-C4A-CHA-C1B
26	eH	201	PEB	NB-C1B-CHA-C4A
26	eH	201	PEB	C2B-C1B-CHA-C4A
26	eH	202	PEB	NA-C4A-CHA-C1B
26	eH	202	PEB	C3A-C4A-CHA-C1B
26	eH	202	PEB	NB-C1B-CHA-C4A
26	eH	202	PEB	C2B-C1B-CHA-C4A
26	eI	201	PEB	NA-C4A-CHA-C1B
26	eI	201	PEB	C3A-C4A-CHA-C1B
26	eI	201	PEB	NB-C1B-CHA-C4A
26	eI	201	PEB	C2B-C1B-CHA-C4A
26	eI	202	PEB	NA-C4A-CHA-C1B
26	eI	202	PEB	C3A-C4A-CHA-C1B
26	eI	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	eI	202	PEB	C2B-C1B-CHA-C4A
26	eJ	201	PEB	NA-C4A-CHA-C1B
26	eJ	201	PEB	C3A-C4A-CHA-C1B
26	eJ	201	PEB	NB-C1B-CHA-C4A
26	eJ	201	PEB	C2B-C1B-CHA-C4A
26	eJ	202	PEB	C1C-C2C-CAC-CBC
26	eJ	202	PEB	C3C-C2C-CAC-CBC
26	eJ	202	PEB	NB-C1B-CHA-C4A
26	eJ	202	PEB	C2B-C1B-CHA-C4A
26	eK	201	PEB	NA-C4A-CHA-C1B
26	eK	201	PEB	C3A-C4A-CHA-C1B
26	eK	201	PEB	NB-C1B-CHA-C4A
26	eK	201	PEB	C2B-C1B-CHA-C4A
26	eK	202	PEB	NA-C4A-CHA-C1B
26	eK	202	PEB	C3A-C4A-CHA-C1B
26	eK	202	PEB	NB-C1B-CHA-C4A
26	eK	202	PEB	C2B-C1B-CHA-C4A
26	eL	201	PEB	NB-C1B-CHA-C4A
26	eL	201	PEB	C2B-C1B-CHA-C4A
26	eL	202	PEB	C1C-C2C-CAC-CBC
26	eL	202	PEB	C3C-C2C-CAC-CBC
26	eL	202	PEB	NB-C1B-CHA-C4A
26	eL	202	PEB	C2B-C1B-CHA-C4A
26	eM	1001	PEB	NA-C4A-CHA-C1B
26	eM	1001	PEB	C3A-C4A-CHA-C1B
26	eM	1001	PEB	NB-C1B-CHA-C4A
26	eM	1001	PEB	C2B-C1B-CHA-C4A
26	eM	1002	PEB	NA-C4A-CHA-C1B
26	eM	1002	PEB	C3A-C4A-CHA-C1B
26	eM	1002	PEB	NB-C1B-CHA-C4A
26	eM	1002	PEB	C2B-C1B-CHA-C4A
26	eN	201	PEB	NA-C4A-CHA-C1B
26	eN	201	PEB	C3A-C4A-CHA-C1B
26	eN	201	PEB	NB-C1B-CHA-C4A
26	eN	201	PEB	C2B-C1B-CHA-C4A
26	eN	202	PEB	C1C-C2C-CAC-CBC
26	eN	202	PEB	C3C-C2C-CAC-CBC
26	eN	202	PEB	NB-C1B-CHA-C4A
26	eN	202	PEB	C2B-C1B-CHA-C4A
26	eO	201	PEB	NA-C4A-CHA-C1B
26	eO	201	PEB	C3A-C4A-CHA-C1B
26	eO	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	eO	201	PEB	C2B-C1B-CHA-C4A
26	eO	202	PEB	NA-C4A-CHA-C1B
26	eO	202	PEB	C3A-C4A-CHA-C1B
26	eO	202	PEB	NB-C1B-CHA-C4A
26	eO	202	PEB	C2B-C1B-CHA-C4A
26	eP	201	PEB	NB-C1B-CHA-C4A
26	eP	201	PEB	C2B-C1B-CHA-C4A
26	eP	202	PEB	NA-C4A-CHA-C1B
26	eP	202	PEB	C3A-C4A-CHA-C1B
26	eP	202	PEB	NB-C1B-CHA-C4A
26	eP	202	PEB	C2B-C1B-CHA-C4A
26	eP	203	PEB	NA-C4A-CHA-C1B
26	eP	203	PEB	C3A-C4A-CHA-C1B
26	eP	203	PEB	NB-C1B-CHA-C4A
26	eP	203	PEB	C2B-C1B-CHA-C4A
26	eQ	201	PEB	NA-C4A-CHA-C1B
26	eQ	201	PEB	C3A-C4A-CHA-C1B
26	eQ	201	PEB	NB-C1B-CHA-C4A
26	eQ	201	PEB	C2B-C1B-CHA-C4A
26	eQ	202	PEB	NA-C4A-CHA-C1B
26	eQ	202	PEB	C3A-C4A-CHA-C1B
26	eQ	202	PEB	NB-C1B-CHA-C4A
26	eQ	202	PEB	C2B-C1B-CHA-C4A
26	eR	201	PEB	NA-C4A-CHA-C1B
26	eR	201	PEB	C3A-C4A-CHA-C1B
26	eR	201	PEB	NB-C1B-CHA-C4A
26	eR	201	PEB	C2B-C1B-CHA-C4A
26	eR	202	PEB	NA-C4A-CHA-C1B
26	eR	202	PEB	C3A-C4A-CHA-C1B
26	eR	202	PEB	NB-C1B-CHA-C4A
26	eR	202	PEB	C2B-C1B-CHA-C4A
26	eS	201	PEB	NA-C4A-CHA-C1B
26	eS	201	PEB	C3A-C4A-CHA-C1B
26	eS	201	PEB	NB-C1B-CHA-C4A
26	eS	201	PEB	C2B-C1B-CHA-C4A
26	eS	202	PEB	NA-C4A-CHA-C1B
26	eS	202	PEB	C3A-C4A-CHA-C1B
26	eS	202	PEB	NB-C1B-CHA-C4A
26	eS	202	PEB	C2B-C1B-CHA-C4A
26	eT	201	PEB	NA-C4A-CHA-C1B
26	eT	201	PEB	C3A-C4A-CHA-C1B
26	eT	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	eT	201	PEB	C2B-C1B-CHA-C4A
26	eT	202	PEB	NA-C4A-CHA-C1B
26	eT	202	PEB	C3A-C4A-CHA-C1B
26	eT	202	PEB	NB-C1B-CHA-C4A
26	eT	202	PEB	C2B-C1B-CHA-C4A
26	eU	201	PEB	NA-C4A-CHA-C1B
26	eU	201	PEB	C3A-C4A-CHA-C1B
26	eU	201	PEB	NB-C1B-CHA-C4A
26	eU	201	PEB	C2B-C1B-CHA-C4A
26	eU	202	PEB	NA-C4A-CHA-C1B
26	eU	202	PEB	C3A-C4A-CHA-C1B
26	eU	202	PEB	NB-C1B-CHA-C4A
26	eU	202	PEB	C2B-C1B-CHA-C4A
26	eV	201	PEB	NA-C4A-CHA-C1B
26	eV	201	PEB	C3A-C4A-CHA-C1B
26	eV	201	PEB	NB-C1B-CHA-C4A
26	eV	201	PEB	C2B-C1B-CHA-C4A
26	eV	202	PEB	C1C-C2C-CAC-CBC
26	eV	202	PEB	C3C-C2C-CAC-CBC
26	eV	202	PEB	NB-C1B-CHA-C4A
26	eV	202	PEB	C2B-C1B-CHA-C4A
26	eW	201	PEB	NA-C4A-CHA-C1B
26	eW	201	PEB	C3A-C4A-CHA-C1B
26	eW	201	PEB	NB-C1B-CHA-C4A
26	eW	201	PEB	C2B-C1B-CHA-C4A
26	eW	202	PEB	NA-C4A-CHA-C1B
26	eW	202	PEB	C3A-C4A-CHA-C1B
26	eW	202	PEB	NB-C1B-CHA-C4A
26	eW	202	PEB	C2B-C1B-CHA-C4A
26	eX	201	PEB	C1C-C2C-CAC-CBC
26	eX	201	PEB	C3C-C2C-CAC-CBC
26	eX	201	PEB	NB-C1B-CHA-C4A
26	eX	201	PEB	C2B-C1B-CHA-C4A
26	eY	401	PEB	NB-C1B-CHA-C4A
26	eY	401	PEB	C2B-C1B-CHA-C4A
26	eY	402	PEB	NA-C4A-CHA-C1B
26	eY	402	PEB	C3A-C4A-CHA-C1B
26	eY	402	PEB	NB-C1B-CHA-C4A
26	eY	402	PEB	C2B-C1B-CHA-C4A
26	eZ	401	PEB	NA-C4A-CHA-C1B
26	eZ	401	PEB	C3A-C4A-CHA-C1B
26	eZ	401	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	eZ	401	PEB	C2B-C1B-CHA-C4A
26	la	1001	PEB	NA-C4A-CHA-C1B
26	la	1001	PEB	C3A-C4A-CHA-C1B
26	la	1001	PEB	NB-C1B-CHA-C4A
26	la	1001	PEB	C2B-C1B-CHA-C4A
26	la	1002	PEB	NA-C4A-CHA-C1B
26	la	1002	PEB	C3A-C4A-CHA-C1B
26	la	1002	PEB	NB-C1B-CHA-C4A
26	la	1002	PEB	C2B-C1B-CHA-C4A
26	lb	201	PEB	NA-C4A-CHA-C1B
26	lb	201	PEB	C3A-C4A-CHA-C1B
26	lb	201	PEB	NB-C1B-CHA-C4A
26	lb	201	PEB	C2B-C1B-CHA-C4A
26	lb	202	PEB	NA-C4A-CHA-C1B
26	lb	202	PEB	C3A-C4A-CHA-C1B
26	lb	202	PEB	NB-C1B-CHA-C4A
26	lb	202	PEB	C2B-C1B-CHA-C4A
26	lc	201	PEB	NA-C4A-CHA-C1B
26	lc	201	PEB	C3A-C4A-CHA-C1B
26	lc	201	PEB	NB-C1B-CHA-C4A
26	lc	201	PEB	C2B-C1B-CHA-C4A
26	lc	202	PEB	NB-C1B-CHA-C4A
26	lc	202	PEB	C2B-C1B-CHA-C4A
26	ld	201	PEB	NB-C1B-CHA-C4A
26	ld	201	PEB	C2B-C1B-CHA-C4A
26	ld	202	PEB	C1C-C2C-CAC-CBC
26	ld	202	PEB	C3C-C2C-CAC-CBC
26	ld	202	PEB	NB-C1B-CHA-C4A
26	ld	202	PEB	C2B-C1B-CHA-C4A
26	le	201	PEB	NA-C4A-CHA-C1B
26	le	201	PEB	C3A-C4A-CHA-C1B
26	le	201	PEB	NB-C1B-CHA-C4A
26	le	201	PEB	C2B-C1B-CHA-C4A
26	le	202	PEB	NB-C1B-CHA-C4A
26	le	202	PEB	C2B-C1B-CHA-C4A
26	lf	201	PEB	NA-C4A-CHA-C1B
26	lf	201	PEB	C3A-C4A-CHA-C1B
26	lf	201	PEB	NB-C1B-CHA-C4A
26	lf	201	PEB	C2B-C1B-CHA-C4A
26	lf	202	PEB	C1C-C2C-CAC-CBC
26	lf	202	PEB	C3C-C2C-CAC-CBC
26	lf	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	lf	202	PEB	C2B-C1B-CHA-C4A
26	lg	201	PEB	NB-C1B-CHA-C4A
26	lg	201	PEB	C2B-C1B-CHA-C4A
26	lg	202	PEB	NB-C1B-CHA-C4A
26	lg	202	PEB	C2B-C1B-CHA-C4A
26	lh	201	PEB	NB-C1B-CHA-C4A
26	lh	201	PEB	C2B-C1B-CHA-C4A
26	lh	202	PEB	C1C-C2C-CAC-CBC
26	lh	202	PEB	C3C-C2C-CAC-CBC
26	lh	202	PEB	NB-C1B-CHA-C4A
26	lh	202	PEB	C2B-C1B-CHA-C4A
26	li	201	PEB	NA-C4A-CHA-C1B
26	li	201	PEB	C3A-C4A-CHA-C1B
26	li	201	PEB	NB-C1B-CHA-C4A
26	li	201	PEB	C2B-C1B-CHA-C4A
26	li	202	PEB	NA-C4A-CHA-C1B
26	li	202	PEB	C3A-C4A-CHA-C1B
26	li	202	PEB	NB-C1B-CHA-C4A
26	li	202	PEB	C2B-C1B-CHA-C4A
26	li	203	PEB	C1C-C2C-CAC-CBC
26	li	203	PEB	C3C-C2C-CAC-CBC
26	li	203	PEB	NB-C1B-CHA-C4A
26	li	203	PEB	C2B-C1B-CHA-C4A
26	lj	201	PEB	NB-C1B-CHA-C4A
26	lj	201	PEB	C2B-C1B-CHA-C4A
26	lk	201	PEB	NA-C4A-CHA-C1B
26	lk	201	PEB	C3A-C4A-CHA-C1B
26	lk	201	PEB	NB-C1B-CHA-C4A
26	lk	201	PEB	C2B-C1B-CHA-C4A
26	lk	202	PEB	NB-C1B-CHA-C4A
26	lk	202	PEB	C2B-C1B-CHA-C4A
26	ll	201	PEB	NA-C4A-CHA-C1B
26	ll	201	PEB	C3A-C4A-CHA-C1B
26	ll	201	PEB	NB-C1B-CHA-C4A
26	ll	201	PEB	C2B-C1B-CHA-C4A
26	ll	202	PEB	C1C-C2C-CAC-CBC
26	ll	202	PEB	C3C-C2C-CAC-CBC
26	ll	202	PEB	NB-C1B-CHA-C4A
26	ll	202	PEB	C2B-C1B-CHA-C4A
26	lm	1001	PEB	NA-C4A-CHA-C1B
26	lm	1001	PEB	C3A-C4A-CHA-C1B
26	lm	1001	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	lm	1001	PEB	C2B-C1B-CHA-C4A
26	lm	1002	PEB	NB-C1B-CHA-C4A
26	lm	1002	PEB	C2B-C1B-CHA-C4A
26	ln	201	PEB	NA-C4A-CHA-C1B
26	ln	201	PEB	C3A-C4A-CHA-C1B
26	ln	201	PEB	NB-C1B-CHA-C4A
26	ln	201	PEB	C2B-C1B-CHA-C4A
26	ln	202	PEB	C1C-C2C-CAC-CBC
26	ln	202	PEB	C3C-C2C-CAC-CBC
26	ln	202	PEB	NB-C1B-CHA-C4A
26	ln	202	PEB	C2B-C1B-CHA-C4A
26	lo	201	PEB	NB-C1B-CHA-C4A
26	lo	201	PEB	C2B-C1B-CHA-C4A
26	lo	202	PEB	NB-C1B-CHA-C4A
26	lo	202	PEB	C2B-C1B-CHA-C4A
26	lo	203	PEB	C1C-C2C-CAC-CBC
26	lo	203	PEB	C3C-C2C-CAC-CBC
26	lo	203	PEB	NB-C1B-CHA-C4A
26	lo	203	PEB	C2B-C1B-CHA-C4A
26	lp	201	PEB	NA-C4A-CHA-C1B
26	lp	201	PEB	C3A-C4A-CHA-C1B
26	lp	201	PEB	NB-C1B-CHA-C4A
26	lp	201	PEB	C2B-C1B-CHA-C4A
26	lp	202	PEB	C1C-C2C-CAC-CBC
26	lp	202	PEB	C3C-C2C-CAC-CBC
26	lp	202	PEB	NB-C1B-CHA-C4A
26	lp	202	PEB	C2B-C1B-CHA-C4A
26	lq	201	PEB	NA-C4A-CHA-C1B
26	lq	201	PEB	C3A-C4A-CHA-C1B
26	lq	201	PEB	NB-C1B-CHA-C4A
26	lq	201	PEB	C2B-C1B-CHA-C4A
26	lq	202	PEB	NA-C4A-CHA-C1B
26	lq	202	PEB	C3A-C4A-CHA-C1B
26	lq	202	PEB	NB-C1B-CHA-C4A
26	lq	202	PEB	C2B-C1B-CHA-C4A
26	lq	203	PEB	NB-C1B-CHA-C4A
26	lq	203	PEB	C2B-C1B-CHA-C4A
26	lr	201	PEB	NA-C4A-CHA-C1B
26	lr	201	PEB	C3A-C4A-CHA-C1B
26	lr	201	PEB	NB-C1B-CHA-C4A
26	lr	201	PEB	C2B-C1B-CHA-C4A
26	lr	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	lr	202	PEB	C3C-C2C-CAC-CBC
26	lr	202	PEB	NB-C1B-CHA-C4A
26	lr	202	PEB	C2B-C1B-CHA-C4A
26	ls	201	PEB	NA-C4A-CHA-C1B
26	ls	201	PEB	C3A-C4A-CHA-C1B
26	ls	201	PEB	NB-C1B-CHA-C4A
26	ls	201	PEB	C2B-C1B-CHA-C4A
26	ls	202	PEB	NB-C1B-CHA-C4A
26	ls	202	PEB	C2B-C1B-CHA-C4A
26	lt	201	PEB	NA-C4A-CHA-C1B
26	lt	201	PEB	C3A-C4A-CHA-C1B
26	lt	201	PEB	NB-C1B-CHA-C4A
26	lt	201	PEB	C2B-C1B-CHA-C4A
26	lt	202	PEB	NB-C1B-CHA-C4A
26	lt	202	PEB	C2B-C1B-CHA-C4A
26	lu	201	PEB	NA-C4A-CHA-C1B
26	lu	201	PEB	C3A-C4A-CHA-C1B
26	lu	201	PEB	NB-C1B-CHA-C4A
26	lu	201	PEB	C2B-C1B-CHA-C4A
26	lu	202	PEB	NB-C1B-CHA-C4A
26	lu	202	PEB	C2B-C1B-CHA-C4A
26	lv	201	PEB	NA-C4A-CHA-C1B
26	lv	201	PEB	C3A-C4A-CHA-C1B
26	lv	201	PEB	NB-C1B-CHA-C4A
26	lv	201	PEB	C2B-C1B-CHA-C4A
26	lw	201	PEB	NB-C1B-CHA-C4A
26	lw	201	PEB	C2B-C1B-CHA-C4A
26	lw	202	PEB	NB-C1B-CHA-C4A
26	lw	202	PEB	C2B-C1B-CHA-C4A
26	lw	203	PEB	C1C-C2C-CAC-CBC
26	lw	203	PEB	C3C-C2C-CAC-CBC
26	lw	203	PEB	NB-C1B-CHA-C4A
26	lw	203	PEB	C2B-C1B-CHA-C4A
26	ly	401	PEB	NA-C4A-CHA-C1B
26	ly	401	PEB	C3A-C4A-CHA-C1B
26	ly	401	PEB	NB-C1B-CHA-C4A
26	ly	401	PEB	C2B-C1B-CHA-C4A
26	ly	402	PEB	NA-C4A-CHA-C1B
26	ly	402	PEB	C3A-C4A-CHA-C1B
26	ly	402	PEB	NB-C1B-CHA-C4A
26	ly	402	PEB	C2B-C1B-CHA-C4A
26	ly	403	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	ly	403	PEB	C3A-C4A-CHA-C1B
26	ly	403	PEB	NB-C1B-CHA-C4A
26	ly	403	PEB	C2B-C1B-CHA-C4A
26	lz	401	PEB	NA-C4A-CHA-C1B
26	lz	401	PEB	C3A-C4A-CHA-C1B
26	lz	401	PEB	NB-C1B-CHA-C4A
26	lz	401	PEB	C2B-C1B-CHA-C4A
26	lz	402	PEB	NA-C4A-CHA-C1B
26	lz	402	PEB	C3A-C4A-CHA-C1B
26	lz	402	PEB	NB-C1B-CHA-C4A
26	lz	402	PEB	C2B-C1B-CHA-C4A
26	fa	201	PEB	NA-C4A-CHA-C1B
26	fa	201	PEB	C3A-C4A-CHA-C1B
26	fa	201	PEB	NB-C1B-CHA-C4A
26	fa	201	PEB	C2B-C1B-CHA-C4A
26	fb	201	PEB	NA-C4A-CHA-C1B
26	fb	201	PEB	C3A-C4A-CHA-C1B
26	fb	201	PEB	NB-C1B-CHA-C4A
26	fb	201	PEB	C2B-C1B-CHA-C4A
26	fb	202	PEB	NB-C1B-CHA-C4A
26	fb	202	PEB	C2B-C1B-CHA-C4A
26	fc	201	PEB	NA-C4A-CHA-C1B
26	fc	201	PEB	C3A-C4A-CHA-C1B
26	fc	201	PEB	NB-C1B-CHA-C4A
26	fc	201	PEB	C2B-C1B-CHA-C4A
26	fc	202	PEB	C1C-C2C-CAC-CBC
26	fc	202	PEB	C3C-C2C-CAC-CBC
26	fc	202	PEB	NB-C1B-CHA-C4A
26	fc	202	PEB	C2B-C1B-CHA-C4A
26	fd	301	PEB	NA-C4A-CHA-C1B
26	fd	301	PEB	C3A-C4A-CHA-C1B
26	fd	301	PEB	NB-C1B-CHA-C4A
26	fd	301	PEB	C2B-C1B-CHA-C4A
26	fd	302	PEB	NA-C4A-CHA-C1B
26	fd	302	PEB	C3A-C4A-CHA-C1B
26	fd	302	PEB	NB-C1B-CHA-C4A
26	fd	302	PEB	C2B-C1B-CHA-C4A
26	fd	303	PEB	NA-C4A-CHA-C1B
26	fd	303	PEB	C3A-C4A-CHA-C1B
26	fd	303	PEB	NB-C1B-CHA-C4A
26	fd	303	PEB	C2B-C1B-CHA-C4A
26	fe	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	fe	201	PEB	C3A-C4A-CHA-C1B
26	fe	201	PEB	NB-C1B-CHA-C4A
26	fe	201	PEB	C2B-C1B-CHA-C4A
26	fe	202	PEB	NB-C1B-CHA-C4A
26	fe	202	PEB	C2B-C1B-CHA-C4A
26	ff	201	PEB	NA-C4A-CHA-C1B
26	ff	201	PEB	C3A-C4A-CHA-C1B
26	ff	201	PEB	NB-C1B-CHA-C4A
26	ff	201	PEB	C2B-C1B-CHA-C4A
26	ff	202	PEB	C1C-C2C-CAC-CBC
26	ff	202	PEB	C3C-C2C-CAC-CBC
26	ff	202	PEB	NB-C1B-CHA-C4A
26	ff	202	PEB	C2B-C1B-CHA-C4A
26	ff	204	PEB	NA-C4A-CHA-C1B
26	ff	204	PEB	C3A-C4A-CHA-C1B
26	ff	204	PEB	NB-C1B-CHA-C4A
26	ff	204	PEB	C2B-C1B-CHA-C4A
26	fg	201	PEB	C1C-C2C-CAC-CBC
26	fg	201	PEB	C3C-C2C-CAC-CBC
26	fg	201	PEB	NB-C1B-CHA-C4A
26	fg	201	PEB	C2B-C1B-CHA-C4A
26	fg	202	PEB	NB-C1B-CHA-C4A
26	fg	202	PEB	C2B-C1B-CHA-C4A
26	fh	1001	PEB	NA-C4A-CHA-C1B
26	fh	1001	PEB	C3A-C4A-CHA-C1B
26	fh	1001	PEB	NB-C1B-CHA-C4A
26	fh	1001	PEB	C2B-C1B-CHA-C4A
26	fh	1002	PEB	NB-C1B-CHA-C4A
26	fh	1002	PEB	C2B-C1B-CHA-C4A
26	fi	201	PEB	NA-C4A-CHA-C1B
26	fi	201	PEB	C3A-C4A-CHA-C1B
26	fi	201	PEB	NB-C1B-CHA-C4A
26	fi	201	PEB	C2B-C1B-CHA-C4A
26	fi	202	PEB	C1C-C2C-CAC-CBC
26	fi	202	PEB	C3C-C2C-CAC-CBC
26	fi	202	PEB	NB-C1B-CHA-C4A
26	fi	202	PEB	C2B-C1B-CHA-C4A
26	fj	201	PEB	NA-C4A-CHA-C1B
26	fj	201	PEB	C3A-C4A-CHA-C1B
26	fj	201	PEB	NB-C1B-CHA-C4A
26	fj	201	PEB	C2B-C1B-CHA-C4A
26	fj	202	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	fj	202	PEB	C3C-C2C-CAC-CBC
26	fj	202	PEB	NB-C1B-CHA-C4A
26	fj	202	PEB	C2B-C1B-CHA-C4A
26	fk	201	PEB	NA-C4A-CHA-C1B
26	fk	201	PEB	C3A-C4A-CHA-C1B
26	fk	201	PEB	NB-C1B-CHA-C4A
26	fk	201	PEB	C2B-C1B-CHA-C4A
26	fk	202	PEB	NB-C1B-CHA-C4A
26	fk	202	PEB	C2B-C1B-CHA-C4A
26	fl	201	PEB	NA-C4A-CHA-C1B
26	fl	201	PEB	C3A-C4A-CHA-C1B
26	fl	201	PEB	NB-C1B-CHA-C4A
26	fl	201	PEB	C2B-C1B-CHA-C4A
26	fl	202	PEB	NB-C1B-CHA-C4A
26	fl	202	PEB	C2B-C1B-CHA-C4A
26	fm	201	PEB	NA-C4A-CHA-C1B
26	fm	201	PEB	C3A-C4A-CHA-C1B
26	fm	201	PEB	NB-C1B-CHA-C4A
26	fm	201	PEB	C2B-C1B-CHA-C4A
26	fm	202	PEB	C1C-C2C-CAC-CBC
26	fm	202	PEB	C3C-C2C-CAC-CBC
26	fm	202	PEB	NB-C1B-CHA-C4A
26	fm	202	PEB	C2B-C1B-CHA-C4A
26	fn	1001	PEB	NA-C4A-CHA-C1B
26	fn	1001	PEB	C3A-C4A-CHA-C1B
26	fn	1001	PEB	NB-C1B-CHA-C4A
26	fn	1001	PEB	C2B-C1B-CHA-C4A
26	fn	1002	PEB	NB-C1B-CHA-C4A
26	fn	1002	PEB	C2B-C1B-CHA-C4A
26	fo	201	PEB	NA-C4A-CHA-C1B
26	fo	201	PEB	C3A-C4A-CHA-C1B
26	fo	201	PEB	NB-C1B-CHA-C4A
26	fo	201	PEB	C2B-C1B-CHA-C4A
26	fo	202	PEB	C1C-C2C-CAC-CBC
26	fo	202	PEB	C3C-C2C-CAC-CBC
26	fo	202	PEB	NB-C1B-CHA-C4A
26	fo	202	PEB	C2B-C1B-CHA-C4A
26	fp	201	PEB	NA-C4A-CHA-C1B
26	fp	201	PEB	C3A-C4A-CHA-C1B
26	fp	201	PEB	NB-C1B-CHA-C4A
26	fp	201	PEB	C2B-C1B-CHA-C4A
26	fp	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	fp	202	PEB	C2B-C1B-CHA-C4A
26	fq	201	PEB	NA-C4A-CHA-C1B
26	fq	201	PEB	C3A-C4A-CHA-C1B
26	fq	201	PEB	NB-C1B-CHA-C4A
26	fq	201	PEB	C2B-C1B-CHA-C4A
26	fq	202	PEB	C1C-C2C-CAC-CBC
26	fq	202	PEB	C3C-C2C-CAC-CBC
26	fq	202	PEB	NB-C1B-CHA-C4A
26	fq	202	PEB	C2B-C1B-CHA-C4A
26	fr	201	PEB	NA-C4A-CHA-C1B
26	fr	201	PEB	C3A-C4A-CHA-C1B
26	fr	201	PEB	NB-C1B-CHA-C4A
26	fr	201	PEB	C2B-C1B-CHA-C4A
26	fr	202	PEB	NB-C1B-CHA-C4A
26	fr	202	PEB	C2B-C1B-CHA-C4A
26	fs	201	PEB	NA-C4A-CHA-C1B
26	fs	201	PEB	C3A-C4A-CHA-C1B
26	fs	201	PEB	NB-C1B-CHA-C4A
26	fs	201	PEB	C2B-C1B-CHA-C4A
26	fs	202	PEB	C1C-C2C-CAC-CBC
26	fs	202	PEB	C3C-C2C-CAC-CBC
26	fs	202	PEB	NB-C1B-CHA-C4A
26	fs	202	PEB	C2B-C1B-CHA-C4A
26	ft	201	PEB	NA-C4A-CHA-C1B
26	ft	201	PEB	C3A-C4A-CHA-C1B
26	ft	201	PEB	NB-C1B-CHA-C4A
26	ft	201	PEB	C2B-C1B-CHA-C4A
26	ft	202	PEB	NB-C1B-CHA-C4A
26	ft	202	PEB	C2B-C1B-CHA-C4A
26	fu	201	PEB	C1C-C2C-CAC-CBC
26	fu	201	PEB	C3C-C2C-CAC-CBC
26	fu	201	PEB	NB-C1B-CHA-C4A
26	fu	201	PEB	C2B-C1B-CHA-C4A
26	fv	201	PEB	NA-C4A-CHA-C1B
26	fv	201	PEB	C3A-C4A-CHA-C1B
26	fv	201	PEB	NB-C1B-CHA-C4A
26	fv	201	PEB	C2B-C1B-CHA-C4A
26	fv	202	PEB	NB-C1B-CHA-C4A
26	fv	202	PEB	C2B-C1B-CHA-C4A
26	fw	201	PEB	NA-C4A-CHA-C1B
26	fw	201	PEB	C3A-C4A-CHA-C1B
26	fw	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	fw	201	PEB	C2B-C1B-CHA-C4A
26	fw	202	PEB	C1C-C2C-CAC-CBC
26	fw	202	PEB	C3C-C2C-CAC-CBC
26	fw	202	PEB	NB-C1B-CHA-C4A
26	fw	202	PEB	C2B-C1B-CHA-C4A
26	fx	201	PEB	NA-C4A-CHA-C1B
26	fx	201	PEB	C3A-C4A-CHA-C1B
26	fx	201	PEB	NB-C1B-CHA-C4A
26	fx	201	PEB	C2B-C1B-CHA-C4A
26	fx	202	PEB	NB-C1B-CHA-C4A
26	fx	202	PEB	C2B-C1B-CHA-C4A
26	fy	201	PEB	C1C-C2C-CAC-CBC
26	fy	201	PEB	C3C-C2C-CAC-CBC
26	fy	201	PEB	NB-C1B-CHA-C4A
26	fy	201	PEB	C2B-C1B-CHA-C4A
26	fz	301	PEB	NB-C1B-CHA-C4A
26	fz	301	PEB	C2B-C1B-CHA-C4A
26	ga	201	PEB	NA-C4A-CHA-C1B
26	ga	201	PEB	C3A-C4A-CHA-C1B
26	ga	201	PEB	NB-C1B-CHA-C4A
26	ga	201	PEB	C2B-C1B-CHA-C4A
26	ga	202	PEB	C1C-C2C-CAC-CBC
26	ga	202	PEB	C3C-C2C-CAC-CBC
26	ga	202	PEB	NB-C1B-CHA-C4A
26	ga	202	PEB	C2B-C1B-CHA-C4A
26	gb	1001	PEB	NA-C4A-CHA-C1B
26	gb	1001	PEB	C3A-C4A-CHA-C1B
26	gb	1001	PEB	NB-C1B-CHA-C4A
26	gb	1001	PEB	C2B-C1B-CHA-C4A
26	gb	1002	PEB	NB-C1B-CHA-C4A
26	gb	1002	PEB	C2B-C1B-CHA-C4A
26	gc	201	PEB	NA-C4A-CHA-C1B
26	gc	201	PEB	C3A-C4A-CHA-C1B
26	gc	201	PEB	NB-C1B-CHA-C4A
26	gc	201	PEB	C2B-C1B-CHA-C4A
26	gc	202	PEB	NB-C1B-CHA-C4A
26	gc	202	PEB	C2B-C1B-CHA-C4A
26	gd	201	PEB	C1C-C2C-CAC-CBC
26	gd	201	PEB	C3C-C2C-CAC-CBC
26	gd	201	PEB	NB-C1B-CHA-C4A
26	gd	201	PEB	C2B-C1B-CHA-C4A
26	ge	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	ge	201	PEB	C3A-C4A-CHA-C1B
26	ge	201	PEB	NB-C1B-CHA-C4A
26	ge	201	PEB	C2B-C1B-CHA-C4A
26	ge	202	PEB	C1C-C2C-CAC-CBC
26	ge	202	PEB	C3C-C2C-CAC-CBC
26	ge	202	PEB	NB-C1B-CHA-C4A
26	ge	202	PEB	C2B-C1B-CHA-C4A
26	gf	201	PEB	NA-C4A-CHA-C1B
26	gf	201	PEB	C3A-C4A-CHA-C1B
26	gf	201	PEB	NB-C1B-CHA-C4A
26	gf	201	PEB	C2B-C1B-CHA-C4A
26	gf	202	PEB	NB-C1B-CHA-C4A
26	gf	202	PEB	C2B-C1B-CHA-C4A
26	gg	201	PEB	NA-C4A-CHA-C1B
26	gg	201	PEB	C3A-C4A-CHA-C1B
26	gg	201	PEB	NB-C1B-CHA-C4A
26	gg	201	PEB	C2B-C1B-CHA-C4A
26	gg	202	PEB	C1C-C2C-CAC-CBC
26	gg	202	PEB	C3C-C2C-CAC-CBC
26	gg	202	PEB	NB-C1B-CHA-C4A
26	gg	202	PEB	C2B-C1B-CHA-C4A
26	gh	201	PEB	NA-C4A-CHA-C1B
26	gh	201	PEB	C3A-C4A-CHA-C1B
26	gh	201	PEB	NB-C1B-CHA-C4A
26	gh	201	PEB	C2B-C1B-CHA-C4A
26	gh	202	PEB	NB-C1B-CHA-C4A
26	gh	202	PEB	C2B-C1B-CHA-C4A
26	gi	201	PEB	NA-C4A-CHA-C1B
26	gi	201	PEB	C3A-C4A-CHA-C1B
26	gi	201	PEB	NB-C1B-CHA-C4A
26	gi	201	PEB	C2B-C1B-CHA-C4A
26	gi	202	PEB	C1C-C2C-CAC-CBC
26	gi	202	PEB	C3C-C2C-CAC-CBC
26	gi	202	PEB	NB-C1B-CHA-C4A
26	gi	202	PEB	C2B-C1B-CHA-C4A
26	gj	201	PEB	NA-C4A-CHA-C1B
26	gj	201	PEB	C3A-C4A-CHA-C1B
26	gj	201	PEB	NB-C1B-CHA-C4A
26	gj	201	PEB	C2B-C1B-CHA-C4A
26	gj	202	PEB	NB-C1B-CHA-C4A
26	gj	202	PEB	C2B-C1B-CHA-C4A
26	gk	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	gk	201	PEB	C3A-C4A-CHA-C1B
26	gk	201	PEB	NB-C1B-CHA-C4A
26	gk	201	PEB	C2B-C1B-CHA-C4A
26	gk	202	PEB	C1C-C2C-CAC-CBC
26	gk	202	PEB	C3C-C2C-CAC-CBC
26	gk	202	PEB	NB-C1B-CHA-C4A
26	gk	202	PEB	C2B-C1B-CHA-C4A
26	gl	201	PEB	NA-C4A-CHA-C1B
26	gl	201	PEB	C3A-C4A-CHA-C1B
26	gl	201	PEB	NB-C1B-CHA-C4A
26	gl	201	PEB	C2B-C1B-CHA-C4A
26	gl	202	PEB	NB-C1B-CHA-C4A
26	gl	202	PEB	C2B-C1B-CHA-C4A
26	gm	1001	PEB	NA-C4A-CHA-C1B
26	gm	1001	PEB	C3A-C4A-CHA-C1B
26	gm	1001	PEB	NB-C1B-CHA-C4A
26	gm	1001	PEB	C2B-C1B-CHA-C4A
26	gm	1002	PEB	NB-C1B-CHA-C4A
26	gm	1002	PEB	C2B-C1B-CHA-C4A
26	gn	201	PEB	NA-C4A-CHA-C1B
26	gn	201	PEB	C3A-C4A-CHA-C1B
26	gn	201	PEB	NB-C1B-CHA-C4A
26	gn	201	PEB	C2B-C1B-CHA-C4A
26	gn	202	PEB	C1C-C2C-CAC-CBC
26	gn	202	PEB	C3C-C2C-CAC-CBC
26	gn	202	PEB	NB-C1B-CHA-C4A
26	gn	202	PEB	C2B-C1B-CHA-C4A
26	go	201	PEB	NA-C4A-CHA-C1B
26	go	201	PEB	C3A-C4A-CHA-C1B
26	go	201	PEB	NB-C1B-CHA-C4A
26	go	201	PEB	C2B-C1B-CHA-C4A
26	go	202	PEB	NB-C1B-CHA-C4A
26	go	202	PEB	C2B-C1B-CHA-C4A
26	gp	201	PEB	NA-C4A-CHA-C1B
26	gp	201	PEB	C3A-C4A-CHA-C1B
26	gp	201	PEB	NB-C1B-CHA-C4A
26	gp	201	PEB	C2B-C1B-CHA-C4A
26	gp	202	PEB	C1C-C2C-CAC-CBC
26	gp	202	PEB	C3C-C2C-CAC-CBC
26	gp	202	PEB	NB-C1B-CHA-C4A
26	gp	202	PEB	C2B-C1B-CHA-C4A
26	gq	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	gq	201	PEB	C3A-C4A-CHA-C1B
26	gq	201	PEB	NB-C1B-CHA-C4A
26	gq	201	PEB	C2B-C1B-CHA-C4A
26	gq	202	PEB	NB-C1B-CHA-C4A
26	gq	202	PEB	C2B-C1B-CHA-C4A
26	gr	201	PEB	C1C-C2C-CAC-CBC
26	gr	201	PEB	C3C-C2C-CAC-CBC
26	gr	201	PEB	NB-C1B-CHA-C4A
26	gr	201	PEB	C2B-C1B-CHA-C4A
26	gs	201	PEB	NA-C4A-CHA-C1B
26	gs	201	PEB	C3A-C4A-CHA-C1B
26	gs	201	PEB	NB-C1B-CHA-C4A
26	gs	201	PEB	C2B-C1B-CHA-C4A
26	gs	202	PEB	NB-C1B-CHA-C4A
26	gs	202	PEB	C2B-C1B-CHA-C4A
26	gt	201	PEB	NA-C4A-CHA-C1B
26	gt	201	PEB	C3A-C4A-CHA-C1B
26	gt	201	PEB	NB-C1B-CHA-C4A
26	gt	201	PEB	C2B-C1B-CHA-C4A
26	gt	202	PEB	C1C-C2C-CAC-CBC
26	gt	202	PEB	C3C-C2C-CAC-CBC
26	gt	202	PEB	NB-C1B-CHA-C4A
26	gt	202	PEB	C2B-C1B-CHA-C4A
26	gu	201	PEB	NA-C4A-CHA-C1B
26	gu	201	PEB	C3A-C4A-CHA-C1B
26	gu	201	PEB	NB-C1B-CHA-C4A
26	gu	201	PEB	C2B-C1B-CHA-C4A
26	gu	202	PEB	NB-C1B-CHA-C4A
26	gu	202	PEB	C2B-C1B-CHA-C4A
26	gv	201	PEB	NA-C4A-CHA-C1B
26	gv	201	PEB	C3A-C4A-CHA-C1B
26	gv	201	PEB	NB-C1B-CHA-C4A
26	gv	201	PEB	C2B-C1B-CHA-C4A
26	gv	202	PEB	C1C-C2C-CAC-CBC
26	gv	202	PEB	C3C-C2C-CAC-CBC
26	gv	202	PEB	NB-C1B-CHA-C4A
26	gv	202	PEB	C2B-C1B-CHA-C4A
26	gw	201	PEB	NA-C4A-CHA-C1B
26	gw	201	PEB	C3A-C4A-CHA-C1B
26	gw	201	PEB	NB-C1B-CHA-C4A
26	gw	201	PEB	C2B-C1B-CHA-C4A
26	gw	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	gw	202	PEB	C2B-C1B-CHA-C4A
26	gx	201	PEB	NA-C4A-CHA-C1B
26	gx	201	PEB	C3A-C4A-CHA-C1B
26	gx	201	PEB	NB-C1B-CHA-C4A
26	gx	201	PEB	C2B-C1B-CHA-C4A
26	gx	202	PEB	C1C-C2C-CAC-CBC
26	gx	202	PEB	C3C-C2C-CAC-CBC
26	gx	202	PEB	NB-C1B-CHA-C4A
26	gx	202	PEB	C2B-C1B-CHA-C4A
26	gy	301	PEB	NA-C4A-CHA-C1B
26	gy	301	PEB	C3A-C4A-CHA-C1B
26	gy	301	PEB	NB-C1B-CHA-C4A
26	gy	301	PEB	C2B-C1B-CHA-C4A
26	gy	302	PEB	NB-C1B-CHA-C4A
26	gy	302	PEB	C2B-C1B-CHA-C4A
26	gy	303	PEB	NA-C4A-CHA-C1B
26	gy	303	PEB	C3A-C4A-CHA-C1B
26	gy	303	PEB	NB-C1B-CHA-C4A
26	gy	303	PEB	C2B-C1B-CHA-C4A
26	gz	301	PEB	NA-C4A-CHA-C1B
26	gz	301	PEB	C3A-C4A-CHA-C1B
26	gz	301	PEB	NB-C1B-CHA-C4A
26	gz	301	PEB	C2B-C1B-CHA-C4A
26	gz	302	PEB	NB-C1B-CHA-C4A
26	gz	302	PEB	C2B-C1B-CHA-C4A
26	gz	303	PEB	NA-C4A-CHA-C1B
26	gz	303	PEB	C3A-C4A-CHA-C1B
26	gz	303	PEB	NB-C1B-CHA-C4A
26	gz	303	PEB	C2B-C1B-CHA-C4A
26	hA	201	PEB	NA-C4A-CHA-C1B
26	hA	201	PEB	C3A-C4A-CHA-C1B
26	hA	201	PEB	NB-C1B-CHA-C4A
26	hA	201	PEB	C2B-C1B-CHA-C4A
26	hA	202	PEB	NB-C1B-CHA-C4A
26	hA	202	PEB	C2B-C1B-CHA-C4A
26	hB	201	PEB	NA-C4A-CHA-C1B
26	hB	201	PEB	C3A-C4A-CHA-C1B
26	hB	201	PEB	NB-C1B-CHA-C4A
26	hB	201	PEB	C2B-C1B-CHA-C4A
26	hB	202	PEB	C1C-C2C-CAC-CBC
26	hB	202	PEB	C3C-C2C-CAC-CBC
26	hB	202	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hB	202	PEB	C2B-C1B-CHA-C4A
26	hC	201	PEB	NA-C4A-CHA-C1B
26	hC	201	PEB	C3A-C4A-CHA-C1B
26	hC	201	PEB	NB-C1B-CHA-C4A
26	hC	201	PEB	C2B-C1B-CHA-C4A
26	hC	202	PEB	NB-C1B-CHA-C4A
26	hC	202	PEB	C2B-C1B-CHA-C4A
26	hD	201	PEB	NA-C4A-CHA-C1B
26	hD	201	PEB	C3A-C4A-CHA-C1B
26	hD	201	PEB	NB-C1B-CHA-C4A
26	hD	201	PEB	C2B-C1B-CHA-C4A
26	hD	202	PEB	C1C-C2C-CAC-CBC
26	hD	202	PEB	C3C-C2C-CAC-CBC
26	hD	202	PEB	NB-C1B-CHA-C4A
26	hD	202	PEB	C2B-C1B-CHA-C4A
26	hE	1001	PEB	NA-C4A-CHA-C1B
26	hE	1001	PEB	C3A-C4A-CHA-C1B
26	hE	1001	PEB	NB-C1B-CHA-C4A
26	hE	1001	PEB	C2B-C1B-CHA-C4A
26	hE	1002	PEB	NB-C1B-CHA-C4A
26	hE	1002	PEB	C2B-C1B-CHA-C4A
26	hF	201	PEB	NA-C4A-CHA-C1B
26	hF	201	PEB	C3A-C4A-CHA-C1B
26	hF	201	PEB	NB-C1B-CHA-C4A
26	hF	201	PEB	C2B-C1B-CHA-C4A
26	hF	202	PEB	NB-C1B-CHA-C4A
26	hF	202	PEB	C2B-C1B-CHA-C4A
26	hG	201	PEB	C1C-C2C-CAC-CBC
26	hG	201	PEB	C3C-C2C-CAC-CBC
26	hG	201	PEB	NB-C1B-CHA-C4A
26	hG	201	PEB	C2B-C1B-CHA-C4A
26	hH	201	PEB	NA-C4A-CHA-C1B
26	hH	201	PEB	C3A-C4A-CHA-C1B
26	hH	201	PEB	NB-C1B-CHA-C4A
26	hH	201	PEB	C2B-C1B-CHA-C4A
26	hH	202	PEB	C1C-C2C-CAC-CBC
26	hH	202	PEB	C3C-C2C-CAC-CBC
26	hH	202	PEB	NB-C1B-CHA-C4A
26	hH	202	PEB	C2B-C1B-CHA-C4A
26	hI	201	PEB	NA-C4A-CHA-C1B
26	hI	201	PEB	C3A-C4A-CHA-C1B
26	hI	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hI	201	PEB	C2B-C1B-CHA-C4A
26	hI	202	PEB	NB-C1B-CHA-C4A
26	hI	202	PEB	C2B-C1B-CHA-C4A
26	hJ	201	PEB	NA-C4A-CHA-C1B
26	hJ	201	PEB	C3A-C4A-CHA-C1B
26	hJ	201	PEB	NB-C1B-CHA-C4A
26	hJ	201	PEB	C2B-C1B-CHA-C4A
26	hJ	202	PEB	C1C-C2C-CAC-CBC
26	hJ	202	PEB	C3C-C2C-CAC-CBC
26	hJ	202	PEB	NB-C1B-CHA-C4A
26	hJ	202	PEB	C2B-C1B-CHA-C4A
26	hK	201	PEB	NA-C4A-CHA-C1B
26	hK	201	PEB	C3A-C4A-CHA-C1B
26	hK	201	PEB	NB-C1B-CHA-C4A
26	hK	201	PEB	C2B-C1B-CHA-C4A
26	hK	202	PEB	NB-C1B-CHA-C4A
26	hK	202	PEB	C2B-C1B-CHA-C4A
26	hL	201	PEB	NA-C4A-CHA-C1B
26	hL	201	PEB	C3A-C4A-CHA-C1B
26	hL	201	PEB	NB-C1B-CHA-C4A
26	hL	201	PEB	C2B-C1B-CHA-C4A
26	hL	202	PEB	C1C-C2C-CAC-CBC
26	hL	202	PEB	C3C-C2C-CAC-CBC
26	hL	202	PEB	NB-C1B-CHA-C4A
26	hL	202	PEB	C2B-C1B-CHA-C4A
26	hM	1001	PEB	NA-C4A-CHA-C1B
26	hM	1001	PEB	C3A-C4A-CHA-C1B
26	hM	1001	PEB	NB-C1B-CHA-C4A
26	hM	1001	PEB	C2B-C1B-CHA-C4A
26	hM	1002	PEB	NB-C1B-CHA-C4A
26	hM	1002	PEB	C2B-C1B-CHA-C4A
26	hN	201	PEB	NA-C4A-CHA-C1B
26	hN	201	PEB	C3A-C4A-CHA-C1B
26	hN	201	PEB	NB-C1B-CHA-C4A
26	hN	201	PEB	C2B-C1B-CHA-C4A
26	hN	202	PEB	C1C-C2C-CAC-CBC
26	hN	202	PEB	C3C-C2C-CAC-CBC
26	hN	202	PEB	NB-C1B-CHA-C4A
26	hN	202	PEB	C2B-C1B-CHA-C4A
26	hO	201	PEB	NA-C4A-CHA-C1B
26	hO	201	PEB	C3A-C4A-CHA-C1B
26	hO	201	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hO	201	PEB	C2B-C1B-CHA-C4A
26	hO	202	PEB	NB-C1B-CHA-C4A
26	hO	202	PEB	C2B-C1B-CHA-C4A
26	hP	201	PEB	NA-C4A-CHA-C1B
26	hP	201	PEB	C3A-C4A-CHA-C1B
26	hP	201	PEB	NB-C1B-CHA-C4A
26	hP	201	PEB	C2B-C1B-CHA-C4A
26	hP	202	PEB	C1C-C2C-CAC-CBC
26	hP	202	PEB	C3C-C2C-CAC-CBC
26	hP	202	PEB	NB-C1B-CHA-C4A
26	hP	202	PEB	C2B-C1B-CHA-C4A
26	hQ	201	PEB	NA-C4A-CHA-C1B
26	hQ	201	PEB	C3A-C4A-CHA-C1B
26	hQ	201	PEB	NB-C1B-CHA-C4A
26	hQ	201	PEB	C2B-C1B-CHA-C4A
26	hQ	202	PEB	NB-C1B-CHA-C4A
26	hQ	202	PEB	C2B-C1B-CHA-C4A
26	hR	201	PEB	NA-C4A-CHA-C1B
26	hR	201	PEB	C3A-C4A-CHA-C1B
26	hR	201	PEB	NB-C1B-CHA-C4A
26	hR	201	PEB	C2B-C1B-CHA-C4A
26	hR	202	PEB	C1C-C2C-CAC-CBC
26	hR	202	PEB	C3C-C2C-CAC-CBC
26	hR	202	PEB	NB-C1B-CHA-C4A
26	hR	202	PEB	C2B-C1B-CHA-C4A
26	hS	201	PEB	NA-C4A-CHA-C1B
26	hS	201	PEB	C3A-C4A-CHA-C1B
26	hS	201	PEB	NB-C1B-CHA-C4A
26	hS	201	PEB	C2B-C1B-CHA-C4A
26	hS	202	PEB	NB-C1B-CHA-C4A
26	hS	202	PEB	C2B-C1B-CHA-C4A
26	hT	201	PEB	NA-C4A-CHA-C1B
26	hT	201	PEB	C3A-C4A-CHA-C1B
26	hT	201	PEB	NB-C1B-CHA-C4A
26	hT	201	PEB	C2B-C1B-CHA-C4A
26	hT	202	PEB	C1C-C2C-CAC-CBC
26	hT	202	PEB	C3C-C2C-CAC-CBC
26	hT	202	PEB	NB-C1B-CHA-C4A
26	hT	202	PEB	C2B-C1B-CHA-C4A
26	hT	204	PEB	NA-C4A-CHA-C1B
26	hT	204	PEB	C3A-C4A-CHA-C1B
26	hT	204	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	hT	204	PEB	C2B-C1B-CHA-C4A
26	hU	201	PEB	NB-C1B-CHA-C4A
26	hU	201	PEB	C2B-C1B-CHA-C4A
26	hV	201	PEB	NA-C4A-CHA-C1B
26	hV	201	PEB	C3A-C4A-CHA-C1B
26	hV	201	PEB	NB-C1B-CHA-C4A
26	hV	201	PEB	C2B-C1B-CHA-C4A
26	hV	202	PEB	C1C-C2C-CAC-CBC
26	hV	202	PEB	C3C-C2C-CAC-CBC
26	hV	202	PEB	NB-C1B-CHA-C4A
26	hV	202	PEB	C2B-C1B-CHA-C4A
26	hW	201	PEB	NA-C4A-CHA-C1B
26	hW	201	PEB	C3A-C4A-CHA-C1B
26	hW	201	PEB	NB-C1B-CHA-C4A
26	hW	201	PEB	C2B-C1B-CHA-C4A
26	hW	202	PEB	NB-C1B-CHA-C4A
26	hW	202	PEB	C2B-C1B-CHA-C4A
26	hX	201	PEB	NA-C4A-CHA-C1B
26	hX	201	PEB	C3A-C4A-CHA-C1B
26	hX	201	PEB	NB-C1B-CHA-C4A
26	hX	201	PEB	C2B-C1B-CHA-C4A
26	hX	202	PEB	C1C-C2C-CAC-CBC
26	hX	202	PEB	C3C-C2C-CAC-CBC
26	hX	202	PEB	NB-C1B-CHA-C4A
26	hX	202	PEB	C2B-C1B-CHA-C4A
26	hY	401	PEB	NA-C4A-CHA-C1B
26	hY	401	PEB	C3A-C4A-CHA-C1B
26	hY	401	PEB	NB-C1B-CHA-C4A
26	hY	401	PEB	C2B-C1B-CHA-C4A
26	hY	402	PEB	NB-C1B-CHA-C4A
26	hY	402	PEB	C2B-C1B-CHA-C4A
26	hY	403	PEB	NA-C4A-CHA-C1B
26	hY	403	PEB	C3A-C4A-CHA-C1B
26	hY	403	PEB	NB-C1B-CHA-C4A
26	hY	403	PEB	C2B-C1B-CHA-C4A
26	hZ	401	PEB	NB-C1B-CHA-C4A
26	hZ	401	PEB	C2B-C1B-CHA-C4A
26	hZ	402	PEB	NA-C4A-CHA-C1B
26	hZ	402	PEB	C3A-C4A-CHA-C1B
26	hZ	402	PEB	NB-C1B-CHA-C4A
26	hZ	402	PEB	C2B-C1B-CHA-C4A
26	iA	1001	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	iA	1001	PEB	C3A-C4A-CHA-C1B
26	iA	1001	PEB	NB-C1B-CHA-C4A
26	iA	1001	PEB	C2B-C1B-CHA-C4A
26	iA	1002	PEB	NB-C1B-CHA-C4A
26	iA	1002	PEB	C2B-C1B-CHA-C4A
26	iB	1001	PEB	NA-C4A-CHA-C1B
26	iB	1001	PEB	C3A-C4A-CHA-C1B
26	iB	1001	PEB	NB-C1B-CHA-C4A
26	iB	1001	PEB	C2B-C1B-CHA-C4A
26	iB	1002	PEB	NB-C1B-CHA-C4A
26	iB	1002	PEB	C2B-C1B-CHA-C4A
26	iC	1001	PEB	NA-C4A-CHA-C1B
26	iC	1001	PEB	C3A-C4A-CHA-C1B
26	iC	1001	PEB	NB-C1B-CHA-C4A
26	iC	1001	PEB	C2B-C1B-CHA-C4A
26	iC	1002	PEB	C1C-C2C-CAC-CBC
26	iC	1002	PEB	C3C-C2C-CAC-CBC
26	iC	1002	PEB	NB-C1B-CHA-C4A
26	iC	1002	PEB	C2B-C1B-CHA-C4A
26	iD	1001	PEB	NA-C4A-CHA-C1B
26	iD	1001	PEB	C3A-C4A-CHA-C1B
26	iD	1001	PEB	NB-C1B-CHA-C4A
26	iD	1001	PEB	C2B-C1B-CHA-C4A
26	iD	1002	PEB	C1C-C2C-CAC-CBC
26	iD	1002	PEB	C3C-C2C-CAC-CBC
26	iD	1002	PEB	NB-C1B-CHA-C4A
26	iD	1002	PEB	C2B-C1B-CHA-C4A
26	iE	1001	PEB	NA-C4A-CHA-C1B
26	iE	1001	PEB	C3A-C4A-CHA-C1B
26	iE	1001	PEB	NB-C1B-CHA-C4A
26	iE	1001	PEB	C2B-C1B-CHA-C4A
26	iE	1002	PEB	C1C-C2C-CAC-CBC
26	iE	1002	PEB	C3C-C2C-CAC-CBC
26	iE	1002	PEB	NB-C1B-CHA-C4A
26	iE	1002	PEB	C2B-C1B-CHA-C4A
26	iF	1001	PEB	NA-C4A-CHA-C1B
26	iF	1001	PEB	C3A-C4A-CHA-C1B
26	iF	1001	PEB	NB-C1B-CHA-C4A
26	iF	1001	PEB	C2B-C1B-CHA-C4A
26	iF	1002	PEB	NB-C1B-CHA-C4A
26	iF	1002	PEB	C2B-C1B-CHA-C4A
26	iG	1001	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	iG	1001	PEB	C3A-C4A-CHA-C1B
26	iG	1001	PEB	NB-C1B-CHA-C4A
26	iG	1001	PEB	C2B-C1B-CHA-C4A
26	iH	1001	PEB	NA-C4A-CHA-C1B
26	iH	1001	PEB	C3A-C4A-CHA-C1B
26	iH	1001	PEB	NB-C1B-CHA-C4A
26	iH	1001	PEB	C2B-C1B-CHA-C4A
26	jI	1001	PEB	NA-C4A-CHA-C1B
26	jI	1001	PEB	C3A-C4A-CHA-C1B
26	jI	1001	PEB	NB-C1B-CHA-C4A
26	jI	1001	PEB	C2B-C1B-CHA-C4A
26	jI	1002	PEB	C1C-C2C-CAC-CBC
26	jI	1002	PEB	C3C-C2C-CAC-CBC
26	jI	1002	PEB	NB-C1B-CHA-C4A
26	jI	1002	PEB	C2B-C1B-CHA-C4A
26	jJ	1001	PEB	NA-C4A-CHA-C1B
26	jJ	1001	PEB	C3A-C4A-CHA-C1B
26	jJ	1001	PEB	NB-C1B-CHA-C4A
26	jJ	1001	PEB	C2B-C1B-CHA-C4A
26	jJ	1002	PEB	C1C-C2C-CAC-CBC
26	jJ	1002	PEB	C3C-C2C-CAC-CBC
26	jJ	1002	PEB	NB-C1B-CHA-C4A
26	jJ	1002	PEB	C2B-C1B-CHA-C4A
26	jK	1001	PEB	NA-C4A-CHA-C1B
26	jK	1001	PEB	C3A-C4A-CHA-C1B
26	jK	1001	PEB	NB-C1B-CHA-C4A
26	jK	1001	PEB	C2B-C1B-CHA-C4A
26	jK	1002	PEB	C1C-C2C-CAC-CBC
26	jK	1002	PEB	C3C-C2C-CAC-CBC
26	jK	1002	PEB	NB-C1B-CHA-C4A
26	jK	1002	PEB	C2B-C1B-CHA-C4A
26	jL	1001	PEB	NA-C4A-CHA-C1B
26	jL	1001	PEB	C3A-C4A-CHA-C1B
26	jL	1001	PEB	NB-C1B-CHA-C4A
26	jL	1001	PEB	C2B-C1B-CHA-C4A
26	jL	1002	PEB	C1C-C2C-CAC-CBC
26	jL	1002	PEB	C3C-C2C-CAC-CBC
26	jL	1002	PEB	NB-C1B-CHA-C4A
26	jL	1002	PEB	C2B-C1B-CHA-C4A
26	jM	1001	PEB	NA-C4A-CHA-C1B
26	jM	1001	PEB	C3A-C4A-CHA-C1B
26	jM	1001	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	jM	1001	PEB	C2B-C1B-CHA-C4A
26	jM	1002	PEB	C1C-C2C-CAC-CBC
26	jM	1002	PEB	C3C-C2C-CAC-CBC
26	jM	1002	PEB	NB-C1B-CHA-C4A
26	jM	1002	PEB	C2B-C1B-CHA-C4A
26	jN	1001	PEB	NA-C4A-CHA-C1B
26	jN	1001	PEB	C3A-C4A-CHA-C1B
26	jN	1001	PEB	NB-C1B-CHA-C4A
26	jN	1001	PEB	C2B-C1B-CHA-C4A
26	jN	1002	PEB	C1C-C2C-CAC-CBC
26	jN	1002	PEB	C3C-C2C-CAC-CBC
26	jN	1002	PEB	NB-C1B-CHA-C4A
26	jN	1002	PEB	C2B-C1B-CHA-C4A
26	jO	1001	PEB	NA-C4A-CHA-C1B
26	jO	1001	PEB	C3A-C4A-CHA-C1B
26	jO	1001	PEB	NB-C1B-CHA-C4A
26	jO	1001	PEB	C2B-C1B-CHA-C4A
26	jO	1002	PEB	C1C-C2C-CAC-CBC
26	jO	1002	PEB	C3C-C2C-CAC-CBC
26	jO	1002	PEB	NB-C1B-CHA-C4A
26	jO	1002	PEB	C2B-C1B-CHA-C4A
26	jP	1001	PEB	NA-C4A-CHA-C1B
26	jP	1001	PEB	C3A-C4A-CHA-C1B
26	jP	1001	PEB	NB-C1B-CHA-C4A
26	jP	1001	PEB	C2B-C1B-CHA-C4A
26	jP	1002	PEB	C1C-C2C-CAC-CBC
26	jP	1002	PEB	C3C-C2C-CAC-CBC
26	jP	1002	PEB	NB-C1B-CHA-C4A
26	jP	1002	PEB	C2B-C1B-CHA-C4A
26	kQ	1001	PEB	NA-C4A-CHA-C1B
26	kQ	1001	PEB	C3A-C4A-CHA-C1B
26	kQ	1001	PEB	NB-C1B-CHA-C4A
26	kQ	1001	PEB	C2B-C1B-CHA-C4A
26	kQ	1002	PEB	C1C-C2C-CAC-CBC
26	kQ	1002	PEB	C3C-C2C-CAC-CBC
26	kQ	1002	PEB	NB-C1B-CHA-C4A
26	kQ	1002	PEB	C2B-C1B-CHA-C4A
26	kR	1001	PEB	NA-C4A-CHA-C1B
26	kR	1001	PEB	C3A-C4A-CHA-C1B
26	kR	1001	PEB	NB-C1B-CHA-C4A
26	kR	1001	PEB	C2B-C1B-CHA-C4A
26	kR	1002	PEB	C1C-C2C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
26	kR	1002	PEB	C3C-C2C-CAC-CBC
26	kR	1002	PEB	NB-C1B-CHA-C4A
26	kR	1002	PEB	C2B-C1B-CHA-C4A
26	kS	1001	PEB	NA-C4A-CHA-C1B
26	kS	1001	PEB	C3A-C4A-CHA-C1B
26	kS	1001	PEB	NB-C1B-CHA-C4A
26	kS	1001	PEB	C2B-C1B-CHA-C4A
26	kS	1002	PEB	C1C-C2C-CAC-CBC
26	kS	1002	PEB	C3C-C2C-CAC-CBC
26	kS	1002	PEB	NB-C1B-CHA-C4A
26	kS	1002	PEB	C2B-C1B-CHA-C4A
26	kT	1001	PEB	NA-C4A-CHA-C1B
26	kT	1001	PEB	C3A-C4A-CHA-C1B
26	kT	1001	PEB	NB-C1B-CHA-C4A
26	kT	1001	PEB	C2B-C1B-CHA-C4A
26	kT	1002	PEB	C1C-C2C-CAC-CBC
26	kT	1002	PEB	C3C-C2C-CAC-CBC
26	kT	1002	PEB	NB-C1B-CHA-C4A
26	kT	1002	PEB	C2B-C1B-CHA-C4A
26	kU	1001	PEB	NA-C4A-CHA-C1B
26	kU	1001	PEB	C3A-C4A-CHA-C1B
26	kU	1001	PEB	NB-C1B-CHA-C4A
26	kU	1001	PEB	C2B-C1B-CHA-C4A
26	kU	1002	PEB	C1C-C2C-CAC-CBC
26	kU	1002	PEB	C3C-C2C-CAC-CBC
26	kU	1002	PEB	NB-C1B-CHA-C4A
26	kU	1002	PEB	C2B-C1B-CHA-C4A
26	kV	1001	PEB	NA-C4A-CHA-C1B
26	kV	1001	PEB	C3A-C4A-CHA-C1B
26	kV	1001	PEB	NB-C1B-CHA-C4A
26	kV	1001	PEB	C2B-C1B-CHA-C4A
26	kV	1002	PEB	C1C-C2C-CAC-CBC
26	kV	1002	PEB	C3C-C2C-CAC-CBC
26	kV	1002	PEB	NB-C1B-CHA-C4A
26	kV	1002	PEB	C2B-C1B-CHA-C4A
26	kW	1001	PEB	NA-C4A-CHA-C1B
26	kW	1001	PEB	C3A-C4A-CHA-C1B
26	kW	1001	PEB	NB-C1B-CHA-C4A
26	kW	1001	PEB	C2B-C1B-CHA-C4A
26	kW	1002	PEB	C1C-C2C-CAC-CBC
26	kW	1002	PEB	C3C-C2C-CAC-CBC
26	kW	1002	PEB	NB-C1B-CHA-C4A

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Mol	Chain	Res	Type	Atoms
26	kW	1002	PEB	C2B-C1B-CHA-C4A
26	kX	1001	PEB	NA-C4A-CHA-C1B
26	kX	1001	PEB	C3A-C4A-CHA-C1B
26	kX	1001	PEB	NB-C1B-CHA-C4A
26	kX	1001	PEB	C2B-C1B-CHA-C4A
26	kX	1002	PEB	C1C-C2C-CAC-CBC
26	kX	1002	PEB	C3C-C2C-CAC-CBC
26	kX	1002	PEB	NB-C1B-CHA-C4A
26	kX	1002	PEB	C2B-C1B-CHA-C4A
27	G1	1001	CYC	ND-C1D-CHD-C4C
27	G1	1001	CYC	C2D-C1D-CHD-C4C
27	H1	201	CYC	NA-C4A-CHB-C1B
27	H1	201	CYC	C4B-C3B-CAB-CBB
27	H1	201	CYC	ND-C1D-CHD-C4C
27	H1	201	CYC	C2D-C1D-CHD-C4C
27	I1	201	CYC	ND-C1D-CHD-C4C
27	I1	201	CYC	C2D-C1D-CHD-C4C
27	J1	201	CYC	NA-C4A-CHB-C1B
27	J1	201	CYC	C4B-C3B-CAB-CBB
27	J1	201	CYC	ND-C1D-CHD-C4C
27	J1	201	CYC	C2D-C1D-CHD-C4C
27	K1	201	CYC	ND-C1D-CHD-C4C
27	K1	201	CYC	C2D-C1D-CHD-C4C
27	L1	201	CYC	ND-C1D-CHD-C4C
27	L1	201	CYC	C2D-C1D-CHD-C4C
27	M1	1001	CYC	NA-C4A-CHB-C1B
27	M1	1001	CYC	C4B-C3B-CAB-CBB
27	M1	1001	CYC	ND-C1D-CHD-C4C
27	M1	1001	CYC	C2D-C1D-CHD-C4C
27	N1	201	CYC	ND-C1D-CHD-C4C
27	N1	201	CYC	C2D-C1D-CHD-C4C
27	O1	201	CYC	ND-C1D-CHD-C4C
27	O1	201	CYC	C2D-C1D-CHD-C4C
27	P1	201	CYC	ND-C1D-CHD-C4C
27	P1	201	CYC	C2D-C1D-CHD-C4C
27	Q1	201	CYC	ND-C1D-CHD-C4C
27	Q1	201	CYC	C2D-C1D-CHD-C4C
27	R1	1001	CYC	ND-C1D-CHD-C4C
27	R1	1001	CYC	C2D-C1D-CHD-C4C
27	S1	201	CYC	NA-C4A-CHB-C1B
27	S1	201	CYC	C4B-C3B-CAB-CBB
27	S1	201	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
27	S1	201	CYC	C2D-C1D-CHD-C4C
27	S1	202	CYC	NA-C4A-CHB-C1B
27	S1	202	CYC	C4B-C3B-CAB-CBB
27	S1	202	CYC	ND-C1D-CHD-C4C
27	S1	202	CYC	C2D-C1D-CHD-C4C
27	U1	201	CYC	ND-C1D-CHD-C4C
27	U1	201	CYC	C2D-C1D-CHD-C4C
27	V1	201	CYC	ND-C1D-CHD-C4C
27	V1	201	CYC	C2D-C1D-CHD-C4C
27	W1	201	CYC	ND-C1D-CHD-C4C
27	W1	201	CYC	C2D-C1D-CHD-C4C
27	X1	201	CYC	ND-C1D-CHD-C4C
27	X1	201	CYC	C2D-C1D-CHD-C4C
27	Y1	201	CYC	NA-C4A-CHB-C1B
27	Y1	201	CYC	C4B-C3B-CAB-CBB
27	Y1	201	CYC	ND-C1D-CHD-C4C
27	Y1	201	CYC	C2D-C1D-CHD-C4C
27	Z1	201	CYC	ND-C1D-CHD-C4C
27	Z1	201	CYC	C2D-C1D-CHD-C4C
27	a1	201	CYC	ND-C1D-CHD-C4C
27	a1	201	CYC	C2D-C1D-CHD-C4C
27	b1	1001	CYC	ND-C1D-CHD-C4C
27	b1	1001	CYC	C2D-C1D-CHD-C4C
27	c1	201	CYC	NA-C4A-CHB-C1B
27	c1	201	CYC	C4B-C3B-CAB-CBB
27	c1	201	CYC	ND-C1D-CHD-C4C
27	c1	201	CYC	C2D-C1D-CHD-C4C
27	d1	1001	CYC	ND-C1D-CHD-C4C
27	d1	1001	CYC	C2D-C1D-CHD-C4C
27	e1	201	CYC	ND-C1D-CHD-C4C
27	e1	201	CYC	C2D-C1D-CHD-C4C
27	f1	201	CYC	ND-C1D-CHD-C4C
27	f1	201	CYC	C2D-C1D-CHD-C4C
27	g1	201	CYC	ND-C1D-CHD-C4C
27	g1	201	CYC	C2D-C1D-CHD-C4C
27	h1	201	CYC	NA-C4A-CHB-C1B
27	h1	201	CYC	C4B-C3B-CAB-CBB
27	h1	201	CYC	ND-C1D-CHD-C4C
27	h1	201	CYC	C2D-C1D-CHD-C4C
27	i1	1001	CYC	ND-C1D-CHD-C4C
27	i1	1001	CYC	C2D-C1D-CHD-C4C
27	j1	201	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
27	j1	201	CYC	C4B-C3B-CAB-CBB
27	j1	201	CYC	ND-C1D-CHD-C4C
27	j1	201	CYC	C2D-C1D-CHD-C4C
27	k1	201	CYC	ND-C1D-CHD-C4C
27	k1	201	CYC	C2D-C1D-CHD-C4C
27	m1	201	CYC	ND-C1D-CHD-C4C
27	m1	201	CYC	C2D-C1D-CHD-C4C
27	n1	201	CYC	ND-C1D-CHD-C4C
27	n1	201	CYC	C2D-C1D-CHD-C4C
27	o1	1001	CYC	ND-C1D-CHD-C4C
27	o1	1001	CYC	C2D-C1D-CHD-C4C
27	p1	201	CYC	NA-C4A-CHB-C1B
27	p1	201	CYC	C4B-C3B-CAB-CBB
27	p1	201	CYC	ND-C1D-CHD-C4C
27	p1	201	CYC	C2D-C1D-CHD-C4C
27	q1	201	CYC	ND-C1D-CHD-C4C
27	q1	201	CYC	C2D-C1D-CHD-C4C
27	r1	201	CYC	NA-C4A-CHB-C1B
27	r1	201	CYC	C4B-C3B-CAB-CBB
27	r1	201	CYC	ND-C1D-CHD-C4C
27	r1	201	CYC	C2D-C1D-CHD-C4C
27	s1	201	CYC	ND-C1D-CHD-C4C
27	s1	201	CYC	C2D-C1D-CHD-C4C
27	t1	201	CYC	NA-C4A-CHB-C1B
27	t1	201	CYC	C4B-C3B-CAB-CBB
27	t1	201	CYC	ND-C1D-CHD-C4C
27	t1	201	CYC	C2D-C1D-CHD-C4C
27	u1	1001	CYC	ND-C1D-CHD-C4C
27	u1	1001	CYC	C2D-C1D-CHD-C4C
27	v1	201	CYC	NA-C4A-CHB-C1B
27	v1	201	CYC	C4B-C3B-CAB-CBB
27	v1	201	CYC	ND-C1D-CHD-C4C
27	v1	201	CYC	C2D-C1D-CHD-C4C
27	w1	201	CYC	ND-C1D-CHD-C4C
27	w1	201	CYC	C2D-C1D-CHD-C4C
27	y1	201	CYC	ND-C1D-CHD-C4C
27	y1	201	CYC	C2D-C1D-CHD-C4C
27	z1	201	CYC	NA-C4A-CHB-C1B
27	z1	201	CYC	C4B-C3B-CAB-CBB
27	z1	201	CYC	ND-C1D-CHD-C4C
27	z1	201	CYC	C2D-C1D-CHD-C4C
27	a2	901	CYC	NA-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
27	a2	901	CYC	C4B-C3B-CAB-CBB
27	a2	901	CYC	ND-C1D-CHD-C4C
27	a2	901	CYC	C2D-C1D-CHD-C4C
27	a2	902	CYC	NA-C4A-CHB-C1B
27	a2	902	CYC	C4B-C3B-CAB-CBB
27	a2	902	CYC	ND-C1D-CHD-C4C
27	a2	902	CYC	C2D-C1D-CHD-C4C
27	b2	1001	CYC	NA-C4A-CHB-C1B
27	b2	1001	CYC	C4B-C3B-CAB-CBB
27	b2	1001	CYC	ND-C1D-CHD-C4C
27	b2	1001	CYC	C2D-C1D-CHD-C4C
27	d2	101	CYC	ND-C1D-CHD-C4C
27	d2	101	CYC	C2D-C1D-CHD-C4C
28	f2	203	PUB	NB-C4B-CHB-C1C
28	h2	203	PUB	NB-C4B-CHB-C1C
28	j2	203	PUB	NB-C4B-CHB-C1C
28	l2	203	PUB	NB-C4B-CHB-C1C
28	n2	203	PUB	NB-C4B-CHB-C1C
28	p2	203	PUB	NB-C4B-CHB-C1C
28	r2	203	PUB	NB-C4B-CHB-C1C
28	t2	203	PUB	NB-C4B-CHB-C1C
28	v2	203	PUB	NB-C4B-CHB-C1C
28	x2	202	PUB	NB-C4B-CHB-C1C
28	z2	203	PUB	NB-C4B-CHB-C1C
28	A2	1005	PUB	NB-C4B-CHB-C1C
28	A2	1006	PUB	NB-C4B-CHB-C1C
28	C2	304	PUB	NB-C4B-CHB-C1C
28	C2	305	PUB	NB-C4B-CHB-C1C
28	D2	304	PUB	NB-C4B-CHB-C1C
28	D2	305	PUB	NB-C4B-CHB-C1C
28	F2	203	PUB	NB-C4B-CHB-C1C
28	H2	202	PUB	NB-C4B-CHB-C1C
28	J2	202	PUB	NB-C4B-CHB-C1C
28	L2	203	PUB	NB-C4B-CHB-C1C
28	N2	203	PUB	NB-C4B-CHB-C1C
28	P2	203	PUB	NB-C4B-CHB-C1C
28	R2	203	PUB	NB-C4B-CHB-C1C
28	T2	203	PUB	NB-C4B-CHB-C1C
28	V2	203	PUB	NB-C4B-CHB-C1C
28	X2	203	PUB	NB-C4B-CHB-C1C
28	Z2	203	PUB	NB-C4B-CHB-C1C
28	B3	203	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	D3	203	PUB	NB-C4B-CHB-C1C
28	F3	203	PUB	NB-C4B-CHB-C1C
28	H3	203	PUB	NB-C4B-CHB-C1C
28	J3	203	PUB	NB-C4B-CHB-C1C
28	L3	203	PUB	NB-C4B-CHB-C1C
28	N3	203	PUB	NB-C4B-CHB-C1C
28	P3	203	PUB	NB-C4B-CHB-C1C
28	R3	203	PUB	NB-C4B-CHB-C1C
28	T3	203	PUB	NB-C4B-CHB-C1C
28	V3	203	PUB	NB-C4B-CHB-C1C
28	X3	202	PUB	NB-C4B-CHB-C1C
28	Z3	203	PUB	NB-C4B-CHB-C1C
28	a3	1005	PUB	NB-C4B-CHB-C1C
28	a3	1006	PUB	NB-C4B-CHB-C1C
28	c3	304	PUB	NB-C4B-CHB-C1C
28	c3	305	PUB	NB-C4B-CHB-C1C
28	d3	303	PUB	NB-C4B-CHB-C1C
28	d3	304	PUB	NB-C4B-CHB-C1C
28	f3	203	PUB	NB-C4B-CHB-C1C
28	h3	202	PUB	NB-C4B-CHB-C1C
28	j3	202	PUB	NB-C4B-CHB-C1C
28	l3	202	PUB	NB-C4B-CHB-C1C
28	n3	203	PUB	NB-C4B-CHB-C1C
28	p3	203	PUB	NB-C4B-CHB-C1C
28	r3	203	PUB	NB-C4B-CHB-C1C
28	t3	203	PUB	NB-C4B-CHB-C1C
28	v3	203	PUB	NB-C4B-CHB-C1C
28	x3	203	PUB	NB-C4B-CHB-C1C
28	z3	203	PUB	NB-C4B-CHB-C1C
28	B4	203	PUB	NB-C4B-CHB-C1C
28	D4	203	PUB	NB-C4B-CHB-C1C
28	F4	203	PUB	NB-C4B-CHB-C1C
28	H4	203	PUB	NB-C4B-CHB-C1C
28	J4	203	PUB	NB-C4B-CHB-C1C
28	L4	203	PUB	NB-C4B-CHB-C1C
28	N4	203	PUB	NB-C4B-CHB-C1C
28	P4	203	PUB	NB-C4B-CHB-C1C
28	R4	203	PUB	NB-C4B-CHB-C1C
28	T4	202	PUB	NB-C4B-CHB-C1C
28	V4	203	PUB	NB-C4B-CHB-C1C
28	X4	203	PUB	NB-C4B-CHB-C1C
28	Z4	203	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	34	1005	PUB	NB-C4B-CHB-C1C
28	34	1006	PUB	NB-C4B-CHB-C1C
28	44	304	PUB	NB-C4B-CHB-C1C
28	44	305	PUB	NB-C4B-CHB-C1C
28	n4	203	PUB	NB-C4B-CHB-C1C
28	p4	203	PUB	NB-C4B-CHB-C1C
28	r4	202	PUB	NB-C4B-CHB-C1C
28	t4	203	PUB	NB-C4B-CHB-C1C
28	v4	203	PUB	NB-C4B-CHB-C1C
28	x4	202	PUB	NB-C4B-CHB-C1C
28	z4	203	PUB	NB-C4B-CHB-C1C
28	B5	203	PUB	NB-C4B-CHB-C1C
28	D5	203	PUB	NB-C4B-CHB-C1C
28	F5	203	PUB	NB-C4B-CHB-C1C
28	H5	202	PUB	NB-C4B-CHB-C1C
28	J5	203	PUB	NB-C4B-CHB-C1C
28	L5	203	PUB	NB-C4B-CHB-C1C
28	N5	203	PUB	NB-C4B-CHB-C1C
28	P5	202	PUB	NB-C4B-CHB-C1C
28	R5	203	PUB	NB-C4B-CHB-C1C
28	T5	202	PUB	NB-C4B-CHB-C1C
28	V5	203	PUB	NB-C4B-CHB-C1C
28	Y5	1005	PUB	NB-C4B-CHB-C1C
28	Y5	1006	PUB	NB-C4B-CHB-C1C
28	Z5	305	PUB	NB-C4B-CHB-C1C
28	Z5	306	PUB	NB-C4B-CHB-C1C
28	n5	203	PUB	NB-C4B-CHB-C1C
28	p5	202	PUB	NB-C4B-CHB-C1C
28	r5	203	PUB	NB-C4B-CHB-C1C
28	t5	203	PUB	NB-C4B-CHB-C1C
28	v5	203	PUB	NB-C4B-CHB-C1C
28	x5	202	PUB	NB-C4B-CHB-C1C
28	z5	203	PUB	NB-C4B-CHB-C1C
28	f8	203	PUB	NB-C4B-CHB-C1C
28	g8	202	PUB	NB-C4B-CHB-C1C
28	h8	203	PUB	NB-C4B-CHB-C1C
28	B6	203	PUB	NB-C4B-CHB-C1C
28	D6	202	PUB	NB-C4B-CHB-C1C
28	F6	203	PUB	NB-C4B-CHB-C1C
28	H6	203	PUB	NB-C4B-CHB-C1C
28	J6	203	PUB	NB-C4B-CHB-C1C
28	L6	202	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	N6	203	PUB	NB-C4B-CHB-C1C
28	P6	203	PUB	NB-C4B-CHB-C1C
28	R6	203	PUB	NB-C4B-CHB-C1C
28	T6	203	PUB	NB-C4B-CHB-C1C
28	V6	203	PUB	NB-C4B-CHB-C1C
28	X6	203	PUB	NB-C4B-CHB-C1C
28	Z6	203	PUB	NB-C4B-CHB-C1C
28	a6	203	PUB	NB-C4B-CHB-C1C
28	b6	203	PUB	NB-C4B-CHB-C1C
28	c6	1004	PUB	NB-C4B-CHB-C1C
28	d6	203	PUB	NB-C4B-CHB-C1C
28	e6	203	PUB	NB-C4B-CHB-C1C
28	l6	203	PUB	NB-C4B-CHB-C1C
28	n6	203	PUB	NB-C4B-CHB-C1C
28	p6	203	PUB	NB-C4B-CHB-C1C
28	r6	203	PUB	NB-C4B-CHB-C1C
28	t6	203	PUB	NB-C4B-CHB-C1C
28	u6	203	PUB	NB-C4B-CHB-C1C
28	v6	203	PUB	NB-C4B-CHB-C1C
28	x6	203	PUB	NB-C4B-CHB-C1C
28	y6	204	PUB	NB-C4B-CHB-C1C
28	z6	203	PUB	NB-C4B-CHB-C1C
28	n8	202	PUB	NB-C4B-CHB-C1C
28	o8	203	PUB	NB-C4B-CHB-C1C
28	p8	203	PUB	NB-C4B-CHB-C1C
28	B7	202	PUB	NB-C4B-CHB-C1C
28	D7	203	PUB	NB-C4B-CHB-C1C
28	F7	202	PUB	NB-C4B-CHB-C1C
28	H7	203	PUB	NB-C4B-CHB-C1C
28	J7	202	PUB	NB-C4B-CHB-C1C
28	L7	202	PUB	NB-C4B-CHB-C1C
28	N7	203	PUB	NB-C4B-CHB-C1C
28	P7	203	PUB	NB-C4B-CHB-C1C
28	R7	203	PUB	NB-C4B-CHB-C1C
28	T7	203	PUB	NB-C4B-CHB-C1C
28	V7	203	PUB	NB-C4B-CHB-C1C
28	X7	203	PUB	NB-C4B-CHB-C1C
28	Z7	203	PUB	NB-C4B-CHB-C1C
28	a7	203	PUB	NB-C4B-CHB-C1C
28	b7	202	PUB	NB-C4B-CHB-C1C
28	c7	203	PUB	NB-C4B-CHB-C1C
28	d7	203	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	e7	203	PUB	NB-C4B-CHB-C1C
28	l7	203	PUB	NB-C4B-CHB-C1C
28	n7	203	PUB	NB-C4B-CHB-C1C
28	p7	202	PUB	NB-C4B-CHB-C1C
28	r7	203	PUB	NB-C4B-CHB-C1C
28	s7	203	PUB	NB-C4B-CHB-C1C
28	t7	203	PUB	NB-C4B-CHB-C1C
28	v7	203	PUB	NB-C4B-CHB-C1C
28	x7	203	PUB	NB-C4B-CHB-C1C
28	y7	203	PUB	NB-C4B-CHB-C1C
28	z7	203	PUB	NB-C4B-CHB-C1C
28	b8	1005	PUB	NB-C4B-CHB-C1C
28	b8	1006	PUB	NB-C4B-CHB-C1C
28	c8	304	PUB	NB-C4B-CHB-C1C
28	c8	305	PUB	NB-C4B-CHB-C1C
28	d8	304	PUB	NB-C4B-CHB-C1C
28	e8	304	PUB	NB-C4B-CHB-C1C
28	e8	305	PUB	NB-C4B-CHB-C1C
28	b9	406	PUB	NB-C4B-CHB-C1C
28	b9	407	PUB	NB-C4B-CHB-C1C
28	c9	304	PUB	NB-C4B-CHB-C1C
28	c9	305	PUB	NB-C4B-CHB-C1C
28	d9	305	PUB	NB-C4B-CHB-C1C
28	e9	305	PUB	NB-C4B-CHB-C1C
28	e9	306	PUB	NB-C4B-CHB-C1C
28	w8	203	PUB	NB-C4B-CHB-C1C
28	y8	203	PUB	NB-C4B-CHB-C1C
28	A8	203	PUB	NB-C4B-CHB-C1C
28	C8	203	PUB	NB-C4B-CHB-C1C
28	E8	203	PUB	NB-C4B-CHB-C1C
28	G8	203	PUB	NB-C4B-CHB-C1C
28	I8	203	PUB	NB-C4B-CHB-C1C
28	K8	203	PUB	NB-C4B-CHB-C1C
28	M8	203	PUB	NB-C4B-CHB-C1C
28	O8	203	PUB	NB-C4B-CHB-C1C
28	Q8	203	PUB	NB-C4B-CHB-C1C
28	T8	304	PUB	NB-C4B-CHB-C1C
28	T8	305	PUB	NB-C4B-CHB-C1C
28	U8	1005	PUB	NB-C4B-CHB-C1C
28	U8	1006	PUB	NB-C4B-CHB-C1C
28	n9	202	PUB	NB-C4B-CHB-C1C
28	p9	203	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	r9	203	PUB	NB-C4B-CHB-C1C
28	t9	203	PUB	NB-C4B-CHB-C1C
28	v9	203	PUB	NB-C4B-CHB-C1C
28	x9	203	PUB	NB-C4B-CHB-C1C
28	z9	203	PUB	NB-C4B-CHB-C1C
28	B9	203	PUB	NB-C4B-CHB-C1C
28	D9	203	PUB	NB-C4B-CHB-C1C
28	F9	203	PUB	NB-C4B-CHB-C1C
28	H9	203	PUB	NB-C4B-CHB-C1C
28	J9	203	PUB	NB-C4B-CHB-C1C
28	L9	203	PUB	NB-C4B-CHB-C1C
28	N9	203	PUB	NB-C4B-CHB-C1C
28	P9	203	PUB	NB-C4B-CHB-C1C
28	R9	203	PUB	NB-C4B-CHB-C1C
28	T9	203	PUB	NB-C4B-CHB-C1C
28	V9	203	PUB	NB-C4B-CHB-C1C
28	Y9	304	PUB	NB-C4B-CHB-C1C
28	Y9	305	PUB	NB-C4B-CHB-C1C
28	Z9	1005	PUB	NB-C4B-CHB-C1C
28	Z9	1006	PUB	NB-C4B-CHB-C1C
28	an	202	PUB	NB-C4B-CHB-C1C
28	ap	203	PUB	NB-C4B-CHB-C1C
28	ar	203	PUB	NB-C4B-CHB-C1C
28	at	203	PUB	NB-C4B-CHB-C1C
28	av	203	PUB	NB-C4B-CHB-C1C
28	ax	202	PUB	NB-C4B-CHB-C1C
28	az	203	PUB	NB-C4B-CHB-C1C
28	aB	203	PUB	NB-C4B-CHB-C1C
28	aD	203	PUB	NB-C4B-CHB-C1C
28	aF	203	PUB	NB-C4B-CHB-C1C
28	aH	203	PUB	NB-C4B-CHB-C1C
28	aJ	203	PUB	NB-C4B-CHB-C1C
28	aL	203	PUB	NB-C4B-CHB-C1C
28	aN	203	PUB	NB-C4B-CHB-C1C
28	aP	203	PUB	NB-C4B-CHB-C1C
28	aR	203	PUB	NB-C4B-CHB-C1C
28	aT	203	PUB	NB-C4B-CHB-C1C
28	aV	203	PUB	NB-C4B-CHB-C1C
28	aY	404	PUB	NB-C4B-CHB-C1C
28	aY	405	PUB	NB-C4B-CHB-C1C
28	aZ	304	PUB	NB-C4B-CHB-C1C
28	aZ	305	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	bn	202	PUB	NB-C4B-CHB-C1C
28	bo	202	PUB	NB-C4B-CHB-C1C
28	bp	202	PUB	NB-C4B-CHB-C1C
28	bq	203	PUB	NB-C4B-CHB-C1C
28	br	203	PUB	NB-C4B-CHB-C1C
28	bs	1004	PUB	NB-C4B-CHB-C1C
28	bz	203	PUB	NB-C4B-CHB-C1C
28	bB	203	PUB	NB-C4B-CHB-C1C
28	bD	203	PUB	NB-C4B-CHB-C1C
28	bF	203	PUB	NB-C4B-CHB-C1C
28	bH	203	PUB	NB-C4B-CHB-C1C
28	bJ	203	PUB	NB-C4B-CHB-C1C
28	bL	203	PUB	NB-C4B-CHB-C1C
28	bN	203	PUB	NB-C4B-CHB-C1C
28	bP	203	PUB	NB-C4B-CHB-C1C
28	bR	202	PUB	NB-C4B-CHB-C1C
28	bT	202	PUB	NB-C4B-CHB-C1C
28	bV	203	PUB	NB-C4B-CHB-C1C
28	bY	1005	PUB	NB-C4B-CHB-C1C
28	bY	1006	PUB	NB-C4B-CHB-C1C
28	bZ	305	PUB	NB-C4B-CHB-C1C
28	bZ	306	PUB	NB-C4B-CHB-C1C
28	cn	202	PUB	NB-C4B-CHB-C1C
28	co	202	PUB	NB-C4B-CHB-C1C
28	cp	203	PUB	NB-C4B-CHB-C1C
28	cq	203	PUB	NB-C4B-CHB-C1C
28	cr	203	PUB	NB-C4B-CHB-C1C
28	cs	203	PUB	NB-C4B-CHB-C1C
28	cz	203	PUB	NB-C4B-CHB-C1C
28	cB	203	PUB	NB-C4B-CHB-C1C
28	cE	203	PUB	NB-C4B-CHB-C1C
28	cF	202	PUB	NB-C4B-CHB-C1C
28	cH	202	PUB	NB-C4B-CHB-C1C
28	cJ	203	PUB	NB-C4B-CHB-C1C
28	cL	203	PUB	NB-C4B-CHB-C1C
28	cM	203	PUB	NB-C4B-CHB-C1C
28	cN	202	PUB	NB-C4B-CHB-C1C
28	cO	203	PUB	NB-C4B-CHB-C1C
28	cP	203	PUB	NB-C4B-CHB-C1C
28	cQ	202	PUB	NB-C4B-CHB-C1C
28	cR	203	PUB	NB-C4B-CHB-C1C
28	cY	203	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	dd	203	PUB	NB-C4B-CHB-C1C
28	df	203	PUB	NB-C4B-CHB-C1C
28	dh	203	PUB	NB-C4B-CHB-C1C
28	di	203	PUB	NB-C4B-CHB-C1C
28	dj	203	PUB	NB-C4B-CHB-C1C
28	dl	203	PUB	NB-C4B-CHB-C1C
28	dn	203	PUB	NB-C4B-CHB-C1C
28	dp	203	PUB	NB-C4B-CHB-C1C
28	dr	203	PUB	NB-C4B-CHB-C1C
28	dt	203	PUB	NB-C4B-CHB-C1C
28	dv	202	PUB	NB-C4B-CHB-C1C
28	dw	405	PUB	NB-C4B-CHB-C1C
28	dw	406	PUB	NB-C4B-CHB-C1C
28	dx	406	PUB	NB-C4B-CHB-C1C
28	dx	407	PUB	NB-C4B-CHB-C1C
28	dB	202	PUB	NB-C4B-CHB-C1C
28	dD	203	PUB	NB-C4B-CHB-C1C
28	dF	203	PUB	NB-C4B-CHB-C1C
28	dH	203	PUB	NB-C4B-CHB-C1C
28	dK	203	PUB	NB-C4B-CHB-C1C
28	dL	203	PUB	NB-C4B-CHB-C1C
28	dN	203	PUB	NB-C4B-CHB-C1C
28	dP	203	PUB	NB-C4B-CHB-C1C
28	dR	203	PUB	NB-C4B-CHB-C1C
28	dT	203	PUB	NB-C4B-CHB-C1C
28	dV	203	PUB	NB-C4B-CHB-C1C
28	dX	203	PUB	NB-C4B-CHB-C1C
28	dY	203	PUB	NB-C4B-CHB-C1C
28	eb	202	PUB	NB-C4B-CHB-C1C
28	ec	203	PUB	NB-C4B-CHB-C1C
28	ee	203	PUB	NB-C4B-CHB-C1C
28	eg	203	PUB	NB-C4B-CHB-C1C
28	ei	203	PUB	NB-C4B-CHB-C1C
28	el	203	PUB	NB-C4B-CHB-C1C
28	en	203	PUB	NB-C4B-CHB-C1C
28	ep	203	PUB	NB-C4B-CHB-C1C
28	er	203	PUB	NB-C4B-CHB-C1C
28	et	203	PUB	NB-C4B-CHB-C1C
28	ev	203	PUB	NB-C4B-CHB-C1C
28	ey	1005	PUB	NB-C4B-CHB-C1C
28	ey	1006	PUB	NB-C4B-CHB-C1C
28	ez	1005	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	ez	1006	PUB	NB-C4B-CHB-C1C
28	eB	204	PUB	NB-C4B-CHB-C1C
28	eD	203	PUB	NB-C4B-CHB-C1C
28	eF	203	PUB	NB-C4B-CHB-C1C
28	eH	203	PUB	NB-C4B-CHB-C1C
28	eJ	203	PUB	NB-C4B-CHB-C1C
28	eL	203	PUB	NB-C4B-CHB-C1C
28	eN	203	PUB	NB-C4B-CHB-C1C
28	eP	204	PUB	NB-C4B-CHB-C1C
28	eR	203	PUB	NB-C4B-CHB-C1C
28	eT	203	PUB	NB-C4B-CHB-C1C
28	eV	203	PUB	NB-C4B-CHB-C1C
28	eX	202	PUB	NB-C4B-CHB-C1C
28	eY	404	PUB	NB-C4B-CHB-C1C
28	eY	405	PUB	NB-C4B-CHB-C1C
28	eZ	403	PUB	NB-C4B-CHB-C1C
28	eZ	404	PUB	NB-C4B-CHB-C1C
28	lb	203	PUB	NB-C4B-CHB-C1C
28	ld	203	PUB	NB-C4B-CHB-C1C
28	lf	203	PUB	NB-C4B-CHB-C1C
28	lh	203	PUB	NB-C4B-CHB-C1C
28	lj	202	PUB	NB-C4B-CHB-C1C
28	ll	203	PUB	NB-C4B-CHB-C1C
28	ln	203	PUB	NB-C4B-CHB-C1C
28	lp	203	PUB	NB-C4B-CHB-C1C
28	lr	203	PUB	NB-C4B-CHB-C1C
28	lt	203	PUB	NB-C4B-CHB-C1C
28	lv	202	PUB	NB-C4B-CHB-C1C
28	lx	201	PUB	NB-C4B-CHB-C1C
28	ly	405	PUB	NB-C4B-CHB-C1C
28	ly	406	PUB	NB-C4B-CHB-C1C
28	lz	404	PUB	NB-C4B-CHB-C1C
28	lz	405	PUB	NB-C4B-CHB-C1C
28	fa	202	PUB	NB-C4B-CHB-C1C
28	fc	203	PUB	NB-C4B-CHB-C1C
28	ff	203	PUB	NB-C4B-CHB-C1C
28	fi	203	PUB	NB-C4B-CHB-C1C
28	fj	203	PUB	NB-C4B-CHB-C1C
28	fm	203	PUB	NB-C4B-CHB-C1C
28	fo	203	PUB	NB-C4B-CHB-C1C
28	fq	203	PUB	NB-C4B-CHB-C1C
28	fs	203	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	fu	202	PUB	NB-C4B-CHB-C1C
28	fw	203	PUB	NB-C4B-CHB-C1C
28	fy	202	PUB	NB-C4B-CHB-C1C
28	ga	203	PUB	NB-C4B-CHB-C1C
28	gd	202	PUB	NB-C4B-CHB-C1C
28	ge	203	PUB	NB-C4B-CHB-C1C
28	gg	203	PUB	NB-C4B-CHB-C1C
28	gi	203	PUB	NB-C4B-CHB-C1C
28	gk	203	PUB	NB-C4B-CHB-C1C
28	gn	203	PUB	NB-C4B-CHB-C1C
28	gp	203	PUB	NB-C4B-CHB-C1C
28	gr	202	PUB	NB-C4B-CHB-C1C
28	gt	203	PUB	NB-C4B-CHB-C1C
28	gv	203	PUB	NB-C4B-CHB-C1C
28	gx	203	PUB	NB-C4B-CHB-C1C
28	gy	305	PUB	NB-C4B-CHB-C1C
28	gy	306	PUB	NB-C4B-CHB-C1C
28	gz	305	PUB	NB-C4B-CHB-C1C
28	gz	306	PUB	NB-C4B-CHB-C1C
28	hB	203	PUB	NB-C4B-CHB-C1C
28	hD	203	PUB	NB-C4B-CHB-C1C
28	hG	202	PUB	NB-C4B-CHB-C1C
28	hH	203	PUB	NB-C4B-CHB-C1C
28	hJ	203	PUB	NB-C4B-CHB-C1C
28	hL	203	PUB	NB-C4B-CHB-C1C
28	hN	203	PUB	NB-C4B-CHB-C1C
28	hP	203	PUB	NB-C4B-CHB-C1C
28	hR	203	PUB	NB-C4B-CHB-C1C
28	hT	203	PUB	NB-C4B-CHB-C1C
28	hV	203	PUB	NB-C4B-CHB-C1C
28	hX	203	PUB	NB-C4B-CHB-C1C
28	hY	405	PUB	NB-C4B-CHB-C1C
28	hY	406	PUB	NB-C4B-CHB-C1C
28	hZ	404	PUB	NB-C4B-CHB-C1C
28	hZ	405	PUB	NB-C4B-CHB-C1C
28	iC	1003	PUB	NB-C4B-CHB-C1C
28	iD	1003	PUB	NB-C4B-CHB-C1C
28	iE	1003	PUB	NB-C4B-CHB-C1C
28	iF	1003	PUB	NB-C4B-CHB-C1C
28	iG	1002	PUB	NB-C4B-CHB-C1C
28	iH	1002	PUB	NB-C4B-CHB-C1C
28	jI	1003	PUB	NB-C4B-CHB-C1C

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Mol	Chain	Res	Type	Atoms
28	jJ	1003	PUB	NB-C4B-CHB-C1C
28	jK	1003	PUB	NB-C4B-CHB-C1C
28	jL	1003	PUB	NB-C4B-CHB-C1C
28	jM	1003	PUB	NB-C4B-CHB-C1C
28	jN	1003	PUB	NB-C4B-CHB-C1C
28	jO	1003	PUB	NB-C4B-CHB-C1C
28	jP	1003	PUB	NB-C4B-CHB-C1C
28	kQ	1003	PUB	NB-C4B-CHB-C1C
28	kR	1003	PUB	NB-C4B-CHB-C1C
28	kS	1003	PUB	NB-C4B-CHB-C1C
28	kT	1003	PUB	NB-C4B-CHB-C1C
28	kU	1003	PUB	NB-C4B-CHB-C1C
28	kV	1003	PUB	NB-C4B-CHB-C1C
28	kW	1003	PUB	NB-C4B-CHB-C1C
28	kX	1003	PUB	NB-C4B-CHB-C1C
29	A2	1004	PVN	C2-C3-C31-C32
29	A2	1004	PVN	N1-C4-C5-C6
29	A2	1004	PVN	C11-C10-C9-N2
29	A2	1004	PVN	C11-C10-C9-C8
29	A2	1004	PVN	N3-C14-C15-C16
29	A2	1004	PVN	C13-C14-C15-C16
29	C2	303	PVN	C3-C4-C5-C6
29	C2	303	PVN	C52-C51-C8-C7
29	C2	303	PVN	C52-C51-C8-C9
29	C2	303	PVN	N3-C14-C15-C16
29	C2	303	PVN	C13-C14-C15-C16
29	D2	303	PVN	C2-C3-C31-C32
29	D2	303	PVN	C3-C4-C5-C6
29	D2	303	PVN	N1-C4-C5-C6
29	D2	303	PVN	N3-C14-C15-C16
29	D2	303	PVN	C13-C14-C15-C16
29	D2	303	PVN	C19-C18-C91-C92
29	a3	1004	PVN	C2-C3-C31-C32
29	a3	1004	PVN	N1-C4-C5-C6
29	a3	1004	PVN	C11-C10-C9-N2
29	a3	1004	PVN	C11-C10-C9-C8
29	a3	1004	PVN	N3-C14-C15-C16
29	a3	1004	PVN	C13-C14-C15-C16
29	c3	303	PVN	C3-C4-C5-C6
29	c3	303	PVN	C52-C51-C8-C7
29	c3	303	PVN	C52-C51-C8-C9
29	c3	303	PVN	N3-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	c3	303	PVN	C13-C14-C15-C16
29	d3	302	PVN	C2-C3-C31-C32
29	d3	302	PVN	C3-C4-C5-C6
29	d3	302	PVN	N1-C4-C5-C6
29	d3	302	PVN	N3-C14-C15-C16
29	d3	302	PVN	C13-C14-C15-C16
29	d3	302	PVN	C19-C18-C91-C92
29	34	1004	PVN	N1-C4-C5-C6
29	34	1004	PVN	N3-C14-C15-C16
29	34	1004	PVN	C13-C14-C15-C16
29	44	303	PVN	N1-C4-C5-C6
29	44	303	PVN	C11-C10-C9-N2
29	44	303	PVN	C11-C10-C9-C8
29	44	303	PVN	C9-C10-C11-C12
29	44	303	PVN	C9-C10-C11-N3
29	44	303	PVN	N3-C14-C15-C16
29	44	303	PVN	C13-C14-C15-C16
29	Y5	1004	PVN	N1-C4-C5-C6
29	Y5	1004	PVN	N3-C14-C15-C16
29	Y5	1004	PVN	C13-C14-C15-C16
29	Z5	304	PVN	N1-C4-C5-C6
29	Z5	304	PVN	C11-C10-C9-N2
29	Z5	304	PVN	C11-C10-C9-C8
29	Z5	304	PVN	C9-C10-C11-C12
29	Z5	304	PVN	C9-C10-C11-N3
29	Z5	304	PVN	N3-C14-C15-C16
29	Z5	304	PVN	C13-C14-C15-C16
29	b8	1004	PVN	C3-C4-C5-C6
29	b8	1004	PVN	C11-C10-C9-N2
29	b8	1004	PVN	C11-C10-C9-C8
29	b8	1004	PVN	N3-C14-C15-C16
29	b8	1004	PVN	C13-C14-C15-C16
29	b8	1004	PVN	C14-C15-C16-C17
29	c8	303	PVN	N1-C4-C5-C6
29	c8	303	PVN	C11-C10-C9-N2
29	c8	303	PVN	C11-C10-C9-C8
29	c8	303	PVN	N3-C14-C15-C16
29	c8	303	PVN	C13-C14-C15-C16
29	c8	303	PVN	C14-C15-C16-N4
29	d8	303	PVN	N1-C4-C5-C6
29	d8	303	PVN	C11-C10-C9-N2
29	d8	303	PVN	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	d8	303	PVN	C9-C10-C11-C12
29	d8	303	PVN	C9-C10-C11-N3
29	d8	303	PVN	N3-C14-C15-C16
29	d8	303	PVN	C13-C14-C15-C16
29	e8	303	PVN	N1-C4-C5-C6
29	e8	303	PVN	C11-C10-C9-N2
29	e8	303	PVN	C11-C10-C9-C8
29	e8	303	PVN	C9-C10-C11-C12
29	e8	303	PVN	C9-C10-C11-N3
29	e8	303	PVN	N3-C14-C15-C16
29	e8	303	PVN	C13-C14-C15-C16
29	b9	405	PVN	C3-C4-C5-C6
29	b9	405	PVN	C11-C10-C9-N2
29	b9	405	PVN	C11-C10-C9-C8
29	b9	405	PVN	N3-C14-C15-C16
29	b9	405	PVN	C13-C14-C15-C16
29	b9	405	PVN	C14-C15-C16-C17
29	c9	303	PVN	N1-C4-C5-C6
29	c9	303	PVN	C11-C10-C9-N2
29	c9	303	PVN	C11-C10-C9-C8
29	c9	303	PVN	N3-C14-C15-C16
29	c9	303	PVN	C13-C14-C15-C16
29	c9	303	PVN	C14-C15-C16-N4
29	d9	304	PVN	N1-C4-C5-C6
29	d9	304	PVN	C11-C10-C9-N2
29	d9	304	PVN	C11-C10-C9-C8
29	d9	304	PVN	C9-C10-C11-C12
29	d9	304	PVN	C9-C10-C11-N3
29	d9	304	PVN	N3-C14-C15-C16
29	d9	304	PVN	C13-C14-C15-C16
29	e9	304	PVN	N1-C4-C5-C6
29	e9	304	PVN	C11-C10-C9-N2
29	e9	304	PVN	C11-C10-C9-C8
29	e9	304	PVN	C9-C10-C11-C12
29	e9	304	PVN	C9-C10-C11-N3
29	e9	304	PVN	N3-C14-C15-C16
29	e9	304	PVN	C13-C14-C15-C16
29	T8	303	PVN	N1-C4-C5-C6
29	T8	303	PVN	C9-C10-C11-N3
29	T8	303	PVN	N3-C14-C15-C16
29	T8	303	PVN	C13-C14-C15-C16
29	T8	303	PVN	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	T8	303	PVN	C14-C15-C16-N4
29	T8	303	PVN	C17-C18-C91-C92
29	U8	1004	PVN	N1-C4-C5-C6
29	U8	1004	PVN	N3-C14-C15-C16
29	U8	1004	PVN	C13-C14-C15-C16
29	U8	1004	PVN	C14-C15-C16-C17
29	Y9	303	PVN	N1-C4-C5-C6
29	Y9	303	PVN	C9-C10-C11-N3
29	Y9	303	PVN	N3-C14-C15-C16
29	Y9	303	PVN	C13-C14-C15-C16
29	Y9	303	PVN	C14-C15-C16-C17
29	Y9	303	PVN	C14-C15-C16-N4
29	Y9	303	PVN	C17-C18-C91-C92
29	Z9	1004	PVN	N1-C4-C5-C6
29	Z9	1004	PVN	N3-C14-C15-C16
29	Z9	1004	PVN	C13-C14-C15-C16
29	Z9	1004	PVN	C14-C15-C16-C17
29	aY	403	PVN	N1-C4-C5-C6
29	aY	403	PVN	N3-C14-C15-C16
29	aY	403	PVN	C13-C14-C15-C16
29	aY	403	PVN	C14-C15-C16-C17
29	aY	403	PVN	C17-C18-C91-C92
29	aZ	303	PVN	C2-C3-C31-C32
29	aZ	303	PVN	N1-C4-C5-C6
29	aZ	303	PVN	N3-C14-C15-C16
29	aZ	303	PVN	C13-C14-C15-C16
29	aZ	303	PVN	C14-C15-C16-N4
29	aZ	303	PVN	C17-C18-C91-C92
29	aZ	303	PVN	C19-C18-C91-C92
29	bY	1004	PVN	N1-C4-C5-C6
29	bY	1004	PVN	N3-C14-C15-C16
29	bY	1004	PVN	C13-C14-C15-C16
29	bY	1004	PVN	C14-C15-C16-C17
29	bY	1004	PVN	C17-C18-C91-C92
29	bZ	304	PVN	C2-C3-C31-C32
29	bZ	304	PVN	N1-C4-C5-C6
29	bZ	304	PVN	C12-C61-C62-C63
29	bZ	304	PVN	N3-C14-C15-C16
29	bZ	304	PVN	C13-C14-C15-C16
29	bZ	304	PVN	C14-C15-C16-N4
29	bZ	304	PVN	C17-C18-C91-C92
29	bZ	304	PVN	C19-C18-C91-C92

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Mol	Chain	Res	Type	Atoms
29	dw	404	PVN	C2-C3-C31-C32
29	dw	404	PVN	N1-C4-C5-C6
29	dw	404	PVN	N3-C14-C15-C16
29	dw	404	PVN	C13-C14-C15-C16
29	dx	405	PVN	C2-C3-C31-C32
29	dx	405	PVN	N1-C4-C5-C6
29	dx	405	PVN	N3-C14-C15-C16
29	dx	405	PVN	C13-C14-C15-C16
29	ey	1004	PVN	C2-C3-C31-C32
29	ey	1004	PVN	C3-C4-C5-C6
29	ey	1004	PVN	N3-C14-C15-C16
29	ey	1004	PVN	C13-C14-C15-C16
29	ey	1004	PVN	C19-C18-C91-C92
29	ez	1004	PVN	C2-C3-C31-C32
29	ez	1004	PVN	C3-C4-C5-C6
29	ez	1004	PVN	N3-C14-C15-C16
29	ez	1004	PVN	C13-C14-C15-C16
29	ez	1004	PVN	C19-C18-C91-C92
29	eY	403	PVN	C2-C3-C31-C32
29	eY	403	PVN	C3-C4-C5-C6
29	eY	403	PVN	C11-C10-C9-N2
29	eY	403	PVN	C11-C10-C9-C8
29	eY	403	PVN	C9-C10-C11-C12
29	eY	403	PVN	C9-C10-C11-N3
29	eY	403	PVN	N3-C14-C15-C16
29	eY	403	PVN	C13-C14-C15-C16
29	eY	403	PVN	C14-C15-C16-C17
29	eZ	402	PVN	C2-C3-C31-C32
29	eZ	402	PVN	C3-C4-C5-C6
29	eZ	402	PVN	C11-C10-C9-N2
29	eZ	402	PVN	C11-C10-C9-C8
29	eZ	402	PVN	C9-C10-C11-C12
29	eZ	402	PVN	C9-C10-C11-N3
29	eZ	402	PVN	N3-C14-C15-C16
29	eZ	402	PVN	C13-C14-C15-C16
29	eZ	402	PVN	C14-C15-C16-C17
29	ly	404	PVN	N1-C4-C5-C6
29	ly	404	PVN	C52-C51-C8-C7
29	ly	404	PVN	C52-C51-C8-C9
29	ly	404	PVN	C9-C10-C11-N3
29	ly	404	PVN	N3-C14-C15-C16
29	ly	404	PVN	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	lz	403	PVN	N1-C4-C5-C6
29	lz	403	PVN	C52-C51-C8-C7
29	lz	403	PVN	C52-C51-C8-C9
29	lz	403	PVN	C9-C10-C11-N3
29	lz	403	PVN	N3-C14-C15-C16
29	lz	403	PVN	C13-C14-C15-C16
29	gy	304	PVN	C2-C3-C31-C32
29	gy	304	PVN	C4-C3-C31-C32
29	gy	304	PVN	C8-C51-C52-C53
29	gy	304	PVN	N3-C14-C15-C16
29	gy	304	PVN	C13-C14-C15-C16
29	gz	304	PVN	C2-C3-C31-C32
29	gz	304	PVN	C4-C3-C31-C32
29	gz	304	PVN	N3-C14-C15-C16
29	gz	304	PVN	C14-C15-C16-C17
29	gz	304	PVN	C14-C15-C16-N4
29	hY	404	PVN	N1-C4-C5-C6
29	hY	404	PVN	N3-C14-C15-C16
29	hY	404	PVN	C13-C14-C15-C16
29	hZ	403	PVN	N1-C4-C5-C6
29	hZ	403	PVN	N3-C14-C15-C16
29	hZ	403	PVN	C13-C14-C15-C16
29	44	303	PVN	C17-C18-C91-C92
29	Z5	304	PVN	C17-C18-C91-C92
29	b8	1004	PVN	C17-C18-C91-C92
29	b9	405	PVN	C17-C18-C91-C92
29	ez	1004	PVN	C17-C18-C91-C92
29	ey	1004	PVN	C17-C18-C91-C92
29	dw	404	PVN	C4-C3-C31-C32
29	A2	1004	PVN	C4-C3-C31-C32
29	a3	1004	PVN	C4-C3-C31-C32
27	H1	201	CYC	C2B-C3B-CAB-CBB
27	J1	201	CYC	C2B-C3B-CAB-CBB
27	M1	1001	CYC	C2B-C3B-CAB-CBB
27	S1	201	CYC	C2B-C3B-CAB-CBB
27	S1	202	CYC	C2B-C3B-CAB-CBB
27	Y1	201	CYC	C2B-C3B-CAB-CBB
27	c1	201	CYC	C2B-C3B-CAB-CBB
27	h1	201	CYC	C2B-C3B-CAB-CBB
27	j1	201	CYC	C2B-C3B-CAB-CBB
27	p1	201	CYC	C2B-C3B-CAB-CBB
27	r1	201	CYC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	t1	201	CYC	C2B-C3B-CAB-CBB
27	v1	201	CYC	C2B-C3B-CAB-CBB
27	z1	201	CYC	C2B-C3B-CAB-CBB
27	a2	901	CYC	C2B-C3B-CAB-CBB
27	a2	902	CYC	C2B-C3B-CAB-CBB
27	b2	1001	CYC	C2B-C3B-CAB-CBB
29	dx	405	PVN	C4-C3-C31-C32
29	eY	403	PVN	C4-C3-C31-C32
29	eZ	402	PVN	C4-C3-C31-C32
29	C2	303	PVN	C17-C18-C91-C92
29	D2	303	PVN	C17-C18-C91-C92
29	c3	303	PVN	C17-C18-C91-C92
29	d3	302	PVN	C17-C18-C91-C92
29	D2	303	PVN	C4-C3-C31-C32
29	d3	302	PVN	C4-C3-C31-C32
29	aZ	303	PVN	C4-C3-C31-C32
29	bZ	304	PVN	C4-C3-C31-C32
29	D2	303	PVN	C14-C15-C16-N4
29	d3	302	PVN	C14-C15-C16-N4
29	A2	1004	PVN	C14-C15-C16-C17
29	C2	303	PVN	C14-C15-C16-C17
29	D2	303	PVN	C14-C15-C16-C17
29	a3	1004	PVN	C14-C15-C16-C17
29	c3	303	PVN	C14-C15-C16-C17
29	d3	302	PVN	C14-C15-C16-C17
29	34	1004	PVN	C14-C15-C16-C17
29	44	303	PVN	C14-C15-C16-C17
29	Y5	1004	PVN	C14-C15-C16-C17
29	Z5	304	PVN	C14-C15-C16-C17
29	c8	303	PVN	C14-C15-C16-C17
29	d8	303	PVN	C14-C15-C16-C17
29	e8	303	PVN	C14-C15-C16-C17
29	c9	303	PVN	C14-C15-C16-C17
29	d9	304	PVN	C14-C15-C16-C17
29	e9	304	PVN	C14-C15-C16-C17
29	aZ	303	PVN	C14-C15-C16-C17
29	bZ	304	PVN	C14-C15-C16-C17
29	dw	404	PVN	C14-C15-C16-C17
29	dx	405	PVN	C14-C15-C16-C17
29	ey	1004	PVN	C14-C15-C16-C17
29	ez	1004	PVN	C14-C15-C16-C17
29	ly	404	PVN	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	lz	403	PVN	C14-C15-C16-C17
29	gy	304	PVN	C14-C15-C16-C17
29	hY	404	PVN	C14-C15-C16-C17
29	hZ	403	PVN	C14-C15-C16-C17
29	ez	1004	PVN	C4-C3-C31-C32
29	dw	404	PVN	C17-C18-C91-C92
29	ey	1004	PVN	C4-C3-C31-C32
29	aY	403	PVN	C4-C3-C31-C32
29	bY	1004	PVN	C4-C3-C31-C32
29	34	1004	PVN	C12-C61-C62-C63
29	Y5	1004	PVN	C12-C61-C62-C63
29	U8	1004	PVN	C12-C61-C62-C63
29	Z9	1004	PVN	C12-C61-C62-C63
29	aZ	303	PVN	C12-C61-C62-C63
29	dx	405	PVN	C12-C61-C62-C63
29	ly	404	PVN	C12-C61-C62-C63
29	lz	403	PVN	C12-C61-C62-C63
29	hY	404	PVN	C12-C61-C62-C63
29	hZ	403	PVN	C12-C61-C62-C63
29	gz	304	PVN	C13-C14-C15-C16
29	C2	303	PVN	C4-C3-C31-C32
29	c3	303	PVN	C4-C3-C31-C32
29	44	303	PVN	C8-C51-C52-C53
29	Z5	304	PVN	C8-C51-C52-C53
29	T8	303	PVN	C8-C51-C52-C53
29	U8	1004	PVN	C8-C51-C52-C53
29	Y9	303	PVN	C8-C51-C52-C53
29	Z9	1004	PVN	C8-C51-C52-C53
29	aY	403	PVN	C8-C51-C52-C53
29	aZ	303	PVN	C8-C51-C52-C53
29	bY	1004	PVN	C8-C51-C52-C53
29	bZ	304	PVN	C8-C51-C52-C53
29	dw	404	PVN	C8-C51-C52-C53
29	ey	1004	PVN	C8-C51-C52-C53
29	eY	403	PVN	C8-C51-C52-C53
29	eZ	402	PVN	C8-C51-C52-C53
29	ly	404	PVN	C8-C51-C52-C53
29	lz	403	PVN	C8-C51-C52-C53
29	D2	303	PVN	C9-C10-C11-N3
29	d3	302	PVN	C9-C10-C11-N3
29	b8	1004	PVN	C9-C10-C11-N3
29	c8	303	PVN	C9-C10-C11-N3

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Mol	Chain	Res	Type	Atoms
29	b9	405	PVN	C9-C10-C11-N3
29	c9	303	PVN	C9-C10-C11-N3
29	gy	304	PVN	C9-C10-C11-N3
29	gz	304	PVN	C9-C10-C11-N3
29	C2	303	PVN	C19-C18-C91-C92
29	c3	303	PVN	C19-C18-C91-C92
29	44	303	PVN	C19-C18-C91-C92
29	Z5	304	PVN	C19-C18-C91-C92
29	b8	1004	PVN	C19-C18-C91-C92
29	b9	405	PVN	C19-C18-C91-C92
29	T8	303	PVN	C19-C18-C91-C92
29	Y9	303	PVN	C19-C18-C91-C92
29	aY	403	PVN	C19-C18-C91-C92
29	bY	1004	PVN	C19-C18-C91-C92
26	A2	1001	PEB	C3B-CAB-CBB-CGB
26	E2	1002	PEB	C3B-CAB-CBB-CGB
26	N2	201	PEB	C3B-CAB-CBB-CGB
26	P2	202	PEB	C3B-CAB-CBB-CGB
26	R2	201	PEB	C3B-CAB-CBB-CGB
26	S2	202	PEB	C3B-CAB-CBB-CGB
26	U2	202	PEB	C3B-CAB-CBB-CGB
26	A3	202	PEB	C3B-CAB-CBB-CGB
26	C3	1002	PEB	C3B-CAB-CBB-CGB
26	E3	202	PEB	C3B-CAB-CBB-CGB
26	G3	202	PEB	C3B-CAB-CBB-CGB
26	I3	202	PEB	C3B-CAB-CBB-CGB
26	K3	202	PEB	C3B-CAB-CBB-CGB
26	M3	202	PEB	C3B-CAB-CBB-CGB
26	O3	1002	PEB	C3B-CAB-CBB-CGB
26	Q3	202	PEB	C3B-CAB-CBB-CGB
26	S3	202	PEB	C3B-CAB-CBB-CGB
26	U3	202	PEB	C3B-CAB-CBB-CGB
26	W3	202	PEB	C3B-CAB-CBB-CGB
26	Y3	202	PEB	C3B-CAB-CBB-CGB
26	a3	1002	PEB	C3B-CAB-CBB-CGB
26	c3	301	PEB	C3B-CAB-CBB-CGB
26	d3	301	PEB	C3B-CAB-CBB-CGB
26	e3	1002	PEB	C3B-CAB-CBB-CGB
26	g3	202	PEB	C3B-CAB-CBB-CGB
26	i3	202	PEB	C3B-CAB-CBB-CGB
26	k3	202	PEB	C3B-CAB-CBB-CGB
26	m3	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	o3	202	PEB	C3B-CAB-CBB-CGB
26	s3	202	PEB	C3B-CAB-CBB-CGB
26	u3	202	PEB	C3B-CAB-CBB-CGB
26	w3	202	PEB	C3B-CAB-CBB-CGB
26	y3	202	PEB	C3B-CAB-CBB-CGB
26	A4	202	PEB	C3B-CAB-CBB-CGB
26	C4	1002	PEB	C3B-CAB-CBB-CGB
26	N4	202	PEB	C3B-CAB-CBB-CGB
26	c4	201	PEB	C3B-CAB-CBB-CGB
26	h4	201	PEB	C3B-CAB-CBB-CGB
26	s4	202	PEB	C3B-CAB-CBB-CGB
26	w4	202	PEB	C3B-CAB-CBB-CGB
26	A5	202	PEB	C3B-CAB-CBB-CGB
26	C5	202	PEB	C3B-CAB-CBB-CGB
26	E5	202	PEB	C3B-CAB-CBB-CGB
26	G5	202	PEB	C3B-CAB-CBB-CGB
26	I5	202	PEB	C3B-CAB-CBB-CGB
26	K5	1002	PEB	C3B-CAB-CBB-CGB
26	M5	202	PEB	C3B-CAB-CBB-CGB
26	O5	202	PEB	C3B-CAB-CBB-CGB
26	Q5	202	PEB	C3B-CAB-CBB-CGB
26	S5	202	PEB	C3B-CAB-CBB-CGB
26	U5	202	PEB	C3B-CAB-CBB-CGB
26	Y5	1002	PEB	C3B-CAB-CBB-CGB
26	Z5	302	PEB	C3B-CAB-CBB-CGB
26	c5	201	PEB	C3B-CAB-CBB-CGB
26	f5	201	PEB	C3B-CAB-CBB-CGB
26	h5	202	PEB	C3B-CAB-CBB-CGB
26	m5	1002	PEB	C3B-CAB-CBB-CGB
26	o5	202	PEB	C3B-CAB-CBB-CGB
26	q5	202	PEB	C3B-CAB-CBB-CGB
26	s5	202	PEB	C3B-CAB-CBB-CGB
26	u5	202	PEB	C3B-CAB-CBB-CGB
26	w5	202	PEB	C3B-CAB-CBB-CGB
26	y5	1002	PEB	C3B-CAB-CBB-CGB
26	G6	202	PEB	C3B-CAB-CBB-CGB
26	H6	201	PEB	C3B-CAB-CBB-CGB
26	N6	202	PEB	C3B-CAB-CBB-CGB
26	U6	202	PEB	C3B-CAB-CBB-CGB
26	V6	202	PEB	C3B-CAB-CBB-CGB
26	a6	202	PEB	C3B-CAB-CBB-CGB
26	d6	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	e6	202	PEB	C3B-CAB-CBB-CGB
26	f6	202	PEB	C3B-CAB-CBB-CGB
26	n6	201	PEB	C3B-CAB-CBB-CGB
26	p6	202	PEB	C3B-CAB-CBB-CGB
26	t6	201	PEB	C3B-CAB-CBB-CGB
26	o8	201	PEB	C3B-CAB-CBB-CGB
26	q8	202	PEB	C3B-CAB-CBB-CGB
26	r8	202	PEB	C3B-CAB-CBB-CGB
26	s8	202	PEB	C3B-CAB-CBB-CGB
26	t8	202	PEB	C3B-CAB-CBB-CGB
26	u8	202	PEB	C3B-CAB-CBB-CGB
26	A7	201	PEB	C3B-CAB-CBB-CGB
26	C7	202	PEB	C3B-CAB-CBB-CGB
26	E7	202	PEB	C3B-CAB-CBB-CGB
26	G7	202	PEB	C3B-CAB-CBB-CGB
26	I7	202	PEB	C3B-CAB-CBB-CGB
26	K7	202	PEB	C3B-CAB-CBB-CGB
26	M7	1003	PEB	C3B-CAB-CBB-CGB
26	O7	202	PEB	C3B-CAB-CBB-CGB
26	Q7	202	PEB	C3B-CAB-CBB-CGB
26	S7	202	PEB	C3B-CAB-CBB-CGB
26	U7	202	PEB	C3B-CAB-CBB-CGB
26	W7	202	PEB	C3B-CAB-CBB-CGB
26	Y7	1002	PEB	C3B-CAB-CBB-CGB
26	f7	202	PEB	C3B-CAB-CBB-CGB
26	g7	202	PEB	C3B-CAB-CBB-CGB
26	h7	202	PEB	C3B-CAB-CBB-CGB
26	i7	202	PEB	C3B-CAB-CBB-CGB
26	j7	202	PEB	C3B-CAB-CBB-CGB
26	k7	1002	PEB	C3B-CAB-CBB-CGB
26	m7	202	PEB	C3B-CAB-CBB-CGB
26	o7	202	PEB	C3B-CAB-CBB-CGB
26	q7	202	PEB	C3B-CAB-CBB-CGB
26	s7	202	PEB	C3B-CAB-CBB-CGB
26	u7	202	PEB	C3B-CAB-CBB-CGB
26	w7	1002	PEB	C3B-CAB-CBB-CGB
26	c8	301	PEB	C3B-CAB-CBB-CGB
26	d8	301	PEB	C3B-CAB-CBB-CGB
26	A9	202	PEB	C3B-CAB-CBB-CGB
26	C9	202	PEB	C3B-CAB-CBB-CGB
26	E9	202	PEB	C3B-CAB-CBB-CGB
26	G9	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	I9	202	PEB	C3B-CAB-CBB-CGB
26	K9	1002	PEB	C3B-CAB-CBB-CGB
26	M9	202	PEB	C3B-CAB-CBB-CGB
26	O9	202	PEB	C3B-CAB-CBB-CGB
26	Q9	202	PEB	C3B-CAB-CBB-CGB
26	S9	202	PEB	C3B-CAB-CBB-CGB
26	U9	202	PEB	C3B-CAB-CBB-CGB
26	Y9	301	PEB	C3B-CAB-CBB-CGB
26	Z9	1002	PEB	C3B-CAB-CBB-CGB
26	ao	202	PEB	C3B-CAB-CBB-CGB
26	aq	202	PEB	C3B-CAB-CBB-CGB
26	as	202	PEB	C3B-CAB-CBB-CGB
26	au	202	PEB	C3B-CAB-CBB-CGB
26	aw	202	PEB	C3B-CAB-CBB-CGB
26	ay	1002	PEB	C3B-CAB-CBB-CGB
26	bA	202	PEB	C3B-CAB-CBB-CGB
26	bC	202	PEB	C3B-CAB-CBB-CGB
26	bE	202	PEB	C3B-CAB-CBB-CGB
26	bG	202	PEB	C3B-CAB-CBB-CGB
26	bI	202	PEB	C3B-CAB-CBB-CGB
26	bK	1002	PEB	C3B-CAB-CBB-CGB
26	bM	202	PEB	C3B-CAB-CBB-CGB
26	bO	202	PEB	C3B-CAB-CBB-CGB
26	bQ	202	PEB	C3B-CAB-CBB-CGB
26	bS	202	PEB	C3B-CAB-CBB-CGB
26	bU	202	PEB	C3B-CAB-CBB-CGB
26	bY	1002	PEB	C3B-CAB-CBB-CGB
26	bZ	302	PEB	C3B-CAB-CBB-CGB
26	cm	1002	PEB	C3B-CAB-CBB-CGB
26	ct	202	PEB	C3B-CAB-CBB-CGB
26	cu	202	PEB	C3B-CAB-CBB-CGB
26	cv	202	PEB	C3B-CAB-CBB-CGB
26	cw	202	PEB	C3B-CAB-CBB-CGB
26	cx	202	PEB	C3B-CAB-CBB-CGB
26	cy	1002	PEB	C3B-CAB-CBB-CGB
26	cA	202	PEB	C3B-CAB-CBB-CGB
26	cC	1002	PEB	C3B-CAB-CBB-CGB
26	cD	202	PEB	C3B-CAB-CBB-CGB
26	cG	202	PEB	C3B-CAB-CBB-CGB
26	cI	202	PEB	C3B-CAB-CBB-CGB
26	cK	202	PEB	C3B-CAB-CBB-CGB
26	cZ	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	da	1002	PEB	C3B-CAB-CBB-CGB
26	db	202	PEB	C3B-CAB-CBB-CGB
26	dc	202	PEB	C3B-CAB-CBB-CGB
26	de	202	PEB	C3B-CAB-CBB-CGB
26	dg	202	PEB	C3B-CAB-CBB-CGB
26	dJ	202	PEB	C3B-CAB-CBB-CGB
26	dU	202	PEB	C3B-CAB-CBB-CGB
26	dZ	1002	PEB	C3B-CAB-CBB-CGB
26	ec	201	PEB	C3B-CAB-CBB-CGB
26	ef	202	PEB	C3B-CAB-CBB-CGB
26	eh	202	PEB	C3B-CAB-CBB-CGB
26	ei	201	PEB	C3B-CAB-CBB-CGB
26	ek	1002	PEB	C3B-CAB-CBB-CGB
26	em	202	PEB	C3B-CAB-CBB-CGB
26	et	201	PEB	C3B-CAB-CBB-CGB
26	eu	202	PEB	C3B-CAB-CBB-CGB
26	ev	201	PEB	C3B-CAB-CBB-CGB
26	ey	1001	PEB	C3B-CAB-CBB-CGB
26	eA	1002	PEB	C3B-CAB-CBB-CGB
26	eB	201	PEB	C3B-CAB-CBB-CGB
26	eL	201	PEB	C3B-CAB-CBB-CGB
26	eP	201	PEB	C3B-CAB-CBB-CGB
26	eY	401	PEB	C3B-CAB-CBB-CGB
26	lc	202	PEB	C3B-CAB-CBB-CGB
26	ld	201	PEB	C3B-CAB-CBB-CGB
26	le	202	PEB	C3B-CAB-CBB-CGB
26	lg	201	PEB	C3B-CAB-CBB-CGB
26	lg	202	PEB	C3B-CAB-CBB-CGB
26	lh	201	PEB	C3B-CAB-CBB-CGB
26	lj	201	PEB	C3B-CAB-CBB-CGB
26	lk	202	PEB	C3B-CAB-CBB-CGB
26	lm	1002	PEB	C3B-CAB-CBB-CGB
26	lo	201	PEB	C3B-CAB-CBB-CGB
26	lo	202	PEB	C3B-CAB-CBB-CGB
26	lq	203	PEB	C3B-CAB-CBB-CGB
26	ls	202	PEB	C3B-CAB-CBB-CGB
26	lt	202	PEB	C3B-CAB-CBB-CGB
26	lu	202	PEB	C3B-CAB-CBB-CGB
26	lw	201	PEB	C3B-CAB-CBB-CGB
26	lw	202	PEB	C3B-CAB-CBB-CGB
26	fb	202	PEB	C3B-CAB-CBB-CGB
26	fe	202	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
26	fg	202	PEB	C3B-CAB-CBB-CGB
26	fh	1002	PEB	C3B-CAB-CBB-CGB
26	fk	202	PEB	C3B-CAB-CBB-CGB
26	fl	202	PEB	C3B-CAB-CBB-CGB
26	fn	1002	PEB	C3B-CAB-CBB-CGB
26	fp	202	PEB	C3B-CAB-CBB-CGB
26	fr	202	PEB	C3B-CAB-CBB-CGB
26	ft	202	PEB	C3B-CAB-CBB-CGB
26	fv	202	PEB	C3B-CAB-CBB-CGB
26	fx	202	PEB	C3B-CAB-CBB-CGB
26	fz	301	PEB	C3B-CAB-CBB-CGB
26	gb	1002	PEB	C3B-CAB-CBB-CGB
26	gc	202	PEB	C3B-CAB-CBB-CGB
26	gf	202	PEB	C3B-CAB-CBB-CGB
26	gh	202	PEB	C3B-CAB-CBB-CGB
26	gj	202	PEB	C3B-CAB-CBB-CGB
26	gl	202	PEB	C3B-CAB-CBB-CGB
26	gm	1002	PEB	C3B-CAB-CBB-CGB
26	go	202	PEB	C3B-CAB-CBB-CGB
26	gq	202	PEB	C3B-CAB-CBB-CGB
26	gs	202	PEB	C3B-CAB-CBB-CGB
26	gu	202	PEB	C3B-CAB-CBB-CGB
26	gw	202	PEB	C3B-CAB-CBB-CGB
26	gy	302	PEB	C3B-CAB-CBB-CGB
26	gz	302	PEB	C3B-CAB-CBB-CGB
26	hA	202	PEB	C3B-CAB-CBB-CGB
26	hC	202	PEB	C3B-CAB-CBB-CGB
26	hE	1002	PEB	C3B-CAB-CBB-CGB
26	hF	202	PEB	C3B-CAB-CBB-CGB
26	hI	202	PEB	C3B-CAB-CBB-CGB
26	hK	202	PEB	C3B-CAB-CBB-CGB
26	hM	1002	PEB	C3B-CAB-CBB-CGB
26	hO	202	PEB	C3B-CAB-CBB-CGB
26	hQ	202	PEB	C3B-CAB-CBB-CGB
26	hS	202	PEB	C3B-CAB-CBB-CGB
26	hU	201	PEB	C3B-CAB-CBB-CGB
26	hW	202	PEB	C3B-CAB-CBB-CGB
26	hY	402	PEB	C3B-CAB-CBB-CGB
26	hZ	401	PEB	C3B-CAB-CBB-CGB
26	iA	1002	PEB	C3B-CAB-CBB-CGB
26	iB	1002	PEB	C3B-CAB-CBB-CGB
26	iF	1002	PEB	C3B-CAB-CBB-CGB

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Mol	Chain	Res	Type	Atoms
27	G1	1001	CYC	C2A-CAA-CBA-CGA
27	I1	201	CYC	C2A-CAA-CBA-CGA
27	K1	201	CYC	C2A-CAA-CBA-CGA
27	L1	201	CYC	C2A-CAA-CBA-CGA
27	N1	201	CYC	C2A-CAA-CBA-CGA
27	O1	201	CYC	C2A-CAA-CBA-CGA
27	P1	201	CYC	C2A-CAA-CBA-CGA
27	Q1	201	CYC	C2A-CAA-CBA-CGA
27	R1	1001	CYC	C2A-CAA-CBA-CGA
27	U1	201	CYC	C2A-CAA-CBA-CGA
27	V1	201	CYC	C2A-CAA-CBA-CGA
27	W1	201	CYC	C2A-CAA-CBA-CGA
27	X1	201	CYC	C2A-CAA-CBA-CGA
27	Z1	201	CYC	C2A-CAA-CBA-CGA
27	a1	201	CYC	C2A-CAA-CBA-CGA
27	b1	1001	CYC	C2A-CAA-CBA-CGA
27	d1	1001	CYC	C2A-CAA-CBA-CGA
27	e1	201	CYC	C2A-CAA-CBA-CGA
27	f1	201	CYC	C2A-CAA-CBA-CGA
27	g1	201	CYC	C2A-CAA-CBA-CGA
27	i1	1001	CYC	C2A-CAA-CBA-CGA
27	k1	201	CYC	C2A-CAA-CBA-CGA
27	m1	201	CYC	C2A-CAA-CBA-CGA
27	n1	201	CYC	C2A-CAA-CBA-CGA
27	o1	1001	CYC	C2A-CAA-CBA-CGA
27	q1	201	CYC	C2A-CAA-CBA-CGA
27	s1	201	CYC	C2A-CAA-CBA-CGA
27	u1	1001	CYC	C2A-CAA-CBA-CGA
27	w1	201	CYC	C2A-CAA-CBA-CGA
27	y1	201	CYC	C2A-CAA-CBA-CGA
27	d2	101	CYC	C2A-CAA-CBA-CGA
29	c8	303	PVN	C12-C61-C62-C63
29	d8	303	PVN	C12-C61-C62-C63
29	e8	303	PVN	C12-C61-C62-C63
29	c9	303	PVN	C12-C61-C62-C63
29	d9	304	PVN	C12-C61-C62-C63
29	e9	304	PVN	C12-C61-C62-C63
29	dw	404	PVN	C12-C61-C62-C63
29	eY	403	PVN	C12-C61-C62-C63
29	eZ	402	PVN	C12-C61-C62-C63
27	G1	1001	CYC	C3A-C4A-CHB-C1B
27	I1	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
27	K1	201	CYC	C3A-C4A-CHB-C1B
27	L1	201	CYC	C3A-C4A-CHB-C1B
27	N1	201	CYC	C3A-C4A-CHB-C1B
27	O1	201	CYC	C3A-C4A-CHB-C1B
27	P1	201	CYC	C3A-C4A-CHB-C1B
27	Q1	201	CYC	C3A-C4A-CHB-C1B
27	R1	1001	CYC	C3A-C4A-CHB-C1B
27	U1	201	CYC	C3A-C4A-CHB-C1B
27	V1	201	CYC	C3A-C4A-CHB-C1B
27	W1	201	CYC	C3A-C4A-CHB-C1B
27	X1	201	CYC	C3A-C4A-CHB-C1B
27	Z1	201	CYC	C3A-C4A-CHB-C1B
27	a1	201	CYC	C3A-C4A-CHB-C1B
27	b1	1001	CYC	C3A-C4A-CHB-C1B
27	d1	1001	CYC	C3A-C4A-CHB-C1B
27	e1	201	CYC	C3A-C4A-CHB-C1B
27	f1	201	CYC	C3A-C4A-CHB-C1B
27	g1	201	CYC	C3A-C4A-CHB-C1B
27	i1	1001	CYC	C3A-C4A-CHB-C1B
27	k1	201	CYC	C3A-C4A-CHB-C1B
27	m1	201	CYC	C3A-C4A-CHB-C1B
27	n1	201	CYC	C3A-C4A-CHB-C1B
27	o1	1001	CYC	C3A-C4A-CHB-C1B
27	q1	201	CYC	C3A-C4A-CHB-C1B
27	s1	201	CYC	C3A-C4A-CHB-C1B
27	u1	1001	CYC	C3A-C4A-CHB-C1B
27	w1	201	CYC	C3A-C4A-CHB-C1B
27	y1	201	CYC	C3A-C4A-CHB-C1B
27	d2	101	CYC	C3A-C4A-CHB-C1B
29	Z9	1004	PVN	C17-C18-C91-C92
29	ly	404	PVN	C17-C18-C91-C92
29	lz	403	PVN	C17-C18-C91-C92
29	U8	1004	PVN	C17-C18-C91-C92
29	A2	1004	PVN	C14-C15-C16-N4
29	C2	303	PVN	C14-C15-C16-N4
29	a3	1004	PVN	C14-C15-C16-N4
29	c3	303	PVN	C14-C15-C16-N4
29	34	1004	PVN	C14-C15-C16-N4
29	44	303	PVN	C14-C15-C16-N4
29	Y5	1004	PVN	C14-C15-C16-N4
29	Z5	304	PVN	C14-C15-C16-N4
29	ey	1004	PVN	C14-C15-C16-N4

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Mol	Chain	Res	Type	Atoms
29	gy	304	PVN	C14-C15-C16-N4
29	hY	404	PVN	C14-C15-C16-N4
29	hZ	403	PVN	C14-C15-C16-N4
27	G1	1001	CYC	NA-C4A-CHB-C1B
27	I1	201	CYC	NA-C4A-CHB-C1B
27	K1	201	CYC	NA-C4A-CHB-C1B
27	L1	201	CYC	NA-C4A-CHB-C1B
27	N1	201	CYC	NA-C4A-CHB-C1B
27	O1	201	CYC	NA-C4A-CHB-C1B
27	P1	201	CYC	NA-C4A-CHB-C1B
27	Q1	201	CYC	NA-C4A-CHB-C1B
27	R1	1001	CYC	NA-C4A-CHB-C1B
27	U1	201	CYC	NA-C4A-CHB-C1B
27	V1	201	CYC	NA-C4A-CHB-C1B
27	W1	201	CYC	NA-C4A-CHB-C1B
27	X1	201	CYC	NA-C4A-CHB-C1B
27	Z1	201	CYC	NA-C4A-CHB-C1B
27	a1	201	CYC	NA-C4A-CHB-C1B
27	b1	1001	CYC	NA-C4A-CHB-C1B
27	d1	1001	CYC	NA-C4A-CHB-C1B
27	e1	201	CYC	NA-C4A-CHB-C1B
27	f1	201	CYC	NA-C4A-CHB-C1B
27	g1	201	CYC	NA-C4A-CHB-C1B
27	i1	1001	CYC	NA-C4A-CHB-C1B
27	k1	201	CYC	NA-C4A-CHB-C1B
27	m1	201	CYC	NA-C4A-CHB-C1B
27	n1	201	CYC	NA-C4A-CHB-C1B
27	o1	1001	CYC	NA-C4A-CHB-C1B
27	q1	201	CYC	NA-C4A-CHB-C1B
27	s1	201	CYC	NA-C4A-CHB-C1B
27	u1	1001	CYC	NA-C4A-CHB-C1B
27	w1	201	CYC	NA-C4A-CHB-C1B
27	y1	201	CYC	NA-C4A-CHB-C1B
27	d2	101	CYC	NA-C4A-CHB-C1B
29	U8	1004	PVN	C14-C15-C16-N4
29	Z9	1004	PVN	C14-C15-C16-N4
27	H1	201	CYC	C3A-C4A-CHB-C1B
27	J1	201	CYC	C3A-C4A-CHB-C1B
27	M1	1001	CYC	C3A-C4A-CHB-C1B
27	S1	201	CYC	C3A-C4A-CHB-C1B
27	S1	202	CYC	C3A-C4A-CHB-C1B
27	Y1	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
27	c1	201	CYC	C3A-C4A-CHB-C1B
27	h1	201	CYC	C3A-C4A-CHB-C1B
27	j1	201	CYC	C3A-C4A-CHB-C1B
27	p1	201	CYC	C3A-C4A-CHB-C1B
27	r1	201	CYC	C3A-C4A-CHB-C1B
27	t1	201	CYC	C3A-C4A-CHB-C1B
27	v1	201	CYC	C3A-C4A-CHB-C1B
27	z1	201	CYC	C3A-C4A-CHB-C1B
27	a2	901	CYC	C3A-C4A-CHB-C1B
27	a2	902	CYC	C3A-C4A-CHB-C1B
27	b2	1001	CYC	C3A-C4A-CHB-C1B
29	dx	405	PVN	C17-C18-C91-C92
29	D2	303	PVN	C8-C51-C52-C53
29	d3	302	PVN	C8-C51-C52-C53
29	dx	405	PVN	C8-C51-C52-C53
29	b8	1004	PVN	C14-C15-C16-N4
29	d8	303	PVN	C14-C15-C16-N4
29	e8	303	PVN	C14-C15-C16-N4
29	b9	405	PVN	C14-C15-C16-N4
29	d9	304	PVN	C14-C15-C16-N4
29	e9	304	PVN	C14-C15-C16-N4
29	aY	403	PVN	C14-C15-C16-N4
29	bY	1004	PVN	C14-C15-C16-N4
29	dw	404	PVN	C14-C15-C16-N4
29	dx	405	PVN	C14-C15-C16-N4
29	ez	1004	PVN	C14-C15-C16-N4
29	eY	403	PVN	C14-C15-C16-N4
29	eZ	402	PVN	C14-C15-C16-N4
29	ly	404	PVN	C14-C15-C16-N4
29	lz	403	PVN	C14-C15-C16-N4
29	A2	1004	PVN	C12-C61-C62-C63
29	a3	1004	PVN	C12-C61-C62-C63
29	b8	1004	PVN	C12-C61-C62-C63
29	b9	405	PVN	C12-C61-C62-C63
29	34	1004	PVN	C17-C18-C91-C92
29	Y5	1004	PVN	C17-C18-C91-C92
29	hY	404	PVN	C17-C18-C91-C92
29	hZ	403	PVN	C17-C18-C91-C92
29	T8	303	PVN	C9-C10-C11-C12
29	Y9	303	PVN	C9-C10-C11-C12
29	ly	404	PVN	C9-C10-C11-C12
29	lz	403	PVN	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	A2	1004	PVN	C8-C51-C52-C53
29	a3	1004	PVN	C8-C51-C52-C53
28	f2	203	PUB	C2A-C3A-CAA-CBA
28	h2	203	PUB	C2A-C3A-CAA-CBA
28	j2	203	PUB	C2A-C3A-CAA-CBA
28	l2	203	PUB	C2A-C3A-CAA-CBA
28	n2	203	PUB	C2A-C3A-CAA-CBA
28	p2	203	PUB	C2A-C3A-CAA-CBA
28	r2	203	PUB	C2A-C3A-CAA-CBA
28	t2	203	PUB	C2A-C3A-CAA-CBA
28	v2	203	PUB	C2A-C3A-CAA-CBA
28	x2	202	PUB	C2A-C3A-CAA-CBA
28	z2	203	PUB	C2A-C3A-CAA-CBA
28	A2	1005	PUB	C2A-C3A-CAA-CBA
28	A2	1006	PUB	C2A-C3A-CAA-CBA
28	C2	304	PUB	C2A-C3A-CAA-CBA
28	C2	305	PUB	C2A-C3A-CAA-CBA
28	D2	304	PUB	C2A-C3A-CAA-CBA
28	D2	305	PUB	C2A-C3A-CAA-CBA
28	F2	203	PUB	C2A-C3A-CAA-CBA
28	H2	202	PUB	C2A-C3A-CAA-CBA
28	J2	202	PUB	C2A-C3A-CAA-CBA
28	L2	203	PUB	C2A-C3A-CAA-CBA
28	N2	203	PUB	C2A-C3A-CAA-CBA
28	P2	203	PUB	C2A-C3A-CAA-CBA
28	R2	203	PUB	C2A-C3A-CAA-CBA
28	T2	203	PUB	C2A-C3A-CAA-CBA
28	V2	203	PUB	C2A-C3A-CAA-CBA
28	X2	203	PUB	C2A-C3A-CAA-CBA
28	Z2	203	PUB	C2A-C3A-CAA-CBA
28	B3	203	PUB	C2A-C3A-CAA-CBA
28	D3	203	PUB	C2A-C3A-CAA-CBA
28	F3	203	PUB	C2A-C3A-CAA-CBA
28	H3	203	PUB	C2A-C3A-CAA-CBA
28	J3	203	PUB	C2A-C3A-CAA-CBA
28	L3	203	PUB	C2A-C3A-CAA-CBA
28	N3	203	PUB	C2A-C3A-CAA-CBA
28	P3	203	PUB	C2A-C3A-CAA-CBA
28	R3	203	PUB	C2A-C3A-CAA-CBA
28	T3	203	PUB	C2A-C3A-CAA-CBA
28	V3	203	PUB	C2A-C3A-CAA-CBA
28	X3	202	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	Z3	203	PUB	C2A-C3A-CAA-CBA
28	a3	1005	PUB	C2A-C3A-CAA-CBA
28	a3	1006	PUB	C2A-C3A-CAA-CBA
28	c3	304	PUB	C2A-C3A-CAA-CBA
28	c3	305	PUB	C2A-C3A-CAA-CBA
28	d3	303	PUB	C2A-C3A-CAA-CBA
28	d3	304	PUB	C2A-C3A-CAA-CBA
28	f3	203	PUB	C2A-C3A-CAA-CBA
28	h3	202	PUB	C2A-C3A-CAA-CBA
28	j3	202	PUB	C2A-C3A-CAA-CBA
28	l3	202	PUB	C2A-C3A-CAA-CBA
28	n3	203	PUB	C2A-C3A-CAA-CBA
28	p3	203	PUB	C2A-C3A-CAA-CBA
28	r3	203	PUB	C2A-C3A-CAA-CBA
28	t3	203	PUB	C2A-C3A-CAA-CBA
28	v3	203	PUB	C2A-C3A-CAA-CBA
28	x3	203	PUB	C2A-C3A-CAA-CBA
28	z3	203	PUB	C2A-C3A-CAA-CBA
28	B4	203	PUB	C2A-C3A-CAA-CBA
28	D4	203	PUB	C2A-C3A-CAA-CBA
28	F4	203	PUB	C2A-C3A-CAA-CBA
28	H4	203	PUB	C2A-C3A-CAA-CBA
28	J4	203	PUB	C2A-C3A-CAA-CBA
28	L4	203	PUB	C2A-C3A-CAA-CBA
28	N4	203	PUB	C2A-C3A-CAA-CBA
28	P4	203	PUB	C2A-C3A-CAA-CBA
28	R4	203	PUB	C2A-C3A-CAA-CBA
28	T4	202	PUB	C2A-C3A-CAA-CBA
28	V4	203	PUB	C2A-C3A-CAA-CBA
28	X4	203	PUB	C2A-C3A-CAA-CBA
28	Z4	203	PUB	C2A-C3A-CAA-CBA
28	34	1005	PUB	C2A-C3A-CAA-CBA
28	34	1006	PUB	C2A-C3A-CAA-CBA
28	44	304	PUB	C2A-C3A-CAA-CBA
28	44	305	PUB	C2A-C3A-CAA-CBA
28	n4	203	PUB	C2A-C3A-CAA-CBA
28	p4	203	PUB	C2A-C3A-CAA-CBA
28	r4	202	PUB	C2A-C3A-CAA-CBA
28	t4	203	PUB	C2A-C3A-CAA-CBA
28	v4	203	PUB	C2A-C3A-CAA-CBA
28	x4	202	PUB	C2A-C3A-CAA-CBA
28	z4	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	B5	203	PUB	C2A-C3A-CAA-CBA
28	D5	203	PUB	C2A-C3A-CAA-CBA
28	F5	203	PUB	C2A-C3A-CAA-CBA
28	H5	202	PUB	C2A-C3A-CAA-CBA
28	J5	203	PUB	C2A-C3A-CAA-CBA
28	L5	203	PUB	C2A-C3A-CAA-CBA
28	N5	203	PUB	C2A-C3A-CAA-CBA
28	P5	202	PUB	C2A-C3A-CAA-CBA
28	R5	203	PUB	C2A-C3A-CAA-CBA
28	T5	202	PUB	C2A-C3A-CAA-CBA
28	V5	203	PUB	C2A-C3A-CAA-CBA
28	Y5	1005	PUB	C2A-C3A-CAA-CBA
28	Y5	1006	PUB	C2A-C3A-CAA-CBA
28	Z5	305	PUB	C2A-C3A-CAA-CBA
28	Z5	306	PUB	C2A-C3A-CAA-CBA
28	n5	203	PUB	C2A-C3A-CAA-CBA
28	p5	202	PUB	C2A-C3A-CAA-CBA
28	r5	203	PUB	C2A-C3A-CAA-CBA
28	t5	203	PUB	C2A-C3A-CAA-CBA
28	v5	203	PUB	C2A-C3A-CAA-CBA
28	x5	202	PUB	C2A-C3A-CAA-CBA
28	z5	203	PUB	C2A-C3A-CAA-CBA
28	f8	203	PUB	C2A-C3A-CAA-CBA
28	g8	202	PUB	C2A-C3A-CAA-CBA
28	h8	203	PUB	C2A-C3A-CAA-CBA
28	B6	203	PUB	C2A-C3A-CAA-CBA
28	D6	202	PUB	C2A-C3A-CAA-CBA
28	F6	203	PUB	C2A-C3A-CAA-CBA
28	H6	203	PUB	C2A-C3A-CAA-CBA
28	J6	203	PUB	C2A-C3A-CAA-CBA
28	L6	202	PUB	C2A-C3A-CAA-CBA
28	N6	203	PUB	C2A-C3A-CAA-CBA
28	P6	203	PUB	C2A-C3A-CAA-CBA
28	R6	203	PUB	C2A-C3A-CAA-CBA
28	T6	203	PUB	C2A-C3A-CAA-CBA
28	V6	203	PUB	C2A-C3A-CAA-CBA
28	X6	203	PUB	C2A-C3A-CAA-CBA
28	Z6	203	PUB	C2A-C3A-CAA-CBA
28	a6	203	PUB	C2A-C3A-CAA-CBA
28	b6	203	PUB	C2A-C3A-CAA-CBA
28	c6	1004	PUB	C2A-C3A-CAA-CBA
28	d6	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	e6	203	PUB	C2A-C3A-CAA-CBA
28	l6	203	PUB	C2A-C3A-CAA-CBA
28	n6	203	PUB	C2A-C3A-CAA-CBA
28	p6	203	PUB	C2A-C3A-CAA-CBA
28	r6	203	PUB	C2A-C3A-CAA-CBA
28	t6	203	PUB	C2A-C3A-CAA-CBA
28	u6	203	PUB	C2A-C3A-CAA-CBA
28	v6	203	PUB	C2A-C3A-CAA-CBA
28	x6	203	PUB	C2A-C3A-CAA-CBA
28	y6	204	PUB	C2A-C3A-CAA-CBA
28	z6	203	PUB	C2A-C3A-CAA-CBA
28	n8	202	PUB	C2A-C3A-CAA-CBA
28	o8	203	PUB	C2A-C3A-CAA-CBA
28	p8	203	PUB	C2A-C3A-CAA-CBA
28	B7	202	PUB	C2A-C3A-CAA-CBA
28	D7	203	PUB	C2A-C3A-CAA-CBA
28	F7	202	PUB	C2A-C3A-CAA-CBA
28	H7	203	PUB	C2A-C3A-CAA-CBA
28	J7	202	PUB	C2A-C3A-CAA-CBA
28	L7	202	PUB	C2A-C3A-CAA-CBA
28	N7	203	PUB	C2A-C3A-CAA-CBA
28	P7	203	PUB	C2A-C3A-CAA-CBA
28	R7	203	PUB	C2A-C3A-CAA-CBA
28	T7	203	PUB	C2A-C3A-CAA-CBA
28	V7	203	PUB	C2A-C3A-CAA-CBA
28	X7	203	PUB	C2A-C3A-CAA-CBA
28	Z7	203	PUB	C2A-C3A-CAA-CBA
28	a7	203	PUB	C2A-C3A-CAA-CBA
28	b7	202	PUB	C2A-C3A-CAA-CBA
28	c7	203	PUB	C2A-C3A-CAA-CBA
28	d7	203	PUB	C2A-C3A-CAA-CBA
28	e7	203	PUB	C2A-C3A-CAA-CBA
28	l7	203	PUB	C2A-C3A-CAA-CBA
28	n7	203	PUB	C2A-C3A-CAA-CBA
28	p7	202	PUB	C2A-C3A-CAA-CBA
28	r7	203	PUB	C2A-C3A-CAA-CBA
28	s7	203	PUB	C2A-C3A-CAA-CBA
28	t7	203	PUB	C2A-C3A-CAA-CBA
28	v7	203	PUB	C2A-C3A-CAA-CBA
28	x7	203	PUB	C2A-C3A-CAA-CBA
28	y7	203	PUB	C2A-C3A-CAA-CBA
28	z7	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	b8	1005	PUB	C2A-C3A-CAA-CBA
28	b8	1006	PUB	C2A-C3A-CAA-CBA
28	c8	304	PUB	C2A-C3A-CAA-CBA
28	c8	305	PUB	C2A-C3A-CAA-CBA
28	d8	304	PUB	C2A-C3A-CAA-CBA
28	e8	304	PUB	C2A-C3A-CAA-CBA
28	e8	305	PUB	C2A-C3A-CAA-CBA
28	b9	406	PUB	C2A-C3A-CAA-CBA
28	b9	407	PUB	C2A-C3A-CAA-CBA
28	c9	304	PUB	C2A-C3A-CAA-CBA
28	c9	305	PUB	C2A-C3A-CAA-CBA
28	d9	305	PUB	C2A-C3A-CAA-CBA
28	e9	305	PUB	C2A-C3A-CAA-CBA
28	e9	306	PUB	C2A-C3A-CAA-CBA
28	w8	203	PUB	C2A-C3A-CAA-CBA
28	y8	203	PUB	C2A-C3A-CAA-CBA
28	A8	203	PUB	C2A-C3A-CAA-CBA
28	C8	203	PUB	C2A-C3A-CAA-CBA
28	E8	203	PUB	C2A-C3A-CAA-CBA
28	G8	203	PUB	C2A-C3A-CAA-CBA
28	I8	203	PUB	C2A-C3A-CAA-CBA
28	K8	203	PUB	C2A-C3A-CAA-CBA
28	M8	203	PUB	C2A-C3A-CAA-CBA
28	O8	203	PUB	C2A-C3A-CAA-CBA
28	Q8	203	PUB	C2A-C3A-CAA-CBA
28	T8	304	PUB	C2A-C3A-CAA-CBA
28	T8	305	PUB	C2A-C3A-CAA-CBA
28	U8	1005	PUB	C2A-C3A-CAA-CBA
28	U8	1006	PUB	C2A-C3A-CAA-CBA
28	n9	202	PUB	C2A-C3A-CAA-CBA
28	p9	203	PUB	C2A-C3A-CAA-CBA
28	r9	203	PUB	C2A-C3A-CAA-CBA
28	t9	203	PUB	C2A-C3A-CAA-CBA
28	v9	203	PUB	C2A-C3A-CAA-CBA
28	x9	203	PUB	C2A-C3A-CAA-CBA
28	z9	203	PUB	C2A-C3A-CAA-CBA
28	B9	203	PUB	C2A-C3A-CAA-CBA
28	D9	203	PUB	C2A-C3A-CAA-CBA
28	F9	203	PUB	C2A-C3A-CAA-CBA
28	H9	203	PUB	C2A-C3A-CAA-CBA
28	J9	203	PUB	C2A-C3A-CAA-CBA
28	L9	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	N9	203	PUB	C2A-C3A-CAA-CBA
28	P9	203	PUB	C2A-C3A-CAA-CBA
28	R9	203	PUB	C2A-C3A-CAA-CBA
28	T9	203	PUB	C2A-C3A-CAA-CBA
28	V9	203	PUB	C2A-C3A-CAA-CBA
28	Y9	304	PUB	C2A-C3A-CAA-CBA
28	Y9	305	PUB	C2A-C3A-CAA-CBA
28	Z9	1005	PUB	C2A-C3A-CAA-CBA
28	Z9	1006	PUB	C2A-C3A-CAA-CBA
28	an	202	PUB	C2A-C3A-CAA-CBA
28	ap	203	PUB	C2A-C3A-CAA-CBA
28	ar	203	PUB	C2A-C3A-CAA-CBA
28	at	203	PUB	C2A-C3A-CAA-CBA
28	av	203	PUB	C2A-C3A-CAA-CBA
28	ax	202	PUB	C2A-C3A-CAA-CBA
28	az	203	PUB	C2A-C3A-CAA-CBA
28	aB	203	PUB	C2A-C3A-CAA-CBA
28	aD	203	PUB	C2A-C3A-CAA-CBA
28	aF	203	PUB	C2A-C3A-CAA-CBA
28	aH	203	PUB	C2A-C3A-CAA-CBA
28	aJ	203	PUB	C2A-C3A-CAA-CBA
28	aL	203	PUB	C2A-C3A-CAA-CBA
28	aN	203	PUB	C2A-C3A-CAA-CBA
28	aP	203	PUB	C2A-C3A-CAA-CBA
28	aR	203	PUB	C2A-C3A-CAA-CBA
28	aT	203	PUB	C2A-C3A-CAA-CBA
28	aV	203	PUB	C2A-C3A-CAA-CBA
28	aY	404	PUB	C2A-C3A-CAA-CBA
28	aY	405	PUB	C2A-C3A-CAA-CBA
28	aZ	304	PUB	C2A-C3A-CAA-CBA
28	aZ	305	PUB	C2A-C3A-CAA-CBA
28	bn	202	PUB	C2A-C3A-CAA-CBA
28	bo	202	PUB	C2A-C3A-CAA-CBA
28	bp	202	PUB	C2A-C3A-CAA-CBA
28	bq	203	PUB	C2A-C3A-CAA-CBA
28	br	203	PUB	C2A-C3A-CAA-CBA
28	bs	1004	PUB	C2A-C3A-CAA-CBA
28	bz	203	PUB	C2A-C3A-CAA-CBA
28	bB	203	PUB	C2A-C3A-CAA-CBA
28	bD	203	PUB	C2A-C3A-CAA-CBA
28	bF	203	PUB	C2A-C3A-CAA-CBA
28	bH	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	bJ	203	PUB	C2A-C3A-CAA-CBA
28	bL	203	PUB	C2A-C3A-CAA-CBA
28	bN	203	PUB	C2A-C3A-CAA-CBA
28	bP	203	PUB	C2A-C3A-CAA-CBA
28	bR	202	PUB	C2A-C3A-CAA-CBA
28	bT	202	PUB	C2A-C3A-CAA-CBA
28	bV	203	PUB	C2A-C3A-CAA-CBA
28	bY	1005	PUB	C2A-C3A-CAA-CBA
28	bY	1006	PUB	C2A-C3A-CAA-CBA
28	bZ	305	PUB	C2A-C3A-CAA-CBA
28	bZ	306	PUB	C2A-C3A-CAA-CBA
28	cn	202	PUB	C2A-C3A-CAA-CBA
28	co	202	PUB	C2A-C3A-CAA-CBA
28	cp	203	PUB	C2A-C3A-CAA-CBA
28	cq	203	PUB	C2A-C3A-CAA-CBA
28	cr	203	PUB	C2A-C3A-CAA-CBA
28	cs	203	PUB	C2A-C3A-CAA-CBA
28	cz	203	PUB	C2A-C3A-CAA-CBA
28	cB	203	PUB	C2A-C3A-CAA-CBA
28	cE	203	PUB	C2A-C3A-CAA-CBA
28	cF	202	PUB	C2A-C3A-CAA-CBA
28	cH	202	PUB	C2A-C3A-CAA-CBA
28	cJ	203	PUB	C2A-C3A-CAA-CBA
28	cL	203	PUB	C2A-C3A-CAA-CBA
28	cM	203	PUB	C2A-C3A-CAA-CBA
28	cN	202	PUB	C2A-C3A-CAA-CBA
28	cO	203	PUB	C2A-C3A-CAA-CBA
28	cP	203	PUB	C2A-C3A-CAA-CBA
28	cQ	202	PUB	C2A-C3A-CAA-CBA
28	cR	203	PUB	C2A-C3A-CAA-CBA
28	cY	203	PUB	C2A-C3A-CAA-CBA
28	dd	203	PUB	C2A-C3A-CAA-CBA
28	df	203	PUB	C2A-C3A-CAA-CBA
28	dh	203	PUB	C2A-C3A-CAA-CBA
28	di	203	PUB	C2A-C3A-CAA-CBA
28	dj	203	PUB	C2A-C3A-CAA-CBA
28	dl	203	PUB	C2A-C3A-CAA-CBA
28	dn	203	PUB	C2A-C3A-CAA-CBA
28	dp	203	PUB	C2A-C3A-CAA-CBA
28	dr	203	PUB	C2A-C3A-CAA-CBA
28	dt	203	PUB	C2A-C3A-CAA-CBA
28	dv	202	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	dw	405	PUB	C2A-C3A-CAA-CBA
28	dw	406	PUB	C2A-C3A-CAA-CBA
28	dx	406	PUB	C2A-C3A-CAA-CBA
28	dx	407	PUB	C2A-C3A-CAA-CBA
28	dB	202	PUB	C2A-C3A-CAA-CBA
28	dD	203	PUB	C2A-C3A-CAA-CBA
28	dF	203	PUB	C2A-C3A-CAA-CBA
28	dH	203	PUB	C2A-C3A-CAA-CBA
28	dK	203	PUB	C2A-C3A-CAA-CBA
28	dL	203	PUB	C2A-C3A-CAA-CBA
28	dN	203	PUB	C2A-C3A-CAA-CBA
28	dP	203	PUB	C2A-C3A-CAA-CBA
28	dR	203	PUB	C2A-C3A-CAA-CBA
28	dT	203	PUB	C2A-C3A-CAA-CBA
28	dV	203	PUB	C2A-C3A-CAA-CBA
28	dX	203	PUB	C2A-C3A-CAA-CBA
28	dY	203	PUB	C2A-C3A-CAA-CBA
28	eb	202	PUB	C2A-C3A-CAA-CBA
28	ec	203	PUB	C2A-C3A-CAA-CBA
28	ee	203	PUB	C2A-C3A-CAA-CBA
28	eg	203	PUB	C2A-C3A-CAA-CBA
28	ei	203	PUB	C2A-C3A-CAA-CBA
28	el	203	PUB	C2A-C3A-CAA-CBA
28	en	203	PUB	C2A-C3A-CAA-CBA
28	ep	203	PUB	C2A-C3A-CAA-CBA
28	er	203	PUB	C2A-C3A-CAA-CBA
28	et	203	PUB	C2A-C3A-CAA-CBA
28	ev	203	PUB	C2A-C3A-CAA-CBA
28	ey	1005	PUB	C2A-C3A-CAA-CBA
28	ey	1006	PUB	C2A-C3A-CAA-CBA
28	ez	1005	PUB	C2A-C3A-CAA-CBA
28	ez	1006	PUB	C2A-C3A-CAA-CBA
28	eB	204	PUB	C2A-C3A-CAA-CBA
28	eD	203	PUB	C2A-C3A-CAA-CBA
28	eF	203	PUB	C2A-C3A-CAA-CBA
28	eH	203	PUB	C2A-C3A-CAA-CBA
28	eJ	203	PUB	C2A-C3A-CAA-CBA
28	eL	203	PUB	C2A-C3A-CAA-CBA
28	eN	203	PUB	C2A-C3A-CAA-CBA
28	eP	204	PUB	C2A-C3A-CAA-CBA
28	eR	203	PUB	C2A-C3A-CAA-CBA
28	eT	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	eV	203	PUB	C2A-C3A-CAA-CBA
28	eX	202	PUB	C2A-C3A-CAA-CBA
28	eY	404	PUB	C2A-C3A-CAA-CBA
28	eY	405	PUB	C2A-C3A-CAA-CBA
28	eZ	403	PUB	C2A-C3A-CAA-CBA
28	eZ	404	PUB	C2A-C3A-CAA-CBA
28	lb	203	PUB	C2A-C3A-CAA-CBA
28	ld	203	PUB	C2A-C3A-CAA-CBA
28	lf	203	PUB	C2A-C3A-CAA-CBA
28	lh	203	PUB	C2A-C3A-CAA-CBA
28	lj	202	PUB	C2A-C3A-CAA-CBA
28	ll	203	PUB	C2A-C3A-CAA-CBA
28	ln	203	PUB	C2A-C3A-CAA-CBA
28	lp	203	PUB	C2A-C3A-CAA-CBA
28	lr	203	PUB	C2A-C3A-CAA-CBA
28	lt	203	PUB	C2A-C3A-CAA-CBA
28	lv	202	PUB	C2A-C3A-CAA-CBA
28	lx	201	PUB	C2A-C3A-CAA-CBA
28	ly	405	PUB	C2A-C3A-CAA-CBA
28	ly	406	PUB	C2A-C3A-CAA-CBA
28	lz	404	PUB	C2A-C3A-CAA-CBA
28	lz	405	PUB	C2A-C3A-CAA-CBA
28	fa	202	PUB	C2A-C3A-CAA-CBA
28	fc	203	PUB	C2A-C3A-CAA-CBA
28	ff	203	PUB	C2A-C3A-CAA-CBA
28	fi	203	PUB	C2A-C3A-CAA-CBA
28	fj	203	PUB	C2A-C3A-CAA-CBA
28	fm	203	PUB	C2A-C3A-CAA-CBA
28	fo	203	PUB	C2A-C3A-CAA-CBA
28	fq	203	PUB	C2A-C3A-CAA-CBA
28	fs	203	PUB	C2A-C3A-CAA-CBA
28	fu	202	PUB	C2A-C3A-CAA-CBA
28	fw	203	PUB	C2A-C3A-CAA-CBA
28	fy	202	PUB	C2A-C3A-CAA-CBA
28	ga	203	PUB	C2A-C3A-CAA-CBA
28	gd	202	PUB	C2A-C3A-CAA-CBA
28	ge	203	PUB	C2A-C3A-CAA-CBA
28	gg	203	PUB	C2A-C3A-CAA-CBA
28	gi	203	PUB	C2A-C3A-CAA-CBA
28	gk	203	PUB	C2A-C3A-CAA-CBA
28	gn	203	PUB	C2A-C3A-CAA-CBA
28	gp	203	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	gr	202	PUB	C2A-C3A-CAA-CBA
28	gt	203	PUB	C2A-C3A-CAA-CBA
28	gv	203	PUB	C2A-C3A-CAA-CBA
28	gx	203	PUB	C2A-C3A-CAA-CBA
28	gy	305	PUB	C2A-C3A-CAA-CBA
28	gy	306	PUB	C2A-C3A-CAA-CBA
28	gz	305	PUB	C2A-C3A-CAA-CBA
28	gz	306	PUB	C2A-C3A-CAA-CBA
28	hB	203	PUB	C2A-C3A-CAA-CBA
28	hD	203	PUB	C2A-C3A-CAA-CBA
28	hG	202	PUB	C2A-C3A-CAA-CBA
28	hH	203	PUB	C2A-C3A-CAA-CBA
28	hJ	203	PUB	C2A-C3A-CAA-CBA
28	hL	203	PUB	C2A-C3A-CAA-CBA
28	hN	203	PUB	C2A-C3A-CAA-CBA
28	hP	203	PUB	C2A-C3A-CAA-CBA
28	hR	203	PUB	C2A-C3A-CAA-CBA
28	hT	203	PUB	C2A-C3A-CAA-CBA
28	hV	203	PUB	C2A-C3A-CAA-CBA
28	hX	203	PUB	C2A-C3A-CAA-CBA
28	hY	405	PUB	C2A-C3A-CAA-CBA
28	hY	406	PUB	C2A-C3A-CAA-CBA
28	hZ	404	PUB	C2A-C3A-CAA-CBA
28	hZ	405	PUB	C2A-C3A-CAA-CBA
28	iC	1003	PUB	C2A-C3A-CAA-CBA
28	iD	1003	PUB	C2A-C3A-CAA-CBA
28	iE	1003	PUB	C2A-C3A-CAA-CBA
28	iF	1003	PUB	C2A-C3A-CAA-CBA
28	iG	1002	PUB	C2A-C3A-CAA-CBA
28	iH	1002	PUB	C2A-C3A-CAA-CBA
28	jI	1003	PUB	C2A-C3A-CAA-CBA
28	jJ	1003	PUB	C2A-C3A-CAA-CBA
28	jK	1003	PUB	C2A-C3A-CAA-CBA
28	jL	1003	PUB	C2A-C3A-CAA-CBA
28	jM	1003	PUB	C2A-C3A-CAA-CBA
28	jN	1003	PUB	C2A-C3A-CAA-CBA
28	jO	1003	PUB	C2A-C3A-CAA-CBA
28	jP	1003	PUB	C2A-C3A-CAA-CBA
28	kQ	1003	PUB	C2A-C3A-CAA-CBA
28	kR	1003	PUB	C2A-C3A-CAA-CBA
28	kS	1003	PUB	C2A-C3A-CAA-CBA
28	kT	1003	PUB	C2A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	kU	1003	PUB	C2A-C3A-CAA-CBA
28	kV	1003	PUB	C2A-C3A-CAA-CBA
28	kW	1003	PUB	C2A-C3A-CAA-CBA
28	kX	1003	PUB	C2A-C3A-CAA-CBA
29	C2	303	PVN	C2-C3-C31-C32
29	c3	303	PVN	C2-C3-C31-C32
27	G1	1001	CYC	C1A-C2A-CAA-CBA
27	I1	201	CYC	C1A-C2A-CAA-CBA
27	K1	201	CYC	C1A-C2A-CAA-CBA
27	L1	201	CYC	C1A-C2A-CAA-CBA
27	N1	201	CYC	C1A-C2A-CAA-CBA
27	O1	201	CYC	C1A-C2A-CAA-CBA
27	P1	201	CYC	C1A-C2A-CAA-CBA
27	Q1	201	CYC	C1A-C2A-CAA-CBA
27	R1	1001	CYC	C1A-C2A-CAA-CBA
27	U1	201	CYC	C1A-C2A-CAA-CBA
27	V1	201	CYC	C1A-C2A-CAA-CBA
27	W1	201	CYC	C1A-C2A-CAA-CBA
27	X1	201	CYC	C1A-C2A-CAA-CBA
27	Z1	201	CYC	C1A-C2A-CAA-CBA
27	a1	201	CYC	C1A-C2A-CAA-CBA
27	b1	1001	CYC	C1A-C2A-CAA-CBA
27	d1	1001	CYC	C1A-C2A-CAA-CBA
27	e1	201	CYC	C1A-C2A-CAA-CBA
27	f1	201	CYC	C1A-C2A-CAA-CBA
27	g1	201	CYC	C1A-C2A-CAA-CBA
27	i1	1001	CYC	C1A-C2A-CAA-CBA
27	k1	201	CYC	C1A-C2A-CAA-CBA
27	m1	201	CYC	C1A-C2A-CAA-CBA
27	n1	201	CYC	C1A-C2A-CAA-CBA
27	o1	1001	CYC	C1A-C2A-CAA-CBA
27	q1	201	CYC	C1A-C2A-CAA-CBA
27	s1	201	CYC	C1A-C2A-CAA-CBA
27	u1	1001	CYC	C1A-C2A-CAA-CBA
27	w1	201	CYC	C1A-C2A-CAA-CBA
27	y1	201	CYC	C1A-C2A-CAA-CBA
27	d2	101	CYC	C1A-C2A-CAA-CBA
29	34	1004	PVN	C3-C4-C5-C6
29	Y5	1004	PVN	C3-C4-C5-C6
29	T8	303	PVN	C3-C4-C5-C6
29	Y9	303	PVN	C3-C4-C5-C6
29	aZ	303	PVN	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	bZ	304	PVN	C3-C4-C5-C6
29	dx	405	PVN	C3-C4-C5-C6
29	gy	304	PVN	C3-C4-C5-C6
29	hY	404	PVN	C3-C4-C5-C6
29	hZ	403	PVN	C3-C4-C5-C6
29	b8	1004	PVN	C9-C10-C11-C12
29	b9	405	PVN	C9-C10-C11-C12
29	gy	304	PVN	C9-C10-C11-C12
29	gz	304	PVN	C9-C10-C11-C12
28	J2	202	PUB	C4A-C3A-CAA-CBA
28	B5	203	PUB	C4A-C3A-CAA-CBA
28	T7	203	PUB	C4A-C3A-CAA-CBA
28	Z7	203	PUB	C4A-C3A-CAA-CBA
28	e7	203	PUB	C4A-C3A-CAA-CBA
28	y7	203	PUB	C4A-C3A-CAA-CBA
28	bD	203	PUB	C4A-C3A-CAA-CBA
28	bR	202	PUB	C4A-C3A-CAA-CBA
28	bT	202	PUB	C4A-C3A-CAA-CBA
28	cH	202	PUB	C4A-C3A-CAA-CBA
28	dp	203	PUB	C4A-C3A-CAA-CBA
28	dT	203	PUB	C4A-C3A-CAA-CBA
28	ei	203	PUB	C4A-C3A-CAA-CBA
28	ev	203	PUB	C4A-C3A-CAA-CBA
28	eR	203	PUB	C4A-C3A-CAA-CBA
28	hB	203	PUB	C4A-C3A-CAA-CBA
28	B7	202	PUB	C4A-C3A-CAA-CBA
28	az	203	PUB	C4A-C3A-CAA-CBA
28	bJ	203	PUB	C4A-C3A-CAA-CBA
28	cY	203	PUB	C4A-C3A-CAA-CBA
28	dx	406	PUB	C4A-C3A-CAA-CBA
28	dH	203	PUB	C4A-C3A-CAA-CBA
28	ec	203	PUB	C4A-C3A-CAA-CBA
28	eJ	203	PUB	C4A-C3A-CAA-CBA
28	fi	203	PUB	C4A-C3A-CAA-CBA
28	f2	203	PUB	C4A-C3A-CAA-CBA
28	h2	203	PUB	C4A-C3A-CAA-CBA
28	j2	203	PUB	C4A-C3A-CAA-CBA
28	l2	203	PUB	C4A-C3A-CAA-CBA
28	n2	203	PUB	C4A-C3A-CAA-CBA
28	p2	203	PUB	C4A-C3A-CAA-CBA
28	r2	203	PUB	C4A-C3A-CAA-CBA
28	t2	203	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	v2	203	PUB	C4A-C3A-CAA-CBA
28	x2	202	PUB	C4A-C3A-CAA-CBA
28	z2	203	PUB	C4A-C3A-CAA-CBA
28	A2	1005	PUB	C4A-C3A-CAA-CBA
28	A2	1006	PUB	C4A-C3A-CAA-CBA
28	C2	304	PUB	C4A-C3A-CAA-CBA
28	C2	305	PUB	C4A-C3A-CAA-CBA
28	D2	304	PUB	C4A-C3A-CAA-CBA
28	D2	305	PUB	C4A-C3A-CAA-CBA
28	F2	203	PUB	C4A-C3A-CAA-CBA
28	H2	202	PUB	C4A-C3A-CAA-CBA
28	L2	203	PUB	C4A-C3A-CAA-CBA
28	N2	203	PUB	C4A-C3A-CAA-CBA
28	P2	203	PUB	C4A-C3A-CAA-CBA
28	R2	203	PUB	C4A-C3A-CAA-CBA
28	T2	203	PUB	C4A-C3A-CAA-CBA
28	V2	203	PUB	C4A-C3A-CAA-CBA
28	X2	203	PUB	C4A-C3A-CAA-CBA
28	Z2	203	PUB	C4A-C3A-CAA-CBA
28	B3	203	PUB	C4A-C3A-CAA-CBA
28	D3	203	PUB	C4A-C3A-CAA-CBA
28	F3	203	PUB	C4A-C3A-CAA-CBA
28	H3	203	PUB	C4A-C3A-CAA-CBA
28	J3	203	PUB	C4A-C3A-CAA-CBA
28	L3	203	PUB	C4A-C3A-CAA-CBA
28	N3	203	PUB	C4A-C3A-CAA-CBA
28	P3	203	PUB	C4A-C3A-CAA-CBA
28	R3	203	PUB	C4A-C3A-CAA-CBA
28	T3	203	PUB	C4A-C3A-CAA-CBA
28	V3	203	PUB	C4A-C3A-CAA-CBA
28	X3	202	PUB	C4A-C3A-CAA-CBA
28	Z3	203	PUB	C4A-C3A-CAA-CBA
28	a3	1005	PUB	C4A-C3A-CAA-CBA
28	a3	1006	PUB	C4A-C3A-CAA-CBA
28	c3	304	PUB	C4A-C3A-CAA-CBA
28	c3	305	PUB	C4A-C3A-CAA-CBA
28	d3	303	PUB	C4A-C3A-CAA-CBA
28	d3	304	PUB	C4A-C3A-CAA-CBA
28	f3	203	PUB	C4A-C3A-CAA-CBA
28	h3	202	PUB	C4A-C3A-CAA-CBA
28	j3	202	PUB	C4A-C3A-CAA-CBA
28	l3	202	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	n3	203	PUB	C4A-C3A-CAA-CBA
28	p3	203	PUB	C4A-C3A-CAA-CBA
28	r3	203	PUB	C4A-C3A-CAA-CBA
28	t3	203	PUB	C4A-C3A-CAA-CBA
28	v3	203	PUB	C4A-C3A-CAA-CBA
28	x3	203	PUB	C4A-C3A-CAA-CBA
28	z3	203	PUB	C4A-C3A-CAA-CBA
28	B4	203	PUB	C4A-C3A-CAA-CBA
28	D4	203	PUB	C4A-C3A-CAA-CBA
28	F4	203	PUB	C4A-C3A-CAA-CBA
28	H4	203	PUB	C4A-C3A-CAA-CBA
28	J4	203	PUB	C4A-C3A-CAA-CBA
28	L4	203	PUB	C4A-C3A-CAA-CBA
28	N4	203	PUB	C4A-C3A-CAA-CBA
28	P4	203	PUB	C4A-C3A-CAA-CBA
28	R4	203	PUB	C4A-C3A-CAA-CBA
28	T4	202	PUB	C4A-C3A-CAA-CBA
28	V4	203	PUB	C4A-C3A-CAA-CBA
28	X4	203	PUB	C4A-C3A-CAA-CBA
28	Z4	203	PUB	C4A-C3A-CAA-CBA
28	34	1005	PUB	C4A-C3A-CAA-CBA
28	34	1006	PUB	C4A-C3A-CAA-CBA
28	44	304	PUB	C4A-C3A-CAA-CBA
28	44	305	PUB	C4A-C3A-CAA-CBA
28	n4	203	PUB	C4A-C3A-CAA-CBA
28	p4	203	PUB	C4A-C3A-CAA-CBA
28	r4	202	PUB	C4A-C3A-CAA-CBA
28	t4	203	PUB	C4A-C3A-CAA-CBA
28	v4	203	PUB	C4A-C3A-CAA-CBA
28	x4	202	PUB	C4A-C3A-CAA-CBA
28	z4	203	PUB	C4A-C3A-CAA-CBA
28	D5	203	PUB	C4A-C3A-CAA-CBA
28	F5	203	PUB	C4A-C3A-CAA-CBA
28	H5	202	PUB	C4A-C3A-CAA-CBA
28	J5	203	PUB	C4A-C3A-CAA-CBA
28	L5	203	PUB	C4A-C3A-CAA-CBA
28	N5	203	PUB	C4A-C3A-CAA-CBA
28	P5	202	PUB	C4A-C3A-CAA-CBA
28	R5	203	PUB	C4A-C3A-CAA-CBA
28	T5	202	PUB	C4A-C3A-CAA-CBA
28	V5	203	PUB	C4A-C3A-CAA-CBA
28	Y5	1005	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	Y5	1006	PUB	C4A-C3A-CAA-CBA
28	Z5	305	PUB	C4A-C3A-CAA-CBA
28	Z5	306	PUB	C4A-C3A-CAA-CBA
28	n5	203	PUB	C4A-C3A-CAA-CBA
28	p5	202	PUB	C4A-C3A-CAA-CBA
28	r5	203	PUB	C4A-C3A-CAA-CBA
28	t5	203	PUB	C4A-C3A-CAA-CBA
28	v5	203	PUB	C4A-C3A-CAA-CBA
28	x5	202	PUB	C4A-C3A-CAA-CBA
28	z5	203	PUB	C4A-C3A-CAA-CBA
28	f8	203	PUB	C4A-C3A-CAA-CBA
28	g8	202	PUB	C4A-C3A-CAA-CBA
28	h8	203	PUB	C4A-C3A-CAA-CBA
28	B6	203	PUB	C4A-C3A-CAA-CBA
28	D6	202	PUB	C4A-C3A-CAA-CBA
28	F6	203	PUB	C4A-C3A-CAA-CBA
28	H6	203	PUB	C4A-C3A-CAA-CBA
28	J6	203	PUB	C4A-C3A-CAA-CBA
28	L6	202	PUB	C4A-C3A-CAA-CBA
28	N6	203	PUB	C4A-C3A-CAA-CBA
28	P6	203	PUB	C4A-C3A-CAA-CBA
28	R6	203	PUB	C4A-C3A-CAA-CBA
28	T6	203	PUB	C4A-C3A-CAA-CBA
28	V6	203	PUB	C4A-C3A-CAA-CBA
28	X6	203	PUB	C4A-C3A-CAA-CBA
28	Z6	203	PUB	C4A-C3A-CAA-CBA
28	a6	203	PUB	C4A-C3A-CAA-CBA
28	b6	203	PUB	C4A-C3A-CAA-CBA
28	c6	1004	PUB	C4A-C3A-CAA-CBA
28	d6	203	PUB	C4A-C3A-CAA-CBA
28	e6	203	PUB	C4A-C3A-CAA-CBA
28	l6	203	PUB	C4A-C3A-CAA-CBA
28	n6	203	PUB	C4A-C3A-CAA-CBA
28	p6	203	PUB	C4A-C3A-CAA-CBA
28	r6	203	PUB	C4A-C3A-CAA-CBA
28	t6	203	PUB	C4A-C3A-CAA-CBA
28	u6	203	PUB	C4A-C3A-CAA-CBA
28	v6	203	PUB	C4A-C3A-CAA-CBA
28	x6	203	PUB	C4A-C3A-CAA-CBA
28	y6	204	PUB	C4A-C3A-CAA-CBA
28	z6	203	PUB	C4A-C3A-CAA-CBA
28	n8	202	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	o8	203	PUB	C4A-C3A-CAA-CBA
28	p8	203	PUB	C4A-C3A-CAA-CBA
28	D7	203	PUB	C4A-C3A-CAA-CBA
28	F7	202	PUB	C4A-C3A-CAA-CBA
28	H7	203	PUB	C4A-C3A-CAA-CBA
28	J7	202	PUB	C4A-C3A-CAA-CBA
28	L7	202	PUB	C4A-C3A-CAA-CBA
28	N7	203	PUB	C4A-C3A-CAA-CBA
28	P7	203	PUB	C4A-C3A-CAA-CBA
28	R7	203	PUB	C4A-C3A-CAA-CBA
28	V7	203	PUB	C4A-C3A-CAA-CBA
28	X7	203	PUB	C4A-C3A-CAA-CBA
28	a7	203	PUB	C4A-C3A-CAA-CBA
28	b7	202	PUB	C4A-C3A-CAA-CBA
28	c7	203	PUB	C4A-C3A-CAA-CBA
28	d7	203	PUB	C4A-C3A-CAA-CBA
28	l7	203	PUB	C4A-C3A-CAA-CBA
28	n7	203	PUB	C4A-C3A-CAA-CBA
28	p7	202	PUB	C4A-C3A-CAA-CBA
28	r7	203	PUB	C4A-C3A-CAA-CBA
28	s7	203	PUB	C4A-C3A-CAA-CBA
28	t7	203	PUB	C4A-C3A-CAA-CBA
28	v7	203	PUB	C4A-C3A-CAA-CBA
28	x7	203	PUB	C4A-C3A-CAA-CBA
28	z7	203	PUB	C4A-C3A-CAA-CBA
28	b8	1005	PUB	C4A-C3A-CAA-CBA
28	b8	1006	PUB	C4A-C3A-CAA-CBA
28	c8	304	PUB	C4A-C3A-CAA-CBA
28	c8	305	PUB	C4A-C3A-CAA-CBA
28	d8	304	PUB	C4A-C3A-CAA-CBA
28	e8	304	PUB	C4A-C3A-CAA-CBA
28	e8	305	PUB	C4A-C3A-CAA-CBA
28	b9	406	PUB	C4A-C3A-CAA-CBA
28	b9	407	PUB	C4A-C3A-CAA-CBA
28	c9	304	PUB	C4A-C3A-CAA-CBA
28	c9	305	PUB	C4A-C3A-CAA-CBA
28	d9	305	PUB	C4A-C3A-CAA-CBA
28	e9	305	PUB	C4A-C3A-CAA-CBA
28	e9	306	PUB	C4A-C3A-CAA-CBA
28	w8	203	PUB	C4A-C3A-CAA-CBA
28	y8	203	PUB	C4A-C3A-CAA-CBA
28	A8	203	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	C8	203	PUB	C4A-C3A-CAA-CBA
28	E8	203	PUB	C4A-C3A-CAA-CBA
28	G8	203	PUB	C4A-C3A-CAA-CBA
28	I8	203	PUB	C4A-C3A-CAA-CBA
28	K8	203	PUB	C4A-C3A-CAA-CBA
28	M8	203	PUB	C4A-C3A-CAA-CBA
28	O8	203	PUB	C4A-C3A-CAA-CBA
28	Q8	203	PUB	C4A-C3A-CAA-CBA
28	T8	304	PUB	C4A-C3A-CAA-CBA
28	T8	305	PUB	C4A-C3A-CAA-CBA
28	U8	1005	PUB	C4A-C3A-CAA-CBA
28	U8	1006	PUB	C4A-C3A-CAA-CBA
28	n9	202	PUB	C4A-C3A-CAA-CBA
28	p9	203	PUB	C4A-C3A-CAA-CBA
28	r9	203	PUB	C4A-C3A-CAA-CBA
28	t9	203	PUB	C4A-C3A-CAA-CBA
28	v9	203	PUB	C4A-C3A-CAA-CBA
28	x9	203	PUB	C4A-C3A-CAA-CBA
28	z9	203	PUB	C4A-C3A-CAA-CBA
28	B9	203	PUB	C4A-C3A-CAA-CBA
28	D9	203	PUB	C4A-C3A-CAA-CBA
28	F9	203	PUB	C4A-C3A-CAA-CBA
28	H9	203	PUB	C4A-C3A-CAA-CBA
28	J9	203	PUB	C4A-C3A-CAA-CBA
28	L9	203	PUB	C4A-C3A-CAA-CBA
28	N9	203	PUB	C4A-C3A-CAA-CBA
28	P9	203	PUB	C4A-C3A-CAA-CBA
28	R9	203	PUB	C4A-C3A-CAA-CBA
28	T9	203	PUB	C4A-C3A-CAA-CBA
28	V9	203	PUB	C4A-C3A-CAA-CBA
28	Y9	304	PUB	C4A-C3A-CAA-CBA
28	Y9	305	PUB	C4A-C3A-CAA-CBA
28	Z9	1005	PUB	C4A-C3A-CAA-CBA
28	Z9	1006	PUB	C4A-C3A-CAA-CBA
28	an	202	PUB	C4A-C3A-CAA-CBA
28	ap	203	PUB	C4A-C3A-CAA-CBA
28	ar	203	PUB	C4A-C3A-CAA-CBA
28	at	203	PUB	C4A-C3A-CAA-CBA
28	av	203	PUB	C4A-C3A-CAA-CBA
28	ax	202	PUB	C4A-C3A-CAA-CBA
28	aB	203	PUB	C4A-C3A-CAA-CBA
28	aD	203	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	aF	203	PUB	C4A-C3A-CAA-CBA
28	aH	203	PUB	C4A-C3A-CAA-CBA
28	aJ	203	PUB	C4A-C3A-CAA-CBA
28	aL	203	PUB	C4A-C3A-CAA-CBA
28	aN	203	PUB	C4A-C3A-CAA-CBA
28	aP	203	PUB	C4A-C3A-CAA-CBA
28	aR	203	PUB	C4A-C3A-CAA-CBA
28	aT	203	PUB	C4A-C3A-CAA-CBA
28	aV	203	PUB	C4A-C3A-CAA-CBA
28	aY	404	PUB	C4A-C3A-CAA-CBA
28	aY	405	PUB	C4A-C3A-CAA-CBA
28	aZ	304	PUB	C4A-C3A-CAA-CBA
28	aZ	305	PUB	C4A-C3A-CAA-CBA
28	bn	202	PUB	C4A-C3A-CAA-CBA
28	bo	202	PUB	C4A-C3A-CAA-CBA
28	bp	202	PUB	C4A-C3A-CAA-CBA
28	bq	203	PUB	C4A-C3A-CAA-CBA
28	br	203	PUB	C4A-C3A-CAA-CBA
28	bs	1004	PUB	C4A-C3A-CAA-CBA
28	bz	203	PUB	C4A-C3A-CAA-CBA
28	bB	203	PUB	C4A-C3A-CAA-CBA
28	bF	203	PUB	C4A-C3A-CAA-CBA
28	bH	203	PUB	C4A-C3A-CAA-CBA
28	bL	203	PUB	C4A-C3A-CAA-CBA
28	bN	203	PUB	C4A-C3A-CAA-CBA
28	bP	203	PUB	C4A-C3A-CAA-CBA
28	bV	203	PUB	C4A-C3A-CAA-CBA
28	bY	1005	PUB	C4A-C3A-CAA-CBA
28	bY	1006	PUB	C4A-C3A-CAA-CBA
28	bZ	305	PUB	C4A-C3A-CAA-CBA
28	bZ	306	PUB	C4A-C3A-CAA-CBA
28	cn	202	PUB	C4A-C3A-CAA-CBA
28	co	202	PUB	C4A-C3A-CAA-CBA
28	cp	203	PUB	C4A-C3A-CAA-CBA
28	cq	203	PUB	C4A-C3A-CAA-CBA
28	cr	203	PUB	C4A-C3A-CAA-CBA
28	cs	203	PUB	C4A-C3A-CAA-CBA
28	cz	203	PUB	C4A-C3A-CAA-CBA
28	cB	203	PUB	C4A-C3A-CAA-CBA
28	cE	203	PUB	C4A-C3A-CAA-CBA
28	cF	202	PUB	C4A-C3A-CAA-CBA
28	cJ	203	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	cL	203	PUB	C4A-C3A-CAA-CBA
28	cM	203	PUB	C4A-C3A-CAA-CBA
28	cN	202	PUB	C4A-C3A-CAA-CBA
28	cO	203	PUB	C4A-C3A-CAA-CBA
28	cP	203	PUB	C4A-C3A-CAA-CBA
28	cQ	202	PUB	C4A-C3A-CAA-CBA
28	cR	203	PUB	C4A-C3A-CAA-CBA
28	dd	203	PUB	C4A-C3A-CAA-CBA
28	df	203	PUB	C4A-C3A-CAA-CBA
28	dh	203	PUB	C4A-C3A-CAA-CBA
28	di	203	PUB	C4A-C3A-CAA-CBA
28	dj	203	PUB	C4A-C3A-CAA-CBA
28	dl	203	PUB	C4A-C3A-CAA-CBA
28	dn	203	PUB	C4A-C3A-CAA-CBA
28	dr	203	PUB	C4A-C3A-CAA-CBA
28	dt	203	PUB	C4A-C3A-CAA-CBA
28	dv	202	PUB	C4A-C3A-CAA-CBA
28	dw	405	PUB	C4A-C3A-CAA-CBA
28	dw	406	PUB	C4A-C3A-CAA-CBA
28	dx	407	PUB	C4A-C3A-CAA-CBA
28	dB	202	PUB	C4A-C3A-CAA-CBA
28	dD	203	PUB	C4A-C3A-CAA-CBA
28	dF	203	PUB	C4A-C3A-CAA-CBA
28	dK	203	PUB	C4A-C3A-CAA-CBA
28	dL	203	PUB	C4A-C3A-CAA-CBA
28	dN	203	PUB	C4A-C3A-CAA-CBA
28	dP	203	PUB	C4A-C3A-CAA-CBA
28	dR	203	PUB	C4A-C3A-CAA-CBA
28	dV	203	PUB	C4A-C3A-CAA-CBA
28	dY	203	PUB	C4A-C3A-CAA-CBA
28	eb	202	PUB	C4A-C3A-CAA-CBA
28	ee	203	PUB	C4A-C3A-CAA-CBA
28	eg	203	PUB	C4A-C3A-CAA-CBA
28	el	203	PUB	C4A-C3A-CAA-CBA
28	en	203	PUB	C4A-C3A-CAA-CBA
28	ep	203	PUB	C4A-C3A-CAA-CBA
28	er	203	PUB	C4A-C3A-CAA-CBA
28	et	203	PUB	C4A-C3A-CAA-CBA
28	ey	1005	PUB	C4A-C3A-CAA-CBA
28	ey	1006	PUB	C4A-C3A-CAA-CBA
28	ez	1005	PUB	C4A-C3A-CAA-CBA
28	ez	1006	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	eB	204	PUB	C4A-C3A-CAA-CBA
28	eD	203	PUB	C4A-C3A-CAA-CBA
28	eF	203	PUB	C4A-C3A-CAA-CBA
28	eH	203	PUB	C4A-C3A-CAA-CBA
28	eL	203	PUB	C4A-C3A-CAA-CBA
28	eN	203	PUB	C4A-C3A-CAA-CBA
28	eP	204	PUB	C4A-C3A-CAA-CBA
28	eV	203	PUB	C4A-C3A-CAA-CBA
28	eX	202	PUB	C4A-C3A-CAA-CBA
28	eY	404	PUB	C4A-C3A-CAA-CBA
28	eY	405	PUB	C4A-C3A-CAA-CBA
28	eZ	403	PUB	C4A-C3A-CAA-CBA
28	eZ	404	PUB	C4A-C3A-CAA-CBA
28	lb	203	PUB	C4A-C3A-CAA-CBA
28	ld	203	PUB	C4A-C3A-CAA-CBA
28	lf	203	PUB	C4A-C3A-CAA-CBA
28	lh	203	PUB	C4A-C3A-CAA-CBA
28	lj	202	PUB	C4A-C3A-CAA-CBA
28	ll	203	PUB	C4A-C3A-CAA-CBA
28	ln	203	PUB	C4A-C3A-CAA-CBA
28	lp	203	PUB	C4A-C3A-CAA-CBA
28	lr	203	PUB	C4A-C3A-CAA-CBA
28	lt	203	PUB	C4A-C3A-CAA-CBA
28	lv	202	PUB	C4A-C3A-CAA-CBA
28	lx	201	PUB	C4A-C3A-CAA-CBA
28	ly	405	PUB	C4A-C3A-CAA-CBA
28	ly	406	PUB	C4A-C3A-CAA-CBA
28	lz	404	PUB	C4A-C3A-CAA-CBA
28	lz	405	PUB	C4A-C3A-CAA-CBA
28	fa	202	PUB	C4A-C3A-CAA-CBA
28	fc	203	PUB	C4A-C3A-CAA-CBA
28	ff	203	PUB	C4A-C3A-CAA-CBA
28	fj	203	PUB	C4A-C3A-CAA-CBA
28	fm	203	PUB	C4A-C3A-CAA-CBA
28	fo	203	PUB	C4A-C3A-CAA-CBA
28	fq	203	PUB	C4A-C3A-CAA-CBA
28	fs	203	PUB	C4A-C3A-CAA-CBA
28	fu	202	PUB	C4A-C3A-CAA-CBA
28	fw	203	PUB	C4A-C3A-CAA-CBA
28	fy	202	PUB	C4A-C3A-CAA-CBA
28	ga	203	PUB	C4A-C3A-CAA-CBA
28	gd	202	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	ge	203	PUB	C4A-C3A-CAA-CBA
28	gg	203	PUB	C4A-C3A-CAA-CBA
28	gi	203	PUB	C4A-C3A-CAA-CBA
28	gk	203	PUB	C4A-C3A-CAA-CBA
28	gn	203	PUB	C4A-C3A-CAA-CBA
28	gp	203	PUB	C4A-C3A-CAA-CBA
28	gr	202	PUB	C4A-C3A-CAA-CBA
28	gt	203	PUB	C4A-C3A-CAA-CBA
28	gv	203	PUB	C4A-C3A-CAA-CBA
28	gx	203	PUB	C4A-C3A-CAA-CBA
28	gy	305	PUB	C4A-C3A-CAA-CBA
28	gy	306	PUB	C4A-C3A-CAA-CBA
28	gz	305	PUB	C4A-C3A-CAA-CBA
28	gz	306	PUB	C4A-C3A-CAA-CBA
28	hD	203	PUB	C4A-C3A-CAA-CBA
28	hG	202	PUB	C4A-C3A-CAA-CBA
28	hH	203	PUB	C4A-C3A-CAA-CBA
28	hJ	203	PUB	C4A-C3A-CAA-CBA
28	hL	203	PUB	C4A-C3A-CAA-CBA
28	hN	203	PUB	C4A-C3A-CAA-CBA
28	hP	203	PUB	C4A-C3A-CAA-CBA
28	hR	203	PUB	C4A-C3A-CAA-CBA
28	hT	203	PUB	C4A-C3A-CAA-CBA
28	hV	203	PUB	C4A-C3A-CAA-CBA
28	hX	203	PUB	C4A-C3A-CAA-CBA
28	hY	405	PUB	C4A-C3A-CAA-CBA
28	hY	406	PUB	C4A-C3A-CAA-CBA
28	hZ	404	PUB	C4A-C3A-CAA-CBA
28	hZ	405	PUB	C4A-C3A-CAA-CBA
28	iC	1003	PUB	C4A-C3A-CAA-CBA
28	iD	1003	PUB	C4A-C3A-CAA-CBA
28	iE	1003	PUB	C4A-C3A-CAA-CBA
28	iF	1003	PUB	C4A-C3A-CAA-CBA
28	iG	1002	PUB	C4A-C3A-CAA-CBA
28	iH	1002	PUB	C4A-C3A-CAA-CBA
28	jI	1003	PUB	C4A-C3A-CAA-CBA
28	jJ	1003	PUB	C4A-C3A-CAA-CBA
28	jK	1003	PUB	C4A-C3A-CAA-CBA
28	jL	1003	PUB	C4A-C3A-CAA-CBA
28	jM	1003	PUB	C4A-C3A-CAA-CBA
28	jN	1003	PUB	C4A-C3A-CAA-CBA
28	jO	1003	PUB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
28	jP	1003	PUB	C4A-C3A-CAA-CBA
28	kQ	1003	PUB	C4A-C3A-CAA-CBA
28	kR	1003	PUB	C4A-C3A-CAA-CBA
28	kS	1003	PUB	C4A-C3A-CAA-CBA
28	kT	1003	PUB	C4A-C3A-CAA-CBA
28	kU	1003	PUB	C4A-C3A-CAA-CBA
28	kV	1003	PUB	C4A-C3A-CAA-CBA
28	kW	1003	PUB	C4A-C3A-CAA-CBA
28	kX	1003	PUB	C4A-C3A-CAA-CBA
29	c8	303	PVN	C4-C3-C31-C32
29	c9	303	PVN	C4-C3-C31-C32
29	b8	1004	PVN	C8-C51-C52-C53
29	b9	405	PVN	C8-C51-C52-C53
28	dX	203	PUB	C4A-C3A-CAA-CBA
28	eT	203	PUB	C4A-C3A-CAA-CBA
29	D2	303	PVN	C12-C61-C62-C63
29	d3	302	PVN	C12-C61-C62-C63
29	T8	303	PVN	C12-C61-C62-C63
29	Y9	303	PVN	C12-C61-C62-C63
29	dw	404	PVN	C19-C18-C91-C92
27	G1	1001	CYC	C3A-C2A-CAA-CBA
27	I1	201	CYC	C3A-C2A-CAA-CBA
27	K1	201	CYC	C3A-C2A-CAA-CBA
27	L1	201	CYC	C3A-C2A-CAA-CBA
27	N1	201	CYC	C3A-C2A-CAA-CBA
27	O1	201	CYC	C3A-C2A-CAA-CBA
27	P1	201	CYC	C3A-C2A-CAA-CBA
27	Q1	201	CYC	C3A-C2A-CAA-CBA
27	R1	1001	CYC	C3A-C2A-CAA-CBA
27	U1	201	CYC	C3A-C2A-CAA-CBA
27	V1	201	CYC	C3A-C2A-CAA-CBA
27	W1	201	CYC	C3A-C2A-CAA-CBA
27	X1	201	CYC	C3A-C2A-CAA-CBA
27	Z1	201	CYC	C3A-C2A-CAA-CBA
27	a1	201	CYC	C3A-C2A-CAA-CBA
27	b1	1001	CYC	C3A-C2A-CAA-CBA
27	d1	1001	CYC	C3A-C2A-CAA-CBA
27	e1	201	CYC	C3A-C2A-CAA-CBA
27	f1	201	CYC	C3A-C2A-CAA-CBA
27	g1	201	CYC	C3A-C2A-CAA-CBA
27	i1	1001	CYC	C3A-C2A-CAA-CBA
27	k1	201	CYC	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
27	m1	201	CYC	C3A-C2A-CAA-CBA
27	n1	201	CYC	C3A-C2A-CAA-CBA
27	o1	1001	CYC	C3A-C2A-CAA-CBA
27	q1	201	CYC	C3A-C2A-CAA-CBA
27	s1	201	CYC	C3A-C2A-CAA-CBA
27	u1	1001	CYC	C3A-C2A-CAA-CBA
27	w1	201	CYC	C3A-C2A-CAA-CBA
27	y1	201	CYC	C3A-C2A-CAA-CBA
27	d2	101	CYC	C3A-C2A-CAA-CBA
28	J2	202	PUB	C2D-C3D-CAD-CBD
28	J3	203	PUB	C2D-C3D-CAD-CBD
28	P3	203	PUB	C2D-C3D-CAD-CBD
28	34	1005	PUB	C2D-C3D-CAD-CBD
28	N6	203	PUB	C2D-C3D-CAD-CBD
28	c6	1004	PUB	C2D-C3D-CAD-CBD
28	T7	203	PUB	C2D-C3D-CAD-CBD
28	d7	203	PUB	C2D-C3D-CAD-CBD
28	r7	203	PUB	C2D-C3D-CAD-CBD
28	c8	305	PUB	C2D-C3D-CAD-CBD
28	c9	304	PUB	C2D-C3D-CAD-CBD
28	I8	203	PUB	C2D-C3D-CAD-CBD
28	L9	203	PUB	C2D-C3D-CAD-CBD
28	N9	203	PUB	C2D-C3D-CAD-CBD
28	ax	202	PUB	C2D-C3D-CAD-CBD
28	aP	203	PUB	C2D-C3D-CAD-CBD
28	bJ	203	PUB	C2D-C3D-CAD-CBD
28	bY	1005	PUB	C2D-C3D-CAD-CBD
28	cH	202	PUB	C2D-C3D-CAD-CBD
28	cL	203	PUB	C2D-C3D-CAD-CBD
28	dr	203	PUB	C2D-C3D-CAD-CBD
28	dw	405	PUB	C2D-C3D-CAD-CBD
28	dw	406	PUB	C2D-C3D-CAD-CBD
28	dT	203	PUB	C2D-C3D-CAD-CBD
28	el	203	PUB	C2D-C3D-CAD-CBD
28	ep	203	PUB	C2D-C3D-CAD-CBD
28	eV	203	PUB	C2D-C3D-CAD-CBD
28	lr	203	PUB	C2D-C3D-CAD-CBD
28	lt	203	PUB	C2D-C3D-CAD-CBD
28	lz	405	PUB	C2D-C3D-CAD-CBD
28	fm	203	PUB	C2D-C3D-CAD-CBD
28	fs	203	PUB	C2D-C3D-CAD-CBD
28	ga	203	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	gk	203	PUB	C2D-C3D-CAD-CBD
28	f2	203	PUB	C2D-C3D-CAD-CBD
28	h2	203	PUB	C2D-C3D-CAD-CBD
28	j2	203	PUB	C2D-C3D-CAD-CBD
28	l2	203	PUB	C2D-C3D-CAD-CBD
28	n2	203	PUB	C2D-C3D-CAD-CBD
28	p2	203	PUB	C2D-C3D-CAD-CBD
28	r2	203	PUB	C2D-C3D-CAD-CBD
28	t2	203	PUB	C2D-C3D-CAD-CBD
28	v2	203	PUB	C2D-C3D-CAD-CBD
28	x2	202	PUB	C2D-C3D-CAD-CBD
28	z2	203	PUB	C2D-C3D-CAD-CBD
28	A2	1005	PUB	C2D-C3D-CAD-CBD
28	A2	1006	PUB	C2D-C3D-CAD-CBD
28	C2	304	PUB	C2D-C3D-CAD-CBD
28	C2	305	PUB	C2D-C3D-CAD-CBD
28	D2	304	PUB	C2D-C3D-CAD-CBD
28	D2	305	PUB	C2D-C3D-CAD-CBD
28	F2	203	PUB	C2D-C3D-CAD-CBD
28	H2	202	PUB	C2D-C3D-CAD-CBD
28	L2	203	PUB	C2D-C3D-CAD-CBD
28	N2	203	PUB	C2D-C3D-CAD-CBD
28	P2	203	PUB	C2D-C3D-CAD-CBD
28	R2	203	PUB	C2D-C3D-CAD-CBD
28	T2	203	PUB	C2D-C3D-CAD-CBD
28	V2	203	PUB	C2D-C3D-CAD-CBD
28	X2	203	PUB	C2D-C3D-CAD-CBD
28	Z2	203	PUB	C2D-C3D-CAD-CBD
28	B3	203	PUB	C2D-C3D-CAD-CBD
28	D3	203	PUB	C2D-C3D-CAD-CBD
28	F3	203	PUB	C2D-C3D-CAD-CBD
28	H3	203	PUB	C2D-C3D-CAD-CBD
28	L3	203	PUB	C2D-C3D-CAD-CBD
28	N3	203	PUB	C2D-C3D-CAD-CBD
28	R3	203	PUB	C2D-C3D-CAD-CBD
28	T3	203	PUB	C2D-C3D-CAD-CBD
28	V3	203	PUB	C2D-C3D-CAD-CBD
28	X3	202	PUB	C2D-C3D-CAD-CBD
28	Z3	203	PUB	C2D-C3D-CAD-CBD
28	a3	1005	PUB	C2D-C3D-CAD-CBD
28	a3	1006	PUB	C2D-C3D-CAD-CBD
28	c3	304	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	c3	305	PUB	C2D-C3D-CAD-CBD
28	d3	303	PUB	C2D-C3D-CAD-CBD
28	d3	304	PUB	C2D-C3D-CAD-CBD
28	f3	203	PUB	C2D-C3D-CAD-CBD
28	h3	202	PUB	C2D-C3D-CAD-CBD
28	j3	202	PUB	C2D-C3D-CAD-CBD
28	l3	202	PUB	C2D-C3D-CAD-CBD
28	n3	203	PUB	C2D-C3D-CAD-CBD
28	p3	203	PUB	C2D-C3D-CAD-CBD
28	r3	203	PUB	C2D-C3D-CAD-CBD
28	t3	203	PUB	C2D-C3D-CAD-CBD
28	v3	203	PUB	C2D-C3D-CAD-CBD
28	x3	203	PUB	C2D-C3D-CAD-CBD
28	z3	203	PUB	C2D-C3D-CAD-CBD
28	B4	203	PUB	C2D-C3D-CAD-CBD
28	D4	203	PUB	C2D-C3D-CAD-CBD
28	F4	203	PUB	C2D-C3D-CAD-CBD
28	H4	203	PUB	C2D-C3D-CAD-CBD
28	J4	203	PUB	C2D-C3D-CAD-CBD
28	L4	203	PUB	C2D-C3D-CAD-CBD
28	N4	203	PUB	C2D-C3D-CAD-CBD
28	P4	203	PUB	C2D-C3D-CAD-CBD
28	R4	203	PUB	C2D-C3D-CAD-CBD
28	T4	202	PUB	C2D-C3D-CAD-CBD
28	V4	203	PUB	C2D-C3D-CAD-CBD
28	X4	203	PUB	C2D-C3D-CAD-CBD
28	Z4	203	PUB	C2D-C3D-CAD-CBD
28	34	1006	PUB	C2D-C3D-CAD-CBD
28	44	304	PUB	C2D-C3D-CAD-CBD
28	44	305	PUB	C2D-C3D-CAD-CBD
28	n4	203	PUB	C2D-C3D-CAD-CBD
28	p4	203	PUB	C2D-C3D-CAD-CBD
28	r4	202	PUB	C2D-C3D-CAD-CBD
28	t4	203	PUB	C2D-C3D-CAD-CBD
28	v4	203	PUB	C2D-C3D-CAD-CBD
28	x4	202	PUB	C2D-C3D-CAD-CBD
28	z4	203	PUB	C2D-C3D-CAD-CBD
28	B5	203	PUB	C2D-C3D-CAD-CBD
28	D5	203	PUB	C2D-C3D-CAD-CBD
28	F5	203	PUB	C2D-C3D-CAD-CBD
28	H5	202	PUB	C2D-C3D-CAD-CBD
28	J5	203	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	L5	203	PUB	C2D-C3D-CAD-CBD
28	N5	203	PUB	C2D-C3D-CAD-CBD
28	P5	202	PUB	C2D-C3D-CAD-CBD
28	R5	203	PUB	C2D-C3D-CAD-CBD
28	T5	202	PUB	C2D-C3D-CAD-CBD
28	V5	203	PUB	C2D-C3D-CAD-CBD
28	Y5	1005	PUB	C2D-C3D-CAD-CBD
28	Y5	1006	PUB	C2D-C3D-CAD-CBD
28	Z5	305	PUB	C2D-C3D-CAD-CBD
28	Z5	306	PUB	C2D-C3D-CAD-CBD
28	n5	203	PUB	C2D-C3D-CAD-CBD
28	p5	202	PUB	C2D-C3D-CAD-CBD
28	r5	203	PUB	C2D-C3D-CAD-CBD
28	t5	203	PUB	C2D-C3D-CAD-CBD
28	v5	203	PUB	C2D-C3D-CAD-CBD
28	x5	202	PUB	C2D-C3D-CAD-CBD
28	z5	203	PUB	C2D-C3D-CAD-CBD
28	f8	203	PUB	C2D-C3D-CAD-CBD
28	g8	202	PUB	C2D-C3D-CAD-CBD
28	h8	203	PUB	C2D-C3D-CAD-CBD
28	B6	203	PUB	C2D-C3D-CAD-CBD
28	D6	202	PUB	C2D-C3D-CAD-CBD
28	F6	203	PUB	C2D-C3D-CAD-CBD
28	H6	203	PUB	C2D-C3D-CAD-CBD
28	J6	203	PUB	C2D-C3D-CAD-CBD
28	L6	202	PUB	C2D-C3D-CAD-CBD
28	P6	203	PUB	C2D-C3D-CAD-CBD
28	R6	203	PUB	C2D-C3D-CAD-CBD
28	T6	203	PUB	C2D-C3D-CAD-CBD
28	V6	203	PUB	C2D-C3D-CAD-CBD
28	X6	203	PUB	C2D-C3D-CAD-CBD
28	Z6	203	PUB	C2D-C3D-CAD-CBD
28	a6	203	PUB	C2D-C3D-CAD-CBD
28	b6	203	PUB	C2D-C3D-CAD-CBD
28	d6	203	PUB	C2D-C3D-CAD-CBD
28	e6	203	PUB	C2D-C3D-CAD-CBD
28	l6	203	PUB	C2D-C3D-CAD-CBD
28	n6	203	PUB	C2D-C3D-CAD-CBD
28	p6	203	PUB	C2D-C3D-CAD-CBD
28	r6	203	PUB	C2D-C3D-CAD-CBD
28	t6	203	PUB	C2D-C3D-CAD-CBD
28	u6	203	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	v6	203	PUB	C2D-C3D-CAD-CBD
28	x6	203	PUB	C2D-C3D-CAD-CBD
28	y6	204	PUB	C2D-C3D-CAD-CBD
28	z6	203	PUB	C2D-C3D-CAD-CBD
28	n8	202	PUB	C2D-C3D-CAD-CBD
28	o8	203	PUB	C2D-C3D-CAD-CBD
28	p8	203	PUB	C2D-C3D-CAD-CBD
28	D7	203	PUB	C2D-C3D-CAD-CBD
28	F7	202	PUB	C2D-C3D-CAD-CBD
28	H7	203	PUB	C2D-C3D-CAD-CBD
28	J7	202	PUB	C2D-C3D-CAD-CBD
28	L7	202	PUB	C2D-C3D-CAD-CBD
28	N7	203	PUB	C2D-C3D-CAD-CBD
28	P7	203	PUB	C2D-C3D-CAD-CBD
28	R7	203	PUB	C2D-C3D-CAD-CBD
28	V7	203	PUB	C2D-C3D-CAD-CBD
28	X7	203	PUB	C2D-C3D-CAD-CBD
28	Z7	203	PUB	C2D-C3D-CAD-CBD
28	a7	203	PUB	C2D-C3D-CAD-CBD
28	b7	202	PUB	C2D-C3D-CAD-CBD
28	c7	203	PUB	C2D-C3D-CAD-CBD
28	e7	203	PUB	C2D-C3D-CAD-CBD
28	l7	203	PUB	C2D-C3D-CAD-CBD
28	n7	203	PUB	C2D-C3D-CAD-CBD
28	p7	202	PUB	C2D-C3D-CAD-CBD
28	s7	203	PUB	C2D-C3D-CAD-CBD
28	t7	203	PUB	C2D-C3D-CAD-CBD
28	v7	203	PUB	C2D-C3D-CAD-CBD
28	x7	203	PUB	C2D-C3D-CAD-CBD
28	y7	203	PUB	C2D-C3D-CAD-CBD
28	z7	203	PUB	C2D-C3D-CAD-CBD
28	b8	1005	PUB	C2D-C3D-CAD-CBD
28	b8	1006	PUB	C2D-C3D-CAD-CBD
28	c8	304	PUB	C2D-C3D-CAD-CBD
28	d8	304	PUB	C2D-C3D-CAD-CBD
28	e8	304	PUB	C2D-C3D-CAD-CBD
28	e8	305	PUB	C2D-C3D-CAD-CBD
28	b9	406	PUB	C2D-C3D-CAD-CBD
28	b9	407	PUB	C2D-C3D-CAD-CBD
28	c9	305	PUB	C2D-C3D-CAD-CBD
28	d9	305	PUB	C2D-C3D-CAD-CBD
28	e9	305	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	e9	306	PUB	C2D-C3D-CAD-CBD
28	w8	203	PUB	C2D-C3D-CAD-CBD
28	y8	203	PUB	C2D-C3D-CAD-CBD
28	A8	203	PUB	C2D-C3D-CAD-CBD
28	C8	203	PUB	C2D-C3D-CAD-CBD
28	E8	203	PUB	C2D-C3D-CAD-CBD
28	G8	203	PUB	C2D-C3D-CAD-CBD
28	K8	203	PUB	C2D-C3D-CAD-CBD
28	M8	203	PUB	C2D-C3D-CAD-CBD
28	O8	203	PUB	C2D-C3D-CAD-CBD
28	Q8	203	PUB	C2D-C3D-CAD-CBD
28	T8	304	PUB	C2D-C3D-CAD-CBD
28	T8	305	PUB	C2D-C3D-CAD-CBD
28	U8	1005	PUB	C2D-C3D-CAD-CBD
28	U8	1006	PUB	C2D-C3D-CAD-CBD
28	n9	202	PUB	C2D-C3D-CAD-CBD
28	p9	203	PUB	C2D-C3D-CAD-CBD
28	r9	203	PUB	C2D-C3D-CAD-CBD
28	t9	203	PUB	C2D-C3D-CAD-CBD
28	v9	203	PUB	C2D-C3D-CAD-CBD
28	x9	203	PUB	C2D-C3D-CAD-CBD
28	z9	203	PUB	C2D-C3D-CAD-CBD
28	B9	203	PUB	C2D-C3D-CAD-CBD
28	D9	203	PUB	C2D-C3D-CAD-CBD
28	F9	203	PUB	C2D-C3D-CAD-CBD
28	H9	203	PUB	C2D-C3D-CAD-CBD
28	J9	203	PUB	C2D-C3D-CAD-CBD
28	P9	203	PUB	C2D-C3D-CAD-CBD
28	R9	203	PUB	C2D-C3D-CAD-CBD
28	T9	203	PUB	C2D-C3D-CAD-CBD
28	V9	203	PUB	C2D-C3D-CAD-CBD
28	Y9	304	PUB	C2D-C3D-CAD-CBD
28	Y9	305	PUB	C2D-C3D-CAD-CBD
28	Z9	1005	PUB	C2D-C3D-CAD-CBD
28	Z9	1006	PUB	C2D-C3D-CAD-CBD
28	an	202	PUB	C2D-C3D-CAD-CBD
28	ap	203	PUB	C2D-C3D-CAD-CBD
28	ar	203	PUB	C2D-C3D-CAD-CBD
28	at	203	PUB	C2D-C3D-CAD-CBD
28	av	203	PUB	C2D-C3D-CAD-CBD
28	az	203	PUB	C2D-C3D-CAD-CBD
28	aB	203	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	aF	203	PUB	C2D-C3D-CAD-CBD
28	aH	203	PUB	C2D-C3D-CAD-CBD
28	aJ	203	PUB	C2D-C3D-CAD-CBD
28	aL	203	PUB	C2D-C3D-CAD-CBD
28	aN	203	PUB	C2D-C3D-CAD-CBD
28	aR	203	PUB	C2D-C3D-CAD-CBD
28	aT	203	PUB	C2D-C3D-CAD-CBD
28	aV	203	PUB	C2D-C3D-CAD-CBD
28	aY	404	PUB	C2D-C3D-CAD-CBD
28	aY	405	PUB	C2D-C3D-CAD-CBD
28	aZ	304	PUB	C2D-C3D-CAD-CBD
28	aZ	305	PUB	C2D-C3D-CAD-CBD
28	bn	202	PUB	C2D-C3D-CAD-CBD
28	bo	202	PUB	C2D-C3D-CAD-CBD
28	bp	202	PUB	C2D-C3D-CAD-CBD
28	bq	203	PUB	C2D-C3D-CAD-CBD
28	br	203	PUB	C2D-C3D-CAD-CBD
28	bs	1004	PUB	C2D-C3D-CAD-CBD
28	bz	203	PUB	C2D-C3D-CAD-CBD
28	bD	203	PUB	C2D-C3D-CAD-CBD
28	bF	203	PUB	C2D-C3D-CAD-CBD
28	bH	203	PUB	C2D-C3D-CAD-CBD
28	bL	203	PUB	C2D-C3D-CAD-CBD
28	bN	203	PUB	C2D-C3D-CAD-CBD
28	bP	203	PUB	C2D-C3D-CAD-CBD
28	bR	202	PUB	C2D-C3D-CAD-CBD
28	bT	202	PUB	C2D-C3D-CAD-CBD
28	bV	203	PUB	C2D-C3D-CAD-CBD
28	bY	1006	PUB	C2D-C3D-CAD-CBD
28	bZ	305	PUB	C2D-C3D-CAD-CBD
28	bZ	306	PUB	C2D-C3D-CAD-CBD
28	cn	202	PUB	C2D-C3D-CAD-CBD
28	co	202	PUB	C2D-C3D-CAD-CBD
28	cp	203	PUB	C2D-C3D-CAD-CBD
28	cq	203	PUB	C2D-C3D-CAD-CBD
28	cr	203	PUB	C2D-C3D-CAD-CBD
28	cz	203	PUB	C2D-C3D-CAD-CBD
28	cB	203	PUB	C2D-C3D-CAD-CBD
28	cE	203	PUB	C2D-C3D-CAD-CBD
28	cF	202	PUB	C2D-C3D-CAD-CBD
28	cJ	203	PUB	C2D-C3D-CAD-CBD
28	cM	203	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	cN	202	PUB	C2D-C3D-CAD-CBD
28	cO	203	PUB	C2D-C3D-CAD-CBD
28	cP	203	PUB	C2D-C3D-CAD-CBD
28	cQ	202	PUB	C2D-C3D-CAD-CBD
28	cR	203	PUB	C2D-C3D-CAD-CBD
28	cY	203	PUB	C2D-C3D-CAD-CBD
28	dd	203	PUB	C2D-C3D-CAD-CBD
28	df	203	PUB	C2D-C3D-CAD-CBD
28	dh	203	PUB	C2D-C3D-CAD-CBD
28	di	203	PUB	C2D-C3D-CAD-CBD
28	dj	203	PUB	C2D-C3D-CAD-CBD
28	dl	203	PUB	C2D-C3D-CAD-CBD
28	dn	203	PUB	C2D-C3D-CAD-CBD
28	dp	203	PUB	C2D-C3D-CAD-CBD
28	dt	203	PUB	C2D-C3D-CAD-CBD
28	dv	202	PUB	C2D-C3D-CAD-CBD
28	dx	406	PUB	C2D-C3D-CAD-CBD
28	dx	407	PUB	C2D-C3D-CAD-CBD
28	dB	202	PUB	C2D-C3D-CAD-CBD
28	dD	203	PUB	C2D-C3D-CAD-CBD
28	dF	203	PUB	C2D-C3D-CAD-CBD
28	dH	203	PUB	C2D-C3D-CAD-CBD
28	dK	203	PUB	C2D-C3D-CAD-CBD
28	dL	203	PUB	C2D-C3D-CAD-CBD
28	dN	203	PUB	C2D-C3D-CAD-CBD
28	dP	203	PUB	C2D-C3D-CAD-CBD
28	dR	203	PUB	C2D-C3D-CAD-CBD
28	dV	203	PUB	C2D-C3D-CAD-CBD
28	dX	203	PUB	C2D-C3D-CAD-CBD
28	dY	203	PUB	C2D-C3D-CAD-CBD
28	eb	202	PUB	C2D-C3D-CAD-CBD
28	ec	203	PUB	C2D-C3D-CAD-CBD
28	ee	203	PUB	C2D-C3D-CAD-CBD
28	eg	203	PUB	C2D-C3D-CAD-CBD
28	ei	203	PUB	C2D-C3D-CAD-CBD
28	en	203	PUB	C2D-C3D-CAD-CBD
28	er	203	PUB	C2D-C3D-CAD-CBD
28	ev	203	PUB	C2D-C3D-CAD-CBD
28	ey	1005	PUB	C2D-C3D-CAD-CBD
28	ey	1006	PUB	C2D-C3D-CAD-CBD
28	ez	1005	PUB	C2D-C3D-CAD-CBD
28	ez	1006	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	eB	204	PUB	C2D-C3D-CAD-CBD
28	eD	203	PUB	C2D-C3D-CAD-CBD
28	eF	203	PUB	C2D-C3D-CAD-CBD
28	eH	203	PUB	C2D-C3D-CAD-CBD
28	eJ	203	PUB	C2D-C3D-CAD-CBD
28	eL	203	PUB	C2D-C3D-CAD-CBD
28	eN	203	PUB	C2D-C3D-CAD-CBD
28	eP	204	PUB	C2D-C3D-CAD-CBD
28	eR	203	PUB	C2D-C3D-CAD-CBD
28	eT	203	PUB	C2D-C3D-CAD-CBD
28	eX	202	PUB	C2D-C3D-CAD-CBD
28	eY	404	PUB	C2D-C3D-CAD-CBD
28	eY	405	PUB	C2D-C3D-CAD-CBD
28	eZ	403	PUB	C2D-C3D-CAD-CBD
28	eZ	404	PUB	C2D-C3D-CAD-CBD
28	lb	203	PUB	C2D-C3D-CAD-CBD
28	ld	203	PUB	C2D-C3D-CAD-CBD
28	lf	203	PUB	C2D-C3D-CAD-CBD
28	lh	203	PUB	C2D-C3D-CAD-CBD
28	lj	202	PUB	C2D-C3D-CAD-CBD
28	ll	203	PUB	C2D-C3D-CAD-CBD
28	ln	203	PUB	C2D-C3D-CAD-CBD
28	lp	203	PUB	C2D-C3D-CAD-CBD
28	lv	202	PUB	C2D-C3D-CAD-CBD
28	lx	201	PUB	C2D-C3D-CAD-CBD
28	ly	405	PUB	C2D-C3D-CAD-CBD
28	ly	406	PUB	C2D-C3D-CAD-CBD
28	lz	404	PUB	C2D-C3D-CAD-CBD
28	fa	202	PUB	C2D-C3D-CAD-CBD
28	fc	203	PUB	C2D-C3D-CAD-CBD
28	ff	203	PUB	C2D-C3D-CAD-CBD
28	fi	203	PUB	C2D-C3D-CAD-CBD
28	fj	203	PUB	C2D-C3D-CAD-CBD
28	fo	203	PUB	C2D-C3D-CAD-CBD
28	fq	203	PUB	C2D-C3D-CAD-CBD
28	fu	202	PUB	C2D-C3D-CAD-CBD
28	fw	203	PUB	C2D-C3D-CAD-CBD
28	gd	202	PUB	C2D-C3D-CAD-CBD
28	ge	203	PUB	C2D-C3D-CAD-CBD
28	gg	203	PUB	C2D-C3D-CAD-CBD
28	gi	203	PUB	C2D-C3D-CAD-CBD
28	gn	203	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	gp	203	PUB	C2D-C3D-CAD-CBD
28	gr	202	PUB	C2D-C3D-CAD-CBD
28	gt	203	PUB	C2D-C3D-CAD-CBD
28	gv	203	PUB	C2D-C3D-CAD-CBD
28	gx	203	PUB	C2D-C3D-CAD-CBD
28	gy	305	PUB	C2D-C3D-CAD-CBD
28	gy	306	PUB	C2D-C3D-CAD-CBD
28	gz	305	PUB	C2D-C3D-CAD-CBD
28	gz	306	PUB	C2D-C3D-CAD-CBD
28	hB	203	PUB	C2D-C3D-CAD-CBD
28	hD	203	PUB	C2D-C3D-CAD-CBD
28	hG	202	PUB	C2D-C3D-CAD-CBD
28	hH	203	PUB	C2D-C3D-CAD-CBD
28	hJ	203	PUB	C2D-C3D-CAD-CBD
28	hL	203	PUB	C2D-C3D-CAD-CBD
28	hN	203	PUB	C2D-C3D-CAD-CBD
28	hP	203	PUB	C2D-C3D-CAD-CBD
28	hR	203	PUB	C2D-C3D-CAD-CBD
28	hV	203	PUB	C2D-C3D-CAD-CBD
28	hX	203	PUB	C2D-C3D-CAD-CBD
28	hY	405	PUB	C2D-C3D-CAD-CBD
28	hY	406	PUB	C2D-C3D-CAD-CBD
28	hZ	404	PUB	C2D-C3D-CAD-CBD
28	hZ	405	PUB	C2D-C3D-CAD-CBD
28	iC	1003	PUB	C2D-C3D-CAD-CBD
28	iD	1003	PUB	C2D-C3D-CAD-CBD
28	iE	1003	PUB	C2D-C3D-CAD-CBD
28	iF	1003	PUB	C2D-C3D-CAD-CBD
28	iG	1002	PUB	C2D-C3D-CAD-CBD
28	iH	1002	PUB	C2D-C3D-CAD-CBD
28	jI	1003	PUB	C2D-C3D-CAD-CBD
28	jJ	1003	PUB	C2D-C3D-CAD-CBD
28	jK	1003	PUB	C2D-C3D-CAD-CBD
28	jL	1003	PUB	C2D-C3D-CAD-CBD
28	jM	1003	PUB	C2D-C3D-CAD-CBD
28	jN	1003	PUB	C2D-C3D-CAD-CBD
28	jO	1003	PUB	C2D-C3D-CAD-CBD
28	jP	1003	PUB	C2D-C3D-CAD-CBD
28	kQ	1003	PUB	C2D-C3D-CAD-CBD
28	kR	1003	PUB	C2D-C3D-CAD-CBD
28	kS	1003	PUB	C2D-C3D-CAD-CBD
28	kT	1003	PUB	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
28	kU	1003	PUB	C2D-C3D-CAD-CBD
28	kV	1003	PUB	C2D-C3D-CAD-CBD
28	kW	1003	PUB	C2D-C3D-CAD-CBD
28	kX	1003	PUB	C2D-C3D-CAD-CBD
28	B7	202	PUB	C2D-C3D-CAD-CBD
28	aD	203	PUB	C2D-C3D-CAD-CBD
28	bB	203	PUB	C2D-C3D-CAD-CBD
28	cs	203	PUB	C2D-C3D-CAD-CBD
28	et	203	PUB	C2D-C3D-CAD-CBD
28	fy	202	PUB	C2D-C3D-CAD-CBD
28	hT	203	PUB	C2D-C3D-CAD-CBD
26	A1	301	PEB	C4A-C3A-CAA-CBA
26	B1	301	PEB	C4A-C3A-CAA-CBA
26	f2	202	PEB	C4A-C3A-CAA-CBA
26	h2	202	PEB	C4A-C3A-CAA-CBA
26	j2	202	PEB	C4A-C3A-CAA-CBA
26	l2	202	PEB	C4A-C3A-CAA-CBA
26	n2	202	PEB	C4A-C3A-CAA-CBA
26	p2	202	PEB	C4A-C3A-CAA-CBA
26	A2	1003	PEB	C4A-C3A-CAA-CBA
26	H2	201	PEB	C4A-C3A-CAA-CBA
26	L2	202	PEB	C4A-C3A-CAA-CBA
26	T2	202	PEB	C4A-C3A-CAA-CBA
26	V2	202	PEB	C4A-C3A-CAA-CBA
26	X2	202	PEB	C4A-C3A-CAA-CBA
26	Z2	202	PEB	C4A-C3A-CAA-CBA
26	B3	202	PEB	C4A-C3A-CAA-CBA
26	D3	202	PEB	C4A-C3A-CAA-CBA
26	F3	202	PEB	C4A-C3A-CAA-CBA
26	H3	202	PEB	C4A-C3A-CAA-CBA
26	J3	202	PEB	C4A-C3A-CAA-CBA
26	L3	202	PEB	C4A-C3A-CAA-CBA
26	N3	202	PEB	C4A-C3A-CAA-CBA
26	P3	202	PEB	C4A-C3A-CAA-CBA
26	R3	202	PEB	C4A-C3A-CAA-CBA
26	T3	202	PEB	C4A-C3A-CAA-CBA
26	V3	202	PEB	C4A-C3A-CAA-CBA
26	W3	203	PEB	C4A-C3A-CAA-CBA
26	Z3	202	PEB	C4A-C3A-CAA-CBA
26	f3	202	PEB	C4A-C3A-CAA-CBA
26	h3	201	PEB	C4A-C3A-CAA-CBA
26	i3	203	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	j3	201	PEB	C4A-C3A-CAA-CBA
26	n3	202	PEB	C4A-C3A-CAA-CBA
26	p3	202	PEB	C4A-C3A-CAA-CBA
26	r3	202	PEB	C4A-C3A-CAA-CBA
26	t3	202	PEB	C4A-C3A-CAA-CBA
26	v3	202	PEB	C4A-C3A-CAA-CBA
26	x3	202	PEB	C4A-C3A-CAA-CBA
26	z3	202	PEB	C4A-C3A-CAA-CBA
26	B4	202	PEB	C4A-C3A-CAA-CBA
26	D4	202	PEB	C4A-C3A-CAA-CBA
26	34	1001	PEB	C4A-C3A-CAA-CBA
26	34	1002	PEB	C4A-C3A-CAA-CBA
26	e4	202	PEB	C4A-C3A-CAA-CBA
26	g4	202	PEB	C4A-C3A-CAA-CBA
26	j4	202	PEB	C4A-C3A-CAA-CBA
26	l4	202	PEB	C4A-C3A-CAA-CBA
26	n4	202	PEB	C4A-C3A-CAA-CBA
26	p4	202	PEB	C4A-C3A-CAA-CBA
26	r4	201	PEB	C4A-C3A-CAA-CBA
26	v4	202	PEB	C4A-C3A-CAA-CBA
26	A5	203	PEB	C4A-C3A-CAA-CBA
26	B5	202	PEB	C4A-C3A-CAA-CBA
26	D5	202	PEB	C4A-C3A-CAA-CBA
26	F5	202	PEB	C4A-C3A-CAA-CBA
26	J5	202	PEB	C4A-C3A-CAA-CBA
26	L5	202	PEB	C4A-C3A-CAA-CBA
26	N5	202	PEB	C4A-C3A-CAA-CBA
26	P5	201	PEB	C4A-C3A-CAA-CBA
26	R5	202	PEB	C4A-C3A-CAA-CBA
26	S5	203	PEB	C4A-C3A-CAA-CBA
26	V5	202	PEB	C4A-C3A-CAA-CBA
26	g5	202	PEB	C4A-C3A-CAA-CBA
26	m5	1003	PEB	C4A-C3A-CAA-CBA
26	n5	202	PEB	C4A-C3A-CAA-CBA
26	p5	201	PEB	C4A-C3A-CAA-CBA
26	r5	202	PEB	C4A-C3A-CAA-CBA
26	t5	202	PEB	C4A-C3A-CAA-CBA
26	v5	202	PEB	C4A-C3A-CAA-CBA
26	z5	202	PEB	C4A-C3A-CAA-CBA
26	h8	202	PEB	C4A-C3A-CAA-CBA
26	B6	202	PEB	C4A-C3A-CAA-CBA
26	J6	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	R6	202	PEB	C4A-C3A-CAA-CBA
26	X6	202	PEB	C4A-C3A-CAA-CBA
26	n6	202	PEB	C4A-C3A-CAA-CBA
26	n8	201	PEB	C4A-C3A-CAA-CBA
26	p8	202	PEB	C4A-C3A-CAA-CBA
26	B7	201	PEB	C4A-C3A-CAA-CBA
26	D7	202	PEB	C4A-C3A-CAA-CBA
26	F7	201	PEB	C4A-C3A-CAA-CBA
26	H7	202	PEB	C4A-C3A-CAA-CBA
26	J7	201	PEB	C4A-C3A-CAA-CBA
26	L7	201	PEB	C4A-C3A-CAA-CBA
26	N7	202	PEB	C4A-C3A-CAA-CBA
26	P7	202	PEB	C4A-C3A-CAA-CBA
26	R7	202	PEB	C4A-C3A-CAA-CBA
26	T7	202	PEB	C4A-C3A-CAA-CBA
26	V7	202	PEB	C4A-C3A-CAA-CBA
26	X7	202	PEB	C4A-C3A-CAA-CBA
26	Y7	1003	PEB	C4A-C3A-CAA-CBA
26	Z7	202	PEB	C4A-C3A-CAA-CBA
26	a7	202	PEB	C4A-C3A-CAA-CBA
26	c7	202	PEB	C4A-C3A-CAA-CBA
26	d7	202	PEB	C4A-C3A-CAA-CBA
26	e7	202	PEB	C4A-C3A-CAA-CBA
26	l7	202	PEB	C4A-C3A-CAA-CBA
26	n7	202	PEB	C4A-C3A-CAA-CBA
26	p7	201	PEB	C4A-C3A-CAA-CBA
26	r7	202	PEB	C4A-C3A-CAA-CBA
26	t7	202	PEB	C4A-C3A-CAA-CBA
26	v7	202	PEB	C4A-C3A-CAA-CBA
26	x7	202	PEB	C4A-C3A-CAA-CBA
26	y7	202	PEB	C4A-C3A-CAA-CBA
26	z7	202	PEB	C4A-C3A-CAA-CBA
26	y8	202	PEB	C4A-C3A-CAA-CBA
26	C8	202	PEB	C4A-C3A-CAA-CBA
26	v9	202	PEB	C4A-C3A-CAA-CBA
26	B9	202	PEB	C4A-C3A-CAA-CBA
26	D9	202	PEB	C4A-C3A-CAA-CBA
26	F9	202	PEB	C4A-C3A-CAA-CBA
26	H9	202	PEB	C4A-C3A-CAA-CBA
26	J9	202	PEB	C4A-C3A-CAA-CBA
26	L9	202	PEB	C4A-C3A-CAA-CBA
26	N9	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	P9	202	PEB	C4A-C3A-CAA-CBA
26	R9	202	PEB	C4A-C3A-CAA-CBA
26	T9	202	PEB	C4A-C3A-CAA-CBA
26	V9	202	PEB	C4A-C3A-CAA-CBA
26	ab	202	PEB	C4A-C3A-CAA-CBA
26	ad	202	PEB	C4A-C3A-CAA-CBA
26	af	202	PEB	C4A-C3A-CAA-CBA
26	ah	202	PEB	C4A-C3A-CAA-CBA
26	aj	202	PEB	C4A-C3A-CAA-CBA
26	al	202	PEB	C4A-C3A-CAA-CBA
26	an	201	PEB	C4A-C3A-CAA-CBA
26	ap	202	PEB	C4A-C3A-CAA-CBA
26	ar	202	PEB	C4A-C3A-CAA-CBA
26	at	202	PEB	C4A-C3A-CAA-CBA
26	av	202	PEB	C4A-C3A-CAA-CBA
26	ax	201	PEB	C4A-C3A-CAA-CBA
26	az	202	PEB	C4A-C3A-CAA-CBA
26	aD	202	PEB	C4A-C3A-CAA-CBA
26	aF	202	PEB	C4A-C3A-CAA-CBA
26	bB	202	PEB	C4A-C3A-CAA-CBA
26	bD	202	PEB	C4A-C3A-CAA-CBA
26	bF	202	PEB	C4A-C3A-CAA-CBA
26	bH	202	PEB	C4A-C3A-CAA-CBA
26	bJ	202	PEB	C4A-C3A-CAA-CBA
26	bL	202	PEB	C4A-C3A-CAA-CBA
26	bN	202	PEB	C4A-C3A-CAA-CBA
26	bP	202	PEB	C4A-C3A-CAA-CBA
26	bQ	203	PEB	C4A-C3A-CAA-CBA
26	bT	201	PEB	C4A-C3A-CAA-CBA
26	bV	202	PEB	C4A-C3A-CAA-CBA
26	cb	202	PEB	C4A-C3A-CAA-CBA
26	cd	202	PEB	C4A-C3A-CAA-CBA
26	cf	201	PEB	C4A-C3A-CAA-CBA
26	ch	202	PEB	C4A-C3A-CAA-CBA
26	cj	202	PEB	C4A-C3A-CAA-CBA
26	cl	202	PEB	C4A-C3A-CAA-CBA
26	cn	201	PEB	C4A-C3A-CAA-CBA
26	co	201	PEB	C4A-C3A-CAA-CBA
26	cp	202	PEB	C4A-C3A-CAA-CBA
26	cq	202	PEB	C4A-C3A-CAA-CBA
26	cr	202	PEB	C4A-C3A-CAA-CBA
26	cs	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	cz	202	PEB	C4A-C3A-CAA-CBA
26	cB	202	PEB	C4A-C3A-CAA-CBA
26	cE	202	PEB	C4A-C3A-CAA-CBA
26	cF	201	PEB	C4A-C3A-CAA-CBA
26	cH	201	PEB	C4A-C3A-CAA-CBA
26	cJ	202	PEB	C4A-C3A-CAA-CBA
26	cL	202	PEB	C4A-C3A-CAA-CBA
26	cY	202	PEB	C4A-C3A-CAA-CBA
26	dd	202	PEB	C4A-C3A-CAA-CBA
26	df	202	PEB	C4A-C3A-CAA-CBA
26	dh	202	PEB	C4A-C3A-CAA-CBA
26	di	202	PEB	C4A-C3A-CAA-CBA
26	dj	202	PEB	C4A-C3A-CAA-CBA
26	dl	202	PEB	C4A-C3A-CAA-CBA
26	dL	202	PEB	C4A-C3A-CAA-CBA
26	dV	202	PEB	C4A-C3A-CAA-CBA
26	dY	202	PEB	C4A-C3A-CAA-CBA
26	ea	203	PEB	C4A-C3A-CAA-CBA
26	ec	202	PEB	C4A-C3A-CAA-CBA
26	ee	202	PEB	C4A-C3A-CAA-CBA
26	eg	202	PEB	C4A-C3A-CAA-CBA
26	ei	202	PEB	C4A-C3A-CAA-CBA
26	el	202	PEB	C4A-C3A-CAA-CBA
26	en	202	PEB	C4A-C3A-CAA-CBA
26	ep	202	PEB	C4A-C3A-CAA-CBA
26	er	202	PEB	C4A-C3A-CAA-CBA
26	et	202	PEB	C4A-C3A-CAA-CBA
26	ev	202	PEB	C4A-C3A-CAA-CBA
26	eB	203	PEB	C4A-C3A-CAA-CBA
26	eJ	202	PEB	C4A-C3A-CAA-CBA
26	eL	202	PEB	C4A-C3A-CAA-CBA
26	eN	202	PEB	C4A-C3A-CAA-CBA
26	eV	202	PEB	C4A-C3A-CAA-CBA
26	eX	201	PEB	C4A-C3A-CAA-CBA
26	ld	202	PEB	C4A-C3A-CAA-CBA
26	lf	202	PEB	C4A-C3A-CAA-CBA
26	lh	202	PEB	C4A-C3A-CAA-CBA
26	li	203	PEB	C4A-C3A-CAA-CBA
26	ll	202	PEB	C4A-C3A-CAA-CBA
26	ln	202	PEB	C4A-C3A-CAA-CBA
26	lo	203	PEB	C4A-C3A-CAA-CBA
26	lp	202	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	lr	202	PEB	C4A-C3A-CAA-CBA
26	lw	203	PEB	C4A-C3A-CAA-CBA
26	fc	202	PEB	C4A-C3A-CAA-CBA
26	ff	202	PEB	C4A-C3A-CAA-CBA
26	fg	201	PEB	C4A-C3A-CAA-CBA
26	fi	202	PEB	C4A-C3A-CAA-CBA
26	fj	202	PEB	C4A-C3A-CAA-CBA
26	fm	202	PEB	C4A-C3A-CAA-CBA
26	fo	202	PEB	C4A-C3A-CAA-CBA
26	fq	202	PEB	C4A-C3A-CAA-CBA
26	fs	202	PEB	C4A-C3A-CAA-CBA
26	fu	201	PEB	C4A-C3A-CAA-CBA
26	fw	202	PEB	C4A-C3A-CAA-CBA
26	fy	201	PEB	C4A-C3A-CAA-CBA
26	ga	202	PEB	C4A-C3A-CAA-CBA
26	gd	201	PEB	C4A-C3A-CAA-CBA
26	ge	202	PEB	C4A-C3A-CAA-CBA
26	gg	202	PEB	C4A-C3A-CAA-CBA
26	gi	202	PEB	C4A-C3A-CAA-CBA
26	gk	202	PEB	C4A-C3A-CAA-CBA
26	gn	202	PEB	C4A-C3A-CAA-CBA
26	gp	202	PEB	C4A-C3A-CAA-CBA
26	gr	201	PEB	C4A-C3A-CAA-CBA
26	gt	202	PEB	C4A-C3A-CAA-CBA
26	gv	202	PEB	C4A-C3A-CAA-CBA
26	gx	202	PEB	C4A-C3A-CAA-CBA
26	hB	202	PEB	C4A-C3A-CAA-CBA
26	hD	202	PEB	C4A-C3A-CAA-CBA
26	hG	201	PEB	C4A-C3A-CAA-CBA
26	hH	202	PEB	C4A-C3A-CAA-CBA
26	hJ	202	PEB	C4A-C3A-CAA-CBA
26	hL	202	PEB	C4A-C3A-CAA-CBA
26	hN	202	PEB	C4A-C3A-CAA-CBA
26	hP	202	PEB	C4A-C3A-CAA-CBA
26	hR	202	PEB	C4A-C3A-CAA-CBA
26	hT	202	PEB	C4A-C3A-CAA-CBA
26	hV	202	PEB	C4A-C3A-CAA-CBA
26	hX	202	PEB	C4A-C3A-CAA-CBA
26	iC	1002	PEB	C4A-C3A-CAA-CBA
26	iD	1002	PEB	C4A-C3A-CAA-CBA
26	iE	1002	PEB	C4A-C3A-CAA-CBA
26	jI	1002	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	jJ	1002	PEB	C4A-C3A-CAA-CBA
26	jK	1002	PEB	C4A-C3A-CAA-CBA
26	jL	1002	PEB	C4A-C3A-CAA-CBA
26	jM	1002	PEB	C4A-C3A-CAA-CBA
26	jN	1002	PEB	C4A-C3A-CAA-CBA
26	jO	1002	PEB	C4A-C3A-CAA-CBA
26	jP	1002	PEB	C4A-C3A-CAA-CBA
26	kQ	1002	PEB	C4A-C3A-CAA-CBA
26	kR	1002	PEB	C4A-C3A-CAA-CBA
26	kS	1002	PEB	C4A-C3A-CAA-CBA
26	kT	1002	PEB	C4A-C3A-CAA-CBA
26	kU	1002	PEB	C4A-C3A-CAA-CBA
26	kV	1002	PEB	C4A-C3A-CAA-CBA
26	kW	1002	PEB	C4A-C3A-CAA-CBA
26	kX	1002	PEB	C4A-C3A-CAA-CBA
29	C2	303	PVN	C9-C10-C11-N3
29	c3	303	PVN	C9-C10-C11-N3
26	A2	1001	PEB	NA-C4A-CHA-C1B
26	E2	1002	PEB	NA-C4A-CHA-C1B
26	N2	201	PEB	NA-C4A-CHA-C1B
26	P2	202	PEB	NA-C4A-CHA-C1B
26	R2	201	PEB	NA-C4A-CHA-C1B
26	S2	202	PEB	NA-C4A-CHA-C1B
26	U2	202	PEB	NA-C4A-CHA-C1B
26	A3	202	PEB	NA-C4A-CHA-C1B
26	C3	1002	PEB	NA-C4A-CHA-C1B
26	E3	202	PEB	NA-C4A-CHA-C1B
26	G3	202	PEB	NA-C4A-CHA-C1B
26	I3	202	PEB	NA-C4A-CHA-C1B
26	K3	202	PEB	NA-C4A-CHA-C1B
26	M3	202	PEB	NA-C4A-CHA-C1B
26	O3	1002	PEB	NA-C4A-CHA-C1B
26	Q3	202	PEB	NA-C4A-CHA-C1B
26	S3	202	PEB	NA-C4A-CHA-C1B
26	U3	202	PEB	NA-C4A-CHA-C1B
26	W3	202	PEB	NA-C4A-CHA-C1B
26	Y3	202	PEB	NA-C4A-CHA-C1B
26	a3	1002	PEB	NA-C4A-CHA-C1B
26	c3	301	PEB	NA-C4A-CHA-C1B
26	d3	301	PEB	NA-C4A-CHA-C1B
26	e3	1002	PEB	NA-C4A-CHA-C1B
26	g3	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	i3	202	PEB	NA-C4A-CHA-C1B
26	k3	202	PEB	NA-C4A-CHA-C1B
26	m3	202	PEB	NA-C4A-CHA-C1B
26	o3	202	PEB	NA-C4A-CHA-C1B
26	s3	202	PEB	NA-C4A-CHA-C1B
26	u3	202	PEB	NA-C4A-CHA-C1B
26	w3	202	PEB	NA-C4A-CHA-C1B
26	y3	202	PEB	NA-C4A-CHA-C1B
26	A4	202	PEB	NA-C4A-CHA-C1B
26	C4	1002	PEB	NA-C4A-CHA-C1B
26	N4	202	PEB	NA-C4A-CHA-C1B
26	c4	201	PEB	NA-C4A-CHA-C1B
26	h4	201	PEB	NA-C4A-CHA-C1B
26	s4	202	PEB	NA-C4A-CHA-C1B
26	w4	202	PEB	NA-C4A-CHA-C1B
26	A5	202	PEB	NA-C4A-CHA-C1B
26	C5	202	PEB	NA-C4A-CHA-C1B
26	E5	202	PEB	NA-C4A-CHA-C1B
26	G5	202	PEB	NA-C4A-CHA-C1B
26	I5	202	PEB	NA-C4A-CHA-C1B
26	K5	1002	PEB	NA-C4A-CHA-C1B
26	M5	202	PEB	NA-C4A-CHA-C1B
26	O5	202	PEB	NA-C4A-CHA-C1B
26	Q5	202	PEB	NA-C4A-CHA-C1B
26	S5	202	PEB	NA-C4A-CHA-C1B
26	U5	202	PEB	NA-C4A-CHA-C1B
26	Y5	1002	PEB	NA-C4A-CHA-C1B
26	Z5	302	PEB	NA-C4A-CHA-C1B
26	c5	201	PEB	NA-C4A-CHA-C1B
26	f5	201	PEB	NA-C4A-CHA-C1B
26	h5	202	PEB	NA-C4A-CHA-C1B
26	m5	1002	PEB	NA-C4A-CHA-C1B
26	o5	202	PEB	NA-C4A-CHA-C1B
26	q5	202	PEB	NA-C4A-CHA-C1B
26	s5	202	PEB	NA-C4A-CHA-C1B
26	u5	202	PEB	NA-C4A-CHA-C1B
26	w5	202	PEB	NA-C4A-CHA-C1B
26	y5	1002	PEB	NA-C4A-CHA-C1B
26	G6	202	PEB	NA-C4A-CHA-C1B
26	H6	201	PEB	NA-C4A-CHA-C1B
26	N6	202	PEB	NA-C4A-CHA-C1B
26	U6	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	V6	202	PEB	NA-C4A-CHA-C1B
26	a6	202	PEB	NA-C4A-CHA-C1B
26	d6	202	PEB	NA-C4A-CHA-C1B
26	e6	202	PEB	NA-C4A-CHA-C1B
26	f6	202	PEB	NA-C4A-CHA-C1B
26	n6	201	PEB	NA-C4A-CHA-C1B
26	p6	202	PEB	NA-C4A-CHA-C1B
26	t6	201	PEB	NA-C4A-CHA-C1B
26	o8	201	PEB	NA-C4A-CHA-C1B
26	q8	202	PEB	NA-C4A-CHA-C1B
26	r8	202	PEB	NA-C4A-CHA-C1B
26	s8	202	PEB	NA-C4A-CHA-C1B
26	t8	202	PEB	NA-C4A-CHA-C1B
26	u8	202	PEB	NA-C4A-CHA-C1B
26	A7	201	PEB	NA-C4A-CHA-C1B
26	C7	202	PEB	NA-C4A-CHA-C1B
26	E7	202	PEB	NA-C4A-CHA-C1B
26	G7	202	PEB	NA-C4A-CHA-C1B
26	I7	202	PEB	NA-C4A-CHA-C1B
26	K7	202	PEB	NA-C4A-CHA-C1B
26	M7	1003	PEB	NA-C4A-CHA-C1B
26	O7	202	PEB	NA-C4A-CHA-C1B
26	Q7	202	PEB	NA-C4A-CHA-C1B
26	S7	202	PEB	NA-C4A-CHA-C1B
26	U7	202	PEB	NA-C4A-CHA-C1B
26	W7	202	PEB	NA-C4A-CHA-C1B
26	Y7	1002	PEB	NA-C4A-CHA-C1B
26	f7	202	PEB	NA-C4A-CHA-C1B
26	g7	202	PEB	NA-C4A-CHA-C1B
26	h7	202	PEB	NA-C4A-CHA-C1B
26	i7	202	PEB	NA-C4A-CHA-C1B
26	j7	202	PEB	NA-C4A-CHA-C1B
26	k7	1002	PEB	NA-C4A-CHA-C1B
26	m7	202	PEB	NA-C4A-CHA-C1B
26	o7	202	PEB	NA-C4A-CHA-C1B
26	q7	202	PEB	NA-C4A-CHA-C1B
26	s7	202	PEB	NA-C4A-CHA-C1B
26	u7	202	PEB	NA-C4A-CHA-C1B
26	w7	1002	PEB	NA-C4A-CHA-C1B
26	c8	301	PEB	NA-C4A-CHA-C1B
26	d8	301	PEB	NA-C4A-CHA-C1B
26	A9	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	C9	202	PEB	NA-C4A-CHA-C1B
26	E9	202	PEB	NA-C4A-CHA-C1B
26	G9	202	PEB	NA-C4A-CHA-C1B
26	I9	202	PEB	NA-C4A-CHA-C1B
26	K9	1002	PEB	NA-C4A-CHA-C1B
26	M9	202	PEB	NA-C4A-CHA-C1B
26	O9	202	PEB	NA-C4A-CHA-C1B
26	Q9	202	PEB	NA-C4A-CHA-C1B
26	S9	202	PEB	NA-C4A-CHA-C1B
26	U9	202	PEB	NA-C4A-CHA-C1B
26	Y9	301	PEB	NA-C4A-CHA-C1B
26	Z9	1002	PEB	NA-C4A-CHA-C1B
26	ao	202	PEB	NA-C4A-CHA-C1B
26	aq	202	PEB	NA-C4A-CHA-C1B
26	as	202	PEB	NA-C4A-CHA-C1B
26	au	202	PEB	NA-C4A-CHA-C1B
26	aw	202	PEB	NA-C4A-CHA-C1B
26	ay	1002	PEB	NA-C4A-CHA-C1B
26	bA	202	PEB	NA-C4A-CHA-C1B
26	bC	202	PEB	NA-C4A-CHA-C1B
26	bE	202	PEB	NA-C4A-CHA-C1B
26	bG	202	PEB	NA-C4A-CHA-C1B
26	bI	202	PEB	NA-C4A-CHA-C1B
26	bK	1002	PEB	NA-C4A-CHA-C1B
26	bM	202	PEB	NA-C4A-CHA-C1B
26	bO	202	PEB	NA-C4A-CHA-C1B
26	bQ	202	PEB	NA-C4A-CHA-C1B
26	bS	202	PEB	NA-C4A-CHA-C1B
26	bU	202	PEB	NA-C4A-CHA-C1B
26	bY	1002	PEB	NA-C4A-CHA-C1B
26	bZ	302	PEB	NA-C4A-CHA-C1B
26	cm	1002	PEB	NA-C4A-CHA-C1B
26	ct	202	PEB	NA-C4A-CHA-C1B
26	cu	202	PEB	NA-C4A-CHA-C1B
26	cv	202	PEB	NA-C4A-CHA-C1B
26	cw	202	PEB	NA-C4A-CHA-C1B
26	cx	202	PEB	NA-C4A-CHA-C1B
26	cy	1002	PEB	NA-C4A-CHA-C1B
26	cA	202	PEB	NA-C4A-CHA-C1B
26	cC	1002	PEB	NA-C4A-CHA-C1B
26	cD	202	PEB	NA-C4A-CHA-C1B
26	cG	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cI	202	PEB	NA-C4A-CHA-C1B
26	cK	202	PEB	NA-C4A-CHA-C1B
26	cZ	202	PEB	NA-C4A-CHA-C1B
26	da	1002	PEB	NA-C4A-CHA-C1B
26	db	202	PEB	NA-C4A-CHA-C1B
26	dc	202	PEB	NA-C4A-CHA-C1B
26	de	202	PEB	NA-C4A-CHA-C1B
26	dg	202	PEB	NA-C4A-CHA-C1B
26	dJ	202	PEB	NA-C4A-CHA-C1B
26	dU	202	PEB	NA-C4A-CHA-C1B
26	dZ	1002	PEB	NA-C4A-CHA-C1B
26	ec	201	PEB	NA-C4A-CHA-C1B
26	ef	202	PEB	NA-C4A-CHA-C1B
26	eh	202	PEB	NA-C4A-CHA-C1B
26	ei	201	PEB	NA-C4A-CHA-C1B
26	ek	1002	PEB	NA-C4A-CHA-C1B
26	em	202	PEB	NA-C4A-CHA-C1B
26	et	201	PEB	NA-C4A-CHA-C1B
26	eu	202	PEB	NA-C4A-CHA-C1B
26	ev	201	PEB	NA-C4A-CHA-C1B
26	ey	1001	PEB	NA-C4A-CHA-C1B
26	eA	1002	PEB	NA-C4A-CHA-C1B
26	eB	201	PEB	NA-C4A-CHA-C1B
26	eL	201	PEB	NA-C4A-CHA-C1B
26	eP	201	PEB	NA-C4A-CHA-C1B
26	eY	401	PEB	NA-C4A-CHA-C1B
26	lc	202	PEB	NA-C4A-CHA-C1B
26	ld	201	PEB	NA-C4A-CHA-C1B
26	le	202	PEB	NA-C4A-CHA-C1B
26	lg	201	PEB	NA-C4A-CHA-C1B
26	lg	202	PEB	NA-C4A-CHA-C1B
26	lh	201	PEB	NA-C4A-CHA-C1B
26	lj	201	PEB	NA-C4A-CHA-C1B
26	lk	202	PEB	NA-C4A-CHA-C1B
26	lm	1002	PEB	NA-C4A-CHA-C1B
26	lo	201	PEB	NA-C4A-CHA-C1B
26	lo	202	PEB	NA-C4A-CHA-C1B
26	lq	203	PEB	NA-C4A-CHA-C1B
26	ls	202	PEB	NA-C4A-CHA-C1B
26	lt	202	PEB	NA-C4A-CHA-C1B
26	lu	202	PEB	NA-C4A-CHA-C1B
26	lw	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	lw	202	PEB	NA-C4A-CHA-C1B
26	fb	202	PEB	NA-C4A-CHA-C1B
26	fe	202	PEB	NA-C4A-CHA-C1B
26	fg	202	PEB	NA-C4A-CHA-C1B
26	fh	1002	PEB	NA-C4A-CHA-C1B
26	fk	202	PEB	NA-C4A-CHA-C1B
26	fl	202	PEB	NA-C4A-CHA-C1B
26	fn	1002	PEB	NA-C4A-CHA-C1B
26	fp	202	PEB	NA-C4A-CHA-C1B
26	fr	202	PEB	NA-C4A-CHA-C1B
26	ft	202	PEB	NA-C4A-CHA-C1B
26	fv	202	PEB	NA-C4A-CHA-C1B
26	fx	202	PEB	NA-C4A-CHA-C1B
26	fz	301	PEB	NA-C4A-CHA-C1B
26	gb	1002	PEB	NA-C4A-CHA-C1B
26	gc	202	PEB	NA-C4A-CHA-C1B
26	gf	202	PEB	NA-C4A-CHA-C1B
26	gh	202	PEB	NA-C4A-CHA-C1B
26	gj	202	PEB	NA-C4A-CHA-C1B
26	gl	202	PEB	NA-C4A-CHA-C1B
26	gm	1002	PEB	NA-C4A-CHA-C1B
26	go	202	PEB	NA-C4A-CHA-C1B
26	gq	202	PEB	NA-C4A-CHA-C1B
26	gs	202	PEB	NA-C4A-CHA-C1B
26	gu	202	PEB	NA-C4A-CHA-C1B
26	gw	202	PEB	NA-C4A-CHA-C1B
26	gy	302	PEB	NA-C4A-CHA-C1B
26	gz	302	PEB	NA-C4A-CHA-C1B
26	hA	202	PEB	NA-C4A-CHA-C1B
26	hC	202	PEB	NA-C4A-CHA-C1B
26	hE	1002	PEB	NA-C4A-CHA-C1B
26	hF	202	PEB	NA-C4A-CHA-C1B
26	hI	202	PEB	NA-C4A-CHA-C1B
26	hK	202	PEB	NA-C4A-CHA-C1B
26	hM	1002	PEB	NA-C4A-CHA-C1B
26	hO	202	PEB	NA-C4A-CHA-C1B
26	hQ	202	PEB	NA-C4A-CHA-C1B
26	hS	202	PEB	NA-C4A-CHA-C1B
26	hU	201	PEB	NA-C4A-CHA-C1B
26	hW	202	PEB	NA-C4A-CHA-C1B
26	hY	402	PEB	NA-C4A-CHA-C1B
26	hZ	401	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	iA	1002	PEB	NA-C4A-CHA-C1B
26	iB	1002	PEB	NA-C4A-CHA-C1B
26	iF	1002	PEB	NA-C4A-CHA-C1B
29	gy	304	PVN	N1-C4-C5-C6
29	ey	1004	PVN	C9-C10-C11-N3
29	D2	303	PVN	C9-C10-C11-C12
29	d3	302	PVN	C9-C10-C11-C12
28	R3	203	PUB	NC-C1C-CHB-C4B
28	d3	303	PUB	NC-C1C-CHB-C4B
28	B7	202	PUB	NC-C1C-CHB-C4B
28	F7	202	PUB	NC-C1C-CHB-C4B
28	an	202	PUB	NC-C1C-CHB-C4B
28	az	203	PUB	NC-C1C-CHB-C4B
28	cq	203	PUB	NC-C1C-CHB-C4B
28	cY	203	PUB	NC-C1C-CHB-C4B
28	et	203	PUB	NC-C1C-CHB-C4B
28	eN	203	PUB	NC-C1C-CHB-C4B
28	eT	203	PUB	NC-C1C-CHB-C4B
26	A1	301	PEB	NA-C4A-CHA-C1B
26	B1	301	PEB	NA-C4A-CHA-C1B
26	f2	202	PEB	NA-C4A-CHA-C1B
26	h2	202	PEB	NA-C4A-CHA-C1B
26	j2	202	PEB	NA-C4A-CHA-C1B
26	l2	202	PEB	NA-C4A-CHA-C1B
26	n2	202	PEB	NA-C4A-CHA-C1B
26	p2	202	PEB	NA-C4A-CHA-C1B
26	A2	1003	PEB	NA-C4A-CHA-C1B
26	H2	201	PEB	NA-C4A-CHA-C1B
26	L2	202	PEB	NA-C4A-CHA-C1B
26	T2	202	PEB	NA-C4A-CHA-C1B
26	V2	202	PEB	NA-C4A-CHA-C1B
26	X2	202	PEB	NA-C4A-CHA-C1B
26	Z2	202	PEB	NA-C4A-CHA-C1B
26	B3	202	PEB	NA-C4A-CHA-C1B
26	D3	202	PEB	NA-C4A-CHA-C1B
26	F3	202	PEB	NA-C4A-CHA-C1B
26	H3	202	PEB	NA-C4A-CHA-C1B
26	J3	202	PEB	NA-C4A-CHA-C1B
26	L3	202	PEB	NA-C4A-CHA-C1B
26	N3	202	PEB	NA-C4A-CHA-C1B
26	P3	202	PEB	NA-C4A-CHA-C1B
26	R3	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	T3	202	PEB	NA-C4A-CHA-C1B
26	V3	202	PEB	NA-C4A-CHA-C1B
26	W3	203	PEB	NA-C4A-CHA-C1B
26	Z3	202	PEB	NA-C4A-CHA-C1B
26	f3	202	PEB	NA-C4A-CHA-C1B
26	h3	201	PEB	NA-C4A-CHA-C1B
26	i3	203	PEB	NA-C4A-CHA-C1B
26	j3	201	PEB	NA-C4A-CHA-C1B
26	n3	202	PEB	NA-C4A-CHA-C1B
26	p3	202	PEB	NA-C4A-CHA-C1B
26	r3	202	PEB	NA-C4A-CHA-C1B
26	t3	202	PEB	NA-C4A-CHA-C1B
26	v3	202	PEB	NA-C4A-CHA-C1B
26	x3	202	PEB	NA-C4A-CHA-C1B
26	z3	202	PEB	NA-C4A-CHA-C1B
26	B4	202	PEB	NA-C4A-CHA-C1B
26	D4	202	PEB	NA-C4A-CHA-C1B
26	34	1001	PEB	NA-C4A-CHA-C1B
26	34	1002	PEB	NA-C4A-CHA-C1B
26	e4	202	PEB	NA-C4A-CHA-C1B
26	g4	202	PEB	NA-C4A-CHA-C1B
26	j4	202	PEB	NA-C4A-CHA-C1B
26	l4	202	PEB	NA-C4A-CHA-C1B
26	n4	202	PEB	NA-C4A-CHA-C1B
26	p4	202	PEB	NA-C4A-CHA-C1B
26	r4	201	PEB	NA-C4A-CHA-C1B
26	v4	202	PEB	NA-C4A-CHA-C1B
26	A5	203	PEB	NA-C4A-CHA-C1B
26	B5	202	PEB	NA-C4A-CHA-C1B
26	D5	202	PEB	NA-C4A-CHA-C1B
26	F5	202	PEB	NA-C4A-CHA-C1B
26	J5	202	PEB	NA-C4A-CHA-C1B
26	L5	202	PEB	NA-C4A-CHA-C1B
26	N5	202	PEB	NA-C4A-CHA-C1B
26	P5	201	PEB	NA-C4A-CHA-C1B
26	R5	202	PEB	NA-C4A-CHA-C1B
26	S5	203	PEB	NA-C4A-CHA-C1B
26	V5	202	PEB	NA-C4A-CHA-C1B
26	g5	202	PEB	NA-C4A-CHA-C1B
26	m5	1003	PEB	NA-C4A-CHA-C1B
26	n5	202	PEB	NA-C4A-CHA-C1B
26	p5	201	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	r5	202	PEB	NA-C4A-CHA-C1B
26	t5	202	PEB	NA-C4A-CHA-C1B
26	v5	202	PEB	NA-C4A-CHA-C1B
26	z5	202	PEB	NA-C4A-CHA-C1B
26	h8	202	PEB	NA-C4A-CHA-C1B
26	B6	202	PEB	NA-C4A-CHA-C1B
26	J6	202	PEB	NA-C4A-CHA-C1B
26	R6	202	PEB	NA-C4A-CHA-C1B
26	X6	202	PEB	NA-C4A-CHA-C1B
26	n6	202	PEB	NA-C4A-CHA-C1B
26	n8	201	PEB	NA-C4A-CHA-C1B
26	p8	202	PEB	NA-C4A-CHA-C1B
26	B7	201	PEB	NA-C4A-CHA-C1B
26	D7	202	PEB	NA-C4A-CHA-C1B
26	F7	201	PEB	NA-C4A-CHA-C1B
26	H7	202	PEB	NA-C4A-CHA-C1B
26	J7	201	PEB	NA-C4A-CHA-C1B
26	L7	201	PEB	NA-C4A-CHA-C1B
26	N7	202	PEB	NA-C4A-CHA-C1B
26	P7	202	PEB	NA-C4A-CHA-C1B
26	R7	202	PEB	NA-C4A-CHA-C1B
26	T7	202	PEB	NA-C4A-CHA-C1B
26	V7	202	PEB	NA-C4A-CHA-C1B
26	X7	202	PEB	NA-C4A-CHA-C1B
26	Y7	1003	PEB	NA-C4A-CHA-C1B
26	Z7	202	PEB	NA-C4A-CHA-C1B
26	a7	202	PEB	NA-C4A-CHA-C1B
26	c7	202	PEB	NA-C4A-CHA-C1B
26	d7	202	PEB	NA-C4A-CHA-C1B
26	e7	202	PEB	NA-C4A-CHA-C1B
26	l7	202	PEB	NA-C4A-CHA-C1B
26	n7	202	PEB	NA-C4A-CHA-C1B
26	p7	201	PEB	NA-C4A-CHA-C1B
26	r7	202	PEB	NA-C4A-CHA-C1B
26	t7	202	PEB	NA-C4A-CHA-C1B
26	v7	202	PEB	NA-C4A-CHA-C1B
26	x7	202	PEB	NA-C4A-CHA-C1B
26	y7	202	PEB	NA-C4A-CHA-C1B
26	z7	202	PEB	NA-C4A-CHA-C1B
26	y8	202	PEB	NA-C4A-CHA-C1B
26	C8	202	PEB	NA-C4A-CHA-C1B
26	v9	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	B9	202	PEB	NA-C4A-CHA-C1B
26	D9	202	PEB	NA-C4A-CHA-C1B
26	F9	202	PEB	NA-C4A-CHA-C1B
26	H9	202	PEB	NA-C4A-CHA-C1B
26	J9	202	PEB	NA-C4A-CHA-C1B
26	L9	202	PEB	NA-C4A-CHA-C1B
26	N9	202	PEB	NA-C4A-CHA-C1B
26	P9	202	PEB	NA-C4A-CHA-C1B
26	R9	202	PEB	NA-C4A-CHA-C1B
26	T9	202	PEB	NA-C4A-CHA-C1B
26	V9	202	PEB	NA-C4A-CHA-C1B
26	ab	202	PEB	NA-C4A-CHA-C1B
26	ad	202	PEB	NA-C4A-CHA-C1B
26	af	202	PEB	NA-C4A-CHA-C1B
26	ah	202	PEB	NA-C4A-CHA-C1B
26	aj	202	PEB	NA-C4A-CHA-C1B
26	al	202	PEB	NA-C4A-CHA-C1B
26	an	201	PEB	NA-C4A-CHA-C1B
26	ap	202	PEB	NA-C4A-CHA-C1B
26	ar	202	PEB	NA-C4A-CHA-C1B
26	at	202	PEB	NA-C4A-CHA-C1B
26	av	202	PEB	NA-C4A-CHA-C1B
26	ax	201	PEB	NA-C4A-CHA-C1B
26	az	202	PEB	NA-C4A-CHA-C1B
26	aD	202	PEB	NA-C4A-CHA-C1B
26	aF	202	PEB	NA-C4A-CHA-C1B
26	bB	202	PEB	NA-C4A-CHA-C1B
26	bD	202	PEB	NA-C4A-CHA-C1B
26	bF	202	PEB	NA-C4A-CHA-C1B
26	bH	202	PEB	NA-C4A-CHA-C1B
26	bJ	202	PEB	NA-C4A-CHA-C1B
26	bL	202	PEB	NA-C4A-CHA-C1B
26	bN	202	PEB	NA-C4A-CHA-C1B
26	bP	202	PEB	NA-C4A-CHA-C1B
26	bQ	203	PEB	NA-C4A-CHA-C1B
26	bT	201	PEB	NA-C4A-CHA-C1B
26	bV	202	PEB	NA-C4A-CHA-C1B
26	cb	202	PEB	NA-C4A-CHA-C1B
26	cd	202	PEB	NA-C4A-CHA-C1B
26	cf	201	PEB	NA-C4A-CHA-C1B
26	ch	202	PEB	NA-C4A-CHA-C1B
26	cj	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	cl	202	PEB	NA-C4A-CHA-C1B
26	cn	201	PEB	NA-C4A-CHA-C1B
26	co	201	PEB	NA-C4A-CHA-C1B
26	cp	202	PEB	NA-C4A-CHA-C1B
26	cq	202	PEB	NA-C4A-CHA-C1B
26	cr	202	PEB	NA-C4A-CHA-C1B
26	cs	202	PEB	NA-C4A-CHA-C1B
26	cz	202	PEB	NA-C4A-CHA-C1B
26	cB	202	PEB	NA-C4A-CHA-C1B
26	cE	202	PEB	NA-C4A-CHA-C1B
26	cF	201	PEB	NA-C4A-CHA-C1B
26	cH	201	PEB	NA-C4A-CHA-C1B
26	cJ	202	PEB	NA-C4A-CHA-C1B
26	cL	202	PEB	NA-C4A-CHA-C1B
26	cY	202	PEB	NA-C4A-CHA-C1B
26	dd	202	PEB	NA-C4A-CHA-C1B
26	df	202	PEB	NA-C4A-CHA-C1B
26	dh	202	PEB	NA-C4A-CHA-C1B
26	di	202	PEB	NA-C4A-CHA-C1B
26	dj	202	PEB	NA-C4A-CHA-C1B
26	dl	202	PEB	NA-C4A-CHA-C1B
26	dL	202	PEB	NA-C4A-CHA-C1B
26	dV	202	PEB	NA-C4A-CHA-C1B
26	dY	202	PEB	NA-C4A-CHA-C1B
26	ea	203	PEB	NA-C4A-CHA-C1B
26	ec	202	PEB	NA-C4A-CHA-C1B
26	ee	202	PEB	NA-C4A-CHA-C1B
26	eg	202	PEB	NA-C4A-CHA-C1B
26	ei	202	PEB	NA-C4A-CHA-C1B
26	el	202	PEB	NA-C4A-CHA-C1B
26	en	202	PEB	NA-C4A-CHA-C1B
26	ep	202	PEB	NA-C4A-CHA-C1B
26	er	202	PEB	NA-C4A-CHA-C1B
26	et	202	PEB	NA-C4A-CHA-C1B
26	ev	202	PEB	NA-C4A-CHA-C1B
26	eB	203	PEB	NA-C4A-CHA-C1B
26	eJ	202	PEB	NA-C4A-CHA-C1B
26	eL	202	PEB	NA-C4A-CHA-C1B
26	eN	202	PEB	NA-C4A-CHA-C1B
26	eV	202	PEB	NA-C4A-CHA-C1B
26	eX	201	PEB	NA-C4A-CHA-C1B
26	ld	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	lf	202	PEB	NA-C4A-CHA-C1B
26	lh	202	PEB	NA-C4A-CHA-C1B
26	li	203	PEB	NA-C4A-CHA-C1B
26	ll	202	PEB	NA-C4A-CHA-C1B
26	ln	202	PEB	NA-C4A-CHA-C1B
26	lo	203	PEB	NA-C4A-CHA-C1B
26	lp	202	PEB	NA-C4A-CHA-C1B
26	lr	202	PEB	NA-C4A-CHA-C1B
26	lw	203	PEB	NA-C4A-CHA-C1B
26	fc	202	PEB	NA-C4A-CHA-C1B
26	ff	202	PEB	NA-C4A-CHA-C1B
26	fg	201	PEB	NA-C4A-CHA-C1B
26	fi	202	PEB	NA-C4A-CHA-C1B
26	fj	202	PEB	NA-C4A-CHA-C1B
26	fm	202	PEB	NA-C4A-CHA-C1B
26	fo	202	PEB	NA-C4A-CHA-C1B
26	fq	202	PEB	NA-C4A-CHA-C1B
26	fs	202	PEB	NA-C4A-CHA-C1B
26	fu	201	PEB	NA-C4A-CHA-C1B
26	fw	202	PEB	NA-C4A-CHA-C1B
26	fy	201	PEB	NA-C4A-CHA-C1B
26	ga	202	PEB	NA-C4A-CHA-C1B
26	gd	201	PEB	NA-C4A-CHA-C1B
26	ge	202	PEB	NA-C4A-CHA-C1B
26	gg	202	PEB	NA-C4A-CHA-C1B
26	gi	202	PEB	NA-C4A-CHA-C1B
26	gk	202	PEB	NA-C4A-CHA-C1B
26	gn	202	PEB	NA-C4A-CHA-C1B
26	gp	202	PEB	NA-C4A-CHA-C1B
26	gr	201	PEB	NA-C4A-CHA-C1B
26	gt	202	PEB	NA-C4A-CHA-C1B
26	gv	202	PEB	NA-C4A-CHA-C1B
26	gx	202	PEB	NA-C4A-CHA-C1B
26	hB	202	PEB	NA-C4A-CHA-C1B
26	hD	202	PEB	NA-C4A-CHA-C1B
26	hG	201	PEB	NA-C4A-CHA-C1B
26	hH	202	PEB	NA-C4A-CHA-C1B
26	hJ	202	PEB	NA-C4A-CHA-C1B
26	hL	202	PEB	NA-C4A-CHA-C1B
26	hN	202	PEB	NA-C4A-CHA-C1B
26	hP	202	PEB	NA-C4A-CHA-C1B
26	hR	202	PEB	NA-C4A-CHA-C1B

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Mol	Chain	Res	Type	Atoms
26	hT	202	PEB	NA-C4A-CHA-C1B
26	hV	202	PEB	NA-C4A-CHA-C1B
26	hX	202	PEB	NA-C4A-CHA-C1B
26	iC	1002	PEB	NA-C4A-CHA-C1B
26	iD	1002	PEB	NA-C4A-CHA-C1B
26	iE	1002	PEB	NA-C4A-CHA-C1B
26	jI	1002	PEB	NA-C4A-CHA-C1B
26	jJ	1002	PEB	NA-C4A-CHA-C1B
26	jK	1002	PEB	NA-C4A-CHA-C1B
26	jL	1002	PEB	NA-C4A-CHA-C1B
26	jM	1002	PEB	NA-C4A-CHA-C1B
26	jN	1002	PEB	NA-C4A-CHA-C1B
26	jO	1002	PEB	NA-C4A-CHA-C1B
26	jP	1002	PEB	NA-C4A-CHA-C1B
26	kQ	1002	PEB	NA-C4A-CHA-C1B
26	kR	1002	PEB	NA-C4A-CHA-C1B
26	kS	1002	PEB	NA-C4A-CHA-C1B
26	kT	1002	PEB	NA-C4A-CHA-C1B
26	kU	1002	PEB	NA-C4A-CHA-C1B
26	kV	1002	PEB	NA-C4A-CHA-C1B
26	kW	1002	PEB	NA-C4A-CHA-C1B
26	kX	1002	PEB	NA-C4A-CHA-C1B
26	e2	201	PEB	CAC-CBC-CGC-O2C
26	f2	201	PEB	CAC-CBC-CGC-O2C
26	g2	201	PEB	CAC-CBC-CGC-O2C
26	h2	201	PEB	CAC-CBC-CGC-O2C
26	i2	201	PEB	CAC-CBC-CGC-O2C
26	i2	202	PEB	CAC-CBC-CGC-O2C
26	j2	201	PEB	CAC-CBC-CGC-O2C
26	k2	201	PEB	CAC-CBC-CGC-O2C
26	k2	202	PEB	CAC-CBC-CGC-O2C
26	l2	201	PEB	CAC-CBC-CGC-O2C
26	m2	201	PEB	CAC-CBC-CGC-O2C
26	m2	202	PEB	CAC-CBC-CGC-O2C
26	n2	201	PEB	CAC-CBC-CGC-O2C
26	o2	1001	PEB	CAC-CBC-CGC-O2C
26	p2	201	PEB	CAC-CBC-CGC-O2C
26	q2	202	PEB	CAC-CBC-CGC-O2C
26	r2	201	PEB	CAC-CBC-CGC-O2C
26	s2	202	PEB	CAC-CBC-CGC-O2C
26	u2	202	PEB	CAC-CBC-CGC-O2C
26	v2	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	w2	201	PEB	CAC-CBC-CGC-O2C
26	w2	202	PEB	CAC-CBC-CGC-O2C
26	w2	203	PEB	CAC-CBC-CGC-O2C
26	x2	201	PEB	CAC-CBC-CGC-O2C
26	y2	201	PEB	CAC-CBC-CGC-O2C
26	y2	202	PEB	CAC-CBC-CGC-O2C
26	z2	202	PEB	CAC-CBC-CGC-O2C
26	A2	1002	PEB	CAC-CBC-CGC-O2C
26	B2	501	PEB	CAC-CBC-CGC-O2C
26	B2	502	PEB	CAC-CBC-CGC-O2C
26	C2	301	PEB	CAC-CBC-CGC-O2C
26	C2	302	PEB	CAC-CBC-CGC-O2C
26	D2	302	PEB	CAC-CBC-CGC-O2C
26	E2	1001	PEB	CAC-CBC-CGC-O2C
26	F2	201	PEB	CAC-CBC-CGC-O2C
26	F2	202	PEB	CAC-CBC-CGC-O2C
26	G2	201	PEB	CAC-CBC-CGC-O2C
26	G2	202	PEB	CAC-CBC-CGC-O2C
26	I2	201	PEB	CAC-CBC-CGC-O2C
26	J2	201	PEB	CAC-CBC-CGC-O2C
26	K2	201	PEB	CAC-CBC-CGC-O2C
26	L2	201	PEB	CAC-CBC-CGC-O2C
26	M2	201	PEB	CAC-CBC-CGC-O2C
26	N2	202	PEB	CAC-CBC-CGC-O2C
26	O2	201	PEB	CAC-CBC-CGC-O2C
26	P2	201	PEB	CAC-CBC-CGC-O2C
26	Q2	1001	PEB	CAC-CBC-CGC-O2C
26	S2	201	PEB	CAC-CBC-CGC-O2C
26	U2	201	PEB	CAC-CBC-CGC-O2C
26	V2	201	PEB	CAC-CBC-CGC-O2C
26	W2	201	PEB	CAC-CBC-CGC-O2C
26	Y2	201	PEB	CAC-CBC-CGC-O2C
26	Y2	202	PEB	CAC-CBC-CGC-O2C
26	A3	201	PEB	CAC-CBC-CGC-O2C
26	C3	1001	PEB	CAC-CBC-CGC-O2C
26	D3	201	PEB	CAC-CBC-CGC-O2C
26	F3	201	PEB	CAC-CBC-CGC-O2C
26	G3	201	PEB	CAC-CBC-CGC-O2C
26	H3	201	PEB	CAC-CBC-CGC-O2C
26	K3	201	PEB	CAC-CBC-CGC-O2C
26	L3	201	PEB	CAC-CBC-CGC-O2C
26	M3	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	N3	201	PEB	CAC-CBC-CGC-O2C
26	O3	1001	PEB	CAC-CBC-CGC-O2C
26	P3	201	PEB	CAC-CBC-CGC-O2C
26	S3	201	PEB	CAC-CBC-CGC-O2C
26	S3	203	PEB	CAC-CBC-CGC-O2C
26	T3	201	PEB	CAC-CBC-CGC-O2C
26	U3	201	PEB	CAC-CBC-CGC-O2C
26	V3	201	PEB	CAC-CBC-CGC-O2C
26	W3	201	PEB	CAC-CBC-CGC-O2C
26	Y3	201	PEB	CAC-CBC-CGC-O2C
26	Z3	201	PEB	CAC-CBC-CGC-O2C
26	a3	1001	PEB	CAC-CBC-CGC-O2C
26	a3	1003	PEB	CAC-CBC-CGC-O2C
26	b3	501	PEB	CAC-CBC-CGC-O2C
26	b3	502	PEB	CAC-CBC-CGC-O2C
26	c3	302	PEB	CAC-CBC-CGC-O2C
26	g3	201	PEB	CAC-CBC-CGC-O2C
26	i3	201	PEB	CAC-CBC-CGC-O2C
26	k3	201	PEB	CAC-CBC-CGC-O2C
26	l3	201	PEB	CAC-CBC-CGC-O2C
26	m3	201	PEB	CAC-CBC-CGC-O2C
26	n3	201	PEB	CAC-CBC-CGC-O2C
26	p3	201	PEB	CAC-CBC-CGC-O2C
26	q3	1001	PEB	CAC-CBC-CGC-O2C
26	r3	201	PEB	CAC-CBC-CGC-O2C
26	u3	201	PEB	CAC-CBC-CGC-O2C
26	v3	201	PEB	CAC-CBC-CGC-O2C
26	w3	201	PEB	CAC-CBC-CGC-O2C
26	x3	201	PEB	CAC-CBC-CGC-O2C
26	y3	201	PEB	CAC-CBC-CGC-O2C
26	z3	201	PEB	CAC-CBC-CGC-O2C
26	A4	201	PEB	CAC-CBC-CGC-O2C
26	B4	201	PEB	CAC-CBC-CGC-O2C
26	C4	1001	PEB	CAC-CBC-CGC-O2C
26	E4	201	PEB	CAC-CBC-CGC-O2C
26	E4	202	PEB	CAC-CBC-CGC-O2C
26	F4	201	PEB	CAC-CBC-CGC-O2C
26	F4	202	PEB	CAC-CBC-CGC-O2C
26	G4	202	PEB	CAC-CBC-CGC-O2C
26	H4	201	PEB	CAC-CBC-CGC-O2C
26	H4	202	PEB	CAC-CBC-CGC-O2C
26	I4	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	J4	201	PEB	CAC-CBC-CGC-O2C
26	L4	201	PEB	CAC-CBC-CGC-O2C
26	L4	202	PEB	CAC-CBC-CGC-O2C
26	M4	202	PEB	CAC-CBC-CGC-O2C
26	N4	201	PEB	CAC-CBC-CGC-O2C
26	O4	1001	PEB	CAC-CBC-CGC-O2C
26	O4	1002	PEB	CAC-CBC-CGC-O2C
26	P4	201	PEB	CAC-CBC-CGC-O2C
26	P4	202	PEB	CAC-CBC-CGC-O2C
26	Q4	201	PEB	CAC-CBC-CGC-O2C
26	Q4	203	PEB	CAC-CBC-CGC-O2C
26	R4	201	PEB	CAC-CBC-CGC-O2C
26	R4	202	PEB	CAC-CBC-CGC-O2C
26	S4	202	PEB	CAC-CBC-CGC-O2C
26	T4	201	PEB	CAC-CBC-CGC-O2C
26	U4	202	PEB	CAC-CBC-CGC-O2C
26	V4	201	PEB	CAC-CBC-CGC-O2C
26	X4	201	PEB	CAC-CBC-CGC-O2C
26	Y4	201	PEB	CAC-CBC-CGC-O2C
26	Z4	201	PEB	CAC-CBC-CGC-O2C
26	34	1007	PEB	CAC-CBC-CGC-O2C
26	44	302	PEB	CAC-CBC-CGC-O2C
26	c4	202	PEB	CAC-CBC-CGC-O2C
26	d4	201	PEB	CAC-CBC-CGC-O2C
26	e4	201	PEB	CAC-CBC-CGC-O2C
26	f4	201	PEB	CAC-CBC-CGC-O2C
26	g4	201	PEB	CAC-CBC-CGC-O2C
26	h4	202	PEB	CAC-CBC-CGC-O2C
26	i4	201	PEB	CAC-CBC-CGC-O2C
26	j4	201	PEB	CAC-CBC-CGC-O2C
26	k4	201	PEB	CAC-CBC-CGC-O2C
26	l4	201	PEB	CAC-CBC-CGC-O2C
26	n4	201	PEB	CAC-CBC-CGC-O2C
26	o4	202	PEB	CAC-CBC-CGC-O2C
26	q4	201	PEB	CAC-CBC-CGC-O2C
26	q4	202	PEB	CAC-CBC-CGC-O2C
26	s4	201	PEB	CAC-CBC-CGC-O2C
26	t4	201	PEB	CAC-CBC-CGC-O2C
26	u4	201	PEB	CAC-CBC-CGC-O2C
26	u4	202	PEB	CAC-CBC-CGC-O2C
26	w4	201	PEB	CAC-CBC-CGC-O2C
26	x4	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	y4	1001	PEB	CAC-CBC-CGC-O2C
26	y4	1002	PEB	CAC-CBC-CGC-O2C
26	B5	201	PEB	CAC-CBC-CGC-O2C
26	D5	201	PEB	CAC-CBC-CGC-O2C
26	E5	201	PEB	CAC-CBC-CGC-O2C
26	F5	201	PEB	CAC-CBC-CGC-O2C
26	G5	201	PEB	CAC-CBC-CGC-O2C
26	H5	201	PEB	CAC-CBC-CGC-O2C
26	I5	201	PEB	CAC-CBC-CGC-O2C
26	M5	201	PEB	CAC-CBC-CGC-O2C
26	N5	201	PEB	CAC-CBC-CGC-O2C
26	O5	201	PEB	CAC-CBC-CGC-O2C
26	Q5	201	PEB	CAC-CBC-CGC-O2C
26	R5	201	PEB	CAC-CBC-CGC-O2C
26	S5	201	PEB	CAC-CBC-CGC-O2C
26	T5	201	PEB	CAC-CBC-CGC-O2C
26	U5	201	PEB	CAC-CBC-CGC-O2C
26	V5	201	PEB	CAC-CBC-CGC-O2C
26	W5	301	PEB	CAC-CBC-CGC-O2C
26	X5	401	PEB	CAC-CBC-CGC-O2C
26	Y5	1001	PEB	CAC-CBC-CGC-O2C
26	Z5	303	PEB	CAC-CBC-CGC-O2C
26	a5	201	PEB	CAC-CBC-CGC-O2C
26	b5	1001	PEB	CAC-CBC-CGC-O2C
26	c5	202	PEB	CAC-CBC-CGC-O2C
26	h5	201	PEB	CAC-CBC-CGC-O2C
26	i5	201	PEB	CAC-CBC-CGC-O2C
26	j5	201	PEB	CAC-CBC-CGC-O2C
26	j5	202	PEB	CAC-CBC-CGC-O2C
26	k5	201	PEB	CAC-CBC-CGC-O2C
26	l5	201	PEB	CAC-CBC-CGC-O2C
26	l5	202	PEB	CAC-CBC-CGC-O2C
26	m5	1001	PEB	CAC-CBC-CGC-O2C
26	n5	201	PEB	CAC-CBC-CGC-O2C
26	o5	201	PEB	CAC-CBC-CGC-O2C
26	t5	201	PEB	CAC-CBC-CGC-O2C
26	v5	201	PEB	CAC-CBC-CGC-O2C
26	w5	201	PEB	CAC-CBC-CGC-O2C
26	x5	201	PEB	CAC-CBC-CGC-O2C
26	y5	1001	PEB	CAC-CBC-CGC-O2C
26	z5	201	PEB	CAC-CBC-CGC-O2C
26	f8	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	f8	202	PEB	CAC-CBC-CGC-O2C
26	g8	201	PEB	CAC-CBC-CGC-O2C
26	i8	201	PEB	CAC-CBC-CGC-O2C
26	j8	202	PEB	CAC-CBC-CGC-O2C
26	k8	201	PEB	CAC-CBC-CGC-O2C
26	k8	202	PEB	CAC-CBC-CGC-O2C
26	k8	203	PEB	CAC-CBC-CGC-O2C
26	l8	201	PEB	CAC-CBC-CGC-O2C
26	m8	201	PEB	CAC-CBC-CGC-O2C
26	A6	1002	PEB	CAC-CBC-CGC-O2C
26	B6	201	PEB	CAC-CBC-CGC-O2C
26	C6	201	PEB	CAC-CBC-CGC-O2C
26	C6	202	PEB	CAC-CBC-CGC-O2C
26	D6	201	PEB	CAC-CBC-CGC-O2C
26	E6	201	PEB	CAC-CBC-CGC-O2C
26	F6	201	PEB	CAC-CBC-CGC-O2C
26	F6	202	PEB	CAC-CBC-CGC-O2C
26	G6	201	PEB	CAC-CBC-CGC-O2C
26	I6	202	PEB	CAC-CBC-CGC-O2C
26	K6	201	PEB	CAC-CBC-CGC-O2C
26	K6	202	PEB	CAC-CBC-CGC-O2C
26	M6	1001	PEB	CAC-CBC-CGC-O2C
26	M6	1002	PEB	CAC-CBC-CGC-O2C
26	N6	201	PEB	CAC-CBC-CGC-O2C
26	O6	201	PEB	CAC-CBC-CGC-O2C
26	O6	202	PEB	CAC-CBC-CGC-O2C
26	P6	202	PEB	CAC-CBC-CGC-O2C
26	Q6	201	PEB	CAC-CBC-CGC-O2C
26	Q6	202	PEB	CAC-CBC-CGC-O2C
26	R6	201	PEB	CAC-CBC-CGC-O2C
26	S6	202	PEB	CAC-CBC-CGC-O2C
26	T6	201	PEB	CAC-CBC-CGC-O2C
26	V6	201	PEB	CAC-CBC-CGC-O2C
26	W6	201	PEB	CAC-CBC-CGC-O2C
26	W6	202	PEB	CAC-CBC-CGC-O2C
26	X6	201	PEB	CAC-CBC-CGC-O2C
26	Y6	201	PEB	CAC-CBC-CGC-O2C
26	Z6	201	PEB	CAC-CBC-CGC-O2C
26	a6	201	PEB	CAC-CBC-CGC-O2C
26	b6	201	PEB	CAC-CBC-CGC-O2C
26	b6	202	PEB	CAC-CBC-CGC-O2C
26	c6	1001	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	c6	1003	PEB	CAC-CBC-CGC-O2C
26	d6	201	PEB	CAC-CBC-CGC-O2C
26	g6	201	PEB	CAC-CBC-CGC-O2C
26	g6	202	PEB	CAC-CBC-CGC-O2C
26	h6	201	PEB	CAC-CBC-CGC-O2C
26	h6	202	PEB	CAC-CBC-CGC-O2C
26	i6	201	PEB	CAC-CBC-CGC-O2C
26	i6	202	PEB	CAC-CBC-CGC-O2C
26	j6	201	PEB	CAC-CBC-CGC-O2C
26	j6	202	PEB	CAC-CBC-CGC-O2C
26	k6	1001	PEB	CAC-CBC-CGC-O2C
26	l6	201	PEB	CAC-CBC-CGC-O2C
26	l6	202	PEB	CAC-CBC-CGC-O2C
26	m6	202	PEB	CAC-CBC-CGC-O2C
26	o6	201	PEB	CAC-CBC-CGC-O2C
26	p6	201	PEB	CAC-CBC-CGC-O2C
26	q6	201	PEB	CAC-CBC-CGC-O2C
26	q6	202	PEB	CAC-CBC-CGC-O2C
26	r6	201	PEB	CAC-CBC-CGC-O2C
26	r6	202	PEB	CAC-CBC-CGC-O2C
26	s6	201	PEB	CAC-CBC-CGC-O2C
26	t6	202	PEB	CAC-CBC-CGC-O2C
26	u6	202	PEB	CAC-CBC-CGC-O2C
26	v6	202	PEB	CAC-CBC-CGC-O2C
26	w6	1001	PEB	CAC-CBC-CGC-O2C
26	w6	1002	PEB	CAC-CBC-CGC-O2C
26	x6	201	PEB	CAC-CBC-CGC-O2C
26	x6	202	PEB	CAC-CBC-CGC-O2C
26	y6	201	PEB	CAC-CBC-CGC-O2C
26	y6	202	PEB	CAC-CBC-CGC-O2C
26	z6	201	PEB	CAC-CBC-CGC-O2C
26	z6	202	PEB	CAC-CBC-CGC-O2C
26	o8	202	PEB	CAC-CBC-CGC-O2C
26	r8	201	PEB	CAC-CBC-CGC-O2C
26	s8	201	PEB	CAC-CBC-CGC-O2C
26	t8	201	PEB	CAC-CBC-CGC-O2C
26	u8	201	PEB	CAC-CBC-CGC-O2C
26	C7	201	PEB	CAC-CBC-CGC-O2C
26	D7	201	PEB	CAC-CBC-CGC-O2C
26	E7	201	PEB	CAC-CBC-CGC-O2C
26	I7	201	PEB	CAC-CBC-CGC-O2C
26	K7	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	M7	1001	PEB	CAC-CBC-CGC-O2C
26	M7	1002	PEB	CAC-CBC-CGC-O2C
26	P7	201	PEB	CAC-CBC-CGC-O2C
26	Q7	201	PEB	CAC-CBC-CGC-O2C
26	R7	201	PEB	CAC-CBC-CGC-O2C
26	T7	201	PEB	CAC-CBC-CGC-O2C
26	U7	201	PEB	CAC-CBC-CGC-O2C
26	V7	201	PEB	CAC-CBC-CGC-O2C
26	X7	201	PEB	CAC-CBC-CGC-O2C
26	Y7	1001	PEB	CAC-CBC-CGC-O2C
26	Z7	201	PEB	CAC-CBC-CGC-O2C
26	b7	201	PEB	CAC-CBC-CGC-O2C
26	c7	201	PEB	CAC-CBC-CGC-O2C
26	d7	201	PEB	CAC-CBC-CGC-O2C
26	g7	201	PEB	CAC-CBC-CGC-O2C
26	h7	201	PEB	CAC-CBC-CGC-O2C
26	i7	201	PEB	CAC-CBC-CGC-O2C
26	k7	1001	PEB	CAC-CBC-CGC-O2C
26	l7	201	PEB	CAC-CBC-CGC-O2C
26	m7	201	PEB	CAC-CBC-CGC-O2C
26	q7	201	PEB	CAC-CBC-CGC-O2C
26	r7	201	PEB	CAC-CBC-CGC-O2C
26	v7	201	PEB	CAC-CBC-CGC-O2C
26	x7	201	PEB	CAC-CBC-CGC-O2C
26	y7	201	PEB	CAC-CBC-CGC-O2C
26	z7	201	PEB	CAC-CBC-CGC-O2C
26	a8	601	PEB	CAC-CBC-CGC-O2C
26	b8	1001	PEB	CAC-CBC-CGC-O2C
26	b8	1002	PEB	CAC-CBC-CGC-O2C
26	b8	1003	PEB	CAC-CBC-CGC-O2C
26	e8	301	PEB	CAC-CBC-CGC-O2C
26	e8	302	PEB	CAC-CBC-CGC-O2C
26	a9	601	PEB	CAC-CBC-CGC-O2C
26	a9	603	PEB	CAC-CBC-CGC-O2C
26	b9	401	PEB	CAC-CBC-CGC-O2C
26	b9	402	PEB	CAC-CBC-CGC-O2C
26	b9	403	PEB	CAC-CBC-CGC-O2C
26	b9	404	PEB	CAC-CBC-CGC-O2C
26	c9	301	PEB	CAC-CBC-CGC-O2C
26	c9	302	PEB	CAC-CBC-CGC-O2C
26	d9	302	PEB	CAC-CBC-CGC-O2C
26	d9	303	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	e9	301	PEB	CAC-CBC-CGC-O2C
26	e9	302	PEB	CAC-CBC-CGC-O2C
26	e9	303	PEB	CAC-CBC-CGC-O2C
26	v8	201	PEB	CAC-CBC-CGC-O2C
26	v8	202	PEB	CAC-CBC-CGC-O2C
26	w8	201	PEB	CAC-CBC-CGC-O2C
26	w8	202	PEB	CAC-CBC-CGC-O2C
26	x8	201	PEB	CAC-CBC-CGC-O2C
26	x8	202	PEB	CAC-CBC-CGC-O2C
26	y8	201	PEB	CAC-CBC-CGC-O2C
26	z8	201	PEB	CAC-CBC-CGC-O2C
26	z8	202	PEB	CAC-CBC-CGC-O2C
26	A8	201	PEB	CAC-CBC-CGC-O2C
26	A8	202	PEB	CAC-CBC-CGC-O2C
26	B8	201	PEB	CAC-CBC-CGC-O2C
26	B8	202	PEB	CAC-CBC-CGC-O2C
26	D8	201	PEB	CAC-CBC-CGC-O2C
26	D8	202	PEB	CAC-CBC-CGC-O2C
26	E8	201	PEB	CAC-CBC-CGC-O2C
26	F8	1001	PEB	CAC-CBC-CGC-O2C
26	G8	201	PEB	CAC-CBC-CGC-O2C
26	G8	202	PEB	CAC-CBC-CGC-O2C
26	H8	201	PEB	CAC-CBC-CGC-O2C
26	H8	202	PEB	CAC-CBC-CGC-O2C
26	I8	202	PEB	CAC-CBC-CGC-O2C
26	J8	201	PEB	CAC-CBC-CGC-O2C
26	J8	202	PEB	CAC-CBC-CGC-O2C
26	K8	201	PEB	CAC-CBC-CGC-O2C
26	K8	202	PEB	CAC-CBC-CGC-O2C
26	L8	201	PEB	CAC-CBC-CGC-O2C
26	L8	202	PEB	CAC-CBC-CGC-O2C
26	M8	201	PEB	CAC-CBC-CGC-O2C
26	M8	202	PEB	CAC-CBC-CGC-O2C
26	N8	201	PEB	CAC-CBC-CGC-O2C
26	N8	202	PEB	CAC-CBC-CGC-O2C
26	Q8	201	PEB	CAC-CBC-CGC-O2C
26	Q8	202	PEB	CAC-CBC-CGC-O2C
26	T8	301	PEB	CAC-CBC-CGC-O2C
26	U8	1002	PEB	CAC-CBC-CGC-O2C
26	U8	1003	PEB	CAC-CBC-CGC-O2C
26	V8	1001	PEB	CAC-CBC-CGC-O2C
26	W8	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	Y8	201	PEB	CAC-CBC-CGC-O2C
26	Z8	201	PEB	CAC-CBC-CGC-O2C
26	h9	201	PEB	CAC-CBC-CGC-O2C
26	h9	202	PEB	CAC-CBC-CGC-O2C
26	i9	201	PEB	CAC-CBC-CGC-O2C
26	j9	201	PEB	CAC-CBC-CGC-O2C
26	j9	202	PEB	CAC-CBC-CGC-O2C
26	k9	201	PEB	CAC-CBC-CGC-O2C
26	l9	201	PEB	CAC-CBC-CGC-O2C
26	m9	1001	PEB	CAC-CBC-CGC-O2C
26	o9	201	PEB	CAC-CBC-CGC-O2C
26	p9	201	PEB	CAC-CBC-CGC-O2C
26	p9	202	PEB	CAC-CBC-CGC-O2C
26	q9	201	PEB	CAC-CBC-CGC-O2C
26	r9	201	PEB	CAC-CBC-CGC-O2C
26	r9	202	PEB	CAC-CBC-CGC-O2C
26	s9	202	PEB	CAC-CBC-CGC-O2C
26	t9	201	PEB	CAC-CBC-CGC-O2C
26	u9	201	PEB	CAC-CBC-CGC-O2C
26	v9	201	PEB	CAC-CBC-CGC-O2C
26	w9	201	PEB	CAC-CBC-CGC-O2C
26	w9	202	PEB	CAC-CBC-CGC-O2C
26	x9	201	PEB	CAC-CBC-CGC-O2C
26	x9	202	PEB	CAC-CBC-CGC-O2C
26	y9	1002	PEB	CAC-CBC-CGC-O2C
26	z9	201	PEB	CAC-CBC-CGC-O2C
26	z9	202	PEB	CAC-CBC-CGC-O2C
26	A9	201	PEB	CAC-CBC-CGC-O2C
26	B9	201	PEB	CAC-CBC-CGC-O2C
26	C9	201	PEB	CAC-CBC-CGC-O2C
26	F9	201	PEB	CAC-CBC-CGC-O2C
26	G9	201	PEB	CAC-CBC-CGC-O2C
26	I9	201	PEB	CAC-CBC-CGC-O2C
26	K9	1001	PEB	CAC-CBC-CGC-O2C
26	N9	201	PEB	CAC-CBC-CGC-O2C
26	O9	201	PEB	CAC-CBC-CGC-O2C
26	P9	201	PEB	CAC-CBC-CGC-O2C
26	Q9	201	PEB	CAC-CBC-CGC-O2C
26	R9	201	PEB	CAC-CBC-CGC-O2C
26	T9	201	PEB	CAC-CBC-CGC-O2C
26	V9	201	PEB	CAC-CBC-CGC-O2C
26	X9	401	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	Y9	302	PEB	CAC-CBC-CGC-O2C
26	Z9	1003	PEB	CAC-CBC-CGC-O2C
26	Z9	1007	PEB	CAC-CBC-CGC-O2C
26	aa	1001	PEB	CAC-CBC-CGC-O2C
26	ab	201	PEB	CAC-CBC-CGC-O2C
26	ac	201	PEB	CAC-CBC-CGC-O2C
26	ad	201	PEB	CAC-CBC-CGC-O2C
26	ae	201	PEB	CAC-CBC-CGC-O2C
26	af	201	PEB	CAC-CBC-CGC-O2C
26	ag	201	PEB	CAC-CBC-CGC-O2C
26	ai	201	PEB	CAC-CBC-CGC-O2C
26	aj	201	PEB	CAC-CBC-CGC-O2C
26	am	1001	PEB	CAC-CBC-CGC-O2C
26	ao	201	PEB	CAC-CBC-CGC-O2C
26	ap	201	PEB	CAC-CBC-CGC-O2C
26	aq	201	PEB	CAC-CBC-CGC-O2C
26	as	201	PEB	CAC-CBC-CGC-O2C
26	at	201	PEB	CAC-CBC-CGC-O2C
26	au	201	PEB	CAC-CBC-CGC-O2C
26	av	201	PEB	CAC-CBC-CGC-O2C
26	aw	201	PEB	CAC-CBC-CGC-O2C
26	ay	1001	PEB	CAC-CBC-CGC-O2C
26	aA	201	PEB	CAC-CBC-CGC-O2C
26	aA	202	PEB	CAC-CBC-CGC-O2C
26	aB	202	PEB	CAC-CBC-CGC-O2C
26	aD	201	PEB	CAC-CBC-CGC-O2C
26	aE	201	PEB	CAC-CBC-CGC-O2C
26	aE	202	PEB	CAC-CBC-CGC-O2C
26	aF	201	PEB	CAC-CBC-CGC-O2C
26	aF	204	PEB	CAC-CBC-CGC-O2C
26	aG	201	PEB	CAC-CBC-CGC-O2C
26	aH	201	PEB	CAC-CBC-CGC-O2C
26	aH	202	PEB	CAC-CBC-CGC-O2C
26	aI	201	PEB	CAC-CBC-CGC-O2C
26	aI	202	PEB	CAC-CBC-CGC-O2C
26	aJ	201	PEB	CAC-CBC-CGC-O2C
26	aJ	202	PEB	CAC-CBC-CGC-O2C
26	aK	1001	PEB	CAC-CBC-CGC-O2C
26	aK	1002	PEB	CAC-CBC-CGC-O2C
26	aL	201	PEB	CAC-CBC-CGC-O2C
26	aL	202	PEB	CAC-CBC-CGC-O2C
26	aM	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	aN	201	PEB	CAC-CBC-CGC-O2C
26	aN	202	PEB	CAC-CBC-CGC-O2C
26	aN	204	PEB	CAC-CBC-CGC-O2C
26	aP	201	PEB	CAC-CBC-CGC-O2C
26	aP	202	PEB	CAC-CBC-CGC-O2C
26	aQ	202	PEB	CAC-CBC-CGC-O2C
26	aR	201	PEB	CAC-CBC-CGC-O2C
26	aR	202	PEB	CAC-CBC-CGC-O2C
26	aS	202	PEB	CAC-CBC-CGC-O2C
26	aT	201	PEB	CAC-CBC-CGC-O2C
26	aT	202	PEB	CAC-CBC-CGC-O2C
26	aU	201	PEB	CAC-CBC-CGC-O2C
26	aU	202	PEB	CAC-CBC-CGC-O2C
26	aV	201	PEB	CAC-CBC-CGC-O2C
26	aV	202	PEB	CAC-CBC-CGC-O2C
26	aW	301	PEB	CAC-CBC-CGC-O2C
26	aW	302	PEB	CAC-CBC-CGC-O2C
26	aX	401	PEB	CAC-CBC-CGC-O2C
26	aX	402	PEB	CAC-CBC-CGC-O2C
26	aY	401	PEB	CAC-CBC-CGC-O2C
26	aY	402	PEB	CAC-CBC-CGC-O2C
26	aZ	301	PEB	CAC-CBC-CGC-O2C
26	aZ	302	PEB	CAC-CBC-CGC-O2C
26	bb	201	PEB	CAC-CBC-CGC-O2C
26	bc	201	PEB	CAC-CBC-CGC-O2C
26	bd	201	PEB	CAC-CBC-CGC-O2C
26	bd	202	PEB	CAC-CBC-CGC-O2C
26	be	201	PEB	CAC-CBC-CGC-O2C
26	bf	201	PEB	CAC-CBC-CGC-O2C
26	bg	201	PEB	CAC-CBC-CGC-O2C
26	bh	201	PEB	CAC-CBC-CGC-O2C
26	bh	202	PEB	CAC-CBC-CGC-O2C
26	bi	201	PEB	CAC-CBC-CGC-O2C
26	bl	201	PEB	CAC-CBC-CGC-O2C
26	bl	202	PEB	CAC-CBC-CGC-O2C
26	bm	1002	PEB	CAC-CBC-CGC-O2C
26	bn	201	PEB	CAC-CBC-CGC-O2C
26	bo	201	PEB	CAC-CBC-CGC-O2C
26	bp	201	PEB	CAC-CBC-CGC-O2C
26	bq	201	PEB	CAC-CBC-CGC-O2C
26	bq	202	PEB	CAC-CBC-CGC-O2C
26	br	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	br	202	PEB	CAC-CBC-CGC-O2C
26	bs	1001	PEB	CAC-CBC-CGC-O2C
26	bs	1002	PEB	CAC-CBC-CGC-O2C
26	bt	201	PEB	CAC-CBC-CGC-O2C
26	bt	202	PEB	CAC-CBC-CGC-O2C
26	bu	201	PEB	CAC-CBC-CGC-O2C
26	bu	202	PEB	CAC-CBC-CGC-O2C
26	bv	202	PEB	CAC-CBC-CGC-O2C
26	bw	201	PEB	CAC-CBC-CGC-O2C
26	bw	202	PEB	CAC-CBC-CGC-O2C
26	bx	201	PEB	CAC-CBC-CGC-O2C
26	bx	202	PEB	CAC-CBC-CGC-O2C
26	bz	201	PEB	CAC-CBC-CGC-O2C
26	bz	202	PEB	CAC-CBC-CGC-O2C
26	bA	201	PEB	CAC-CBC-CGC-O2C
26	bC	201	PEB	CAC-CBC-CGC-O2C
26	bD	201	PEB	CAC-CBC-CGC-O2C
26	bI	201	PEB	CAC-CBC-CGC-O2C
26	bL	201	PEB	CAC-CBC-CGC-O2C
26	bN	201	PEB	CAC-CBC-CGC-O2C
26	bO	201	PEB	CAC-CBC-CGC-O2C
26	bP	201	PEB	CAC-CBC-CGC-O2C
26	bR	201	PEB	CAC-CBC-CGC-O2C
26	bV	201	PEB	CAC-CBC-CGC-O2C
26	bW	301	PEB	CAC-CBC-CGC-O2C
26	bX	401	PEB	CAC-CBC-CGC-O2C
26	bX	402	PEB	CAC-CBC-CGC-O2C
26	bY	1001	PEB	CAC-CBC-CGC-O2C
26	bY	1003	PEB	CAC-CBC-CGC-O2C
26	bZ	303	PEB	CAC-CBC-CGC-O2C
26	ca	1001	PEB	CAC-CBC-CGC-O2C
26	cb	201	PEB	CAC-CBC-CGC-O2C
26	cc	201	PEB	CAC-CBC-CGC-O2C
26	ch	201	PEB	CAC-CBC-CGC-O2C
26	ci	201	PEB	CAC-CBC-CGC-O2C
26	ck	201	PEB	CAC-CBC-CGC-O2C
26	cl	201	PEB	CAC-CBC-CGC-O2C
26	cm	1001	PEB	CAC-CBC-CGC-O2C
26	cr	201	PEB	CAC-CBC-CGC-O2C
26	cs	201	PEB	CAC-CBC-CGC-O2C
26	cu	201	PEB	CAC-CBC-CGC-O2C
26	cv	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	cw	201	PEB	CAC-CBC-CGC-O2C
26	cB	201	PEB	CAC-CBC-CGC-O2C
26	cC	1003	PEB	CAC-CBC-CGC-O2C
26	cE	201	PEB	CAC-CBC-CGC-O2C
26	cG	201	PEB	CAC-CBC-CGC-O2C
26	cI	201	PEB	CAC-CBC-CGC-O2C
26	cJ	201	PEB	CAC-CBC-CGC-O2C
26	cK	201	PEB	CAC-CBC-CGC-O2C
26	cM	201	PEB	CAC-CBC-CGC-O2C
26	cM	202	PEB	CAC-CBC-CGC-O2C
26	cN	201	PEB	CAC-CBC-CGC-O2C
26	cO	201	PEB	CAC-CBC-CGC-O2C
26	cP	201	PEB	CAC-CBC-CGC-O2C
26	cQ	201	PEB	CAC-CBC-CGC-O2C
26	cR	201	PEB	CAC-CBC-CGC-O2C
26	cR	202	PEB	CAC-CBC-CGC-O2C
26	cS	201	PEB	CAC-CBC-CGC-O2C
26	cS	202	PEB	CAC-CBC-CGC-O2C
26	cT	1002	PEB	CAC-CBC-CGC-O2C
26	cV	201	PEB	CAC-CBC-CGC-O2C
26	cV	203	PEB	CAC-CBC-CGC-O2C
26	cW	201	PEB	CAC-CBC-CGC-O2C
26	cW	202	PEB	CAC-CBC-CGC-O2C
26	cX	201	PEB	CAC-CBC-CGC-O2C
26	cX	202	PEB	CAC-CBC-CGC-O2C
26	cY	201	PEB	CAC-CBC-CGC-O2C
26	cZ	201	PEB	CAC-CBC-CGC-O2C
26	da	1001	PEB	CAC-CBC-CGC-O2C
26	db	201	PEB	CAC-CBC-CGC-O2C
26	dc	201	PEB	CAC-CBC-CGC-O2C
26	dc	203	PEB	CAC-CBC-CGC-O2C
26	dd	201	PEB	CAC-CBC-CGC-O2C
26	de	201	PEB	CAC-CBC-CGC-O2C
26	df	201	PEB	CAC-CBC-CGC-O2C
26	dh	201	PEB	CAC-CBC-CGC-O2C
26	di	201	PEB	CAC-CBC-CGC-O2C
26	dk	1001	PEB	CAC-CBC-CGC-O2C
26	dm	202	PEB	CAC-CBC-CGC-O2C
26	dn	201	PEB	CAC-CBC-CGC-O2C
26	dn	202	PEB	CAC-CBC-CGC-O2C
26	do	201	PEB	CAC-CBC-CGC-O2C
26	do	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	dp	202	PEB	CAC-CBC-CGC-O2C
26	dq	201	PEB	CAC-CBC-CGC-O2C
26	dq	202	PEB	CAC-CBC-CGC-O2C
26	dr	202	PEB	CAC-CBC-CGC-O2C
26	ds	201	PEB	CAC-CBC-CGC-O2C
26	ds	202	PEB	CAC-CBC-CGC-O2C
26	dt	201	PEB	CAC-CBC-CGC-O2C
26	dt	202	PEB	CAC-CBC-CGC-O2C
26	du	201	PEB	CAC-CBC-CGC-O2C
26	du	202	PEB	CAC-CBC-CGC-O2C
26	du	203	PEB	CAC-CBC-CGC-O2C
26	dv	201	PEB	CAC-CBC-CGC-O2C
26	dw	401	PEB	CAC-CBC-CGC-O2C
26	dw	402	PEB	CAC-CBC-CGC-O2C
26	dw	403	PEB	CAC-CBC-CGC-O2C
26	dx	402	PEB	CAC-CBC-CGC-O2C
26	dx	403	PEB	CAC-CBC-CGC-O2C
26	dy	401	PEB	CAC-CBC-CGC-O2C
26	dz	401	PEB	CAC-CBC-CGC-O2C
26	dz	402	PEB	CAC-CBC-CGC-O2C
26	dA	201	PEB	CAC-CBC-CGC-O2C
26	dA	202	PEB	CAC-CBC-CGC-O2C
26	dB	201	PEB	CAC-CBC-CGC-O2C
26	dC	201	PEB	CAC-CBC-CGC-O2C
26	dC	202	PEB	CAC-CBC-CGC-O2C
26	dD	201	PEB	CAC-CBC-CGC-O2C
26	dE	201	PEB	CAC-CBC-CGC-O2C
26	dF	202	PEB	CAC-CBC-CGC-O2C
26	dG	202	PEB	CAC-CBC-CGC-O2C
26	dH	201	PEB	CAC-CBC-CGC-O2C
26	dH	202	PEB	CAC-CBC-CGC-O2C
26	dI	1001	PEB	CAC-CBC-CGC-O2C
26	dI	1002	PEB	CAC-CBC-CGC-O2C
26	dJ	201	PEB	CAC-CBC-CGC-O2C
26	dK	201	PEB	CAC-CBC-CGC-O2C
26	dL	201	PEB	CAC-CBC-CGC-O2C
26	dM	1001	PEB	CAC-CBC-CGC-O2C
26	dM	1002	PEB	CAC-CBC-CGC-O2C
26	dN	201	PEB	CAC-CBC-CGC-O2C
26	dO	202	PEB	CAC-CBC-CGC-O2C
26	dP	201	PEB	CAC-CBC-CGC-O2C
26	dQ	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	dR	202	PEB	CAC-CBC-CGC-O2C
26	dS	201	PEB	CAC-CBC-CGC-O2C
26	dT	201	PEB	CAC-CBC-CGC-O2C
26	dT	202	PEB	CAC-CBC-CGC-O2C
26	dU	201	PEB	CAC-CBC-CGC-O2C
26	dW	202	PEB	CAC-CBC-CGC-O2C
26	dY	201	PEB	CAC-CBC-CGC-O2C
26	dZ	1001	PEB	CAC-CBC-CGC-O2C
26	ed	201	PEB	CAC-CBC-CGC-O2C
26	ed	202	PEB	CAC-CBC-CGC-O2C
26	ee	201	PEB	CAC-CBC-CGC-O2C
26	ef	201	PEB	CAC-CBC-CGC-O2C
26	eg	201	PEB	CAC-CBC-CGC-O2C
26	eh	201	PEB	CAC-CBC-CGC-O2C
26	ej	202	PEB	CAC-CBC-CGC-O2C
26	ek	1001	PEB	CAC-CBC-CGC-O2C
26	el	201	PEB	CAC-CBC-CGC-O2C
26	em	201	PEB	CAC-CBC-CGC-O2C
26	ep	201	PEB	CAC-CBC-CGC-O2C
26	eq	201	PEB	CAC-CBC-CGC-O2C
26	eq	202	PEB	CAC-CBC-CGC-O2C
26	er	201	PEB	CAC-CBC-CGC-O2C
26	eu	201	PEB	CAC-CBC-CGC-O2C
26	ey	1003	PEB	CAC-CBC-CGC-O2C
26	ez	1001	PEB	CAC-CBC-CGC-O2C
26	ez	1002	PEB	CAC-CBC-CGC-O2C
26	ez	1003	PEB	CAC-CBC-CGC-O2C
26	eA	1001	PEB	CAC-CBC-CGC-O2C
26	eC	202	PEB	CAC-CBC-CGC-O2C
26	eD	201	PEB	CAC-CBC-CGC-O2C
26	eD	202	PEB	CAC-CBC-CGC-O2C
26	eE	201	PEB	CAC-CBC-CGC-O2C
26	eF	202	PEB	CAC-CBC-CGC-O2C
26	eG	201	PEB	CAC-CBC-CGC-O2C
26	eH	201	PEB	CAC-CBC-CGC-O2C
26	eH	202	PEB	CAC-CBC-CGC-O2C
26	eI	202	PEB	CAC-CBC-CGC-O2C
26	eJ	201	PEB	CAC-CBC-CGC-O2C
26	eK	201	PEB	CAC-CBC-CGC-O2C
26	eM	1001	PEB	CAC-CBC-CGC-O2C
26	eM	1002	PEB	CAC-CBC-CGC-O2C
26	eN	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	eO	202	PEB	CAC-CBC-CGC-O2C
26	eP	202	PEB	CAC-CBC-CGC-O2C
26	eP	203	PEB	CAC-CBC-CGC-O2C
26	eQ	202	PEB	CAC-CBC-CGC-O2C
26	eR	201	PEB	CAC-CBC-CGC-O2C
26	eR	202	PEB	CAC-CBC-CGC-O2C
26	eS	201	PEB	CAC-CBC-CGC-O2C
26	eT	201	PEB	CAC-CBC-CGC-O2C
26	eT	202	PEB	CAC-CBC-CGC-O2C
26	eV	201	PEB	CAC-CBC-CGC-O2C
26	eW	201	PEB	CAC-CBC-CGC-O2C
26	eY	402	PEB	CAC-CBC-CGC-O2C
26	eZ	401	PEB	CAC-CBC-CGC-O2C
26	la	1002	PEB	CAC-CBC-CGC-O2C
26	lb	201	PEB	CAC-CBC-CGC-O2C
26	lc	201	PEB	CAC-CBC-CGC-O2C
26	le	201	PEB	CAC-CBC-CGC-O2C
26	lf	201	PEB	CAC-CBC-CGC-O2C
26	li	201	PEB	CAC-CBC-CGC-O2C
26	ll	201	PEB	CAC-CBC-CGC-O2C
26	lp	201	PEB	CAC-CBC-CGC-O2C
26	lq	201	PEB	CAC-CBC-CGC-O2C
26	lq	202	PEB	CAC-CBC-CGC-O2C
26	ls	201	PEB	CAC-CBC-CGC-O2C
26	lt	201	PEB	CAC-CBC-CGC-O2C
26	ly	402	PEB	CAC-CBC-CGC-O2C
26	ly	403	PEB	CAC-CBC-CGC-O2C
26	lz	401	PEB	CAC-CBC-CGC-O2C
26	lz	402	PEB	CAC-CBC-CGC-O2C
26	fb	201	PEB	CAC-CBC-CGC-O2C
26	fd	301	PEB	CAC-CBC-CGC-O2C
26	fd	302	PEB	CAC-CBC-CGC-O2C
26	ff	204	PEB	CAC-CBC-CGC-O2C
26	fh	1001	PEB	CAC-CBC-CGC-O2C
26	fi	201	PEB	CAC-CBC-CGC-O2C
26	fj	201	PEB	CAC-CBC-CGC-O2C
26	fk	201	PEB	CAC-CBC-CGC-O2C
26	fl	201	PEB	CAC-CBC-CGC-O2C
26	fm	201	PEB	CAC-CBC-CGC-O2C
26	fn	1001	PEB	CAC-CBC-CGC-O2C
26	fo	201	PEB	CAC-CBC-CGC-O2C
26	fp	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	fr	201	PEB	CAC-CBC-CGC-O2C
26	fs	201	PEB	CAC-CBC-CGC-O2C
26	ft	201	PEB	CAC-CBC-CGC-O2C
26	fv	201	PEB	CAC-CBC-CGC-O2C
26	fw	201	PEB	CAC-CBC-CGC-O2C
26	fx	201	PEB	CAC-CBC-CGC-O2C
26	gb	1001	PEB	CAC-CBC-CGC-O2C
26	gc	201	PEB	CAC-CBC-CGC-O2C
26	gf	201	PEB	CAC-CBC-CGC-O2C
26	gg	201	PEB	CAC-CBC-CGC-O2C
26	gh	201	PEB	CAC-CBC-CGC-O2C
26	gi	201	PEB	CAC-CBC-CGC-O2C
26	gj	201	PEB	CAC-CBC-CGC-O2C
26	gk	201	PEB	CAC-CBC-CGC-O2C
26	gm	1001	PEB	CAC-CBC-CGC-O2C
26	gn	201	PEB	CAC-CBC-CGC-O2C
26	go	201	PEB	CAC-CBC-CGC-O2C
26	gp	201	PEB	CAC-CBC-CGC-O2C
26	gs	201	PEB	CAC-CBC-CGC-O2C
26	gt	201	PEB	CAC-CBC-CGC-O2C
26	gu	201	PEB	CAC-CBC-CGC-O2C
26	gv	201	PEB	CAC-CBC-CGC-O2C
26	gx	201	PEB	CAC-CBC-CGC-O2C
26	gy	301	PEB	CAC-CBC-CGC-O2C
26	gy	303	PEB	CAC-CBC-CGC-O2C
26	hA	201	PEB	CAC-CBC-CGC-O2C
26	hB	201	PEB	CAC-CBC-CGC-O2C
26	hC	201	PEB	CAC-CBC-CGC-O2C
26	hD	201	PEB	CAC-CBC-CGC-O2C
26	hF	201	PEB	CAC-CBC-CGC-O2C
26	hI	201	PEB	CAC-CBC-CGC-O2C
26	hJ	201	PEB	CAC-CBC-CGC-O2C
26	hK	201	PEB	CAC-CBC-CGC-O2C
26	hL	201	PEB	CAC-CBC-CGC-O2C
26	hN	201	PEB	CAC-CBC-CGC-O2C
26	hO	201	PEB	CAC-CBC-CGC-O2C
26	hP	201	PEB	CAC-CBC-CGC-O2C
26	hQ	201	PEB	CAC-CBC-CGC-O2C
26	hR	201	PEB	CAC-CBC-CGC-O2C
26	hS	201	PEB	CAC-CBC-CGC-O2C
26	hT	201	PEB	CAC-CBC-CGC-O2C
26	hT	204	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	hW	201	PEB	CAC-CBC-CGC-O2C
26	hX	201	PEB	CAC-CBC-CGC-O2C
26	hY	401	PEB	CAC-CBC-CGC-O2C
26	hY	403	PEB	CAC-CBC-CGC-O2C
26	hZ	402	PEB	CAC-CBC-CGC-O2C
26	iB	1001	PEB	CAC-CBC-CGC-O2C
26	iD	1001	PEB	CAC-CBC-CGC-O2C
26	iE	1001	PEB	CAC-CBC-CGC-O2C
26	iG	1001	PEB	CAC-CBC-CGC-O2C
26	jJ	1001	PEB	CAC-CBC-CGC-O2C
26	jK	1001	PEB	CAC-CBC-CGC-O2C
26	jL	1001	PEB	CAC-CBC-CGC-O2C
26	jN	1001	PEB	CAC-CBC-CGC-O2C
26	jP	1001	PEB	CAC-CBC-CGC-O2C
26	kQ	1001	PEB	CAC-CBC-CGC-O2C
26	kR	1001	PEB	CAC-CBC-CGC-O2C
26	kS	1001	PEB	CAC-CBC-CGC-O2C
26	kV	1001	PEB	CAC-CBC-CGC-O2C
26	kX	1001	PEB	CAC-CBC-CGC-O2C
29	C2	303	PVN	C61-C62-C63-O65
29	c3	303	PVN	C61-C62-C63-O65
29	eY	403	PVN	C51-C52-C53-O55
29	eZ	402	PVN	C51-C52-C53-O55
26	Q3	201	PEB	CAC-CBC-CGC-O2C
26	X3	201	PEB	CAC-CBC-CGC-O2C
26	V4	202	PEB	CAC-CBC-CGC-O2C
26	W4	201	PEB	CAC-CBC-CGC-O2C
26	J5	201	PEB	CAC-CBC-CGC-O2C
26	s5	201	PEB	CAC-CBC-CGC-O2C
26	eU	202	PEB	CAC-CBC-CGC-O2C
26	fq	201	PEB	CAC-CBC-CGC-O2C
26	kT	1001	PEB	CAC-CBC-CGC-O2C
29	ez	1004	PVN	C51-C52-C53-O55
26	e2	202	PEB	CAC-CBC-CGC-O2C
26	o2	1002	PEB	CAC-CBC-CGC-O2C
26	s2	201	PEB	CAC-CBC-CGC-O2C
26	z2	201	PEB	CAC-CBC-CGC-O2C
26	M2	202	PEB	CAC-CBC-CGC-O2C
26	O2	202	PEB	CAC-CBC-CGC-O2C
26	W2	202	PEB	CAC-CBC-CGC-O2C
26	I3	201	PEB	CAC-CBC-CGC-O2C
26	K3	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	e3	1001	PEB	CAC-CBC-CGC-O2C
26	g3	202	PEB	CAB-CBB-CGB-O2B
26	o3	201	PEB	CAC-CBC-CGC-O2C
26	s3	202	PEB	CAB-CBB-CGB-O2B
26	G4	201	PEB	CAC-CBC-CGC-O2C
26	I4	202	PEB	CAC-CBC-CGC-O2C
26	M4	201	PEB	CAC-CBC-CGC-O2C
26	S4	201	PEB	CAC-CBC-CGC-O2C
26	U4	201	PEB	CAC-CBC-CGC-O2C
26	W4	202	PEB	CAC-CBC-CGC-O2C
26	X4	202	PEB	CAC-CBC-CGC-O2C
26	Y4	202	PEB	CAC-CBC-CGC-O2C
26	Z4	202	PEB	CAC-CBC-CGC-O2C
26	24	401	PEB	CAC-CBC-CGC-O2C
26	34	1003	PEB	CAC-CBC-CGC-O2C
26	44	301	PEB	CAC-CBC-CGC-O2C
26	a4	201	PEB	CAC-CBC-CGC-O2C
26	m4	1001	PEB	CAC-CBC-CGC-O2C
26	A5	201	PEB	CAC-CBC-CGC-O2C
26	C5	201	PEB	CAC-CBC-CGC-O2C
26	I5	202	PEB	CAB-CBB-CGB-O2B
26	K5	1002	PEB	CAB-CBB-CGB-O2B
26	Y5	1002	PEB	CAB-CBB-CGB-O2B
26	g5	201	PEB	CAC-CBC-CGC-O2C
26	h5	202	PEB	CAB-CBB-CGB-O2B
26	r5	201	PEB	CAC-CBC-CGC-O2C
26	u5	201	PEB	CAC-CBC-CGC-O2C
26	h8	201	PEB	CAC-CBC-CGC-O2C
26	j8	201	PEB	CAC-CBC-CGC-O2C
26	A6	1001	PEB	CAC-CBC-CGC-O2C
26	E6	202	PEB	CAC-CBC-CGC-O2C
26	H6	202	PEB	CAC-CBC-CGC-O2C
26	J6	201	PEB	CAC-CBC-CGC-O2C
26	T6	202	PEB	CAC-CBC-CGC-O2C
26	U6	201	PEB	CAC-CBC-CGC-O2C
26	V6	202	PEB	CAB-CBB-CGB-O2B
26	e6	201	PEB	CAC-CBC-CGC-O2C
26	f6	201	PEB	CAC-CBC-CGC-O2C
26	n6	201	PEB	CAB-CBB-CGB-O2B
26	s6	202	PEB	CAC-CBC-CGC-O2C
26	q8	201	PEB	CAC-CBC-CGC-O2C
26	A7	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	C7	202	PEB	CAB-CBB-CGB-O2B
26	G7	201	PEB	CAC-CBC-CGC-O2C
26	K7	202	PEB	CAB-CBB-CGB-O2B
26	O7	201	PEB	CAC-CBC-CGC-O2C
26	O7	202	PEB	CAB-CBB-CGB-O2B
26	Q7	202	PEB	CAB-CBB-CGB-O2B
26	S7	201	PEB	CAC-CBC-CGC-O2C
26	Y7	1002	PEB	CAB-CBB-CGB-O2B
26	a7	201	PEB	CAC-CBC-CGC-O2C
26	e7	201	PEB	CAC-CBC-CGC-O2C
26	f7	201	PEB	CAC-CBC-CGC-O2C
26	j7	201	PEB	CAC-CBC-CGC-O2C
26	n7	201	PEB	CAC-CBC-CGC-O2C
26	o7	201	PEB	CAC-CBC-CGC-O2C
26	o7	202	PEB	CAB-CBB-CGB-O2B
26	q7	202	PEB	CAB-CBB-CGB-O2B
26	s7	202	PEB	CAB-CBB-CGB-O2B
26	w7	1002	PEB	CAB-CBB-CGB-O2B
26	d9	301	PEB	CAC-CBC-CGC-O2C
26	F8	1002	PEB	CAC-CBC-CGC-O2C
26	I8	201	PEB	CAC-CBC-CGC-O2C
26	O8	201	PEB	CAC-CBC-CGC-O2C
26	O8	202	PEB	CAC-CBC-CGC-O2C
26	P8	201	PEB	CAC-CBC-CGC-O2C
26	S8	401	PEB	CAC-CBC-CGC-O2C
26	T8	302	PEB	CAC-CBC-CGC-O2C
26	U8	1001	PEB	CAC-CBC-CGC-O2C
26	W8	201	PEB	CAC-CBC-CGC-O2C
26	f9	201	PEB	CAC-CBC-CGC-O2C
26	f9	202	PEB	CAC-CBC-CGC-O2C
26	g9	201	PEB	CAC-CBC-CGC-O2C
26	l9	202	PEB	CAC-CBC-CGC-O2C
26	s9	201	PEB	CAC-CBC-CGC-O2C
26	u9	202	PEB	CAC-CBC-CGC-O2C
26	y9	1001	PEB	CAC-CBC-CGC-O2C
26	E9	202	PEB	CAB-CBB-CGB-O2B
26	H9	201	PEB	CAC-CBC-CGC-O2C
26	J9	201	PEB	CAC-CBC-CGC-O2C
26	L9	201	PEB	CAC-CBC-CGC-O2C
26	M9	201	PEB	CAC-CBC-CGC-O2C
26	U9	201	PEB	CAC-CBC-CGC-O2C
26	ah	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	ar	201	PEB	CAC-CBC-CGC-O2C
26	az	201	PEB	CAC-CBC-CGC-O2C
26	aC	201	PEB	CAC-CBC-CGC-O2C
26	aM	202	PEB	CAC-CBC-CGC-O2C
26	aO	201	PEB	CAC-CBC-CGC-O2C
26	aS	201	PEB	CAC-CBC-CGC-O2C
26	bj	202	PEB	CAC-CBC-CGC-O2C
26	by	1002	PEB	CAC-CBC-CGC-O2C
26	bB	201	PEB	CAC-CBC-CGC-O2C
26	bM	201	PEB	CAC-CBC-CGC-O2C
26	bM	202	PEB	CAB-CBB-CGB-O2B
26	bS	201	PEB	CAC-CBC-CGC-O2C
26	bU	201	PEB	CAC-CBC-CGC-O2C
26	bY	1002	PEB	CAB-CBB-CGB-O2B
26	cd	201	PEB	CAC-CBC-CGC-O2C
26	cg	201	PEB	CAC-CBC-CGC-O2C
26	cp	201	PEB	CAC-CBC-CGC-O2C
26	cq	201	PEB	CAC-CBC-CGC-O2C
26	ct	201	PEB	CAC-CBC-CGC-O2C
26	ct	202	PEB	CAB-CBB-CGB-O2B
26	cu	202	PEB	CAB-CBB-CGB-O2B
26	cx	201	PEB	CAC-CBC-CGC-O2C
26	cy	1001	PEB	CAC-CBC-CGC-O2C
26	cz	201	PEB	CAC-CBC-CGC-O2C
26	cD	201	PEB	CAC-CBC-CGC-O2C
26	cL	201	PEB	CAC-CBC-CGC-O2C
26	cO	202	PEB	CAC-CBC-CGC-O2C
26	dk	1002	PEB	CAC-CBC-CGC-O2C
26	dl	201	PEB	CAC-CBC-CGC-O2C
26	dx	404	PEB	CAC-CBC-CGC-O2C
26	dG	201	PEB	CAC-CBC-CGC-O2C
26	dK	202	PEB	CAC-CBC-CGC-O2C
26	dQ	201	PEB	CAC-CBC-CGC-O2C
26	dW	201	PEB	CAC-CBC-CGC-O2C
26	ea	202	PEB	CAC-CBC-CGC-O2C
26	ec	201	PEB	CAB-CBB-CGB-O2B
26	eo	202	PEB	CAC-CBC-CGC-O2C
26	es	201	PEB	CAC-CBC-CGC-O2C
26	eu	202	PEB	CAB-CBB-CGB-O2B
26	ev	201	PEB	CAB-CBB-CGB-O2B
26	eB	201	PEB	CAB-CBB-CGB-O2B
26	eB	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	eC	201	PEB	CAC-CBC-CGC-O2C
26	eI	201	PEB	CAC-CBC-CGC-O2C
26	eK	202	PEB	CAC-CBC-CGC-O2C
26	eO	201	PEB	CAC-CBC-CGC-O2C
26	eS	202	PEB	CAC-CBC-CGC-O2C
26	eW	202	PEB	CAC-CBC-CGC-O2C
26	eY	401	PEB	CAB-CBB-CGB-O2B
26	la	1001	PEB	CAC-CBC-CGC-O2C
26	lb	202	PEB	CAC-CBC-CGC-O2C
26	ln	201	PEB	CAC-CBC-CGC-O2C
26	ly	401	PEB	CAC-CBC-CGC-O2C
26	fa	201	PEB	CAC-CBC-CGC-O2C
26	fe	201	PEB	CAC-CBC-CGC-O2C
26	ff	201	PEB	CAC-CBC-CGC-O2C
26	fp	202	PEB	CAB-CBB-CGB-O2B
26	gq	201	PEB	CAC-CBC-CGC-O2C
26	gw	201	PEB	CAC-CBC-CGC-O2C
26	gz	301	PEB	CAC-CBC-CGC-O2C
26	gz	303	PEB	CAC-CBC-CGC-O2C
26	hC	202	PEB	CAB-CBB-CGB-O2B
26	hE	1001	PEB	CAC-CBC-CGC-O2C
26	hE	1002	PEB	CAB-CBB-CGB-O2B
26	hU	201	PEB	CAB-CBB-CGB-O2B
26	hZ	401	PEB	CAB-CBB-CGB-O2B
26	iA	1002	PEB	CAB-CBB-CGB-O2B
26	iC	1001	PEB	CAC-CBC-CGC-O2C
26	jM	1001	PEB	CAC-CBC-CGC-O2C
26	jO	1001	PEB	CAC-CBC-CGC-O2C
26	kU	1001	PEB	CAC-CBC-CGC-O2C
29	ly	404	PVN	C61-C62-C63-O65
29	gz	304	PVN	C61-C62-C63-O65
26	g2	202	PEB	CAC-CBC-CGC-O2C
26	q2	201	PEB	CAC-CBC-CGC-O2C
26	r2	202	PEB	CAC-CBC-CGC-O2C
26	t2	201	PEB	CAC-CBC-CGC-O2C
26	t2	202	PEB	CAC-CBC-CGC-O2C
26	u2	201	PEB	CAC-CBC-CGC-O2C
26	v2	202	PEB	CAC-CBC-CGC-O2C
26	A2	1001	PEB	CAB-CBB-CGB-O2B
26	D2	301	PEB	CAC-CBC-CGC-O2C
26	E2	1002	PEB	CAB-CBB-CGB-O2B
26	I2	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	K2	202	PEB	CAC-CBC-CGC-O2C
26	N2	201	PEB	CAB-CBB-CGB-O2B
26	P2	202	PEB	CAB-CBB-CGB-O2B
26	R2	201	PEB	CAB-CBB-CGB-O2B
26	R2	202	PEB	CAC-CBC-CGC-O2C
26	S2	202	PEB	CAB-CBB-CGB-O2B
26	T2	201	PEB	CAC-CBC-CGC-O2C
26	U2	202	PEB	CAB-CBB-CGB-O2B
26	X2	201	PEB	CAC-CBC-CGC-O2C
26	Z2	201	PEB	CAC-CBC-CGC-O2C
26	A3	202	PEB	CAB-CBB-CGB-O2B
26	B3	201	PEB	CAC-CBC-CGC-O2C
26	C3	1002	PEB	CAB-CBB-CGB-O2B
26	E3	201	PEB	CAC-CBC-CGC-O2C
26	E3	202	PEB	CAB-CBB-CGB-O2B
26	G3	202	PEB	CAB-CBB-CGB-O2B
26	I3	202	PEB	CAB-CBB-CGB-O2B
26	J3	201	PEB	CAC-CBC-CGC-O2C
26	M3	202	PEB	CAB-CBB-CGB-O2B
26	O3	1002	PEB	CAB-CBB-CGB-O2B
26	Q3	202	PEB	CAB-CBB-CGB-O2B
26	R3	201	PEB	CAC-CBC-CGC-O2C
26	S3	202	PEB	CAB-CBB-CGB-O2B
26	U3	202	PEB	CAB-CBB-CGB-O2B
26	W3	202	PEB	CAB-CBB-CGB-O2B
26	Y3	202	PEB	CAB-CBB-CGB-O2B
26	a3	1002	PEB	CAB-CBB-CGB-O2B
26	c3	301	PEB	CAB-CBB-CGB-O2B
26	d3	301	PEB	CAB-CBB-CGB-O2B
26	f3	201	PEB	CAC-CBC-CGC-O2C
26	i3	202	PEB	CAB-CBB-CGB-O2B
26	k3	202	PEB	CAB-CBB-CGB-O2B
26	m3	202	PEB	CAB-CBB-CGB-O2B
26	o3	202	PEB	CAB-CBB-CGB-O2B
26	s3	201	PEB	CAC-CBC-CGC-O2C
26	t3	201	PEB	CAC-CBC-CGC-O2C
26	u3	202	PEB	CAB-CBB-CGB-O2B
26	w3	202	PEB	CAB-CBB-CGB-O2B
26	y3	202	PEB	CAB-CBB-CGB-O2B
26	A4	202	PEB	CAB-CBB-CGB-O2B
26	C4	1002	PEB	CAB-CBB-CGB-O2B
26	D4	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	J4	202	PEB	CAC-CBC-CGC-O2C
26	K4	201	PEB	CAC-CBC-CGC-O2C
26	K4	202	PEB	CAC-CBC-CGC-O2C
26	N4	202	PEB	CAB-CBB-CGB-O2B
26	Q4	202	PEB	CAC-CBC-CGC-O2C
26	b4	1001	PEB	CAC-CBC-CGC-O2C
26	c4	201	PEB	CAB-CBB-CGB-O2B
26	h4	201	PEB	CAB-CBB-CGB-O2B
26	o4	201	PEB	CAC-CBC-CGC-O2C
26	p4	201	PEB	CAC-CBC-CGC-O2C
26	s4	202	PEB	CAB-CBB-CGB-O2B
26	t4	202	PEB	CAC-CBC-CGC-O2C
26	v4	201	PEB	CAC-CBC-CGC-O2C
26	w4	202	PEB	CAB-CBB-CGB-O2B
26	z4	201	PEB	CAC-CBC-CGC-O2C
26	z4	202	PEB	CAC-CBC-CGC-O2C
26	A5	202	PEB	CAB-CBB-CGB-O2B
26	C5	202	PEB	CAB-CBB-CGB-O2B
26	E5	202	PEB	CAB-CBB-CGB-O2B
26	G5	202	PEB	CAB-CBB-CGB-O2B
26	K5	1001	PEB	CAC-CBC-CGC-O2C
26	L5	201	PEB	CAC-CBC-CGC-O2C
26	M5	202	PEB	CAB-CBB-CGB-O2B
26	O5	202	PEB	CAB-CBB-CGB-O2B
26	Q5	202	PEB	CAB-CBB-CGB-O2B
26	S5	202	PEB	CAB-CBB-CGB-O2B
26	U5	202	PEB	CAB-CBB-CGB-O2B
26	Y5	1003	PEB	CAC-CBC-CGC-O2C
26	Z5	301	PEB	CAC-CBC-CGC-O2C
26	Z5	302	PEB	CAB-CBB-CGB-O2B
26	c5	201	PEB	CAB-CBB-CGB-O2B
26	d5	201	PEB	CAC-CBC-CGC-O2C
26	e5	201	PEB	CAC-CBC-CGC-O2C
26	f5	201	PEB	CAB-CBB-CGB-O2B
26	m5	1002	PEB	CAB-CBB-CGB-O2B
26	o5	202	PEB	CAB-CBB-CGB-O2B
26	q5	201	PEB	CAC-CBC-CGC-O2C
26	q5	202	PEB	CAB-CBB-CGB-O2B
26	s5	202	PEB	CAB-CBB-CGB-O2B
26	u5	202	PEB	CAB-CBB-CGB-O2B
26	w5	202	PEB	CAB-CBB-CGB-O2B
26	y5	1002	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	l8	202	PEB	CAC-CBC-CGC-O2C
26	m8	202	PEB	CAC-CBC-CGC-O2C
26	G6	202	PEB	CAB-CBB-CGB-O2B
26	H6	201	PEB	CAB-CBB-CGB-O2B
26	I6	201	PEB	CAC-CBC-CGC-O2C
26	L6	201	PEB	CAC-CBC-CGC-O2C
26	N6	202	PEB	CAB-CBB-CGB-O2B
26	P6	201	PEB	CAC-CBC-CGC-O2C
26	S6	201	PEB	CAC-CBC-CGC-O2C
26	U6	202	PEB	CAB-CBB-CGB-O2B
26	Z6	202	PEB	CAC-CBC-CGC-O2C
26	a6	202	PEB	CAB-CBB-CGB-O2B
26	c6	1002	PEB	CAC-CBC-CGC-O2C
26	d6	202	PEB	CAB-CBB-CGB-O2B
26	e6	202	PEB	CAB-CBB-CGB-O2B
26	f6	202	PEB	CAB-CBB-CGB-O2B
26	k6	1002	PEB	CAC-CBC-CGC-O2C
26	m6	201	PEB	CAC-CBC-CGC-O2C
26	o6	202	PEB	CAC-CBC-CGC-O2C
26	p6	202	PEB	CAB-CBB-CGB-O2B
26	t6	201	PEB	CAB-CBB-CGB-O2B
26	u6	201	PEB	CAC-CBC-CGC-O2C
26	v6	201	PEB	CAC-CBC-CGC-O2C
26	y6	203	PEB	CAC-CBC-CGC-O2C
26	o8	201	PEB	CAB-CBB-CGB-O2B
26	p8	201	PEB	CAC-CBC-CGC-O2C
26	q8	202	PEB	CAB-CBB-CGB-O2B
26	r8	202	PEB	CAB-CBB-CGB-O2B
26	s8	202	PEB	CAB-CBB-CGB-O2B
26	t8	202	PEB	CAB-CBB-CGB-O2B
26	u8	202	PEB	CAB-CBB-CGB-O2B
26	E7	202	PEB	CAB-CBB-CGB-O2B
26	G7	202	PEB	CAB-CBB-CGB-O2B
26	H7	201	PEB	CAC-CBC-CGC-O2C
26	I7	202	PEB	CAB-CBB-CGB-O2B
26	N7	201	PEB	CAC-CBC-CGC-O2C
26	S7	202	PEB	CAB-CBB-CGB-O2B
26	U7	202	PEB	CAB-CBB-CGB-O2B
26	W7	201	PEB	CAC-CBC-CGC-O2C
26	W7	202	PEB	CAB-CBB-CGB-O2B
26	f7	202	PEB	CAB-CBB-CGB-O2B
26	g7	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	h7	202	PEB	CAB-CBB-CGB-O2B
26	i7	202	PEB	CAB-CBB-CGB-O2B
26	j7	202	PEB	CAB-CBB-CGB-O2B
26	k7	1002	PEB	CAB-CBB-CGB-O2B
26	m7	202	PEB	CAB-CBB-CGB-O2B
26	s7	201	PEB	CAC-CBC-CGC-O2C
26	t7	201	PEB	CAC-CBC-CGC-O2C
26	u7	201	PEB	CAC-CBC-CGC-O2C
26	u7	202	PEB	CAB-CBB-CGB-O2B
26	w7	1001	PEB	CAC-CBC-CGC-O2C
26	a8	602	PEB	CAC-CBC-CGC-O2C
26	c8	301	PEB	CAB-CBB-CGB-O2B
26	c8	302	PEB	CAC-CBC-CGC-O2C
26	d8	301	PEB	CAB-CBB-CGB-O2B
26	d8	302	PEB	CAC-CBC-CGC-O2C
26	a9	602	PEB	CAC-CBC-CGC-O2C
26	C8	201	PEB	CAC-CBC-CGC-O2C
26	E8	202	PEB	CAC-CBC-CGC-O2C
26	P8	202	PEB	CAC-CBC-CGC-O2C
26	X8	201	PEB	CAC-CBC-CGC-O2C
26	Y8	202	PEB	CAC-CBC-CGC-O2C
26	n9	201	PEB	CAC-CBC-CGC-O2C
26	q9	202	PEB	CAC-CBC-CGC-O2C
26	t9	202	PEB	CAC-CBC-CGC-O2C
26	A9	202	PEB	CAB-CBB-CGB-O2B
26	C9	202	PEB	CAB-CBB-CGB-O2B
26	D9	201	PEB	CAC-CBC-CGC-O2C
26	E9	201	PEB	CAC-CBC-CGC-O2C
26	G9	202	PEB	CAB-CBB-CGB-O2B
26	I9	202	PEB	CAB-CBB-CGB-O2B
26	K9	1002	PEB	CAB-CBB-CGB-O2B
26	M9	202	PEB	CAB-CBB-CGB-O2B
26	O9	202	PEB	CAB-CBB-CGB-O2B
26	Q9	202	PEB	CAB-CBB-CGB-O2B
26	S9	201	PEB	CAC-CBC-CGC-O2C
26	S9	202	PEB	CAB-CBB-CGB-O2B
26	U9	202	PEB	CAB-CBB-CGB-O2B
26	Y9	301	PEB	CAB-CBB-CGB-O2B
26	Z9	1001	PEB	CAC-CBC-CGC-O2C
26	Z9	1002	PEB	CAB-CBB-CGB-O2B
26	ak	201	PEB	CAC-CBC-CGC-O2C
26	al	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	ao	202	PEB	CAB-CBB-CGB-O2B
26	aq	202	PEB	CAB-CBB-CGB-O2B
26	as	202	PEB	CAB-CBB-CGB-O2B
26	au	202	PEB	CAB-CBB-CGB-O2B
26	aw	202	PEB	CAB-CBB-CGB-O2B
26	ay	1002	PEB	CAB-CBB-CGB-O2B
26	aB	201	PEB	CAC-CBC-CGC-O2C
26	aC	202	PEB	CAC-CBC-CGC-O2C
26	aQ	201	PEB	CAC-CBC-CGC-O2C
26	aY	406	PEB	CAC-CBC-CGC-O2C
26	ba	1001	PEB	CAC-CBC-CGC-O2C
26	bj	201	PEB	CAC-CBC-CGC-O2C
26	bk	201	PEB	CAC-CBC-CGC-O2C
26	bm	1001	PEB	CAC-CBC-CGC-O2C
26	bs	1003	PEB	CAC-CBC-CGC-O2C
26	bv	201	PEB	CAC-CBC-CGC-O2C
26	by	1001	PEB	CAC-CBC-CGC-O2C
26	bA	202	PEB	CAB-CBB-CGB-O2B
26	bC	202	PEB	CAB-CBB-CGB-O2B
26	bE	201	PEB	CAC-CBC-CGC-O2C
26	bF	201	PEB	CAC-CBC-CGC-O2C
26	bG	201	PEB	CAC-CBC-CGC-O2C
26	bG	202	PEB	CAB-CBB-CGB-O2B
26	bH	201	PEB	CAC-CBC-CGC-O2C
26	bI	202	PEB	CAB-CBB-CGB-O2B
26	bJ	201	PEB	CAC-CBC-CGC-O2C
26	bK	1001	PEB	CAC-CBC-CGC-O2C
26	bK	1002	PEB	CAB-CBB-CGB-O2B
26	bQ	201	PEB	CAC-CBC-CGC-O2C
26	bQ	202	PEB	CAB-CBB-CGB-O2B
26	bS	202	PEB	CAB-CBB-CGB-O2B
26	bU	202	PEB	CAB-CBB-CGB-O2B
26	bZ	301	PEB	CAC-CBC-CGC-O2C
26	bZ	302	PEB	CAB-CBB-CGB-O2B
26	ce	201	PEB	CAC-CBC-CGC-O2C
26	cj	201	PEB	CAC-CBC-CGC-O2C
26	cm	1002	PEB	CAB-CBB-CGB-O2B
26	cv	202	PEB	CAB-CBB-CGB-O2B
26	cw	202	PEB	CAB-CBB-CGB-O2B
26	cx	202	PEB	CAB-CBB-CGB-O2B
26	cy	1002	PEB	CAB-CBB-CGB-O2B
26	cA	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	cA	202	PEB	CAB-CBB-CGB-O2B
26	cC	1001	PEB	CAC-CBC-CGC-O2C
26	cC	1002	PEB	CAB-CBB-CGB-O2B
26	cD	202	PEB	CAB-CBB-CGB-O2B
26	cG	202	PEB	CAB-CBB-CGB-O2B
26	cI	202	PEB	CAB-CBB-CGB-O2B
26	cK	202	PEB	CAB-CBB-CGB-O2B
26	cP	202	PEB	CAC-CBC-CGC-O2C
26	cT	1001	PEB	CAC-CBC-CGC-O2C
26	cU	201	PEB	CAC-CBC-CGC-O2C
26	cU	202	PEB	CAC-CBC-CGC-O2C
26	cV	202	PEB	CAC-CBC-CGC-O2C
26	cZ	202	PEB	CAB-CBB-CGB-O2B
26	da	1002	PEB	CAB-CBB-CGB-O2B
26	db	202	PEB	CAB-CBB-CGB-O2B
26	dc	202	PEB	CAB-CBB-CGB-O2B
26	de	202	PEB	CAB-CBB-CGB-O2B
26	dg	201	PEB	CAC-CBC-CGC-O2C
26	dg	202	PEB	CAB-CBB-CGB-O2B
26	dj	201	PEB	CAC-CBC-CGC-O2C
26	dm	201	PEB	CAC-CBC-CGC-O2C
26	dp	201	PEB	CAC-CBC-CGC-O2C
26	dr	201	PEB	CAC-CBC-CGC-O2C
26	dx	401	PEB	CAC-CBC-CGC-O2C
26	dD	202	PEB	CAC-CBC-CGC-O2C
26	dF	201	PEB	CAC-CBC-CGC-O2C
26	dJ	202	PEB	CAB-CBB-CGB-O2B
26	dN	202	PEB	CAC-CBC-CGC-O2C
26	dO	201	PEB	CAC-CBC-CGC-O2C
26	dP	202	PEB	CAC-CBC-CGC-O2C
26	dR	201	PEB	CAC-CBC-CGC-O2C
26	dU	202	PEB	CAB-CBB-CGB-O2B
26	dV	201	PEB	CAC-CBC-CGC-O2C
26	dX	201	PEB	CAC-CBC-CGC-O2C
26	dX	202	PEB	CAC-CBC-CGC-O2C
26	dZ	1002	PEB	CAB-CBB-CGB-O2B
26	ea	201	PEB	CAC-CBC-CGC-O2C
26	eb	201	PEB	CAC-CBC-CGC-O2C
26	ef	202	PEB	CAB-CBB-CGB-O2B
26	eh	202	PEB	CAB-CBB-CGB-O2B
26	ei	201	PEB	CAB-CBB-CGB-O2B
26	ej	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	ek	1002	PEB	CAB-CBB-CGB-O2B
26	em	202	PEB	CAB-CBB-CGB-O2B
26	en	201	PEB	CAC-CBC-CGC-O2C
26	eo	201	PEB	CAC-CBC-CGC-O2C
26	es	202	PEB	CAC-CBC-CGC-O2C
26	et	201	PEB	CAB-CBB-CGB-O2B
26	ew	301	PEB	CAC-CBC-CGC-O2C
26	ey	1001	PEB	CAB-CBB-CGB-O2B
26	ey	1002	PEB	CAC-CBC-CGC-O2C
26	eA	1002	PEB	CAB-CBB-CGB-O2B
26	eE	202	PEB	CAC-CBC-CGC-O2C
26	eF	201	PEB	CAC-CBC-CGC-O2C
26	eG	202	PEB	CAC-CBC-CGC-O2C
26	eL	201	PEB	CAB-CBB-CGB-O2B
26	eQ	201	PEB	CAC-CBC-CGC-O2C
26	eU	201	PEB	CAC-CBC-CGC-O2C
26	lc	202	PEB	CAB-CBB-CGB-O2B
26	ld	201	PEB	CAB-CBB-CGB-O2B
26	le	202	PEB	CAB-CBB-CGB-O2B
26	lg	201	PEB	CAB-CBB-CGB-O2B
26	lg	202	PEB	CAB-CBB-CGB-O2B
26	lh	201	PEB	CAB-CBB-CGB-O2B
26	li	202	PEB	CAC-CBC-CGC-O2C
26	lj	201	PEB	CAB-CBB-CGB-O2B
26	lk	201	PEB	CAC-CBC-CGC-O2C
26	lk	202	PEB	CAB-CBB-CGB-O2B
26	lm	1001	PEB	CAC-CBC-CGC-O2C
26	lm	1002	PEB	CAB-CBB-CGB-O2B
26	lo	201	PEB	CAB-CBB-CGB-O2B
26	lo	202	PEB	CAB-CBB-CGB-O2B
26	lq	203	PEB	CAB-CBB-CGB-O2B
26	lr	201	PEB	CAC-CBC-CGC-O2C
26	ls	202	PEB	CAB-CBB-CGB-O2B
26	lt	202	PEB	CAB-CBB-CGB-O2B
26	lu	201	PEB	CAC-CBC-CGC-O2C
26	lu	202	PEB	CAB-CBB-CGB-O2B
26	lv	201	PEB	CAC-CBC-CGC-O2C
26	lw	201	PEB	CAB-CBB-CGB-O2B
26	lw	202	PEB	CAB-CBB-CGB-O2B
26	fb	202	PEB	CAB-CBB-CGB-O2B
26	fc	201	PEB	CAC-CBC-CGC-O2C
26	fd	303	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	fe	202	PEB	CAB-CBB-CGB-O2B
26	fg	202	PEB	CAB-CBB-CGB-O2B
26	fh	1002	PEB	CAB-CBB-CGB-O2B
26	fk	202	PEB	CAB-CBB-CGB-O2B
26	fl	202	PEB	CAB-CBB-CGB-O2B
26	fn	1002	PEB	CAB-CBB-CGB-O2B
26	fr	202	PEB	CAB-CBB-CGB-O2B
26	ft	202	PEB	CAB-CBB-CGB-O2B
26	fv	202	PEB	CAB-CBB-CGB-O2B
26	fx	202	PEB	CAB-CBB-CGB-O2B
26	fz	301	PEB	CAB-CBB-CGB-O2B
26	ga	201	PEB	CAC-CBC-CGC-O2C
26	gb	1002	PEB	CAB-CBB-CGB-O2B
26	gc	202	PEB	CAB-CBB-CGB-O2B
26	ge	201	PEB	CAC-CBC-CGC-O2C
26	gf	202	PEB	CAB-CBB-CGB-O2B
26	gh	202	PEB	CAB-CBB-CGB-O2B
26	gj	202	PEB	CAB-CBB-CGB-O2B
26	gl	201	PEB	CAC-CBC-CGC-O2C
26	gl	202	PEB	CAB-CBB-CGB-O2B
26	gm	1002	PEB	CAB-CBB-CGB-O2B
26	go	202	PEB	CAB-CBB-CGB-O2B
26	gq	202	PEB	CAB-CBB-CGB-O2B
26	gs	202	PEB	CAB-CBB-CGB-O2B
26	gu	202	PEB	CAB-CBB-CGB-O2B
26	gw	202	PEB	CAB-CBB-CGB-O2B
26	gy	302	PEB	CAB-CBB-CGB-O2B
26	gz	302	PEB	CAB-CBB-CGB-O2B
26	hA	202	PEB	CAB-CBB-CGB-O2B
26	hF	202	PEB	CAB-CBB-CGB-O2B
26	hH	201	PEB	CAC-CBC-CGC-O2C
26	hI	202	PEB	CAB-CBB-CGB-O2B
26	hK	202	PEB	CAB-CBB-CGB-O2B
26	hM	1001	PEB	CAC-CBC-CGC-O2C
26	hM	1002	PEB	CAB-CBB-CGB-O2B
26	hO	202	PEB	CAB-CBB-CGB-O2B
26	hQ	202	PEB	CAB-CBB-CGB-O2B
26	hS	202	PEB	CAB-CBB-CGB-O2B
26	hV	201	PEB	CAC-CBC-CGC-O2C
26	hW	202	PEB	CAB-CBB-CGB-O2B
26	hY	402	PEB	CAB-CBB-CGB-O2B
26	iA	1001	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	iB	1002	PEB	CAB-CBB-CGB-O2B
26	iF	1001	PEB	CAC-CBC-CGC-O2C
26	iF	1002	PEB	CAB-CBB-CGB-O2B
26	iH	1001	PEB	CAC-CBC-CGC-O2C
26	jI	1001	PEB	CAC-CBC-CGC-O2C
26	kW	1001	PEB	CAC-CBC-CGC-O2C
29	lz	403	PVN	C61-C62-C63-O65
26	e3	1002	PEB	CAB-CBB-CGB-O2B
26	M7	1003	PEB	CAB-CBB-CGB-O2B
26	bE	202	PEB	CAB-CBB-CGB-O2B
26	bO	202	PEB	CAB-CBB-CGB-O2B
26	eP	201	PEB	CAB-CBB-CGB-O2B
29	A2	1004	PVN	C61-C62-C63-O65
29	a3	1004	PVN	C61-C62-C63-O65
29	dw	404	PVN	C61-C62-C63-O65
29	ly	404	PVN	C61-C62-C63-O64
29	lz	403	PVN	C61-C62-C63-O64
26	e2	201	PEB	CAC-CBC-CGC-O1C
26	e2	202	PEB	CAC-CBC-CGC-O1C
26	f2	201	PEB	CAC-CBC-CGC-O1C
26	g2	201	PEB	CAC-CBC-CGC-O1C
26	g2	202	PEB	CAC-CBC-CGC-O1C
26	h2	201	PEB	CAC-CBC-CGC-O1C
26	i2	201	PEB	CAC-CBC-CGC-O1C
26	i2	202	PEB	CAC-CBC-CGC-O1C
26	j2	201	PEB	CAC-CBC-CGC-O1C
26	k2	201	PEB	CAC-CBC-CGC-O1C
26	k2	202	PEB	CAC-CBC-CGC-O1C
26	l2	201	PEB	CAC-CBC-CGC-O1C
26	m2	201	PEB	CAC-CBC-CGC-O1C
26	m2	202	PEB	CAC-CBC-CGC-O1C
26	n2	201	PEB	CAC-CBC-CGC-O1C
26	o2	1001	PEB	CAC-CBC-CGC-O1C
26	o2	1002	PEB	CAC-CBC-CGC-O1C
26	p2	201	PEB	CAC-CBC-CGC-O1C
26	q2	201	PEB	CAC-CBC-CGC-O1C
26	q2	202	PEB	CAC-CBC-CGC-O1C
26	r2	201	PEB	CAC-CBC-CGC-O1C
26	r2	202	PEB	CAC-CBC-CGC-O1C
26	s2	201	PEB	CAC-CBC-CGC-O1C
26	s2	202	PEB	CAC-CBC-CGC-O1C
26	t2	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	t2	202	PEB	CAC-CBC-CGC-O1C
26	u2	201	PEB	CAC-CBC-CGC-O1C
26	u2	202	PEB	CAC-CBC-CGC-O1C
26	v2	201	PEB	CAC-CBC-CGC-O1C
26	v2	202	PEB	CAC-CBC-CGC-O1C
26	w2	201	PEB	CAC-CBC-CGC-O1C
26	w2	202	PEB	CAC-CBC-CGC-O1C
26	w2	203	PEB	CAC-CBC-CGC-O1C
26	x2	201	PEB	CAC-CBC-CGC-O1C
26	y2	201	PEB	CAC-CBC-CGC-O1C
26	y2	202	PEB	CAC-CBC-CGC-O1C
26	z2	201	PEB	CAC-CBC-CGC-O1C
26	z2	202	PEB	CAC-CBC-CGC-O1C
26	A2	1002	PEB	CAC-CBC-CGC-O1C
26	B2	501	PEB	CAC-CBC-CGC-O1C
26	B2	502	PEB	CAC-CBC-CGC-O1C
26	C2	301	PEB	CAC-CBC-CGC-O1C
26	C2	302	PEB	CAC-CBC-CGC-O1C
26	D2	301	PEB	CAC-CBC-CGC-O1C
26	D2	302	PEB	CAC-CBC-CGC-O1C
26	E2	1001	PEB	CAC-CBC-CGC-O1C
26	F2	201	PEB	CAC-CBC-CGC-O1C
26	F2	202	PEB	CAC-CBC-CGC-O1C
26	G2	201	PEB	CAC-CBC-CGC-O1C
26	G2	202	PEB	CAC-CBC-CGC-O1C
26	I2	201	PEB	CAC-CBC-CGC-O1C
26	I2	202	PEB	CAC-CBC-CGC-O1C
26	J2	201	PEB	CAC-CBC-CGC-O1C
26	K2	201	PEB	CAC-CBC-CGC-O1C
26	K2	202	PEB	CAC-CBC-CGC-O1C
26	L2	201	PEB	CAC-CBC-CGC-O1C
26	M2	201	PEB	CAC-CBC-CGC-O1C
26	M2	202	PEB	CAC-CBC-CGC-O1C
26	N2	202	PEB	CAC-CBC-CGC-O1C
26	O2	201	PEB	CAC-CBC-CGC-O1C
26	O2	202	PEB	CAC-CBC-CGC-O1C
26	P2	201	PEB	CAC-CBC-CGC-O1C
26	Q2	1001	PEB	CAC-CBC-CGC-O1C
26	R2	202	PEB	CAC-CBC-CGC-O1C
26	S2	201	PEB	CAC-CBC-CGC-O1C
26	T2	201	PEB	CAC-CBC-CGC-O1C
26	U2	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	V2	201	PEB	CAC-CBC-CGC-O1C
26	W2	201	PEB	CAC-CBC-CGC-O1C
26	W2	202	PEB	CAC-CBC-CGC-O1C
26	X2	201	PEB	CAC-CBC-CGC-O1C
26	Y2	201	PEB	CAC-CBC-CGC-O1C
26	Y2	202	PEB	CAC-CBC-CGC-O1C
26	Z2	201	PEB	CAC-CBC-CGC-O1C
26	A3	201	PEB	CAC-CBC-CGC-O1C
26	B3	201	PEB	CAC-CBC-CGC-O1C
26	C3	1001	PEB	CAC-CBC-CGC-O1C
26	D3	201	PEB	CAC-CBC-CGC-O1C
26	E3	201	PEB	CAC-CBC-CGC-O1C
26	F3	201	PEB	CAC-CBC-CGC-O1C
26	G3	201	PEB	CAC-CBC-CGC-O1C
26	H3	201	PEB	CAC-CBC-CGC-O1C
26	I3	201	PEB	CAC-CBC-CGC-O1C
26	J3	201	PEB	CAC-CBC-CGC-O1C
26	K3	201	PEB	CAC-CBC-CGC-O1C
26	L3	201	PEB	CAC-CBC-CGC-O1C
26	M3	201	PEB	CAC-CBC-CGC-O1C
26	N3	201	PEB	CAC-CBC-CGC-O1C
26	O3	1001	PEB	CAC-CBC-CGC-O1C
26	P3	201	PEB	CAC-CBC-CGC-O1C
26	Q3	201	PEB	CAC-CBC-CGC-O1C
26	R3	201	PEB	CAC-CBC-CGC-O1C
26	S3	201	PEB	CAC-CBC-CGC-O1C
26	S3	203	PEB	CAC-CBC-CGC-O1C
26	T3	201	PEB	CAC-CBC-CGC-O1C
26	U3	201	PEB	CAC-CBC-CGC-O1C
26	V3	201	PEB	CAC-CBC-CGC-O1C
26	W3	201	PEB	CAC-CBC-CGC-O1C
26	X3	201	PEB	CAC-CBC-CGC-O1C
26	Y3	201	PEB	CAC-CBC-CGC-O1C
26	Z3	201	PEB	CAC-CBC-CGC-O1C
26	a3	1001	PEB	CAC-CBC-CGC-O1C
26	a3	1003	PEB	CAC-CBC-CGC-O1C
26	b3	501	PEB	CAC-CBC-CGC-O1C
26	b3	502	PEB	CAC-CBC-CGC-O1C
26	c3	302	PEB	CAC-CBC-CGC-O1C
26	e3	1001	PEB	CAC-CBC-CGC-O1C
26	f3	201	PEB	CAC-CBC-CGC-O1C
26	g3	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	i3	201	PEB	CAC-CBC-CGC-O1C
26	k3	201	PEB	CAC-CBC-CGC-O1C
26	l3	201	PEB	CAC-CBC-CGC-O1C
26	m3	201	PEB	CAC-CBC-CGC-O1C
26	n3	201	PEB	CAC-CBC-CGC-O1C
26	o3	201	PEB	CAC-CBC-CGC-O1C
26	p3	201	PEB	CAC-CBC-CGC-O1C
26	q3	1001	PEB	CAC-CBC-CGC-O1C
26	r3	201	PEB	CAC-CBC-CGC-O1C
26	s3	201	PEB	CAC-CBC-CGC-O1C
26	t3	201	PEB	CAC-CBC-CGC-O1C
26	u3	201	PEB	CAC-CBC-CGC-O1C
26	v3	201	PEB	CAC-CBC-CGC-O1C
26	w3	201	PEB	CAC-CBC-CGC-O1C
26	x3	201	PEB	CAC-CBC-CGC-O1C
26	y3	201	PEB	CAC-CBC-CGC-O1C
26	z3	201	PEB	CAC-CBC-CGC-O1C
26	A4	201	PEB	CAC-CBC-CGC-O1C
26	B4	201	PEB	CAC-CBC-CGC-O1C
26	C4	1001	PEB	CAC-CBC-CGC-O1C
26	D4	201	PEB	CAC-CBC-CGC-O1C
26	E4	201	PEB	CAC-CBC-CGC-O1C
26	E4	202	PEB	CAC-CBC-CGC-O1C
26	F4	201	PEB	CAC-CBC-CGC-O1C
26	F4	202	PEB	CAC-CBC-CGC-O1C
26	G4	201	PEB	CAC-CBC-CGC-O1C
26	G4	202	PEB	CAC-CBC-CGC-O1C
26	H4	201	PEB	CAC-CBC-CGC-O1C
26	H4	202	PEB	CAC-CBC-CGC-O1C
26	I4	201	PEB	CAC-CBC-CGC-O1C
26	I4	202	PEB	CAC-CBC-CGC-O1C
26	J4	201	PEB	CAC-CBC-CGC-O1C
26	J4	202	PEB	CAC-CBC-CGC-O1C
26	K4	201	PEB	CAC-CBC-CGC-O1C
26	K4	202	PEB	CAC-CBC-CGC-O1C
26	L4	201	PEB	CAC-CBC-CGC-O1C
26	L4	202	PEB	CAC-CBC-CGC-O1C
26	M4	201	PEB	CAC-CBC-CGC-O1C
26	M4	202	PEB	CAC-CBC-CGC-O1C
26	N4	201	PEB	CAC-CBC-CGC-O1C
26	O4	1001	PEB	CAC-CBC-CGC-O1C
26	O4	1002	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	P4	201	PEB	CAC-CBC-CGC-O1C
26	P4	202	PEB	CAC-CBC-CGC-O1C
26	Q4	201	PEB	CAC-CBC-CGC-O1C
26	Q4	202	PEB	CAC-CBC-CGC-O1C
26	Q4	203	PEB	CAC-CBC-CGC-O1C
26	R4	201	PEB	CAC-CBC-CGC-O1C
26	R4	202	PEB	CAC-CBC-CGC-O1C
26	S4	201	PEB	CAC-CBC-CGC-O1C
26	S4	202	PEB	CAC-CBC-CGC-O1C
26	T4	201	PEB	CAC-CBC-CGC-O1C
26	U4	201	PEB	CAC-CBC-CGC-O1C
26	U4	202	PEB	CAC-CBC-CGC-O1C
26	V4	201	PEB	CAC-CBC-CGC-O1C
26	V4	202	PEB	CAC-CBC-CGC-O1C
26	W4	201	PEB	CAC-CBC-CGC-O1C
26	W4	202	PEB	CAC-CBC-CGC-O1C
26	X4	201	PEB	CAC-CBC-CGC-O1C
26	X4	202	PEB	CAC-CBC-CGC-O1C
26	Y4	201	PEB	CAC-CBC-CGC-O1C
26	Y4	202	PEB	CAC-CBC-CGC-O1C
26	Z4	201	PEB	CAC-CBC-CGC-O1C
26	Z4	202	PEB	CAC-CBC-CGC-O1C
26	24	401	PEB	CAC-CBC-CGC-O1C
26	34	1003	PEB	CAC-CBC-CGC-O1C
26	34	1007	PEB	CAC-CBC-CGC-O1C
26	44	301	PEB	CAC-CBC-CGC-O1C
26	44	302	PEB	CAC-CBC-CGC-O1C
26	a4	201	PEB	CAC-CBC-CGC-O1C
26	b4	1001	PEB	CAC-CBC-CGC-O1C
26	c4	202	PEB	CAC-CBC-CGC-O1C
26	d4	201	PEB	CAC-CBC-CGC-O1C
26	e4	201	PEB	CAC-CBC-CGC-O1C
26	f4	201	PEB	CAC-CBC-CGC-O1C
26	g4	201	PEB	CAC-CBC-CGC-O1C
26	h4	202	PEB	CAC-CBC-CGC-O1C
26	i4	201	PEB	CAC-CBC-CGC-O1C
26	j4	201	PEB	CAC-CBC-CGC-O1C
26	k4	201	PEB	CAC-CBC-CGC-O1C
26	l4	201	PEB	CAC-CBC-CGC-O1C
26	m4	1001	PEB	CAC-CBC-CGC-O1C
26	n4	201	PEB	CAC-CBC-CGC-O1C
26	o4	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	o4	202	PEB	CAC-CBC-CGC-O1C
26	p4	201	PEB	CAC-CBC-CGC-O1C
26	q4	201	PEB	CAC-CBC-CGC-O1C
26	q4	202	PEB	CAC-CBC-CGC-O1C
26	s4	201	PEB	CAC-CBC-CGC-O1C
26	t4	201	PEB	CAC-CBC-CGC-O1C
26	t4	202	PEB	CAC-CBC-CGC-O1C
26	u4	201	PEB	CAC-CBC-CGC-O1C
26	u4	202	PEB	CAC-CBC-CGC-O1C
26	v4	201	PEB	CAC-CBC-CGC-O1C
26	w4	201	PEB	CAC-CBC-CGC-O1C
26	x4	201	PEB	CAC-CBC-CGC-O1C
26	y4	1001	PEB	CAC-CBC-CGC-O1C
26	y4	1002	PEB	CAC-CBC-CGC-O1C
26	z4	201	PEB	CAC-CBC-CGC-O1C
26	z4	202	PEB	CAC-CBC-CGC-O1C
26	A5	201	PEB	CAC-CBC-CGC-O1C
26	B5	201	PEB	CAC-CBC-CGC-O1C
26	C5	201	PEB	CAC-CBC-CGC-O1C
26	D5	201	PEB	CAC-CBC-CGC-O1C
26	E5	201	PEB	CAC-CBC-CGC-O1C
26	F5	201	PEB	CAC-CBC-CGC-O1C
26	G5	201	PEB	CAC-CBC-CGC-O1C
26	H5	201	PEB	CAC-CBC-CGC-O1C
26	I5	201	PEB	CAC-CBC-CGC-O1C
26	J5	201	PEB	CAC-CBC-CGC-O1C
26	K5	1001	PEB	CAC-CBC-CGC-O1C
26	L5	201	PEB	CAC-CBC-CGC-O1C
26	M5	201	PEB	CAC-CBC-CGC-O1C
26	N5	201	PEB	CAC-CBC-CGC-O1C
26	O5	201	PEB	CAC-CBC-CGC-O1C
26	Q5	201	PEB	CAC-CBC-CGC-O1C
26	R5	201	PEB	CAC-CBC-CGC-O1C
26	S5	201	PEB	CAC-CBC-CGC-O1C
26	T5	201	PEB	CAC-CBC-CGC-O1C
26	U5	201	PEB	CAC-CBC-CGC-O1C
26	V5	201	PEB	CAC-CBC-CGC-O1C
26	W5	301	PEB	CAC-CBC-CGC-O1C
26	X5	401	PEB	CAC-CBC-CGC-O1C
26	Y5	1001	PEB	CAC-CBC-CGC-O1C
26	Y5	1003	PEB	CAC-CBC-CGC-O1C
26	Z5	301	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	Z5	303	PEB	CAC-CBC-CGC-O1C
26	a5	201	PEB	CAC-CBC-CGC-O1C
26	b5	1001	PEB	CAC-CBC-CGC-O1C
26	c5	202	PEB	CAC-CBC-CGC-O1C
26	d5	201	PEB	CAC-CBC-CGC-O1C
26	e5	201	PEB	CAC-CBC-CGC-O1C
26	g5	201	PEB	CAC-CBC-CGC-O1C
26	h5	201	PEB	CAC-CBC-CGC-O1C
26	i5	201	PEB	CAC-CBC-CGC-O1C
26	j5	201	PEB	CAC-CBC-CGC-O1C
26	j5	202	PEB	CAC-CBC-CGC-O1C
26	k5	201	PEB	CAC-CBC-CGC-O1C
26	l5	201	PEB	CAC-CBC-CGC-O1C
26	l5	202	PEB	CAC-CBC-CGC-O1C
26	m5	1001	PEB	CAC-CBC-CGC-O1C
26	n5	201	PEB	CAC-CBC-CGC-O1C
26	o5	201	PEB	CAC-CBC-CGC-O1C
26	q5	201	PEB	CAC-CBC-CGC-O1C
26	r5	201	PEB	CAC-CBC-CGC-O1C
26	s5	201	PEB	CAC-CBC-CGC-O1C
26	t5	201	PEB	CAC-CBC-CGC-O1C
26	u5	201	PEB	CAC-CBC-CGC-O1C
26	v5	201	PEB	CAC-CBC-CGC-O1C
26	w5	201	PEB	CAC-CBC-CGC-O1C
26	x5	201	PEB	CAC-CBC-CGC-O1C
26	y5	1001	PEB	CAC-CBC-CGC-O1C
26	z5	201	PEB	CAC-CBC-CGC-O1C
26	f8	201	PEB	CAC-CBC-CGC-O1C
26	f8	202	PEB	CAC-CBC-CGC-O1C
26	g8	201	PEB	CAC-CBC-CGC-O1C
26	h8	201	PEB	CAC-CBC-CGC-O1C
26	i8	201	PEB	CAC-CBC-CGC-O1C
26	j8	201	PEB	CAC-CBC-CGC-O1C
26	j8	202	PEB	CAC-CBC-CGC-O1C
26	k8	201	PEB	CAC-CBC-CGC-O1C
26	k8	202	PEB	CAC-CBC-CGC-O1C
26	k8	203	PEB	CAC-CBC-CGC-O1C
26	l8	201	PEB	CAC-CBC-CGC-O1C
26	l8	202	PEB	CAC-CBC-CGC-O1C
26	m8	201	PEB	CAC-CBC-CGC-O1C
26	m8	202	PEB	CAC-CBC-CGC-O1C
26	A6	1001	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	A6	1002	PEB	CAC-CBC-CGC-O1C
26	B6	201	PEB	CAC-CBC-CGC-O1C
26	C6	201	PEB	CAC-CBC-CGC-O1C
26	C6	202	PEB	CAC-CBC-CGC-O1C
26	D6	201	PEB	CAC-CBC-CGC-O1C
26	E6	201	PEB	CAC-CBC-CGC-O1C
26	E6	202	PEB	CAC-CBC-CGC-O1C
26	F6	201	PEB	CAC-CBC-CGC-O1C
26	F6	202	PEB	CAC-CBC-CGC-O1C
26	G6	201	PEB	CAC-CBC-CGC-O1C
26	H6	202	PEB	CAC-CBC-CGC-O1C
26	I6	201	PEB	CAC-CBC-CGC-O1C
26	I6	202	PEB	CAC-CBC-CGC-O1C
26	J6	201	PEB	CAC-CBC-CGC-O1C
26	K6	201	PEB	CAC-CBC-CGC-O1C
26	K6	202	PEB	CAC-CBC-CGC-O1C
26	L6	201	PEB	CAC-CBC-CGC-O1C
26	M6	1001	PEB	CAC-CBC-CGC-O1C
26	M6	1002	PEB	CAC-CBC-CGC-O1C
26	N6	201	PEB	CAC-CBC-CGC-O1C
26	O6	201	PEB	CAC-CBC-CGC-O1C
26	O6	202	PEB	CAC-CBC-CGC-O1C
26	P6	201	PEB	CAC-CBC-CGC-O1C
26	P6	202	PEB	CAC-CBC-CGC-O1C
26	Q6	201	PEB	CAC-CBC-CGC-O1C
26	Q6	202	PEB	CAC-CBC-CGC-O1C
26	R6	201	PEB	CAC-CBC-CGC-O1C
26	S6	201	PEB	CAC-CBC-CGC-O1C
26	S6	202	PEB	CAC-CBC-CGC-O1C
26	T6	201	PEB	CAC-CBC-CGC-O1C
26	T6	202	PEB	CAC-CBC-CGC-O1C
26	U6	201	PEB	CAC-CBC-CGC-O1C
26	V6	201	PEB	CAC-CBC-CGC-O1C
26	W6	201	PEB	CAC-CBC-CGC-O1C
26	W6	202	PEB	CAC-CBC-CGC-O1C
26	X6	201	PEB	CAC-CBC-CGC-O1C
26	Y6	201	PEB	CAC-CBC-CGC-O1C
26	Z6	201	PEB	CAC-CBC-CGC-O1C
26	Z6	202	PEB	CAC-CBC-CGC-O1C
26	a6	201	PEB	CAC-CBC-CGC-O1C
26	b6	201	PEB	CAC-CBC-CGC-O1C
26	b6	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	c6	1001	PEB	CAC-CBC-CGC-O1C
26	c6	1002	PEB	CAC-CBC-CGC-O1C
26	c6	1003	PEB	CAC-CBC-CGC-O1C
26	d6	201	PEB	CAC-CBC-CGC-O1C
26	e6	201	PEB	CAC-CBC-CGC-O1C
26	f6	201	PEB	CAC-CBC-CGC-O1C
26	g6	201	PEB	CAC-CBC-CGC-O1C
26	g6	202	PEB	CAC-CBC-CGC-O1C
26	h6	201	PEB	CAC-CBC-CGC-O1C
26	h6	202	PEB	CAC-CBC-CGC-O1C
26	i6	201	PEB	CAC-CBC-CGC-O1C
26	i6	202	PEB	CAC-CBC-CGC-O1C
26	j6	201	PEB	CAC-CBC-CGC-O1C
26	j6	202	PEB	CAC-CBC-CGC-O1C
26	k6	1001	PEB	CAC-CBC-CGC-O1C
26	k6	1002	PEB	CAC-CBC-CGC-O1C
26	l6	201	PEB	CAC-CBC-CGC-O1C
26	l6	202	PEB	CAC-CBC-CGC-O1C
26	m6	201	PEB	CAC-CBC-CGC-O1C
26	m6	202	PEB	CAC-CBC-CGC-O1C
26	o6	201	PEB	CAC-CBC-CGC-O1C
26	o6	202	PEB	CAC-CBC-CGC-O1C
26	p6	201	PEB	CAC-CBC-CGC-O1C
26	q6	201	PEB	CAC-CBC-CGC-O1C
26	q6	202	PEB	CAC-CBC-CGC-O1C
26	r6	201	PEB	CAC-CBC-CGC-O1C
26	r6	202	PEB	CAC-CBC-CGC-O1C
26	s6	201	PEB	CAC-CBC-CGC-O1C
26	s6	202	PEB	CAC-CBC-CGC-O1C
26	t6	202	PEB	CAC-CBC-CGC-O1C
26	u6	201	PEB	CAC-CBC-CGC-O1C
26	u6	202	PEB	CAC-CBC-CGC-O1C
26	v6	201	PEB	CAC-CBC-CGC-O1C
26	v6	202	PEB	CAC-CBC-CGC-O1C
26	w6	1001	PEB	CAC-CBC-CGC-O1C
26	w6	1002	PEB	CAC-CBC-CGC-O1C
26	x6	201	PEB	CAC-CBC-CGC-O1C
26	x6	202	PEB	CAC-CBC-CGC-O1C
26	y6	201	PEB	CAC-CBC-CGC-O1C
26	y6	202	PEB	CAC-CBC-CGC-O1C
26	y6	203	PEB	CAC-CBC-CGC-O1C
26	z6	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	z6	202	PEB	CAC-CBC-CGC-O1C
26	o8	202	PEB	CAC-CBC-CGC-O1C
26	p8	201	PEB	CAC-CBC-CGC-O1C
26	q8	201	PEB	CAC-CBC-CGC-O1C
26	r8	201	PEB	CAC-CBC-CGC-O1C
26	s8	201	PEB	CAC-CBC-CGC-O1C
26	t8	201	PEB	CAC-CBC-CGC-O1C
26	u8	201	PEB	CAC-CBC-CGC-O1C
26	C7	201	PEB	CAC-CBC-CGC-O1C
26	D7	201	PEB	CAC-CBC-CGC-O1C
26	E7	201	PEB	CAC-CBC-CGC-O1C
26	G7	201	PEB	CAC-CBC-CGC-O1C
26	H7	201	PEB	CAC-CBC-CGC-O1C
26	I7	201	PEB	CAC-CBC-CGC-O1C
26	K7	201	PEB	CAC-CBC-CGC-O1C
26	M7	1001	PEB	CAC-CBC-CGC-O1C
26	M7	1002	PEB	CAC-CBC-CGC-O1C
26	N7	201	PEB	CAC-CBC-CGC-O1C
26	O7	201	PEB	CAC-CBC-CGC-O1C
26	P7	201	PEB	CAC-CBC-CGC-O1C
26	Q7	201	PEB	CAC-CBC-CGC-O1C
26	R7	201	PEB	CAC-CBC-CGC-O1C
26	S7	201	PEB	CAC-CBC-CGC-O1C
26	T7	201	PEB	CAC-CBC-CGC-O1C
26	U7	201	PEB	CAC-CBC-CGC-O1C
26	V7	201	PEB	CAC-CBC-CGC-O1C
26	W7	201	PEB	CAC-CBC-CGC-O1C
26	X7	201	PEB	CAC-CBC-CGC-O1C
26	Y7	1001	PEB	CAC-CBC-CGC-O1C
26	Z7	201	PEB	CAC-CBC-CGC-O1C
26	a7	201	PEB	CAC-CBC-CGC-O1C
26	b7	201	PEB	CAC-CBC-CGC-O1C
26	c7	201	PEB	CAC-CBC-CGC-O1C
26	d7	201	PEB	CAC-CBC-CGC-O1C
26	e7	201	PEB	CAC-CBC-CGC-O1C
26	f7	201	PEB	CAC-CBC-CGC-O1C
26	g7	201	PEB	CAC-CBC-CGC-O1C
26	h7	201	PEB	CAC-CBC-CGC-O1C
26	i7	201	PEB	CAC-CBC-CGC-O1C
26	j7	201	PEB	CAC-CBC-CGC-O1C
26	k7	1001	PEB	CAC-CBC-CGC-O1C
26	l7	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	m7	201	PEB	CAC-CBC-CGC-O1C
26	n7	201	PEB	CAC-CBC-CGC-O1C
26	o7	201	PEB	CAC-CBC-CGC-O1C
26	q7	201	PEB	CAC-CBC-CGC-O1C
26	r7	201	PEB	CAC-CBC-CGC-O1C
26	s7	201	PEB	CAC-CBC-CGC-O1C
26	t7	201	PEB	CAC-CBC-CGC-O1C
26	u7	201	PEB	CAC-CBC-CGC-O1C
26	v7	201	PEB	CAC-CBC-CGC-O1C
26	w7	1001	PEB	CAC-CBC-CGC-O1C
26	x7	201	PEB	CAC-CBC-CGC-O1C
26	y7	201	PEB	CAC-CBC-CGC-O1C
26	z7	201	PEB	CAC-CBC-CGC-O1C
26	a8	601	PEB	CAC-CBC-CGC-O1C
26	a8	602	PEB	CAC-CBC-CGC-O1C
26	b8	1001	PEB	CAC-CBC-CGC-O1C
26	b8	1002	PEB	CAC-CBC-CGC-O1C
26	b8	1003	PEB	CAC-CBC-CGC-O1C
26	c8	302	PEB	CAC-CBC-CGC-O1C
26	d8	302	PEB	CAC-CBC-CGC-O1C
26	e8	301	PEB	CAC-CBC-CGC-O1C
26	e8	302	PEB	CAC-CBC-CGC-O1C
26	a9	601	PEB	CAC-CBC-CGC-O1C
26	a9	602	PEB	CAC-CBC-CGC-O1C
26	a9	603	PEB	CAC-CBC-CGC-O1C
26	b9	401	PEB	CAC-CBC-CGC-O1C
26	b9	402	PEB	CAC-CBC-CGC-O1C
26	b9	403	PEB	CAC-CBC-CGC-O1C
26	b9	404	PEB	CAC-CBC-CGC-O1C
26	c9	301	PEB	CAC-CBC-CGC-O1C
26	c9	302	PEB	CAC-CBC-CGC-O1C
26	d9	301	PEB	CAC-CBC-CGC-O1C
26	d9	302	PEB	CAC-CBC-CGC-O1C
26	d9	303	PEB	CAC-CBC-CGC-O1C
26	e9	301	PEB	CAC-CBC-CGC-O1C
26	e9	302	PEB	CAC-CBC-CGC-O1C
26	e9	303	PEB	CAC-CBC-CGC-O1C
26	v8	201	PEB	CAC-CBC-CGC-O1C
26	v8	202	PEB	CAC-CBC-CGC-O1C
26	w8	201	PEB	CAC-CBC-CGC-O1C
26	w8	202	PEB	CAC-CBC-CGC-O1C
26	x8	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	x8	202	PEB	CAC-CBC-CGC-O1C
26	y8	201	PEB	CAC-CBC-CGC-O1C
26	z8	201	PEB	CAC-CBC-CGC-O1C
26	z8	202	PEB	CAC-CBC-CGC-O1C
26	A8	201	PEB	CAC-CBC-CGC-O1C
26	A8	202	PEB	CAC-CBC-CGC-O1C
26	B8	201	PEB	CAC-CBC-CGC-O1C
26	B8	202	PEB	CAC-CBC-CGC-O1C
26	C8	201	PEB	CAC-CBC-CGC-O1C
26	D8	201	PEB	CAC-CBC-CGC-O1C
26	D8	202	PEB	CAC-CBC-CGC-O1C
26	E8	201	PEB	CAC-CBC-CGC-O1C
26	E8	202	PEB	CAC-CBC-CGC-O1C
26	F8	1001	PEB	CAC-CBC-CGC-O1C
26	F8	1002	PEB	CAC-CBC-CGC-O1C
26	G8	201	PEB	CAC-CBC-CGC-O1C
26	G8	202	PEB	CAC-CBC-CGC-O1C
26	H8	201	PEB	CAC-CBC-CGC-O1C
26	H8	202	PEB	CAC-CBC-CGC-O1C
26	I8	201	PEB	CAC-CBC-CGC-O1C
26	I8	202	PEB	CAC-CBC-CGC-O1C
26	J8	201	PEB	CAC-CBC-CGC-O1C
26	J8	202	PEB	CAC-CBC-CGC-O1C
26	K8	201	PEB	CAC-CBC-CGC-O1C
26	K8	202	PEB	CAC-CBC-CGC-O1C
26	L8	201	PEB	CAC-CBC-CGC-O1C
26	L8	202	PEB	CAC-CBC-CGC-O1C
26	M8	201	PEB	CAC-CBC-CGC-O1C
26	M8	202	PEB	CAC-CBC-CGC-O1C
26	N8	201	PEB	CAC-CBC-CGC-O1C
26	N8	202	PEB	CAC-CBC-CGC-O1C
26	O8	201	PEB	CAC-CBC-CGC-O1C
26	O8	202	PEB	CAC-CBC-CGC-O1C
26	P8	201	PEB	CAC-CBC-CGC-O1C
26	P8	202	PEB	CAC-CBC-CGC-O1C
26	Q8	201	PEB	CAC-CBC-CGC-O1C
26	Q8	202	PEB	CAC-CBC-CGC-O1C
26	S8	401	PEB	CAC-CBC-CGC-O1C
26	T8	301	PEB	CAC-CBC-CGC-O1C
26	T8	302	PEB	CAC-CBC-CGC-O1C
26	U8	1001	PEB	CAC-CBC-CGC-O1C
26	U8	1002	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	U8	1003	PEB	CAC-CBC-CGC-O1C
26	V8	1001	PEB	CAC-CBC-CGC-O1C
26	W8	201	PEB	CAC-CBC-CGC-O1C
26	W8	202	PEB	CAC-CBC-CGC-O1C
26	X8	201	PEB	CAC-CBC-CGC-O1C
26	Y8	201	PEB	CAC-CBC-CGC-O1C
26	Y8	202	PEB	CAC-CBC-CGC-O1C
26	Z8	201	PEB	CAC-CBC-CGC-O1C
26	f9	201	PEB	CAC-CBC-CGC-O1C
26	f9	202	PEB	CAC-CBC-CGC-O1C
26	g9	201	PEB	CAC-CBC-CGC-O1C
26	h9	201	PEB	CAC-CBC-CGC-O1C
26	h9	202	PEB	CAC-CBC-CGC-O1C
26	i9	201	PEB	CAC-CBC-CGC-O1C
26	j9	201	PEB	CAC-CBC-CGC-O1C
26	j9	202	PEB	CAC-CBC-CGC-O1C
26	k9	201	PEB	CAC-CBC-CGC-O1C
26	l9	201	PEB	CAC-CBC-CGC-O1C
26	l9	202	PEB	CAC-CBC-CGC-O1C
26	m9	1001	PEB	CAC-CBC-CGC-O1C
26	n9	201	PEB	CAC-CBC-CGC-O1C
26	o9	201	PEB	CAC-CBC-CGC-O1C
26	p9	201	PEB	CAC-CBC-CGC-O1C
26	p9	202	PEB	CAC-CBC-CGC-O1C
26	q9	201	PEB	CAC-CBC-CGC-O1C
26	q9	202	PEB	CAC-CBC-CGC-O1C
26	r9	201	PEB	CAC-CBC-CGC-O1C
26	r9	202	PEB	CAC-CBC-CGC-O1C
26	s9	201	PEB	CAC-CBC-CGC-O1C
26	s9	202	PEB	CAC-CBC-CGC-O1C
26	t9	201	PEB	CAC-CBC-CGC-O1C
26	t9	202	PEB	CAC-CBC-CGC-O1C
26	u9	201	PEB	CAC-CBC-CGC-O1C
26	u9	202	PEB	CAC-CBC-CGC-O1C
26	v9	201	PEB	CAC-CBC-CGC-O1C
26	w9	201	PEB	CAC-CBC-CGC-O1C
26	w9	202	PEB	CAC-CBC-CGC-O1C
26	x9	201	PEB	CAC-CBC-CGC-O1C
26	x9	202	PEB	CAC-CBC-CGC-O1C
26	y9	1001	PEB	CAC-CBC-CGC-O1C
26	y9	1002	PEB	CAC-CBC-CGC-O1C
26	z9	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	z9	202	PEB	CAC-CBC-CGC-O1C
26	A9	201	PEB	CAC-CBC-CGC-O1C
26	B9	201	PEB	CAC-CBC-CGC-O1C
26	C9	201	PEB	CAC-CBC-CGC-O1C
26	D9	201	PEB	CAC-CBC-CGC-O1C
26	E9	201	PEB	CAC-CBC-CGC-O1C
26	F9	201	PEB	CAC-CBC-CGC-O1C
26	G9	201	PEB	CAC-CBC-CGC-O1C
26	H9	201	PEB	CAC-CBC-CGC-O1C
26	I9	201	PEB	CAC-CBC-CGC-O1C
26	J9	201	PEB	CAC-CBC-CGC-O1C
26	K9	1001	PEB	CAC-CBC-CGC-O1C
26	L9	201	PEB	CAC-CBC-CGC-O1C
26	M9	201	PEB	CAC-CBC-CGC-O1C
26	N9	201	PEB	CAC-CBC-CGC-O1C
26	O9	201	PEB	CAC-CBC-CGC-O1C
26	P9	201	PEB	CAC-CBC-CGC-O1C
26	Q9	201	PEB	CAC-CBC-CGC-O1C
26	R9	201	PEB	CAC-CBC-CGC-O1C
26	S9	201	PEB	CAC-CBC-CGC-O1C
26	T9	201	PEB	CAC-CBC-CGC-O1C
26	U9	201	PEB	CAC-CBC-CGC-O1C
26	V9	201	PEB	CAC-CBC-CGC-O1C
26	X9	401	PEB	CAC-CBC-CGC-O1C
26	Y9	302	PEB	CAC-CBC-CGC-O1C
26	Z9	1001	PEB	CAC-CBC-CGC-O1C
26	Z9	1003	PEB	CAC-CBC-CGC-O1C
26	Z9	1007	PEB	CAC-CBC-CGC-O1C
26	aa	1001	PEB	CAC-CBC-CGC-O1C
26	ab	201	PEB	CAC-CBC-CGC-O1C
26	ac	201	PEB	CAC-CBC-CGC-O1C
26	ad	201	PEB	CAC-CBC-CGC-O1C
26	ae	201	PEB	CAC-CBC-CGC-O1C
26	af	201	PEB	CAC-CBC-CGC-O1C
26	ag	201	PEB	CAC-CBC-CGC-O1C
26	ah	201	PEB	CAC-CBC-CGC-O1C
26	ai	201	PEB	CAC-CBC-CGC-O1C
26	aj	201	PEB	CAC-CBC-CGC-O1C
26	ak	201	PEB	CAC-CBC-CGC-O1C
26	al	201	PEB	CAC-CBC-CGC-O1C
26	am	1001	PEB	CAC-CBC-CGC-O1C
26	ao	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	ap	201	PEB	CAC-CBC-CGC-O1C
26	aq	201	PEB	CAC-CBC-CGC-O1C
26	ar	201	PEB	CAC-CBC-CGC-O1C
26	as	201	PEB	CAC-CBC-CGC-O1C
26	at	201	PEB	CAC-CBC-CGC-O1C
26	au	201	PEB	CAC-CBC-CGC-O1C
26	av	201	PEB	CAC-CBC-CGC-O1C
26	aw	201	PEB	CAC-CBC-CGC-O1C
26	ay	1001	PEB	CAC-CBC-CGC-O1C
26	az	201	PEB	CAC-CBC-CGC-O1C
26	aA	201	PEB	CAC-CBC-CGC-O1C
26	aA	202	PEB	CAC-CBC-CGC-O1C
26	aB	201	PEB	CAC-CBC-CGC-O1C
26	aB	202	PEB	CAC-CBC-CGC-O1C
26	aC	201	PEB	CAC-CBC-CGC-O1C
26	aC	202	PEB	CAC-CBC-CGC-O1C
26	aD	201	PEB	CAC-CBC-CGC-O1C
26	aE	201	PEB	CAC-CBC-CGC-O1C
26	aE	202	PEB	CAC-CBC-CGC-O1C
26	aF	201	PEB	CAC-CBC-CGC-O1C
26	aF	204	PEB	CAC-CBC-CGC-O1C
26	aG	201	PEB	CAC-CBC-CGC-O1C
26	aH	201	PEB	CAC-CBC-CGC-O1C
26	aH	202	PEB	CAC-CBC-CGC-O1C
26	aI	201	PEB	CAC-CBC-CGC-O1C
26	aI	202	PEB	CAC-CBC-CGC-O1C
26	aJ	201	PEB	CAC-CBC-CGC-O1C
26	aJ	202	PEB	CAC-CBC-CGC-O1C
26	aK	1001	PEB	CAC-CBC-CGC-O1C
26	aK	1002	PEB	CAC-CBC-CGC-O1C
26	aL	201	PEB	CAC-CBC-CGC-O1C
26	aL	202	PEB	CAC-CBC-CGC-O1C
26	aM	201	PEB	CAC-CBC-CGC-O1C
26	aM	202	PEB	CAC-CBC-CGC-O1C
26	aN	201	PEB	CAC-CBC-CGC-O1C
26	aN	202	PEB	CAC-CBC-CGC-O1C
26	aN	204	PEB	CAC-CBC-CGC-O1C
26	aO	201	PEB	CAC-CBC-CGC-O1C
26	aP	201	PEB	CAC-CBC-CGC-O1C
26	aP	202	PEB	CAC-CBC-CGC-O1C
26	aQ	201	PEB	CAC-CBC-CGC-O1C
26	aQ	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	aR	201	PEB	CAC-CBC-CGC-O1C
26	aR	202	PEB	CAC-CBC-CGC-O1C
26	aS	201	PEB	CAC-CBC-CGC-O1C
26	aS	202	PEB	CAC-CBC-CGC-O1C
26	aT	201	PEB	CAC-CBC-CGC-O1C
26	aT	202	PEB	CAC-CBC-CGC-O1C
26	aU	201	PEB	CAC-CBC-CGC-O1C
26	aU	202	PEB	CAC-CBC-CGC-O1C
26	aV	201	PEB	CAC-CBC-CGC-O1C
26	aV	202	PEB	CAC-CBC-CGC-O1C
26	aW	301	PEB	CAC-CBC-CGC-O1C
26	aW	302	PEB	CAC-CBC-CGC-O1C
26	aX	401	PEB	CAC-CBC-CGC-O1C
26	aX	402	PEB	CAC-CBC-CGC-O1C
26	aY	401	PEB	CAC-CBC-CGC-O1C
26	aY	402	PEB	CAC-CBC-CGC-O1C
26	aY	406	PEB	CAC-CBC-CGC-O1C
26	aZ	301	PEB	CAC-CBC-CGC-O1C
26	aZ	302	PEB	CAC-CBC-CGC-O1C
26	ba	1001	PEB	CAC-CBC-CGC-O1C
26	bb	201	PEB	CAC-CBC-CGC-O1C
26	bc	201	PEB	CAC-CBC-CGC-O1C
26	bd	201	PEB	CAC-CBC-CGC-O1C
26	bd	202	PEB	CAC-CBC-CGC-O1C
26	be	201	PEB	CAC-CBC-CGC-O1C
26	bf	201	PEB	CAC-CBC-CGC-O1C
26	bg	201	PEB	CAC-CBC-CGC-O1C
26	bh	201	PEB	CAC-CBC-CGC-O1C
26	bh	202	PEB	CAC-CBC-CGC-O1C
26	bi	201	PEB	CAC-CBC-CGC-O1C
26	bj	201	PEB	CAC-CBC-CGC-O1C
26	bj	202	PEB	CAC-CBC-CGC-O1C
26	bk	201	PEB	CAC-CBC-CGC-O1C
26	bl	201	PEB	CAC-CBC-CGC-O1C
26	bl	202	PEB	CAC-CBC-CGC-O1C
26	bm	1001	PEB	CAC-CBC-CGC-O1C
26	bm	1002	PEB	CAC-CBC-CGC-O1C
26	bn	201	PEB	CAC-CBC-CGC-O1C
26	bo	201	PEB	CAC-CBC-CGC-O1C
26	bp	201	PEB	CAC-CBC-CGC-O1C
26	bq	201	PEB	CAC-CBC-CGC-O1C
26	bq	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	br	201	PEB	CAC-CBC-CGC-O1C
26	br	202	PEB	CAC-CBC-CGC-O1C
26	bs	1001	PEB	CAC-CBC-CGC-O1C
26	bs	1002	PEB	CAC-CBC-CGC-O1C
26	bs	1003	PEB	CAC-CBC-CGC-O1C
26	bt	201	PEB	CAC-CBC-CGC-O1C
26	bt	202	PEB	CAC-CBC-CGC-O1C
26	bu	201	PEB	CAC-CBC-CGC-O1C
26	bu	202	PEB	CAC-CBC-CGC-O1C
26	bv	201	PEB	CAC-CBC-CGC-O1C
26	bv	202	PEB	CAC-CBC-CGC-O1C
26	bw	201	PEB	CAC-CBC-CGC-O1C
26	bw	202	PEB	CAC-CBC-CGC-O1C
26	bx	201	PEB	CAC-CBC-CGC-O1C
26	bx	202	PEB	CAC-CBC-CGC-O1C
26	by	1001	PEB	CAC-CBC-CGC-O1C
26	by	1002	PEB	CAC-CBC-CGC-O1C
26	bz	201	PEB	CAC-CBC-CGC-O1C
26	bz	202	PEB	CAC-CBC-CGC-O1C
26	bA	201	PEB	CAC-CBC-CGC-O1C
26	bB	201	PEB	CAC-CBC-CGC-O1C
26	bC	201	PEB	CAC-CBC-CGC-O1C
26	bD	201	PEB	CAC-CBC-CGC-O1C
26	bE	201	PEB	CAC-CBC-CGC-O1C
26	bF	201	PEB	CAC-CBC-CGC-O1C
26	bG	201	PEB	CAC-CBC-CGC-O1C
26	bH	201	PEB	CAC-CBC-CGC-O1C
26	bI	201	PEB	CAC-CBC-CGC-O1C
26	bJ	201	PEB	CAC-CBC-CGC-O1C
26	bK	1001	PEB	CAC-CBC-CGC-O1C
26	bL	201	PEB	CAC-CBC-CGC-O1C
26	bM	201	PEB	CAC-CBC-CGC-O1C
26	bN	201	PEB	CAC-CBC-CGC-O1C
26	bO	201	PEB	CAC-CBC-CGC-O1C
26	bP	201	PEB	CAC-CBC-CGC-O1C
26	bQ	201	PEB	CAC-CBC-CGC-O1C
26	bR	201	PEB	CAC-CBC-CGC-O1C
26	bS	201	PEB	CAC-CBC-CGC-O1C
26	bU	201	PEB	CAC-CBC-CGC-O1C
26	bV	201	PEB	CAC-CBC-CGC-O1C
26	bW	301	PEB	CAC-CBC-CGC-O1C
26	bX	401	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	bX	402	PEB	CAC-CBC-CGC-O1C
26	bY	1001	PEB	CAC-CBC-CGC-O1C
26	bY	1003	PEB	CAC-CBC-CGC-O1C
26	bZ	301	PEB	CAC-CBC-CGC-O1C
26	bZ	303	PEB	CAC-CBC-CGC-O1C
26	ca	1001	PEB	CAC-CBC-CGC-O1C
26	cb	201	PEB	CAC-CBC-CGC-O1C
26	cc	201	PEB	CAC-CBC-CGC-O1C
26	cd	201	PEB	CAC-CBC-CGC-O1C
26	ce	201	PEB	CAC-CBC-CGC-O1C
26	cg	201	PEB	CAC-CBC-CGC-O1C
26	ch	201	PEB	CAC-CBC-CGC-O1C
26	ci	201	PEB	CAC-CBC-CGC-O1C
26	cj	201	PEB	CAC-CBC-CGC-O1C
26	ck	201	PEB	CAC-CBC-CGC-O1C
26	cl	201	PEB	CAC-CBC-CGC-O1C
26	cm	1001	PEB	CAC-CBC-CGC-O1C
26	cp	201	PEB	CAC-CBC-CGC-O1C
26	cq	201	PEB	CAC-CBC-CGC-O1C
26	cr	201	PEB	CAC-CBC-CGC-O1C
26	cs	201	PEB	CAC-CBC-CGC-O1C
26	ct	201	PEB	CAC-CBC-CGC-O1C
26	cu	201	PEB	CAC-CBC-CGC-O1C
26	cv	201	PEB	CAC-CBC-CGC-O1C
26	cw	201	PEB	CAC-CBC-CGC-O1C
26	cx	201	PEB	CAC-CBC-CGC-O1C
26	cy	1001	PEB	CAC-CBC-CGC-O1C
26	cz	201	PEB	CAC-CBC-CGC-O1C
26	cA	201	PEB	CAC-CBC-CGC-O1C
26	cB	201	PEB	CAC-CBC-CGC-O1C
26	cC	1001	PEB	CAC-CBC-CGC-O1C
26	cC	1003	PEB	CAC-CBC-CGC-O1C
26	cD	201	PEB	CAC-CBC-CGC-O1C
26	cE	201	PEB	CAC-CBC-CGC-O1C
26	cG	201	PEB	CAC-CBC-CGC-O1C
26	cI	201	PEB	CAC-CBC-CGC-O1C
26	cJ	201	PEB	CAC-CBC-CGC-O1C
26	cK	201	PEB	CAC-CBC-CGC-O1C
26	cL	201	PEB	CAC-CBC-CGC-O1C
26	cM	201	PEB	CAC-CBC-CGC-O1C
26	cM	202	PEB	CAC-CBC-CGC-O1C
26	cN	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	cO	201	PEB	CAC-CBC-CGC-O1C
26	cO	202	PEB	CAC-CBC-CGC-O1C
26	cP	201	PEB	CAC-CBC-CGC-O1C
26	cP	202	PEB	CAC-CBC-CGC-O1C
26	cQ	201	PEB	CAC-CBC-CGC-O1C
26	cR	201	PEB	CAC-CBC-CGC-O1C
26	cR	202	PEB	CAC-CBC-CGC-O1C
26	cS	201	PEB	CAC-CBC-CGC-O1C
26	cS	202	PEB	CAC-CBC-CGC-O1C
26	cT	1001	PEB	CAC-CBC-CGC-O1C
26	cT	1002	PEB	CAC-CBC-CGC-O1C
26	cU	201	PEB	CAC-CBC-CGC-O1C
26	cU	202	PEB	CAC-CBC-CGC-O1C
26	cV	201	PEB	CAC-CBC-CGC-O1C
26	cV	202	PEB	CAC-CBC-CGC-O1C
26	cV	203	PEB	CAC-CBC-CGC-O1C
26	cW	201	PEB	CAC-CBC-CGC-O1C
26	cW	202	PEB	CAC-CBC-CGC-O1C
26	cX	201	PEB	CAC-CBC-CGC-O1C
26	cX	202	PEB	CAC-CBC-CGC-O1C
26	cY	201	PEB	CAC-CBC-CGC-O1C
26	cZ	201	PEB	CAC-CBC-CGC-O1C
26	da	1001	PEB	CAC-CBC-CGC-O1C
26	db	201	PEB	CAC-CBC-CGC-O1C
26	dc	201	PEB	CAC-CBC-CGC-O1C
26	dc	203	PEB	CAC-CBC-CGC-O1C
26	dd	201	PEB	CAC-CBC-CGC-O1C
26	de	201	PEB	CAC-CBC-CGC-O1C
26	df	201	PEB	CAC-CBC-CGC-O1C
26	dg	201	PEB	CAC-CBC-CGC-O1C
26	dh	201	PEB	CAC-CBC-CGC-O1C
26	di	201	PEB	CAC-CBC-CGC-O1C
26	dj	201	PEB	CAC-CBC-CGC-O1C
26	dk	1001	PEB	CAC-CBC-CGC-O1C
26	dk	1002	PEB	CAC-CBC-CGC-O1C
26	dl	201	PEB	CAC-CBC-CGC-O1C
26	dm	201	PEB	CAC-CBC-CGC-O1C
26	dm	202	PEB	CAC-CBC-CGC-O1C
26	dn	201	PEB	CAC-CBC-CGC-O1C
26	dn	202	PEB	CAC-CBC-CGC-O1C
26	do	201	PEB	CAC-CBC-CGC-O1C
26	do	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	dp	201	PEB	CAC-CBC-CGC-O1C
26	dp	202	PEB	CAC-CBC-CGC-O1C
26	dq	201	PEB	CAC-CBC-CGC-O1C
26	dq	202	PEB	CAC-CBC-CGC-O1C
26	dr	201	PEB	CAC-CBC-CGC-O1C
26	dr	202	PEB	CAC-CBC-CGC-O1C
26	ds	201	PEB	CAC-CBC-CGC-O1C
26	ds	202	PEB	CAC-CBC-CGC-O1C
26	dt	201	PEB	CAC-CBC-CGC-O1C
26	dt	202	PEB	CAC-CBC-CGC-O1C
26	du	201	PEB	CAC-CBC-CGC-O1C
26	du	202	PEB	CAC-CBC-CGC-O1C
26	du	203	PEB	CAC-CBC-CGC-O1C
26	dv	201	PEB	CAC-CBC-CGC-O1C
26	dw	401	PEB	CAC-CBC-CGC-O1C
26	dw	402	PEB	CAC-CBC-CGC-O1C
26	dw	403	PEB	CAC-CBC-CGC-O1C
26	dx	401	PEB	CAC-CBC-CGC-O1C
26	dx	402	PEB	CAC-CBC-CGC-O1C
26	dx	403	PEB	CAC-CBC-CGC-O1C
26	dx	404	PEB	CAC-CBC-CGC-O1C
26	dy	401	PEB	CAC-CBC-CGC-O1C
26	dz	401	PEB	CAC-CBC-CGC-O1C
26	dz	402	PEB	CAC-CBC-CGC-O1C
26	dA	201	PEB	CAC-CBC-CGC-O1C
26	dA	202	PEB	CAC-CBC-CGC-O1C
26	dB	201	PEB	CAC-CBC-CGC-O1C
26	dC	201	PEB	CAC-CBC-CGC-O1C
26	dC	202	PEB	CAC-CBC-CGC-O1C
26	dD	201	PEB	CAC-CBC-CGC-O1C
26	dD	202	PEB	CAC-CBC-CGC-O1C
26	dE	201	PEB	CAC-CBC-CGC-O1C
26	dF	201	PEB	CAC-CBC-CGC-O1C
26	dF	202	PEB	CAC-CBC-CGC-O1C
26	dG	201	PEB	CAC-CBC-CGC-O1C
26	dG	202	PEB	CAC-CBC-CGC-O1C
26	dH	201	PEB	CAC-CBC-CGC-O1C
26	dH	202	PEB	CAC-CBC-CGC-O1C
26	dI	1001	PEB	CAC-CBC-CGC-O1C
26	dI	1002	PEB	CAC-CBC-CGC-O1C
26	dJ	201	PEB	CAC-CBC-CGC-O1C
26	dK	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	dK	202	PEB	CAC-CBC-CGC-O1C
26	dL	201	PEB	CAC-CBC-CGC-O1C
26	dM	1001	PEB	CAC-CBC-CGC-O1C
26	dM	1002	PEB	CAC-CBC-CGC-O1C
26	dN	201	PEB	CAC-CBC-CGC-O1C
26	dN	202	PEB	CAC-CBC-CGC-O1C
26	dO	201	PEB	CAC-CBC-CGC-O1C
26	dO	202	PEB	CAC-CBC-CGC-O1C
26	dP	201	PEB	CAC-CBC-CGC-O1C
26	dP	202	PEB	CAC-CBC-CGC-O1C
26	dQ	201	PEB	CAC-CBC-CGC-O1C
26	dQ	202	PEB	CAC-CBC-CGC-O1C
26	dR	201	PEB	CAC-CBC-CGC-O1C
26	dR	202	PEB	CAC-CBC-CGC-O1C
26	dS	201	PEB	CAC-CBC-CGC-O1C
26	dT	201	PEB	CAC-CBC-CGC-O1C
26	dT	202	PEB	CAC-CBC-CGC-O1C
26	dU	201	PEB	CAC-CBC-CGC-O1C
26	dV	201	PEB	CAC-CBC-CGC-O1C
26	dW	201	PEB	CAC-CBC-CGC-O1C
26	dW	202	PEB	CAC-CBC-CGC-O1C
26	dX	201	PEB	CAC-CBC-CGC-O1C
26	dX	202	PEB	CAC-CBC-CGC-O1C
26	dY	201	PEB	CAC-CBC-CGC-O1C
26	dZ	1001	PEB	CAC-CBC-CGC-O1C
26	ea	201	PEB	CAC-CBC-CGC-O1C
26	ea	202	PEB	CAC-CBC-CGC-O1C
26	eb	201	PEB	CAC-CBC-CGC-O1C
26	ed	201	PEB	CAC-CBC-CGC-O1C
26	ed	202	PEB	CAC-CBC-CGC-O1C
26	ee	201	PEB	CAC-CBC-CGC-O1C
26	ef	201	PEB	CAC-CBC-CGC-O1C
26	eg	201	PEB	CAC-CBC-CGC-O1C
26	eh	201	PEB	CAC-CBC-CGC-O1C
26	ej	201	PEB	CAC-CBC-CGC-O1C
26	ej	202	PEB	CAC-CBC-CGC-O1C
26	ek	1001	PEB	CAC-CBC-CGC-O1C
26	el	201	PEB	CAC-CBC-CGC-O1C
26	em	201	PEB	CAC-CBC-CGC-O1C
26	en	201	PEB	CAC-CBC-CGC-O1C
26	eo	201	PEB	CAC-CBC-CGC-O1C
26	eo	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	ep	201	PEB	CAC-CBC-CGC-O1C
26	eq	201	PEB	CAC-CBC-CGC-O1C
26	eq	202	PEB	CAC-CBC-CGC-O1C
26	er	201	PEB	CAC-CBC-CGC-O1C
26	es	201	PEB	CAC-CBC-CGC-O1C
26	es	202	PEB	CAC-CBC-CGC-O1C
26	eu	201	PEB	CAC-CBC-CGC-O1C
26	ew	301	PEB	CAC-CBC-CGC-O1C
26	ey	1002	PEB	CAC-CBC-CGC-O1C
26	ey	1003	PEB	CAC-CBC-CGC-O1C
26	ez	1001	PEB	CAC-CBC-CGC-O1C
26	ez	1002	PEB	CAC-CBC-CGC-O1C
26	ez	1003	PEB	CAC-CBC-CGC-O1C
26	eA	1001	PEB	CAC-CBC-CGC-O1C
26	eB	202	PEB	CAC-CBC-CGC-O1C
26	eC	201	PEB	CAC-CBC-CGC-O1C
26	eC	202	PEB	CAC-CBC-CGC-O1C
26	eD	201	PEB	CAC-CBC-CGC-O1C
26	eD	202	PEB	CAC-CBC-CGC-O1C
26	eE	201	PEB	CAC-CBC-CGC-O1C
26	eE	202	PEB	CAC-CBC-CGC-O1C
26	eF	201	PEB	CAC-CBC-CGC-O1C
26	eF	202	PEB	CAC-CBC-CGC-O1C
26	eG	201	PEB	CAC-CBC-CGC-O1C
26	eG	202	PEB	CAC-CBC-CGC-O1C
26	eH	201	PEB	CAC-CBC-CGC-O1C
26	eH	202	PEB	CAC-CBC-CGC-O1C
26	eI	201	PEB	CAC-CBC-CGC-O1C
26	eI	202	PEB	CAC-CBC-CGC-O1C
26	eJ	201	PEB	CAC-CBC-CGC-O1C
26	eK	201	PEB	CAC-CBC-CGC-O1C
26	eK	202	PEB	CAC-CBC-CGC-O1C
26	eM	1001	PEB	CAC-CBC-CGC-O1C
26	eM	1002	PEB	CAC-CBC-CGC-O1C
26	eN	201	PEB	CAC-CBC-CGC-O1C
26	eO	201	PEB	CAC-CBC-CGC-O1C
26	eO	202	PEB	CAC-CBC-CGC-O1C
26	eP	202	PEB	CAC-CBC-CGC-O1C
26	eP	203	PEB	CAC-CBC-CGC-O1C
26	eQ	201	PEB	CAC-CBC-CGC-O1C
26	eQ	202	PEB	CAC-CBC-CGC-O1C
26	eR	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	eR	202	PEB	CAC-CBC-CGC-O1C
26	eS	201	PEB	CAC-CBC-CGC-O1C
26	eS	202	PEB	CAC-CBC-CGC-O1C
26	eT	201	PEB	CAC-CBC-CGC-O1C
26	eT	202	PEB	CAC-CBC-CGC-O1C
26	eU	201	PEB	CAC-CBC-CGC-O1C
26	eU	202	PEB	CAC-CBC-CGC-O1C
26	eV	201	PEB	CAC-CBC-CGC-O1C
26	eW	201	PEB	CAC-CBC-CGC-O1C
26	eW	202	PEB	CAC-CBC-CGC-O1C
26	eY	402	PEB	CAC-CBC-CGC-O1C
26	eZ	401	PEB	CAC-CBC-CGC-O1C
26	la	1001	PEB	CAC-CBC-CGC-O1C
26	la	1002	PEB	CAC-CBC-CGC-O1C
26	lb	201	PEB	CAC-CBC-CGC-O1C
26	lb	202	PEB	CAC-CBC-CGC-O1C
26	lc	201	PEB	CAC-CBC-CGC-O1C
26	le	201	PEB	CAC-CBC-CGC-O1C
26	lf	201	PEB	CAC-CBC-CGC-O1C
26	li	201	PEB	CAC-CBC-CGC-O1C
26	li	202	PEB	CAC-CBC-CGC-O1C
26	lk	201	PEB	CAC-CBC-CGC-O1C
26	ll	201	PEB	CAC-CBC-CGC-O1C
26	lm	1001	PEB	CAC-CBC-CGC-O1C
26	ln	201	PEB	CAC-CBC-CGC-O1C
26	lp	201	PEB	CAC-CBC-CGC-O1C
26	lq	201	PEB	CAC-CBC-CGC-O1C
26	lq	202	PEB	CAC-CBC-CGC-O1C
26	lr	201	PEB	CAC-CBC-CGC-O1C
26	ls	201	PEB	CAC-CBC-CGC-O1C
26	lt	201	PEB	CAC-CBC-CGC-O1C
26	lu	201	PEB	CAC-CBC-CGC-O1C
26	lv	201	PEB	CAC-CBC-CGC-O1C
26	ly	401	PEB	CAC-CBC-CGC-O1C
26	ly	402	PEB	CAC-CBC-CGC-O1C
26	ly	403	PEB	CAC-CBC-CGC-O1C
26	lz	401	PEB	CAC-CBC-CGC-O1C
26	lz	402	PEB	CAC-CBC-CGC-O1C
26	fa	201	PEB	CAC-CBC-CGC-O1C
26	fb	201	PEB	CAC-CBC-CGC-O1C
26	fc	201	PEB	CAC-CBC-CGC-O1C
26	fd	301	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	fd	302	PEB	CAC-CBC-CGC-O1C
26	fd	303	PEB	CAC-CBC-CGC-O1C
26	fe	201	PEB	CAC-CBC-CGC-O1C
26	ff	201	PEB	CAC-CBC-CGC-O1C
26	ff	204	PEB	CAC-CBC-CGC-O1C
26	fh	1001	PEB	CAC-CBC-CGC-O1C
26	fi	201	PEB	CAC-CBC-CGC-O1C
26	fj	201	PEB	CAC-CBC-CGC-O1C
26	fk	201	PEB	CAC-CBC-CGC-O1C
26	fl	201	PEB	CAC-CBC-CGC-O1C
26	fm	201	PEB	CAC-CBC-CGC-O1C
26	fn	1001	PEB	CAC-CBC-CGC-O1C
26	fo	201	PEB	CAC-CBC-CGC-O1C
26	fp	201	PEB	CAC-CBC-CGC-O1C
26	fq	201	PEB	CAC-CBC-CGC-O1C
26	fr	201	PEB	CAC-CBC-CGC-O1C
26	fs	201	PEB	CAC-CBC-CGC-O1C
26	ft	201	PEB	CAC-CBC-CGC-O1C
26	fv	201	PEB	CAC-CBC-CGC-O1C
26	fw	201	PEB	CAC-CBC-CGC-O1C
26	fx	201	PEB	CAC-CBC-CGC-O1C
26	ga	201	PEB	CAC-CBC-CGC-O1C
26	gb	1001	PEB	CAC-CBC-CGC-O1C
26	gc	201	PEB	CAC-CBC-CGC-O1C
26	ge	201	PEB	CAC-CBC-CGC-O1C
26	gf	201	PEB	CAC-CBC-CGC-O1C
26	gg	201	PEB	CAC-CBC-CGC-O1C
26	gh	201	PEB	CAC-CBC-CGC-O1C
26	gi	201	PEB	CAC-CBC-CGC-O1C
26	gj	201	PEB	CAC-CBC-CGC-O1C
26	gk	201	PEB	CAC-CBC-CGC-O1C
26	gl	201	PEB	CAC-CBC-CGC-O1C
26	gm	1001	PEB	CAC-CBC-CGC-O1C
26	gn	201	PEB	CAC-CBC-CGC-O1C
26	go	201	PEB	CAC-CBC-CGC-O1C
26	gp	201	PEB	CAC-CBC-CGC-O1C
26	gq	201	PEB	CAC-CBC-CGC-O1C
26	gs	201	PEB	CAC-CBC-CGC-O1C
26	gt	201	PEB	CAC-CBC-CGC-O1C
26	gu	201	PEB	CAC-CBC-CGC-O1C
26	gv	201	PEB	CAC-CBC-CGC-O1C
26	gw	201	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	gx	201	PEB	CAC-CBC-CGC-O1C
26	gy	301	PEB	CAC-CBC-CGC-O1C
26	gy	303	PEB	CAC-CBC-CGC-O1C
26	gz	301	PEB	CAC-CBC-CGC-O1C
26	gz	303	PEB	CAC-CBC-CGC-O1C
26	hA	201	PEB	CAC-CBC-CGC-O1C
26	hB	201	PEB	CAC-CBC-CGC-O1C
26	hC	201	PEB	CAC-CBC-CGC-O1C
26	hD	201	PEB	CAC-CBC-CGC-O1C
26	hE	1001	PEB	CAC-CBC-CGC-O1C
26	hF	201	PEB	CAC-CBC-CGC-O1C
26	hH	201	PEB	CAC-CBC-CGC-O1C
26	hI	201	PEB	CAC-CBC-CGC-O1C
26	hJ	201	PEB	CAC-CBC-CGC-O1C
26	hK	201	PEB	CAC-CBC-CGC-O1C
26	hL	201	PEB	CAC-CBC-CGC-O1C
26	hM	1001	PEB	CAC-CBC-CGC-O1C
26	hN	201	PEB	CAC-CBC-CGC-O1C
26	hO	201	PEB	CAC-CBC-CGC-O1C
26	hP	201	PEB	CAC-CBC-CGC-O1C
26	hQ	201	PEB	CAC-CBC-CGC-O1C
26	hR	201	PEB	CAC-CBC-CGC-O1C
26	hS	201	PEB	CAC-CBC-CGC-O1C
26	hT	201	PEB	CAC-CBC-CGC-O1C
26	hT	204	PEB	CAC-CBC-CGC-O1C
26	hV	201	PEB	CAC-CBC-CGC-O1C
26	hW	201	PEB	CAC-CBC-CGC-O1C
26	hX	201	PEB	CAC-CBC-CGC-O1C
26	hY	401	PEB	CAC-CBC-CGC-O1C
26	hY	403	PEB	CAC-CBC-CGC-O1C
26	hZ	402	PEB	CAC-CBC-CGC-O1C
26	iA	1001	PEB	CAC-CBC-CGC-O1C
26	iB	1001	PEB	CAC-CBC-CGC-O1C
26	iC	1001	PEB	CAC-CBC-CGC-O1C
26	iD	1001	PEB	CAC-CBC-CGC-O1C
26	iE	1001	PEB	CAC-CBC-CGC-O1C
26	iF	1001	PEB	CAC-CBC-CGC-O1C
26	iG	1001	PEB	CAC-CBC-CGC-O1C
26	iH	1001	PEB	CAC-CBC-CGC-O1C
26	jI	1001	PEB	CAC-CBC-CGC-O1C
26	jJ	1001	PEB	CAC-CBC-CGC-O1C
26	jK	1001	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	jL	1001	PEB	CAC-CBC-CGC-O1C
26	jM	1001	PEB	CAC-CBC-CGC-O1C
26	jN	1001	PEB	CAC-CBC-CGC-O1C
26	jO	1001	PEB	CAC-CBC-CGC-O1C
26	jP	1001	PEB	CAC-CBC-CGC-O1C
26	kQ	1001	PEB	CAC-CBC-CGC-O1C
26	kR	1001	PEB	CAC-CBC-CGC-O1C
26	kS	1001	PEB	CAC-CBC-CGC-O1C
26	kT	1001	PEB	CAC-CBC-CGC-O1C
26	kU	1001	PEB	CAC-CBC-CGC-O1C
26	kV	1001	PEB	CAC-CBC-CGC-O1C
26	kW	1001	PEB	CAC-CBC-CGC-O1C
26	kX	1001	PEB	CAC-CBC-CGC-O1C
29	c3	303	PVN	C51-C52-C53-O55
29	U8	1004	PVN	C61-C62-C63-O65
29	ez	1004	PVN	C51-C52-C53-O54
28	h2	203	PUB	NC-C1C-CHB-C4B
28	l2	203	PUB	NC-C1C-CHB-C4B
28	v2	203	PUB	NC-C1C-CHB-C4B
28	x2	202	PUB	NC-C1C-CHB-C4B
28	C2	305	PUB	NC-C1C-CHB-C4B
28	D2	304	PUB	NC-C1C-CHB-C4B
28	F2	203	PUB	NC-C1C-CHB-C4B
28	P2	203	PUB	NC-C1C-CHB-C4B
28	R2	203	PUB	NC-C1C-CHB-C4B
28	V2	203	PUB	NC-C1C-CHB-C4B
28	B3	203	PUB	NC-C1C-CHB-C4B
28	F3	203	PUB	NC-C1C-CHB-C4B
28	L3	203	PUB	NC-C1C-CHB-C4B
28	T3	203	PUB	NC-C1C-CHB-C4B
28	V3	203	PUB	NC-C1C-CHB-C4B
28	X3	202	PUB	NC-C1C-CHB-C4B
28	a3	1005	PUB	NC-C1C-CHB-C4B
28	c3	305	PUB	NC-C1C-CHB-C4B
28	h3	202	PUB	NC-C1C-CHB-C4B
28	l3	202	PUB	NC-C1C-CHB-C4B
28	p3	203	PUB	NC-C1C-CHB-C4B
28	t3	203	PUB	NC-C1C-CHB-C4B
28	v3	203	PUB	NC-C1C-CHB-C4B
28	x3	203	PUB	NC-C1C-CHB-C4B
28	z3	203	PUB	NC-C1C-CHB-C4B
28	B4	203	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	D4	203	PUB	NC-C1C-CHB-C4B
28	F4	203	PUB	NC-C1C-CHB-C4B
28	H4	203	PUB	NC-C1C-CHB-C4B
28	J4	203	PUB	NC-C1C-CHB-C4B
28	L4	203	PUB	NC-C1C-CHB-C4B
28	N4	203	PUB	NC-C1C-CHB-C4B
28	P4	203	PUB	NC-C1C-CHB-C4B
28	R4	203	PUB	NC-C1C-CHB-C4B
28	T4	202	PUB	NC-C1C-CHB-C4B
28	V4	203	PUB	NC-C1C-CHB-C4B
28	X4	203	PUB	NC-C1C-CHB-C4B
28	34	1005	PUB	NC-C1C-CHB-C4B
28	44	304	PUB	NC-C1C-CHB-C4B
28	n4	203	PUB	NC-C1C-CHB-C4B
28	p4	203	PUB	NC-C1C-CHB-C4B
28	t4	203	PUB	NC-C1C-CHB-C4B
28	v4	203	PUB	NC-C1C-CHB-C4B
28	x4	202	PUB	NC-C1C-CHB-C4B
28	B5	203	PUB	NC-C1C-CHB-C4B
28	H5	202	PUB	NC-C1C-CHB-C4B
28	J5	203	PUB	NC-C1C-CHB-C4B
28	R5	203	PUB	NC-C1C-CHB-C4B
28	V5	203	PUB	NC-C1C-CHB-C4B
28	Y5	1006	PUB	NC-C1C-CHB-C4B
28	Z5	306	PUB	NC-C1C-CHB-C4B
28	n5	203	PUB	NC-C1C-CHB-C4B
28	r5	203	PUB	NC-C1C-CHB-C4B
28	v5	203	PUB	NC-C1C-CHB-C4B
28	x5	202	PUB	NC-C1C-CHB-C4B
28	f8	203	PUB	NC-C1C-CHB-C4B
28	B6	203	PUB	NC-C1C-CHB-C4B
28	H6	203	PUB	NC-C1C-CHB-C4B
28	N6	203	PUB	NC-C1C-CHB-C4B
28	P6	203	PUB	NC-C1C-CHB-C4B
28	T6	203	PUB	NC-C1C-CHB-C4B
28	V6	203	PUB	NC-C1C-CHB-C4B
28	Z6	203	PUB	NC-C1C-CHB-C4B
28	c6	1004	PUB	NC-C1C-CHB-C4B
28	e6	203	PUB	NC-C1C-CHB-C4B
28	l6	203	PUB	NC-C1C-CHB-C4B
28	p6	203	PUB	NC-C1C-CHB-C4B
28	r6	203	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	v6	203	PUB	NC-C1C-CHB-C4B
28	z6	203	PUB	NC-C1C-CHB-C4B
28	o8	203	PUB	NC-C1C-CHB-C4B
28	D7	203	PUB	NC-C1C-CHB-C4B
28	H7	203	PUB	NC-C1C-CHB-C4B
28	J7	202	PUB	NC-C1C-CHB-C4B
28	N7	203	PUB	NC-C1C-CHB-C4B
28	P7	203	PUB	NC-C1C-CHB-C4B
28	T7	203	PUB	NC-C1C-CHB-C4B
28	a7	203	PUB	NC-C1C-CHB-C4B
28	d7	203	PUB	NC-C1C-CHB-C4B
28	p7	202	PUB	NC-C1C-CHB-C4B
28	t7	203	PUB	NC-C1C-CHB-C4B
28	v7	203	PUB	NC-C1C-CHB-C4B
28	x7	203	PUB	NC-C1C-CHB-C4B
28	b8	1006	PUB	NC-C1C-CHB-C4B
28	c8	304	PUB	NC-C1C-CHB-C4B
28	d8	304	PUB	NC-C1C-CHB-C4B
28	e8	305	PUB	NC-C1C-CHB-C4B
28	e9	305	PUB	NC-C1C-CHB-C4B
28	e9	306	PUB	NC-C1C-CHB-C4B
28	y8	203	PUB	NC-C1C-CHB-C4B
28	A8	203	PUB	NC-C1C-CHB-C4B
28	G8	203	PUB	NC-C1C-CHB-C4B
28	I8	203	PUB	NC-C1C-CHB-C4B
28	O8	203	PUB	NC-C1C-CHB-C4B
28	T8	304	PUB	NC-C1C-CHB-C4B
28	U8	1006	PUB	NC-C1C-CHB-C4B
28	n9	202	PUB	NC-C1C-CHB-C4B
28	p9	203	PUB	NC-C1C-CHB-C4B
28	v9	203	PUB	NC-C1C-CHB-C4B
28	x9	203	PUB	NC-C1C-CHB-C4B
28	z9	203	PUB	NC-C1C-CHB-C4B
28	B9	203	PUB	NC-C1C-CHB-C4B
28	F9	203	PUB	NC-C1C-CHB-C4B
28	H9	203	PUB	NC-C1C-CHB-C4B
28	J9	203	PUB	NC-C1C-CHB-C4B
28	P9	203	PUB	NC-C1C-CHB-C4B
28	R9	203	PUB	NC-C1C-CHB-C4B
28	T9	203	PUB	NC-C1C-CHB-C4B
28	Y9	304	PUB	NC-C1C-CHB-C4B
28	Z9	1005	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	Z9	1006	PUB	NC-C1C-CHB-C4B
28	at	203	PUB	NC-C1C-CHB-C4B
28	aD	203	PUB	NC-C1C-CHB-C4B
28	aF	203	PUB	NC-C1C-CHB-C4B
28	aH	203	PUB	NC-C1C-CHB-C4B
28	aJ	203	PUB	NC-C1C-CHB-C4B
28	aN	203	PUB	NC-C1C-CHB-C4B
28	aP	203	PUB	NC-C1C-CHB-C4B
28	aR	203	PUB	NC-C1C-CHB-C4B
28	aT	203	PUB	NC-C1C-CHB-C4B
28	aV	203	PUB	NC-C1C-CHB-C4B
28	aY	404	PUB	NC-C1C-CHB-C4B
28	aY	405	PUB	NC-C1C-CHB-C4B
28	aZ	305	PUB	NC-C1C-CHB-C4B
28	bo	202	PUB	NC-C1C-CHB-C4B
28	br	203	PUB	NC-C1C-CHB-C4B
28	bs	1004	PUB	NC-C1C-CHB-C4B
28	bD	203	PUB	NC-C1C-CHB-C4B
28	bL	203	PUB	NC-C1C-CHB-C4B
28	bN	203	PUB	NC-C1C-CHB-C4B
28	bP	203	PUB	NC-C1C-CHB-C4B
28	bV	203	PUB	NC-C1C-CHB-C4B
28	bY	1005	PUB	NC-C1C-CHB-C4B
28	bY	1006	PUB	NC-C1C-CHB-C4B
28	bZ	305	PUB	NC-C1C-CHB-C4B
28	cn	202	PUB	NC-C1C-CHB-C4B
28	cs	203	PUB	NC-C1C-CHB-C4B
28	cz	203	PUB	NC-C1C-CHB-C4B
28	cB	203	PUB	NC-C1C-CHB-C4B
28	cE	203	PUB	NC-C1C-CHB-C4B
28	cH	202	PUB	NC-C1C-CHB-C4B
28	cJ	203	PUB	NC-C1C-CHB-C4B
28	cM	203	PUB	NC-C1C-CHB-C4B
28	cN	202	PUB	NC-C1C-CHB-C4B
28	cP	203	PUB	NC-C1C-CHB-C4B
28	cR	203	PUB	NC-C1C-CHB-C4B
28	dd	203	PUB	NC-C1C-CHB-C4B
28	df	203	PUB	NC-C1C-CHB-C4B
28	dj	203	PUB	NC-C1C-CHB-C4B
28	dl	203	PUB	NC-C1C-CHB-C4B
28	dp	203	PUB	NC-C1C-CHB-C4B
28	dt	203	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	dv	202	PUB	NC-C1C-CHB-C4B
28	dw	406	PUB	NC-C1C-CHB-C4B
28	dx	407	PUB	NC-C1C-CHB-C4B
28	dB	202	PUB	NC-C1C-CHB-C4B
28	dK	203	PUB	NC-C1C-CHB-C4B
28	dP	203	PUB	NC-C1C-CHB-C4B
28	dR	203	PUB	NC-C1C-CHB-C4B
28	dT	203	PUB	NC-C1C-CHB-C4B
28	eb	202	PUB	NC-C1C-CHB-C4B
28	el	203	PUB	NC-C1C-CHB-C4B
28	en	203	PUB	NC-C1C-CHB-C4B
28	ev	203	PUB	NC-C1C-CHB-C4B
28	ey	1005	PUB	NC-C1C-CHB-C4B
28	ey	1006	PUB	NC-C1C-CHB-C4B
28	eB	204	PUB	NC-C1C-CHB-C4B
28	eF	203	PUB	NC-C1C-CHB-C4B
28	eL	203	PUB	NC-C1C-CHB-C4B
28	eR	203	PUB	NC-C1C-CHB-C4B
28	eX	202	PUB	NC-C1C-CHB-C4B
28	eY	405	PUB	NC-C1C-CHB-C4B
28	eZ	404	PUB	NC-C1C-CHB-C4B
28	lb	203	PUB	NC-C1C-CHB-C4B
28	ld	203	PUB	NC-C1C-CHB-C4B
28	lh	203	PUB	NC-C1C-CHB-C4B
28	ln	203	PUB	NC-C1C-CHB-C4B
28	lp	203	PUB	NC-C1C-CHB-C4B
28	lr	203	PUB	NC-C1C-CHB-C4B
28	lv	202	PUB	NC-C1C-CHB-C4B
28	ly	405	PUB	NC-C1C-CHB-C4B
28	lz	404	PUB	NC-C1C-CHB-C4B
28	lz	405	PUB	NC-C1C-CHB-C4B
28	fa	202	PUB	NC-C1C-CHB-C4B
28	fc	203	PUB	NC-C1C-CHB-C4B
28	fi	203	PUB	NC-C1C-CHB-C4B
28	fo	203	PUB	NC-C1C-CHB-C4B
28	fq	203	PUB	NC-C1C-CHB-C4B
28	fs	203	PUB	NC-C1C-CHB-C4B
28	fu	202	PUB	NC-C1C-CHB-C4B
28	gd	202	PUB	NC-C1C-CHB-C4B
28	ge	203	PUB	NC-C1C-CHB-C4B
28	gk	203	PUB	NC-C1C-CHB-C4B
28	gr	202	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	gt	203	PUB	NC-C1C-CHB-C4B
28	gx	203	PUB	NC-C1C-CHB-C4B
28	hB	203	PUB	NC-C1C-CHB-C4B
28	hD	203	PUB	NC-C1C-CHB-C4B
28	hG	202	PUB	NC-C1C-CHB-C4B
28	hJ	203	PUB	NC-C1C-CHB-C4B
28	hN	203	PUB	NC-C1C-CHB-C4B
28	hP	203	PUB	NC-C1C-CHB-C4B
28	hV	203	PUB	NC-C1C-CHB-C4B
28	hZ	404	PUB	NC-C1C-CHB-C4B
28	iC	1003	PUB	NC-C1C-CHB-C4B
28	iE	1003	PUB	NC-C1C-CHB-C4B
28	iF	1003	PUB	NC-C1C-CHB-C4B
28	iH	1002	PUB	NC-C1C-CHB-C4B
28	jK	1003	PUB	NC-C1C-CHB-C4B
28	jM	1003	PUB	NC-C1C-CHB-C4B
28	kU	1003	PUB	NC-C1C-CHB-C4B
28	kW	1003	PUB	NC-C1C-CHB-C4B
26	A2	1001	PEB	CAC-CBC-CGC-O2C
26	E2	1002	PEB	CAC-CBC-CGC-O2C
26	N2	201	PEB	CAC-CBC-CGC-O2C
26	P2	202	PEB	CAC-CBC-CGC-O2C
26	R2	201	PEB	CAC-CBC-CGC-O2C
26	S2	202	PEB	CAC-CBC-CGC-O2C
26	U2	202	PEB	CAC-CBC-CGC-O2C
26	A3	202	PEB	CAC-CBC-CGC-O2C
26	E3	202	PEB	CAC-CBC-CGC-O2C
26	G3	202	PEB	CAC-CBC-CGC-O2C
26	I3	202	PEB	CAC-CBC-CGC-O2C
26	K3	202	PEB	CAC-CBC-CGC-O2C
26	M3	202	PEB	CAC-CBC-CGC-O2C
26	O3	1002	PEB	CAC-CBC-CGC-O2C
26	Q3	202	PEB	CAC-CBC-CGC-O2C
26	S3	202	PEB	CAC-CBC-CGC-O2C
26	U3	202	PEB	CAC-CBC-CGC-O2C
26	W3	202	PEB	CAC-CBC-CGC-O2C
26	a3	1002	PEB	CAC-CBC-CGC-O2C
26	c3	301	PEB	CAC-CBC-CGC-O2C
26	e3	1002	PEB	CAC-CBC-CGC-O2C
26	g3	202	PEB	CAC-CBC-CGC-O2C
26	i3	202	PEB	CAC-CBC-CGC-O2C
26	k3	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	m3	202	PEB	CAC-CBC-CGC-O2C
26	s3	202	PEB	CAC-CBC-CGC-O2C
26	u3	202	PEB	CAC-CBC-CGC-O2C
26	w3	202	PEB	CAC-CBC-CGC-O2C
26	y3	202	PEB	CAC-CBC-CGC-O2C
26	A4	202	PEB	CAC-CBC-CGC-O2C
26	C4	1002	PEB	CAC-CBC-CGC-O2C
26	N4	202	PEB	CAC-CBC-CGC-O2C
26	c4	201	PEB	CAC-CBC-CGC-O2C
26	h4	201	PEB	CAC-CBC-CGC-O2C
26	s4	202	PEB	CAC-CBC-CGC-O2C
26	w4	202	PEB	CAC-CBC-CGC-O2C
26	A5	202	PEB	CAC-CBC-CGC-O2C
26	C5	202	PEB	CAC-CBC-CGC-O2C
26	E5	202	PEB	CAC-CBC-CGC-O2C
26	G5	202	PEB	CAC-CBC-CGC-O2C
26	O5	202	PEB	CAC-CBC-CGC-O2C
26	Q5	202	PEB	CAC-CBC-CGC-O2C
26	U5	202	PEB	CAC-CBC-CGC-O2C
26	Y5	1002	PEB	CAC-CBC-CGC-O2C
26	Z5	302	PEB	CAC-CBC-CGC-O2C
26	c5	201	PEB	CAC-CBC-CGC-O2C
26	f5	201	PEB	CAC-CBC-CGC-O2C
26	h5	202	PEB	CAC-CBC-CGC-O2C
26	m5	1002	PEB	CAC-CBC-CGC-O2C
26	o5	202	PEB	CAC-CBC-CGC-O2C
26	q5	202	PEB	CAC-CBC-CGC-O2C
26	s5	202	PEB	CAC-CBC-CGC-O2C
26	u5	202	PEB	CAC-CBC-CGC-O2C
26	w5	202	PEB	CAC-CBC-CGC-O2C
26	y5	1002	PEB	CAC-CBC-CGC-O2C
26	G6	202	PEB	CAC-CBC-CGC-O2C
26	H6	201	PEB	CAC-CBC-CGC-O2C
26	N6	202	PEB	CAC-CBC-CGC-O2C
26	U6	202	PEB	CAC-CBC-CGC-O2C
26	V6	202	PEB	CAC-CBC-CGC-O2C
26	a6	202	PEB	CAC-CBC-CGC-O2C
26	d6	202	PEB	CAC-CBC-CGC-O2C
26	e6	202	PEB	CAC-CBC-CGC-O2C
26	n6	201	PEB	CAC-CBC-CGC-O2C
26	p6	202	PEB	CAC-CBC-CGC-O2C
26	o8	201	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	q8	202	PEB	CAC-CBC-CGC-O2C
26	r8	202	PEB	CAC-CBC-CGC-O2C
26	s8	202	PEB	CAC-CBC-CGC-O2C
26	t8	202	PEB	CAC-CBC-CGC-O2C
26	u8	202	PEB	CAC-CBC-CGC-O2C
26	A7	201	PEB	CAC-CBC-CGC-O2C
26	C7	202	PEB	CAC-CBC-CGC-O2C
26	E7	202	PEB	CAC-CBC-CGC-O2C
26	G7	202	PEB	CAC-CBC-CGC-O2C
26	I7	202	PEB	CAC-CBC-CGC-O2C
26	K7	202	PEB	CAC-CBC-CGC-O2C
26	M7	1003	PEB	CAC-CBC-CGC-O2C
26	O7	202	PEB	CAC-CBC-CGC-O2C
26	Q7	202	PEB	CAC-CBC-CGC-O2C
26	S7	202	PEB	CAC-CBC-CGC-O2C
26	U7	202	PEB	CAC-CBC-CGC-O2C
26	W7	202	PEB	CAC-CBC-CGC-O2C
26	Y7	1002	PEB	CAC-CBC-CGC-O2C
26	f7	202	PEB	CAC-CBC-CGC-O2C
26	g7	202	PEB	CAC-CBC-CGC-O2C
26	h7	202	PEB	CAC-CBC-CGC-O2C
26	i7	202	PEB	CAC-CBC-CGC-O2C
26	j7	202	PEB	CAC-CBC-CGC-O2C
26	k7	1002	PEB	CAC-CBC-CGC-O2C
26	m7	202	PEB	CAC-CBC-CGC-O2C
26	o7	202	PEB	CAC-CBC-CGC-O2C
26	q7	202	PEB	CAC-CBC-CGC-O2C
26	s7	202	PEB	CAC-CBC-CGC-O2C
26	u7	202	PEB	CAC-CBC-CGC-O2C
26	w7	1002	PEB	CAC-CBC-CGC-O2C
26	d8	301	PEB	CAC-CBC-CGC-O2C
26	A9	202	PEB	CAC-CBC-CGC-O2C
26	C9	202	PEB	CAC-CBC-CGC-O2C
26	E9	202	PEB	CAC-CBC-CGC-O2C
26	G9	202	PEB	CAC-CBC-CGC-O2C
26	K9	1002	PEB	CAC-CBC-CGC-O2C
26	M9	202	PEB	CAC-CBC-CGC-O2C
26	O9	202	PEB	CAC-CBC-CGC-O2C
26	S9	202	PEB	CAC-CBC-CGC-O2C
26	U9	202	PEB	CAC-CBC-CGC-O2C
26	Y9	301	PEB	CAC-CBC-CGC-O2C
26	Z9	1002	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	ao	202	PEB	CAC-CBC-CGC-O2C
26	aq	202	PEB	CAC-CBC-CGC-O2C
26	as	202	PEB	CAC-CBC-CGC-O2C
26	au	202	PEB	CAC-CBC-CGC-O2C
26	aw	202	PEB	CAC-CBC-CGC-O2C
26	ay	1002	PEB	CAC-CBC-CGC-O2C
26	bA	202	PEB	CAC-CBC-CGC-O2C
26	bC	202	PEB	CAC-CBC-CGC-O2C
26	bE	202	PEB	CAC-CBC-CGC-O2C
26	bG	202	PEB	CAC-CBC-CGC-O2C
26	bI	202	PEB	CAC-CBC-CGC-O2C
26	bK	1002	PEB	CAC-CBC-CGC-O2C
26	bM	202	PEB	CAC-CBC-CGC-O2C
26	bO	202	PEB	CAC-CBC-CGC-O2C
26	bQ	202	PEB	CAC-CBC-CGC-O2C
26	bS	202	PEB	CAC-CBC-CGC-O2C
26	bU	202	PEB	CAC-CBC-CGC-O2C
26	bY	1002	PEB	CAC-CBC-CGC-O2C
26	bZ	302	PEB	CAC-CBC-CGC-O2C
26	cm	1002	PEB	CAC-CBC-CGC-O2C
26	cu	202	PEB	CAC-CBC-CGC-O2C
26	cv	202	PEB	CAC-CBC-CGC-O2C
26	cw	202	PEB	CAC-CBC-CGC-O2C
26	cx	202	PEB	CAC-CBC-CGC-O2C
26	cy	1002	PEB	CAC-CBC-CGC-O2C
26	cA	202	PEB	CAC-CBC-CGC-O2C
26	cD	202	PEB	CAC-CBC-CGC-O2C
26	cG	202	PEB	CAC-CBC-CGC-O2C
26	cI	202	PEB	CAC-CBC-CGC-O2C
26	cK	202	PEB	CAC-CBC-CGC-O2C
26	cZ	202	PEB	CAC-CBC-CGC-O2C
26	da	1002	PEB	CAC-CBC-CGC-O2C
26	db	202	PEB	CAC-CBC-CGC-O2C
26	dc	202	PEB	CAC-CBC-CGC-O2C
26	de	202	PEB	CAC-CBC-CGC-O2C
26	dg	202	PEB	CAC-CBC-CGC-O2C
26	dJ	202	PEB	CAC-CBC-CGC-O2C
26	dU	202	PEB	CAC-CBC-CGC-O2C
26	dZ	1002	PEB	CAC-CBC-CGC-O2C
26	ec	201	PEB	CAC-CBC-CGC-O2C
26	ef	202	PEB	CAC-CBC-CGC-O2C
26	eh	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	ei	201	PEB	CAC-CBC-CGC-O2C
26	ek	1002	PEB	CAC-CBC-CGC-O2C
26	em	202	PEB	CAC-CBC-CGC-O2C
26	et	201	PEB	CAC-CBC-CGC-O2C
26	eu	202	PEB	CAC-CBC-CGC-O2C
26	ev	201	PEB	CAC-CBC-CGC-O2C
26	ey	1001	PEB	CAC-CBC-CGC-O2C
26	eA	1002	PEB	CAC-CBC-CGC-O2C
26	eB	201	PEB	CAC-CBC-CGC-O2C
26	eL	201	PEB	CAC-CBC-CGC-O2C
26	eP	201	PEB	CAC-CBC-CGC-O2C
26	eY	401	PEB	CAC-CBC-CGC-O2C
26	lc	202	PEB	CAC-CBC-CGC-O2C
26	ld	201	PEB	CAC-CBC-CGC-O2C
26	le	202	PEB	CAC-CBC-CGC-O2C
26	lg	201	PEB	CAC-CBC-CGC-O2C
26	lh	201	PEB	CAC-CBC-CGC-O2C
26	lj	201	PEB	CAC-CBC-CGC-O2C
26	lk	202	PEB	CAC-CBC-CGC-O2C
26	lm	1002	PEB	CAC-CBC-CGC-O2C
26	lq	203	PEB	CAC-CBC-CGC-O2C
26	ls	202	PEB	CAC-CBC-CGC-O2C
26	lt	202	PEB	CAC-CBC-CGC-O2C
26	lu	202	PEB	CAC-CBC-CGC-O2C
26	lw	201	PEB	CAC-CBC-CGC-O2C
26	lw	202	PEB	CAC-CBC-CGC-O2C
26	fb	202	PEB	CAC-CBC-CGC-O2C
26	fe	202	PEB	CAC-CBC-CGC-O2C
26	fg	202	PEB	CAC-CBC-CGC-O2C
26	fh	1002	PEB	CAC-CBC-CGC-O2C
26	fk	202	PEB	CAC-CBC-CGC-O2C
26	fl	202	PEB	CAC-CBC-CGC-O2C
26	fn	1002	PEB	CAC-CBC-CGC-O2C
26	fp	202	PEB	CAC-CBC-CGC-O2C
26	fr	202	PEB	CAC-CBC-CGC-O2C
26	ft	202	PEB	CAC-CBC-CGC-O2C
26	fx	202	PEB	CAC-CBC-CGC-O2C
26	fz	301	PEB	CAC-CBC-CGC-O2C
26	gb	1002	PEB	CAC-CBC-CGC-O2C
26	gc	202	PEB	CAC-CBC-CGC-O2C
26	gf	202	PEB	CAC-CBC-CGC-O2C
26	gh	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	gj	202	PEB	CAC-CBC-CGC-O2C
26	gl	202	PEB	CAC-CBC-CGC-O2C
26	gm	1002	PEB	CAC-CBC-CGC-O2C
26	go	202	PEB	CAC-CBC-CGC-O2C
26	gq	202	PEB	CAC-CBC-CGC-O2C
26	gs	202	PEB	CAC-CBC-CGC-O2C
26	gu	202	PEB	CAC-CBC-CGC-O2C
26	gw	202	PEB	CAC-CBC-CGC-O2C
26	gz	302	PEB	CAC-CBC-CGC-O2C
26	hA	202	PEB	CAC-CBC-CGC-O2C
26	hF	202	PEB	CAC-CBC-CGC-O2C
26	hI	202	PEB	CAC-CBC-CGC-O2C
26	hK	202	PEB	CAC-CBC-CGC-O2C
26	hM	1002	PEB	CAC-CBC-CGC-O2C
26	hQ	202	PEB	CAC-CBC-CGC-O2C
26	hS	202	PEB	CAC-CBC-CGC-O2C
26	hU	201	PEB	CAC-CBC-CGC-O2C
26	hW	202	PEB	CAC-CBC-CGC-O2C
26	hY	402	PEB	CAC-CBC-CGC-O2C
26	hZ	401	PEB	CAC-CBC-CGC-O2C
26	iA	1002	PEB	CAC-CBC-CGC-O2C
26	iB	1002	PEB	CAC-CBC-CGC-O2C
26	iF	1002	PEB	CAC-CBC-CGC-O2C
29	C2	303	PVN	C51-C52-C53-O55
29	c8	303	PVN	C51-C52-C53-O55
29	c9	303	PVN	C51-C52-C53-O55
29	eY	403	PVN	C61-C62-C63-O64
29	eZ	402	PVN	C61-C62-C63-O64
26	C3	1002	PEB	CAC-CBC-CGC-O2C
26	Y3	202	PEB	CAC-CBC-CGC-O2C
26	d3	301	PEB	CAC-CBC-CGC-O2C
26	o3	202	PEB	CAC-CBC-CGC-O2C
26	I5	202	PEB	CAC-CBC-CGC-O2C
26	K5	1002	PEB	CAC-CBC-CGC-O2C
26	M5	202	PEB	CAC-CBC-CGC-O2C
26	S5	202	PEB	CAC-CBC-CGC-O2C
26	f6	202	PEB	CAC-CBC-CGC-O2C
26	t6	201	PEB	CAC-CBC-CGC-O2C
26	c8	301	PEB	CAC-CBC-CGC-O2C
26	I9	202	PEB	CAC-CBC-CGC-O2C
26	Q9	202	PEB	CAC-CBC-CGC-O2C
26	ct	202	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
26	cC	1002	PEB	CAC-CBC-CGC-O2C
26	lg	202	PEB	CAC-CBC-CGC-O2C
26	lo	201	PEB	CAC-CBC-CGC-O2C
26	lo	202	PEB	CAC-CBC-CGC-O2C
26	fv	202	PEB	CAC-CBC-CGC-O2C
26	gy	302	PEB	CAC-CBC-CGC-O2C
26	hC	202	PEB	CAC-CBC-CGC-O2C
26	hE	1002	PEB	CAC-CBC-CGC-O2C
26	hO	202	PEB	CAC-CBC-CGC-O2C
29	44	303	PVN	C51-C52-C53-O55
29	Z5	304	PVN	C51-C52-C53-O55
27	H1	201	CYC	CAA-CBA-CGA-O1A
27	J1	201	CYC	CAA-CBA-CGA-O1A
27	M1	1001	CYC	CAA-CBA-CGA-O1A
27	S1	201	CYC	CAA-CBA-CGA-O1A
27	S1	202	CYC	CAA-CBA-CGA-O1A
27	Y1	201	CYC	CAA-CBA-CGA-O1A
27	c1	201	CYC	CAA-CBA-CGA-O1A
27	h1	201	CYC	CAA-CBA-CGA-O1A
27	j1	201	CYC	CAA-CBA-CGA-O1A
27	p1	201	CYC	CAA-CBA-CGA-O1A
27	r1	201	CYC	CAA-CBA-CGA-O1A
27	t1	201	CYC	CAA-CBA-CGA-O1A
27	v1	201	CYC	CAA-CBA-CGA-O1A
27	z1	201	CYC	CAA-CBA-CGA-O1A
27	a2	901	CYC	CAA-CBA-CGA-O1A
27	a2	902	CYC	CAA-CBA-CGA-O1A
27	b2	1001	CYC	CAA-CBA-CGA-O1A
29	Z9	1004	PVN	C61-C62-C63-O65
29	eY	403	PVN	C51-C52-C53-O54
29	eZ	402	PVN	C51-C52-C53-O54
29	Z9	1004	PVN	C61-C62-C63-O64
29	D2	303	PVN	C61-C62-C63-O64
29	d3	302	PVN	C61-C62-C63-O64
29	e8	303	PVN	C61-C62-C63-O65
29	e9	304	PVN	C61-C62-C63-O65
26	E2	1002	PEB	CAC-CBC-CGC-O1C
26	O3	1002	PEB	CAC-CBC-CGC-O1C
26	S3	202	PEB	CAC-CBC-CGC-O1C
26	e3	1002	PEB	CAC-CBC-CGC-O1C
26	g3	202	PEB	CAC-CBC-CGC-O1C
26	A4	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	h4	201	PEB	CAC-CBC-CGC-O1C
26	A5	202	PEB	CAC-CBC-CGC-O1C
26	U5	202	PEB	CAC-CBC-CGC-O1C
26	w5	202	PEB	CAC-CBC-CGC-O1C
26	f6	202	PEB	CAC-CBC-CGC-O1C
26	n6	201	PEB	CAC-CBC-CGC-O1C
26	q8	202	PEB	CAC-CBC-CGC-O1C
26	r8	202	PEB	CAC-CBC-CGC-O1C
26	W7	202	PEB	CAC-CBC-CGC-O1C
26	o7	202	PEB	CAC-CBC-CGC-O1C
26	u7	202	PEB	CAC-CBC-CGC-O1C
26	Q9	202	PEB	CAC-CBC-CGC-O1C
26	U9	202	PEB	CAC-CBC-CGC-O1C
26	Y9	301	PEB	CAC-CBC-CGC-O1C
26	as	202	PEB	CAC-CBC-CGC-O1C
26	bA	202	PEB	CAC-CBC-CGC-O1C
26	bM	202	PEB	CAC-CBC-CGC-O1C
26	bU	202	PEB	CAC-CBC-CGC-O1C
26	bZ	302	PEB	CAC-CBC-CGC-O1C
26	cw	202	PEB	CAC-CBC-CGC-O1C
26	cy	1002	PEB	CAC-CBC-CGC-O1C
26	cA	202	PEB	CAC-CBC-CGC-O1C
26	cD	202	PEB	CAC-CBC-CGC-O1C
26	cI	202	PEB	CAC-CBC-CGC-O1C
26	dg	202	PEB	CAC-CBC-CGC-O1C
26	dZ	1002	PEB	CAC-CBC-CGC-O1C
26	et	201	PEB	CAC-CBC-CGC-O1C
26	ld	201	PEB	CAC-CBC-CGC-O1C
26	lg	201	PEB	CAC-CBC-CGC-O1C
26	lo	202	PEB	CAC-CBC-CGC-O1C
26	lt	202	PEB	CAC-CBC-CGC-O1C
26	lw	201	PEB	CAC-CBC-CGC-O1C
26	fn	1002	PEB	CAC-CBC-CGC-O1C
26	fp	202	PEB	CAC-CBC-CGC-O1C
26	fr	202	PEB	CAC-CBC-CGC-O1C
26	ft	202	PEB	CAC-CBC-CGC-O1C
26	hC	202	PEB	CAC-CBC-CGC-O1C
26	hE	1002	PEB	CAC-CBC-CGC-O1C
26	hM	1002	PEB	CAC-CBC-CGC-O1C
29	A2	1004	PVN	C51-C52-C53-O55
29	C2	303	PVN	C51-C52-C53-O54
29	a3	1004	PVN	C51-C52-C53-O55

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Mol	Chain	Res	Type	Atoms
29	c3	303	PVN	C51-C52-C53-O54
29	U8	1004	PVN	C61-C62-C63-O64
29	dw	404	PVN	C61-C62-C63-O64
26	A2	1001	PEB	CAC-CBC-CGC-O1C
26	N2	201	PEB	CAC-CBC-CGC-O1C
26	P2	202	PEB	CAC-CBC-CGC-O1C
26	R2	201	PEB	CAC-CBC-CGC-O1C
26	S2	202	PEB	CAC-CBC-CGC-O1C
26	U2	202	PEB	CAC-CBC-CGC-O1C
26	A3	202	PEB	CAC-CBC-CGC-O1C
26	C3	1002	PEB	CAC-CBC-CGC-O1C
26	E3	202	PEB	CAC-CBC-CGC-O1C
26	G3	202	PEB	CAC-CBC-CGC-O1C
26	I3	202	PEB	CAC-CBC-CGC-O1C
26	K3	202	PEB	CAC-CBC-CGC-O1C
26	M3	202	PEB	CAC-CBC-CGC-O1C
26	Q3	202	PEB	CAC-CBC-CGC-O1C
26	U3	202	PEB	CAC-CBC-CGC-O1C
26	W3	202	PEB	CAC-CBC-CGC-O1C
26	Y3	202	PEB	CAC-CBC-CGC-O1C
26	a3	1002	PEB	CAC-CBC-CGC-O1C
26	c3	301	PEB	CAC-CBC-CGC-O1C
26	d3	301	PEB	CAC-CBC-CGC-O1C
26	i3	202	PEB	CAC-CBC-CGC-O1C
26	k3	202	PEB	CAC-CBC-CGC-O1C
26	m3	202	PEB	CAC-CBC-CGC-O1C
26	o3	202	PEB	CAC-CBC-CGC-O1C
26	s3	202	PEB	CAC-CBC-CGC-O1C
26	u3	202	PEB	CAC-CBC-CGC-O1C
26	w3	202	PEB	CAC-CBC-CGC-O1C
26	y3	202	PEB	CAC-CBC-CGC-O1C
26	C4	1002	PEB	CAC-CBC-CGC-O1C
26	N4	202	PEB	CAC-CBC-CGC-O1C
26	c4	201	PEB	CAC-CBC-CGC-O1C
26	s4	202	PEB	CAC-CBC-CGC-O1C
26	w4	202	PEB	CAC-CBC-CGC-O1C
26	C5	202	PEB	CAC-CBC-CGC-O1C
26	E5	202	PEB	CAC-CBC-CGC-O1C
26	G5	202	PEB	CAC-CBC-CGC-O1C
26	I5	202	PEB	CAC-CBC-CGC-O1C
26	K5	1002	PEB	CAC-CBC-CGC-O1C
26	M5	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	O5	202	PEB	CAC-CBC-CGC-O1C
26	Q5	202	PEB	CAC-CBC-CGC-O1C
26	S5	202	PEB	CAC-CBC-CGC-O1C
26	Y5	1002	PEB	CAC-CBC-CGC-O1C
26	Z5	302	PEB	CAC-CBC-CGC-O1C
26	c5	201	PEB	CAC-CBC-CGC-O1C
26	f5	201	PEB	CAC-CBC-CGC-O1C
26	h5	202	PEB	CAC-CBC-CGC-O1C
26	m5	1002	PEB	CAC-CBC-CGC-O1C
26	o5	202	PEB	CAC-CBC-CGC-O1C
26	q5	202	PEB	CAC-CBC-CGC-O1C
26	s5	202	PEB	CAC-CBC-CGC-O1C
26	u5	202	PEB	CAC-CBC-CGC-O1C
26	y5	1002	PEB	CAC-CBC-CGC-O1C
26	G6	202	PEB	CAC-CBC-CGC-O1C
26	H6	201	PEB	CAC-CBC-CGC-O1C
26	N6	202	PEB	CAC-CBC-CGC-O1C
26	U6	202	PEB	CAC-CBC-CGC-O1C
26	V6	202	PEB	CAC-CBC-CGC-O1C
26	a6	202	PEB	CAC-CBC-CGC-O1C
26	d6	202	PEB	CAC-CBC-CGC-O1C
26	e6	202	PEB	CAC-CBC-CGC-O1C
26	p6	202	PEB	CAC-CBC-CGC-O1C
26	t6	201	PEB	CAC-CBC-CGC-O1C
26	o8	201	PEB	CAC-CBC-CGC-O1C
26	s8	202	PEB	CAC-CBC-CGC-O1C
26	t8	202	PEB	CAC-CBC-CGC-O1C
26	u8	202	PEB	CAC-CBC-CGC-O1C
26	A7	201	PEB	CAC-CBC-CGC-O1C
26	C7	202	PEB	CAC-CBC-CGC-O1C
26	E7	202	PEB	CAC-CBC-CGC-O1C
26	G7	202	PEB	CAC-CBC-CGC-O1C
26	I7	202	PEB	CAC-CBC-CGC-O1C
26	K7	202	PEB	CAC-CBC-CGC-O1C
26	M7	1003	PEB	CAC-CBC-CGC-O1C
26	O7	202	PEB	CAC-CBC-CGC-O1C
26	Q7	202	PEB	CAC-CBC-CGC-O1C
26	S7	202	PEB	CAC-CBC-CGC-O1C
26	U7	202	PEB	CAC-CBC-CGC-O1C
26	Y7	1002	PEB	CAC-CBC-CGC-O1C
26	f7	202	PEB	CAC-CBC-CGC-O1C
26	g7	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	h7	202	PEB	CAC-CBC-CGC-O1C
26	i7	202	PEB	CAC-CBC-CGC-O1C
26	j7	202	PEB	CAC-CBC-CGC-O1C
26	k7	1002	PEB	CAC-CBC-CGC-O1C
26	m7	202	PEB	CAC-CBC-CGC-O1C
26	q7	202	PEB	CAC-CBC-CGC-O1C
26	s7	202	PEB	CAC-CBC-CGC-O1C
26	w7	1002	PEB	CAC-CBC-CGC-O1C
26	c8	301	PEB	CAC-CBC-CGC-O1C
26	d8	301	PEB	CAC-CBC-CGC-O1C
26	A9	202	PEB	CAC-CBC-CGC-O1C
26	C9	202	PEB	CAC-CBC-CGC-O1C
26	E9	202	PEB	CAC-CBC-CGC-O1C
26	G9	202	PEB	CAC-CBC-CGC-O1C
26	I9	202	PEB	CAC-CBC-CGC-O1C
26	K9	1002	PEB	CAC-CBC-CGC-O1C
26	M9	202	PEB	CAC-CBC-CGC-O1C
26	O9	202	PEB	CAC-CBC-CGC-O1C
26	S9	202	PEB	CAC-CBC-CGC-O1C
26	Z9	1002	PEB	CAC-CBC-CGC-O1C
26	ao	202	PEB	CAC-CBC-CGC-O1C
26	aq	202	PEB	CAC-CBC-CGC-O1C
26	au	202	PEB	CAC-CBC-CGC-O1C
26	aw	202	PEB	CAC-CBC-CGC-O1C
26	ay	1002	PEB	CAC-CBC-CGC-O1C
26	bC	202	PEB	CAC-CBC-CGC-O1C
26	bE	202	PEB	CAC-CBC-CGC-O1C
26	bG	202	PEB	CAC-CBC-CGC-O1C
26	bI	202	PEB	CAC-CBC-CGC-O1C
26	bK	1002	PEB	CAC-CBC-CGC-O1C
26	bO	202	PEB	CAC-CBC-CGC-O1C
26	bQ	202	PEB	CAC-CBC-CGC-O1C
26	bS	202	PEB	CAC-CBC-CGC-O1C
26	bY	1002	PEB	CAC-CBC-CGC-O1C
26	cm	1002	PEB	CAC-CBC-CGC-O1C
26	ct	202	PEB	CAC-CBC-CGC-O1C
26	cu	202	PEB	CAC-CBC-CGC-O1C
26	cv	202	PEB	CAC-CBC-CGC-O1C
26	cx	202	PEB	CAC-CBC-CGC-O1C
26	cC	1002	PEB	CAC-CBC-CGC-O1C
26	cG	202	PEB	CAC-CBC-CGC-O1C
26	cK	202	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	cZ	202	PEB	CAC-CBC-CGC-O1C
26	da	1002	PEB	CAC-CBC-CGC-O1C
26	db	202	PEB	CAC-CBC-CGC-O1C
26	dc	202	PEB	CAC-CBC-CGC-O1C
26	de	202	PEB	CAC-CBC-CGC-O1C
26	dJ	202	PEB	CAC-CBC-CGC-O1C
26	dU	202	PEB	CAC-CBC-CGC-O1C
26	ec	201	PEB	CAC-CBC-CGC-O1C
26	ef	202	PEB	CAC-CBC-CGC-O1C
26	eh	202	PEB	CAC-CBC-CGC-O1C
26	ei	201	PEB	CAC-CBC-CGC-O1C
26	ek	1002	PEB	CAC-CBC-CGC-O1C
26	em	202	PEB	CAC-CBC-CGC-O1C
26	eu	202	PEB	CAC-CBC-CGC-O1C
26	ev	201	PEB	CAC-CBC-CGC-O1C
26	ey	1001	PEB	CAC-CBC-CGC-O1C
26	eA	1002	PEB	CAC-CBC-CGC-O1C
26	eB	201	PEB	CAC-CBC-CGC-O1C
26	eL	201	PEB	CAC-CBC-CGC-O1C
26	eP	201	PEB	CAC-CBC-CGC-O1C
26	eY	401	PEB	CAC-CBC-CGC-O1C
26	lc	202	PEB	CAC-CBC-CGC-O1C
26	le	202	PEB	CAC-CBC-CGC-O1C
26	lg	202	PEB	CAC-CBC-CGC-O1C
26	lh	201	PEB	CAC-CBC-CGC-O1C
26	lj	201	PEB	CAC-CBC-CGC-O1C
26	lk	202	PEB	CAC-CBC-CGC-O1C
26	lm	1002	PEB	CAC-CBC-CGC-O1C
26	lo	201	PEB	CAC-CBC-CGC-O1C
26	lq	203	PEB	CAC-CBC-CGC-O1C
26	ls	202	PEB	CAC-CBC-CGC-O1C
26	lu	202	PEB	CAC-CBC-CGC-O1C
26	lw	202	PEB	CAC-CBC-CGC-O1C
26	fb	202	PEB	CAC-CBC-CGC-O1C
26	fe	202	PEB	CAC-CBC-CGC-O1C
26	fg	202	PEB	CAC-CBC-CGC-O1C
26	fh	1002	PEB	CAC-CBC-CGC-O1C
26	fk	202	PEB	CAC-CBC-CGC-O1C
26	fl	202	PEB	CAC-CBC-CGC-O1C
26	fv	202	PEB	CAC-CBC-CGC-O1C
26	fx	202	PEB	CAC-CBC-CGC-O1C
26	fz	301	PEB	CAC-CBC-CGC-O1C

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Mol	Chain	Res	Type	Atoms
26	gb	1002	PEB	CAC-CBC-CGC-O1C
26	gc	202	PEB	CAC-CBC-CGC-O1C
26	gf	202	PEB	CAC-CBC-CGC-O1C
26	gh	202	PEB	CAC-CBC-CGC-O1C
26	gj	202	PEB	CAC-CBC-CGC-O1C
26	gl	202	PEB	CAC-CBC-CGC-O1C
26	gm	1002	PEB	CAC-CBC-CGC-O1C
26	go	202	PEB	CAC-CBC-CGC-O1C
26	gq	202	PEB	CAC-CBC-CGC-O1C
26	gs	202	PEB	CAC-CBC-CGC-O1C
26	gu	202	PEB	CAC-CBC-CGC-O1C
26	gw	202	PEB	CAC-CBC-CGC-O1C
26	gy	302	PEB	CAC-CBC-CGC-O1C
26	gz	302	PEB	CAC-CBC-CGC-O1C
26	hA	202	PEB	CAC-CBC-CGC-O1C
26	hF	202	PEB	CAC-CBC-CGC-O1C
26	hI	202	PEB	CAC-CBC-CGC-O1C
26	hK	202	PEB	CAC-CBC-CGC-O1C
26	hO	202	PEB	CAC-CBC-CGC-O1C
26	hQ	202	PEB	CAC-CBC-CGC-O1C
26	hS	202	PEB	CAC-CBC-CGC-O1C
26	hU	201	PEB	CAC-CBC-CGC-O1C
26	hW	202	PEB	CAC-CBC-CGC-O1C
26	hY	402	PEB	CAC-CBC-CGC-O1C
26	hZ	401	PEB	CAC-CBC-CGC-O1C
26	iA	1002	PEB	CAC-CBC-CGC-O1C
26	iB	1002	PEB	CAC-CBC-CGC-O1C
26	iF	1002	PEB	CAC-CBC-CGC-O1C
29	A2	1004	PVN	C51-C52-C53-O54
29	a3	1004	PVN	C51-C52-C53-O54
29	c8	303	PVN	C51-C52-C53-O54
29	d8	303	PVN	C51-C52-C53-O55
29	c9	303	PVN	C51-C52-C53-O54
29	d9	304	PVN	C51-C52-C53-O55
29	dx	405	PVN	C61-C62-C63-O65
29	d8	303	PVN	C61-C62-C63-O64
29	d9	304	PVN	C61-C62-C63-O64
27	M1	1001	CYC	CAD-CBD-CGD-O2D
27	S1	202	CYC	CAD-CBD-CGD-O2D
27	Y1	201	CYC	CAD-CBD-CGD-O2D
27	c1	201	CYC	CAD-CBD-CGD-O2D
27	r1	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	z1	201	CYC	CAD-CBD-CGD-O2D
27	a2	901	CYC	CAD-CBD-CGD-O2D
29	C2	303	PVN	C61-C62-C63-O64
29	c3	303	PVN	C61-C62-C63-O64
29	c8	303	PVN	C61-C62-C63-O65
29	e8	303	PVN	C61-C62-C63-O64
29	c9	303	PVN	C61-C62-C63-O65
29	e9	304	PVN	C61-C62-C63-O64
26	A2	1001	PEB	CAB-CBB-CGB-O1B
26	E2	1002	PEB	CAB-CBB-CGB-O1B
26	N2	201	PEB	CAB-CBB-CGB-O1B
26	P2	202	PEB	CAB-CBB-CGB-O1B
26	R2	201	PEB	CAB-CBB-CGB-O1B
26	S2	202	PEB	CAB-CBB-CGB-O1B
26	U2	202	PEB	CAB-CBB-CGB-O1B
26	A3	202	PEB	CAB-CBB-CGB-O1B
26	C3	1002	PEB	CAB-CBB-CGB-O1B
26	E3	202	PEB	CAB-CBB-CGB-O1B
26	G3	202	PEB	CAB-CBB-CGB-O1B
26	I3	202	PEB	CAB-CBB-CGB-O1B
26	K3	202	PEB	CAB-CBB-CGB-O1B
26	O3	1002	PEB	CAB-CBB-CGB-O1B
26	Q3	202	PEB	CAB-CBB-CGB-O1B
26	S3	202	PEB	CAB-CBB-CGB-O1B
26	U3	202	PEB	CAB-CBB-CGB-O1B
26	W3	202	PEB	CAB-CBB-CGB-O1B
26	Y3	202	PEB	CAB-CBB-CGB-O1B
26	a3	1002	PEB	CAB-CBB-CGB-O1B
26	c3	301	PEB	CAB-CBB-CGB-O1B
26	d3	301	PEB	CAB-CBB-CGB-O1B
26	e3	1002	PEB	CAB-CBB-CGB-O1B
26	g3	202	PEB	CAB-CBB-CGB-O1B
26	i3	202	PEB	CAB-CBB-CGB-O1B
26	k3	202	PEB	CAB-CBB-CGB-O1B
26	m3	202	PEB	CAB-CBB-CGB-O1B
26	o3	202	PEB	CAB-CBB-CGB-O1B
26	s3	202	PEB	CAB-CBB-CGB-O1B
26	u3	202	PEB	CAB-CBB-CGB-O1B
26	w3	202	PEB	CAB-CBB-CGB-O1B
26	y3	202	PEB	CAB-CBB-CGB-O1B
26	A4	202	PEB	CAB-CBB-CGB-O1B
26	C4	1002	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	N4	202	PEB	CAB-CBB-CGB-O1B
26	c4	201	PEB	CAB-CBB-CGB-O1B
26	h4	201	PEB	CAB-CBB-CGB-O1B
26	s4	202	PEB	CAB-CBB-CGB-O1B
26	w4	202	PEB	CAB-CBB-CGB-O1B
26	A5	202	PEB	CAB-CBB-CGB-O1B
26	C5	202	PEB	CAB-CBB-CGB-O1B
26	E5	202	PEB	CAB-CBB-CGB-O1B
26	G5	202	PEB	CAB-CBB-CGB-O1B
26	I5	202	PEB	CAB-CBB-CGB-O1B
26	K5	1002	PEB	CAB-CBB-CGB-O1B
26	M5	202	PEB	CAB-CBB-CGB-O1B
26	O5	202	PEB	CAB-CBB-CGB-O1B
26	Q5	202	PEB	CAB-CBB-CGB-O1B
26	S5	202	PEB	CAB-CBB-CGB-O1B
26	U5	202	PEB	CAB-CBB-CGB-O1B
26	Y5	1002	PEB	CAB-CBB-CGB-O1B
26	Z5	302	PEB	CAB-CBB-CGB-O1B
26	c5	201	PEB	CAB-CBB-CGB-O1B
26	f5	201	PEB	CAB-CBB-CGB-O1B
26	h5	202	PEB	CAB-CBB-CGB-O1B
26	m5	1002	PEB	CAB-CBB-CGB-O1B
26	o5	202	PEB	CAB-CBB-CGB-O1B
26	q5	202	PEB	CAB-CBB-CGB-O1B
26	s5	202	PEB	CAB-CBB-CGB-O1B
26	u5	202	PEB	CAB-CBB-CGB-O1B
26	w5	202	PEB	CAB-CBB-CGB-O1B
26	y5	1002	PEB	CAB-CBB-CGB-O1B
26	G6	202	PEB	CAB-CBB-CGB-O1B
26	H6	201	PEB	CAB-CBB-CGB-O1B
26	N6	202	PEB	CAB-CBB-CGB-O1B
26	U6	202	PEB	CAB-CBB-CGB-O1B
26	V6	202	PEB	CAB-CBB-CGB-O1B
26	a6	202	PEB	CAB-CBB-CGB-O1B
26	d6	202	PEB	CAB-CBB-CGB-O1B
26	n6	201	PEB	CAB-CBB-CGB-O1B
26	p6	202	PEB	CAB-CBB-CGB-O1B
26	t6	201	PEB	CAB-CBB-CGB-O1B
26	o8	201	PEB	CAB-CBB-CGB-O1B
26	q8	202	PEB	CAB-CBB-CGB-O1B
26	r8	202	PEB	CAB-CBB-CGB-O1B
26	s8	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	t8	202	PEB	CAB-CBB-CGB-O1B
26	u8	202	PEB	CAB-CBB-CGB-O1B
26	A7	201	PEB	CAB-CBB-CGB-O1B
26	C7	202	PEB	CAB-CBB-CGB-O1B
26	E7	202	PEB	CAB-CBB-CGB-O1B
26	G7	202	PEB	CAB-CBB-CGB-O1B
26	I7	202	PEB	CAB-CBB-CGB-O1B
26	K7	202	PEB	CAB-CBB-CGB-O1B
26	M7	1003	PEB	CAB-CBB-CGB-O1B
26	O7	202	PEB	CAB-CBB-CGB-O1B
26	Q7	202	PEB	CAB-CBB-CGB-O1B
26	S7	202	PEB	CAB-CBB-CGB-O1B
26	U7	202	PEB	CAB-CBB-CGB-O1B
26	W7	202	PEB	CAB-CBB-CGB-O1B
26	Y7	1002	PEB	CAB-CBB-CGB-O1B
26	f7	202	PEB	CAB-CBB-CGB-O1B
26	g7	202	PEB	CAB-CBB-CGB-O1B
26	h7	202	PEB	CAB-CBB-CGB-O1B
26	i7	202	PEB	CAB-CBB-CGB-O1B
26	j7	202	PEB	CAB-CBB-CGB-O1B
26	k7	1002	PEB	CAB-CBB-CGB-O1B
26	m7	202	PEB	CAB-CBB-CGB-O1B
26	o7	202	PEB	CAB-CBB-CGB-O1B
26	q7	202	PEB	CAB-CBB-CGB-O1B
26	s7	202	PEB	CAB-CBB-CGB-O1B
26	u7	202	PEB	CAB-CBB-CGB-O1B
26	w7	1002	PEB	CAB-CBB-CGB-O1B
26	c8	301	PEB	CAB-CBB-CGB-O1B
26	d8	301	PEB	CAB-CBB-CGB-O1B
26	E9	202	PEB	CAB-CBB-CGB-O1B
26	G9	202	PEB	CAB-CBB-CGB-O1B
26	I9	202	PEB	CAB-CBB-CGB-O1B
26	K9	1002	PEB	CAB-CBB-CGB-O1B
26	M9	202	PEB	CAB-CBB-CGB-O1B
26	O9	202	PEB	CAB-CBB-CGB-O1B
26	Q9	202	PEB	CAB-CBB-CGB-O1B
26	S9	202	PEB	CAB-CBB-CGB-O1B
26	U9	202	PEB	CAB-CBB-CGB-O1B
26	Y9	301	PEB	CAB-CBB-CGB-O1B
26	Z9	1002	PEB	CAB-CBB-CGB-O1B
26	ao	202	PEB	CAB-CBB-CGB-O1B
26	aq	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	as	202	PEB	CAB-CBB-CGB-O1B
26	au	202	PEB	CAB-CBB-CGB-O1B
26	aw	202	PEB	CAB-CBB-CGB-O1B
26	ay	1002	PEB	CAB-CBB-CGB-O1B
26	bA	202	PEB	CAB-CBB-CGB-O1B
26	bC	202	PEB	CAB-CBB-CGB-O1B
26	bE	202	PEB	CAB-CBB-CGB-O1B
26	bG	202	PEB	CAB-CBB-CGB-O1B
26	bI	202	PEB	CAB-CBB-CGB-O1B
26	bK	1002	PEB	CAB-CBB-CGB-O1B
26	bM	202	PEB	CAB-CBB-CGB-O1B
26	bO	202	PEB	CAB-CBB-CGB-O1B
26	bQ	202	PEB	CAB-CBB-CGB-O1B
26	bS	202	PEB	CAB-CBB-CGB-O1B
26	bU	202	PEB	CAB-CBB-CGB-O1B
26	bY	1002	PEB	CAB-CBB-CGB-O1B
26	bZ	302	PEB	CAB-CBB-CGB-O1B
26	cm	1002	PEB	CAB-CBB-CGB-O1B
26	ct	202	PEB	CAB-CBB-CGB-O1B
26	cu	202	PEB	CAB-CBB-CGB-O1B
26	cv	202	PEB	CAB-CBB-CGB-O1B
26	cw	202	PEB	CAB-CBB-CGB-O1B
26	cx	202	PEB	CAB-CBB-CGB-O1B
26	cy	1002	PEB	CAB-CBB-CGB-O1B
26	cA	202	PEB	CAB-CBB-CGB-O1B
26	cC	1002	PEB	CAB-CBB-CGB-O1B
26	cD	202	PEB	CAB-CBB-CGB-O1B
26	cG	202	PEB	CAB-CBB-CGB-O1B
26	cI	202	PEB	CAB-CBB-CGB-O1B
26	cK	202	PEB	CAB-CBB-CGB-O1B
26	cZ	202	PEB	CAB-CBB-CGB-O1B
26	da	1002	PEB	CAB-CBB-CGB-O1B
26	db	202	PEB	CAB-CBB-CGB-O1B
26	dc	202	PEB	CAB-CBB-CGB-O1B
26	de	202	PEB	CAB-CBB-CGB-O1B
26	dg	202	PEB	CAB-CBB-CGB-O1B
26	dJ	202	PEB	CAB-CBB-CGB-O1B
26	dU	202	PEB	CAB-CBB-CGB-O1B
26	dZ	1002	PEB	CAB-CBB-CGB-O1B
26	ec	201	PEB	CAB-CBB-CGB-O1B
26	ef	202	PEB	CAB-CBB-CGB-O1B
26	eh	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	ei	201	PEB	CAB-CBB-CGB-O1B
26	ek	1002	PEB	CAB-CBB-CGB-O1B
26	em	202	PEB	CAB-CBB-CGB-O1B
26	et	201	PEB	CAB-CBB-CGB-O1B
26	ev	201	PEB	CAB-CBB-CGB-O1B
26	ey	1001	PEB	CAB-CBB-CGB-O1B
26	eA	1002	PEB	CAB-CBB-CGB-O1B
26	eB	201	PEB	CAB-CBB-CGB-O1B
26	eL	201	PEB	CAB-CBB-CGB-O1B
26	eP	201	PEB	CAB-CBB-CGB-O1B
26	eY	401	PEB	CAB-CBB-CGB-O1B
26	lc	202	PEB	CAB-CBB-CGB-O1B
26	ld	201	PEB	CAB-CBB-CGB-O1B
26	le	202	PEB	CAB-CBB-CGB-O1B
26	lg	201	PEB	CAB-CBB-CGB-O1B
26	lg	202	PEB	CAB-CBB-CGB-O1B
26	lh	201	PEB	CAB-CBB-CGB-O1B
26	lj	201	PEB	CAB-CBB-CGB-O1B
26	lk	202	PEB	CAB-CBB-CGB-O1B
26	lm	1002	PEB	CAB-CBB-CGB-O1B
26	lo	201	PEB	CAB-CBB-CGB-O1B
26	lo	202	PEB	CAB-CBB-CGB-O1B
26	ls	202	PEB	CAB-CBB-CGB-O1B
26	lt	202	PEB	CAB-CBB-CGB-O1B
26	lu	202	PEB	CAB-CBB-CGB-O1B
26	lw	201	PEB	CAB-CBB-CGB-O1B
26	lw	202	PEB	CAB-CBB-CGB-O1B
26	fb	202	PEB	CAB-CBB-CGB-O1B
26	fe	202	PEB	CAB-CBB-CGB-O1B
26	fg	202	PEB	CAB-CBB-CGB-O1B
26	fh	1002	PEB	CAB-CBB-CGB-O1B
26	fk	202	PEB	CAB-CBB-CGB-O1B
26	fl	202	PEB	CAB-CBB-CGB-O1B
26	fn	1002	PEB	CAB-CBB-CGB-O1B
26	fp	202	PEB	CAB-CBB-CGB-O1B
26	fr	202	PEB	CAB-CBB-CGB-O1B
26	ft	202	PEB	CAB-CBB-CGB-O1B
26	fv	202	PEB	CAB-CBB-CGB-O1B
26	fx	202	PEB	CAB-CBB-CGB-O1B
26	fz	301	PEB	CAB-CBB-CGB-O1B
26	gb	1002	PEB	CAB-CBB-CGB-O1B
26	gc	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	gf	202	PEB	CAB-CBB-CGB-O1B
26	gh	202	PEB	CAB-CBB-CGB-O1B
26	gj	202	PEB	CAB-CBB-CGB-O1B
26	gl	202	PEB	CAB-CBB-CGB-O1B
26	gm	1002	PEB	CAB-CBB-CGB-O1B
26	go	202	PEB	CAB-CBB-CGB-O1B
26	gq	202	PEB	CAB-CBB-CGB-O1B
26	gs	202	PEB	CAB-CBB-CGB-O1B
26	gu	202	PEB	CAB-CBB-CGB-O1B
26	gw	202	PEB	CAB-CBB-CGB-O1B
26	gy	302	PEB	CAB-CBB-CGB-O1B
26	gz	302	PEB	CAB-CBB-CGB-O1B
26	hA	202	PEB	CAB-CBB-CGB-O1B
26	hC	202	PEB	CAB-CBB-CGB-O1B
26	hE	1002	PEB	CAB-CBB-CGB-O1B
26	hF	202	PEB	CAB-CBB-CGB-O1B
26	hI	202	PEB	CAB-CBB-CGB-O1B
26	hK	202	PEB	CAB-CBB-CGB-O1B
26	hM	1002	PEB	CAB-CBB-CGB-O1B
26	hO	202	PEB	CAB-CBB-CGB-O1B
26	hQ	202	PEB	CAB-CBB-CGB-O1B
26	hS	202	PEB	CAB-CBB-CGB-O1B
26	hU	201	PEB	CAB-CBB-CGB-O1B
26	hW	202	PEB	CAB-CBB-CGB-O1B
26	hY	402	PEB	CAB-CBB-CGB-O1B
26	hZ	401	PEB	CAB-CBB-CGB-O1B
26	iA	1002	PEB	CAB-CBB-CGB-O1B
26	iB	1002	PEB	CAB-CBB-CGB-O1B
26	iF	1002	PEB	CAB-CBB-CGB-O1B
27	H1	201	CYC	CAD-CBD-CGD-O2D
27	h1	201	CYC	CAD-CBD-CGD-O2D
27	p1	201	CYC	CAD-CBD-CGD-O2D
27	t1	201	CYC	CAD-CBD-CGD-O2D
27	v1	201	CYC	CAD-CBD-CGD-O2D
27	a2	902	CYC	CAD-CBD-CGD-O2D
27	b2	1001	CYC	CAD-CBD-CGD-O2D
29	d8	303	PVN	C61-C62-C63-O65
29	d9	304	PVN	C61-C62-C63-O65
29	dx	405	PVN	C61-C62-C63-O64
26	M3	202	PEB	CAB-CBB-CGB-O1B
26	e6	202	PEB	CAB-CBB-CGB-O1B
26	f6	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	A9	202	PEB	CAB-CBB-CGB-O1B
26	C9	202	PEB	CAB-CBB-CGB-O1B
26	eu	202	PEB	CAB-CBB-CGB-O1B
26	lq	203	PEB	CAB-CBB-CGB-O1B
27	J1	201	CYC	CAD-CBD-CGD-O2D
27	S1	201	CYC	CAD-CBD-CGD-O2D
27	j1	201	CYC	CAD-CBD-CGD-O2D
29	D2	303	PVN	C61-C62-C63-O65
29	d3	302	PVN	C61-C62-C63-O65
29	e8	303	PVN	C51-C52-C53-O55
29	d9	304	PVN	C51-C52-C53-O54
29	e9	304	PVN	C51-C52-C53-O55
29	aY	403	PVN	C61-C62-C63-O65
29	bY	1004	PVN	C61-C62-C63-O65
29	gz	304	PVN	C61-C62-C63-O64
29	ez	1004	PVN	C8-C51-C52-C53
29	34	1004	PVN	C61-C62-C63-O65
29	Y5	1004	PVN	C61-C62-C63-O65
29	b9	405	PVN	C61-C62-C63-O65
29	hY	404	PVN	C61-C62-C63-O65
29	hZ	403	PVN	C61-C62-C63-O65
29	c8	303	PVN	C9-C10-C11-C12
29	c9	303	PVN	C9-C10-C11-C12
27	H1	201	CYC	CAA-CBA-CGA-O2A
27	c1	201	CYC	CAA-CBA-CGA-O2A
29	A2	1004	PVN	C61-C62-C63-O64
29	a3	1004	PVN	C61-C62-C63-O64
29	b8	1004	PVN	C61-C62-C63-O65
29	c8	303	PVN	C61-C62-C63-O64
29	c9	303	PVN	C61-C62-C63-O64
27	J1	201	CYC	CAA-CBA-CGA-O2A
27	M1	1001	CYC	CAA-CBA-CGA-O2A
27	S1	201	CYC	CAA-CBA-CGA-O2A
27	S1	202	CYC	CAA-CBA-CGA-O2A
27	Y1	201	CYC	CAA-CBA-CGA-O2A
27	h1	201	CYC	CAA-CBA-CGA-O2A
27	j1	201	CYC	CAA-CBA-CGA-O2A
27	p1	201	CYC	CAA-CBA-CGA-O2A
27	r1	201	CYC	CAA-CBA-CGA-O2A
27	t1	201	CYC	CAA-CBA-CGA-O2A
27	v1	201	CYC	CAA-CBA-CGA-O2A
27	z1	201	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	a2	901	CYC	CAA-CBA-CGA-O2A
27	a2	902	CYC	CAA-CBA-CGA-O2A
27	b2	1001	CYC	CAA-CBA-CGA-O2A
29	d8	303	PVN	C51-C52-C53-O54
29	eY	403	PVN	C61-C62-C63-O65
28	f2	203	PUB	NC-C1C-CHB-C4B
28	j2	203	PUB	NC-C1C-CHB-C4B
28	n2	203	PUB	NC-C1C-CHB-C4B
28	p2	203	PUB	NC-C1C-CHB-C4B
28	r2	203	PUB	NC-C1C-CHB-C4B
28	t2	203	PUB	NC-C1C-CHB-C4B
28	z2	203	PUB	NC-C1C-CHB-C4B
28	A2	1005	PUB	NC-C1C-CHB-C4B
28	A2	1006	PUB	NC-C1C-CHB-C4B
28	C2	304	PUB	NC-C1C-CHB-C4B
28	D2	305	PUB	NC-C1C-CHB-C4B
28	H2	202	PUB	NC-C1C-CHB-C4B
28	J2	202	PUB	NC-C1C-CHB-C4B
28	L2	203	PUB	NC-C1C-CHB-C4B
28	N2	203	PUB	NC-C1C-CHB-C4B
28	T2	203	PUB	NC-C1C-CHB-C4B
28	X2	203	PUB	NC-C1C-CHB-C4B
28	Z2	203	PUB	NC-C1C-CHB-C4B
28	D3	203	PUB	NC-C1C-CHB-C4B
28	H3	203	PUB	NC-C1C-CHB-C4B
28	J3	203	PUB	NC-C1C-CHB-C4B
28	N3	203	PUB	NC-C1C-CHB-C4B
28	P3	203	PUB	NC-C1C-CHB-C4B
28	Z3	203	PUB	NC-C1C-CHB-C4B
28	a3	1006	PUB	NC-C1C-CHB-C4B
28	c3	304	PUB	NC-C1C-CHB-C4B
28	d3	304	PUB	NC-C1C-CHB-C4B
28	f3	203	PUB	NC-C1C-CHB-C4B
28	j3	202	PUB	NC-C1C-CHB-C4B
28	n3	203	PUB	NC-C1C-CHB-C4B
28	r3	203	PUB	NC-C1C-CHB-C4B
28	Z4	203	PUB	NC-C1C-CHB-C4B
28	34	1006	PUB	NC-C1C-CHB-C4B
28	44	305	PUB	NC-C1C-CHB-C4B
28	r4	202	PUB	NC-C1C-CHB-C4B
28	z4	203	PUB	NC-C1C-CHB-C4B
28	D5	203	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	F5	203	PUB	NC-C1C-CHB-C4B
28	L5	203	PUB	NC-C1C-CHB-C4B
28	N5	203	PUB	NC-C1C-CHB-C4B
28	P5	202	PUB	NC-C1C-CHB-C4B
28	T5	202	PUB	NC-C1C-CHB-C4B
28	Y5	1005	PUB	NC-C1C-CHB-C4B
28	Z5	305	PUB	NC-C1C-CHB-C4B
28	p5	202	PUB	NC-C1C-CHB-C4B
28	t5	203	PUB	NC-C1C-CHB-C4B
28	z5	203	PUB	NC-C1C-CHB-C4B
28	g8	202	PUB	NC-C1C-CHB-C4B
28	h8	203	PUB	NC-C1C-CHB-C4B
28	D6	202	PUB	NC-C1C-CHB-C4B
28	F6	203	PUB	NC-C1C-CHB-C4B
28	J6	203	PUB	NC-C1C-CHB-C4B
28	L6	202	PUB	NC-C1C-CHB-C4B
28	R6	203	PUB	NC-C1C-CHB-C4B
28	X6	203	PUB	NC-C1C-CHB-C4B
28	a6	203	PUB	NC-C1C-CHB-C4B
28	b6	203	PUB	NC-C1C-CHB-C4B
28	d6	203	PUB	NC-C1C-CHB-C4B
28	n6	203	PUB	NC-C1C-CHB-C4B
28	t6	203	PUB	NC-C1C-CHB-C4B
28	u6	203	PUB	NC-C1C-CHB-C4B
28	x6	203	PUB	NC-C1C-CHB-C4B
28	y6	204	PUB	NC-C1C-CHB-C4B
28	n8	202	PUB	NC-C1C-CHB-C4B
28	p8	203	PUB	NC-C1C-CHB-C4B
28	L7	202	PUB	NC-C1C-CHB-C4B
28	R7	203	PUB	NC-C1C-CHB-C4B
28	V7	203	PUB	NC-C1C-CHB-C4B
28	X7	203	PUB	NC-C1C-CHB-C4B
28	Z7	203	PUB	NC-C1C-CHB-C4B
28	b7	202	PUB	NC-C1C-CHB-C4B
28	c7	203	PUB	NC-C1C-CHB-C4B
28	e7	203	PUB	NC-C1C-CHB-C4B
28	l7	203	PUB	NC-C1C-CHB-C4B
28	n7	203	PUB	NC-C1C-CHB-C4B
28	r7	203	PUB	NC-C1C-CHB-C4B
28	s7	203	PUB	NC-C1C-CHB-C4B
28	y7	203	PUB	NC-C1C-CHB-C4B
28	z7	203	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	b8	1005	PUB	NC-C1C-CHB-C4B
28	c8	305	PUB	NC-C1C-CHB-C4B
28	e8	304	PUB	NC-C1C-CHB-C4B
28	b9	406	PUB	NC-C1C-CHB-C4B
28	b9	407	PUB	NC-C1C-CHB-C4B
28	c9	304	PUB	NC-C1C-CHB-C4B
28	c9	305	PUB	NC-C1C-CHB-C4B
28	d9	305	PUB	NC-C1C-CHB-C4B
28	w8	203	PUB	NC-C1C-CHB-C4B
28	C8	203	PUB	NC-C1C-CHB-C4B
28	E8	203	PUB	NC-C1C-CHB-C4B
28	K8	203	PUB	NC-C1C-CHB-C4B
28	M8	203	PUB	NC-C1C-CHB-C4B
28	Q8	203	PUB	NC-C1C-CHB-C4B
28	T8	305	PUB	NC-C1C-CHB-C4B
28	U8	1005	PUB	NC-C1C-CHB-C4B
28	r9	203	PUB	NC-C1C-CHB-C4B
28	t9	203	PUB	NC-C1C-CHB-C4B
28	D9	203	PUB	NC-C1C-CHB-C4B
28	L9	203	PUB	NC-C1C-CHB-C4B
28	N9	203	PUB	NC-C1C-CHB-C4B
28	V9	203	PUB	NC-C1C-CHB-C4B
28	Y9	305	PUB	NC-C1C-CHB-C4B
28	ap	203	PUB	NC-C1C-CHB-C4B
28	ar	203	PUB	NC-C1C-CHB-C4B
28	av	203	PUB	NC-C1C-CHB-C4B
28	ax	202	PUB	NC-C1C-CHB-C4B
28	aB	203	PUB	NC-C1C-CHB-C4B
28	aL	203	PUB	NC-C1C-CHB-C4B
28	aZ	304	PUB	NC-C1C-CHB-C4B
28	bn	202	PUB	NC-C1C-CHB-C4B
28	bp	202	PUB	NC-C1C-CHB-C4B
28	bq	203	PUB	NC-C1C-CHB-C4B
28	bz	203	PUB	NC-C1C-CHB-C4B
28	bB	203	PUB	NC-C1C-CHB-C4B
28	bF	203	PUB	NC-C1C-CHB-C4B
28	bH	203	PUB	NC-C1C-CHB-C4B
28	bJ	203	PUB	NC-C1C-CHB-C4B
28	bR	202	PUB	NC-C1C-CHB-C4B
28	bT	202	PUB	NC-C1C-CHB-C4B
28	bZ	306	PUB	NC-C1C-CHB-C4B
28	co	202	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	cp	203	PUB	NC-C1C-CHB-C4B
28	cr	203	PUB	NC-C1C-CHB-C4B
28	cF	202	PUB	NC-C1C-CHB-C4B
28	cL	203	PUB	NC-C1C-CHB-C4B
28	cO	203	PUB	NC-C1C-CHB-C4B
28	cQ	202	PUB	NC-C1C-CHB-C4B
28	dh	203	PUB	NC-C1C-CHB-C4B
28	di	203	PUB	NC-C1C-CHB-C4B
28	dn	203	PUB	NC-C1C-CHB-C4B
28	dr	203	PUB	NC-C1C-CHB-C4B
28	dw	405	PUB	NC-C1C-CHB-C4B
28	dx	406	PUB	NC-C1C-CHB-C4B
28	dD	203	PUB	NC-C1C-CHB-C4B
28	dF	203	PUB	NC-C1C-CHB-C4B
28	dH	203	PUB	NC-C1C-CHB-C4B
28	dL	203	PUB	NC-C1C-CHB-C4B
28	dN	203	PUB	NC-C1C-CHB-C4B
28	dV	203	PUB	NC-C1C-CHB-C4B
28	dX	203	PUB	NC-C1C-CHB-C4B
28	dY	203	PUB	NC-C1C-CHB-C4B
28	ec	203	PUB	NC-C1C-CHB-C4B
28	ee	203	PUB	NC-C1C-CHB-C4B
28	eg	203	PUB	NC-C1C-CHB-C4B
28	ei	203	PUB	NC-C1C-CHB-C4B
28	ep	203	PUB	NC-C1C-CHB-C4B
28	er	203	PUB	NC-C1C-CHB-C4B
28	ez	1005	PUB	NC-C1C-CHB-C4B
28	ez	1006	PUB	NC-C1C-CHB-C4B
28	eD	203	PUB	NC-C1C-CHB-C4B
28	eH	203	PUB	NC-C1C-CHB-C4B
28	eJ	203	PUB	NC-C1C-CHB-C4B
28	eP	204	PUB	NC-C1C-CHB-C4B
28	eV	203	PUB	NC-C1C-CHB-C4B
28	eY	404	PUB	NC-C1C-CHB-C4B
28	eZ	403	PUB	NC-C1C-CHB-C4B
28	lf	203	PUB	NC-C1C-CHB-C4B
28	lj	202	PUB	NC-C1C-CHB-C4B
28	ll	203	PUB	NC-C1C-CHB-C4B
28	lt	203	PUB	NC-C1C-CHB-C4B
28	lx	201	PUB	NC-C1C-CHB-C4B
28	ly	406	PUB	NC-C1C-CHB-C4B
28	ff	203	PUB	NC-C1C-CHB-C4B

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Mol	Chain	Res	Type	Atoms
28	fj	203	PUB	NC-C1C-CHB-C4B
28	fm	203	PUB	NC-C1C-CHB-C4B
28	fw	203	PUB	NC-C1C-CHB-C4B
28	fy	202	PUB	NC-C1C-CHB-C4B
28	ga	203	PUB	NC-C1C-CHB-C4B
28	gg	203	PUB	NC-C1C-CHB-C4B
28	gi	203	PUB	NC-C1C-CHB-C4B
28	gn	203	PUB	NC-C1C-CHB-C4B
28	gp	203	PUB	NC-C1C-CHB-C4B
28	gv	203	PUB	NC-C1C-CHB-C4B
28	gy	305	PUB	NC-C1C-CHB-C4B
28	gy	306	PUB	NC-C1C-CHB-C4B
28	gz	305	PUB	NC-C1C-CHB-C4B
28	gz	306	PUB	NC-C1C-CHB-C4B
28	hH	203	PUB	NC-C1C-CHB-C4B
28	hL	203	PUB	NC-C1C-CHB-C4B
28	hR	203	PUB	NC-C1C-CHB-C4B
28	hT	203	PUB	NC-C1C-CHB-C4B
28	hX	203	PUB	NC-C1C-CHB-C4B
28	hY	405	PUB	NC-C1C-CHB-C4B
28	hY	406	PUB	NC-C1C-CHB-C4B
28	hZ	405	PUB	NC-C1C-CHB-C4B
28	iD	1003	PUB	NC-C1C-CHB-C4B
28	iG	1002	PUB	NC-C1C-CHB-C4B
28	jI	1003	PUB	NC-C1C-CHB-C4B
28	jJ	1003	PUB	NC-C1C-CHB-C4B
28	jL	1003	PUB	NC-C1C-CHB-C4B
28	jN	1003	PUB	NC-C1C-CHB-C4B
28	jO	1003	PUB	NC-C1C-CHB-C4B
28	jP	1003	PUB	NC-C1C-CHB-C4B
28	kQ	1003	PUB	NC-C1C-CHB-C4B
28	kR	1003	PUB	NC-C1C-CHB-C4B
28	kS	1003	PUB	NC-C1C-CHB-C4B
28	kT	1003	PUB	NC-C1C-CHB-C4B
28	kV	1003	PUB	NC-C1C-CHB-C4B
28	kX	1003	PUB	NC-C1C-CHB-C4B
29	34	1004	PVN	C51-C52-C53-O55
29	Y5	1004	PVN	C51-C52-C53-O55
29	bY	1004	PVN	C61-C62-C63-O64
29	eZ	402	PVN	C61-C62-C63-O65
29	hY	404	PVN	C51-C52-C53-O55
29	hZ	403	PVN	C51-C52-C53-O55

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Mol	Chain	Res	Type	Atoms
29	aY	403	PVN	C61-C62-C63-O64
29	44	303	PVN	C61-C62-C63-O65
29	Z5	304	PVN	C61-C62-C63-O65
29	ez	1004	PVN	C61-C62-C63-O65
29	b8	1004	PVN	C61-C62-C63-O64
29	b9	405	PVN	C61-C62-C63-O64
29	hY	404	PVN	C61-C62-C63-O64
29	hZ	403	PVN	C61-C62-C63-O64
29	34	1004	PVN	C61-C62-C63-O64
29	gy	304	PVN	C61-C62-C63-O64
29	gy	304	PVN	C61-C62-C63-O65
29	44	303	PVN	C61-C62-C63-O64
29	Y5	1004	PVN	C61-C62-C63-O64
29	Z5	304	PVN	C61-C62-C63-O64
29	ez	1004	PVN	C61-C62-C63-O64
28	f2	203	PUB	CAB-CBB-CGB-O1B
28	f2	203	PUB	CAB-CBB-CGB-O2B
28	h2	203	PUB	CAB-CBB-CGB-O1B
28	h2	203	PUB	CAB-CBB-CGB-O2B
28	j2	203	PUB	CAB-CBB-CGB-O1B
28	j2	203	PUB	CAB-CBB-CGB-O2B
28	l2	203	PUB	CAB-CBB-CGB-O1B
28	l2	203	PUB	CAB-CBB-CGB-O2B
28	n2	203	PUB	CAB-CBB-CGB-O1B
28	n2	203	PUB	CAB-CBB-CGB-O2B
28	p2	203	PUB	CAB-CBB-CGB-O1B
28	p2	203	PUB	CAB-CBB-CGB-O2B
28	r2	203	PUB	CAB-CBB-CGB-O1B
28	r2	203	PUB	CAB-CBB-CGB-O2B
28	t2	203	PUB	CAB-CBB-CGB-O1B
28	t2	203	PUB	CAB-CBB-CGB-O2B
28	v2	203	PUB	CAB-CBB-CGB-O1B
28	v2	203	PUB	CAB-CBB-CGB-O2B
28	x2	202	PUB	CAB-CBB-CGB-O1B
28	x2	202	PUB	CAB-CBB-CGB-O2B
28	z2	203	PUB	CAB-CBB-CGB-O1B
28	z2	203	PUB	CAB-CBB-CGB-O2B
28	A2	1005	PUB	CAB-CBB-CGB-O1B
28	A2	1005	PUB	CAB-CBB-CGB-O2B
28	A2	1006	PUB	CAB-CBB-CGB-O1B
28	A2	1006	PUB	CAB-CBB-CGB-O2B
28	C2	304	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	C2	304	PUB	CAB-CBB-CGB-O2B
28	C2	305	PUB	CAB-CBB-CGB-O1B
28	C2	305	PUB	CAB-CBB-CGB-O2B
28	D2	304	PUB	CAB-CBB-CGB-O1B
28	D2	304	PUB	CAB-CBB-CGB-O2B
28	D2	305	PUB	CAB-CBB-CGB-O1B
28	D2	305	PUB	CAB-CBB-CGB-O2B
28	F2	203	PUB	CAB-CBB-CGB-O1B
28	F2	203	PUB	CAB-CBB-CGB-O2B
28	H2	202	PUB	CAB-CBB-CGB-O1B
28	H2	202	PUB	CAB-CBB-CGB-O2B
28	J2	202	PUB	CAB-CBB-CGB-O1B
28	J2	202	PUB	CAB-CBB-CGB-O2B
28	L2	203	PUB	CAB-CBB-CGB-O1B
28	L2	203	PUB	CAB-CBB-CGB-O2B
28	N2	203	PUB	CAB-CBB-CGB-O1B
28	P2	203	PUB	CAB-CBB-CGB-O1B
28	P2	203	PUB	CAB-CBB-CGB-O2B
28	R2	203	PUB	CAB-CBB-CGB-O1B
28	R2	203	PUB	CAB-CBB-CGB-O2B
28	T2	203	PUB	CAB-CBB-CGB-O1B
28	T2	203	PUB	CAB-CBB-CGB-O2B
28	V2	203	PUB	CAB-CBB-CGB-O1B
28	V2	203	PUB	CAB-CBB-CGB-O2B
28	X2	203	PUB	CAB-CBB-CGB-O1B
28	X2	203	PUB	CAB-CBB-CGB-O2B
28	Z2	203	PUB	CAB-CBB-CGB-O1B
28	Z2	203	PUB	CAB-CBB-CGB-O2B
28	B3	203	PUB	CAB-CBB-CGB-O1B
28	B3	203	PUB	CAB-CBB-CGB-O2B
28	D3	203	PUB	CAB-CBB-CGB-O1B
28	D3	203	PUB	CAB-CBB-CGB-O2B
28	F3	203	PUB	CAB-CBB-CGB-O1B
28	F3	203	PUB	CAB-CBB-CGB-O2B
28	H3	203	PUB	CAB-CBB-CGB-O1B
28	H3	203	PUB	CAB-CBB-CGB-O2B
28	J3	203	PUB	CAB-CBB-CGB-O1B
28	J3	203	PUB	CAB-CBB-CGB-O2B
28	L3	203	PUB	CAB-CBB-CGB-O1B
28	L3	203	PUB	CAB-CBB-CGB-O2B
28	N3	203	PUB	CAB-CBB-CGB-O1B
28	N3	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	P3	203	PUB	CAB-CBB-CGB-O1B
28	P3	203	PUB	CAB-CBB-CGB-O2B
28	R3	203	PUB	CAB-CBB-CGB-O1B
28	R3	203	PUB	CAB-CBB-CGB-O2B
28	T3	203	PUB	CAB-CBB-CGB-O1B
28	T3	203	PUB	CAB-CBB-CGB-O2B
28	V3	203	PUB	CAB-CBB-CGB-O1B
28	V3	203	PUB	CAB-CBB-CGB-O2B
28	X3	202	PUB	CAB-CBB-CGB-O1B
28	X3	202	PUB	CAB-CBB-CGB-O2B
28	Z3	203	PUB	CAB-CBB-CGB-O1B
28	Z3	203	PUB	CAB-CBB-CGB-O2B
28	a3	1005	PUB	CAB-CBB-CGB-O1B
28	a3	1005	PUB	CAB-CBB-CGB-O2B
28	a3	1006	PUB	CAB-CBB-CGB-O1B
28	a3	1006	PUB	CAB-CBB-CGB-O2B
28	c3	304	PUB	CAB-CBB-CGB-O1B
28	c3	304	PUB	CAB-CBB-CGB-O2B
28	c3	305	PUB	CAB-CBB-CGB-O1B
28	c3	305	PUB	CAB-CBB-CGB-O2B
28	d3	303	PUB	CAB-CBB-CGB-O1B
28	d3	304	PUB	CAB-CBB-CGB-O1B
28	d3	304	PUB	CAB-CBB-CGB-O2B
28	f3	203	PUB	CAB-CBB-CGB-O1B
28	f3	203	PUB	CAB-CBB-CGB-O2B
28	h3	202	PUB	CAB-CBB-CGB-O1B
28	h3	202	PUB	CAB-CBB-CGB-O2B
28	j3	202	PUB	CAB-CBB-CGB-O1B
28	j3	202	PUB	CAB-CBB-CGB-O2B
28	l3	202	PUB	CAB-CBB-CGB-O1B
28	l3	202	PUB	CAB-CBB-CGB-O2B
28	n3	203	PUB	CAB-CBB-CGB-O1B
28	n3	203	PUB	CAB-CBB-CGB-O2B
28	p3	203	PUB	CAB-CBB-CGB-O1B
28	p3	203	PUB	CAB-CBB-CGB-O2B
28	r3	203	PUB	CAB-CBB-CGB-O1B
28	r3	203	PUB	CAB-CBB-CGB-O2B
28	t3	203	PUB	CAB-CBB-CGB-O1B
28	t3	203	PUB	CAB-CBB-CGB-O2B
28	v3	203	PUB	CAB-CBB-CGB-O1B
28	v3	203	PUB	CAB-CBB-CGB-O2B
28	x3	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	x3	203	PUB	CAB-CBB-CGB-O2B
28	z3	203	PUB	CAB-CBB-CGB-O1B
28	z3	203	PUB	CAB-CBB-CGB-O2B
28	B4	203	PUB	CAB-CBB-CGB-O1B
28	B4	203	PUB	CAB-CBB-CGB-O2B
28	D4	203	PUB	CAB-CBB-CGB-O1B
28	D4	203	PUB	CAB-CBB-CGB-O2B
28	F4	203	PUB	CAB-CBB-CGB-O1B
28	F4	203	PUB	CAB-CBB-CGB-O2B
28	H4	203	PUB	CAB-CBB-CGB-O1B
28	H4	203	PUB	CAB-CBB-CGB-O2B
28	J4	203	PUB	CAB-CBB-CGB-O1B
28	J4	203	PUB	CAB-CBB-CGB-O2B
28	L4	203	PUB	CAB-CBB-CGB-O1B
28	L4	203	PUB	CAB-CBB-CGB-O2B
28	N4	203	PUB	CAB-CBB-CGB-O1B
28	N4	203	PUB	CAB-CBB-CGB-O2B
28	P4	203	PUB	CAB-CBB-CGB-O1B
28	P4	203	PUB	CAB-CBB-CGB-O2B
28	R4	203	PUB	CAB-CBB-CGB-O1B
28	R4	203	PUB	CAB-CBB-CGB-O2B
28	T4	202	PUB	CAB-CBB-CGB-O1B
28	T4	202	PUB	CAB-CBB-CGB-O2B
28	V4	203	PUB	CAB-CBB-CGB-O1B
28	V4	203	PUB	CAB-CBB-CGB-O2B
28	X4	203	PUB	CAB-CBB-CGB-O1B
28	X4	203	PUB	CAB-CBB-CGB-O2B
28	Z4	203	PUB	CAB-CBB-CGB-O1B
28	Z4	203	PUB	CAB-CBB-CGB-O2B
28	34	1005	PUB	CAB-CBB-CGB-O1B
28	34	1005	PUB	CAB-CBB-CGB-O2B
28	34	1006	PUB	CAB-CBB-CGB-O2B
28	44	304	PUB	CAB-CBB-CGB-O1B
28	44	304	PUB	CAB-CBB-CGB-O2B
28	44	305	PUB	CAB-CBB-CGB-O1B
28	44	305	PUB	CAB-CBB-CGB-O2B
28	n4	203	PUB	CAB-CBB-CGB-O1B
28	n4	203	PUB	CAB-CBB-CGB-O2B
28	p4	203	PUB	CAB-CBB-CGB-O1B
28	p4	203	PUB	CAB-CBB-CGB-O2B
28	r4	202	PUB	CAB-CBB-CGB-O1B
28	t4	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	t4	203	PUB	CAB-CBB-CGB-O2B
28	v4	203	PUB	CAB-CBB-CGB-O1B
28	v4	203	PUB	CAB-CBB-CGB-O2B
28	x4	202	PUB	CAB-CBB-CGB-O1B
28	x4	202	PUB	CAB-CBB-CGB-O2B
28	z4	203	PUB	CAB-CBB-CGB-O1B
28	z4	203	PUB	CAB-CBB-CGB-O2B
28	B5	203	PUB	CAB-CBB-CGB-O1B
28	B5	203	PUB	CAB-CBB-CGB-O2B
28	D5	203	PUB	CAB-CBB-CGB-O1B
28	D5	203	PUB	CAB-CBB-CGB-O2B
28	F5	203	PUB	CAB-CBB-CGB-O1B
28	F5	203	PUB	CAB-CBB-CGB-O2B
28	H5	202	PUB	CAB-CBB-CGB-O1B
28	H5	202	PUB	CAB-CBB-CGB-O2B
28	J5	203	PUB	CAB-CBB-CGB-O1B
28	J5	203	PUB	CAB-CBB-CGB-O2B
28	L5	203	PUB	CAB-CBB-CGB-O1B
28	L5	203	PUB	CAB-CBB-CGB-O2B
28	N5	203	PUB	CAB-CBB-CGB-O1B
28	N5	203	PUB	CAB-CBB-CGB-O2B
28	P5	202	PUB	CAB-CBB-CGB-O1B
28	P5	202	PUB	CAB-CBB-CGB-O2B
28	R5	203	PUB	CAB-CBB-CGB-O1B
28	R5	203	PUB	CAB-CBB-CGB-O2B
28	T5	202	PUB	CAB-CBB-CGB-O1B
28	T5	202	PUB	CAB-CBB-CGB-O2B
28	V5	203	PUB	CAB-CBB-CGB-O1B
28	V5	203	PUB	CAB-CBB-CGB-O2B
28	Y5	1005	PUB	CAB-CBB-CGB-O1B
28	Y5	1005	PUB	CAB-CBB-CGB-O2B
28	Y5	1006	PUB	CAB-CBB-CGB-O1B
28	Y5	1006	PUB	CAB-CBB-CGB-O2B
28	Z5	305	PUB	CAB-CBB-CGB-O1B
28	Z5	305	PUB	CAB-CBB-CGB-O2B
28	Z5	306	PUB	CAB-CBB-CGB-O1B
28	Z5	306	PUB	CAB-CBB-CGB-O2B
28	n5	203	PUB	CAB-CBB-CGB-O1B
28	n5	203	PUB	CAB-CBB-CGB-O2B
28	p5	202	PUB	CAB-CBB-CGB-O1B
28	p5	202	PUB	CAB-CBB-CGB-O2B
28	r5	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	t5	203	PUB	CAB-CBB-CGB-O1B
28	t5	203	PUB	CAB-CBB-CGB-O2B
28	v5	203	PUB	CAB-CBB-CGB-O1B
28	v5	203	PUB	CAB-CBB-CGB-O2B
28	x5	202	PUB	CAB-CBB-CGB-O1B
28	x5	202	PUB	CAB-CBB-CGB-O2B
28	z5	203	PUB	CAB-CBB-CGB-O1B
28	z5	203	PUB	CAB-CBB-CGB-O2B
28	f8	203	PUB	CAB-CBB-CGB-O1B
28	f8	203	PUB	CAB-CBB-CGB-O2B
28	g8	202	PUB	CAB-CBB-CGB-O1B
28	g8	202	PUB	CAB-CBB-CGB-O2B
28	h8	203	PUB	CAB-CBB-CGB-O1B
28	h8	203	PUB	CAB-CBB-CGB-O2B
28	B6	203	PUB	CAB-CBB-CGB-O1B
28	D6	202	PUB	CAB-CBB-CGB-O1B
28	D6	202	PUB	CAB-CBB-CGB-O2B
28	F6	203	PUB	CAB-CBB-CGB-O1B
28	F6	203	PUB	CAB-CBB-CGB-O2B
28	H6	203	PUB	CAB-CBB-CGB-O1B
28	H6	203	PUB	CAB-CBB-CGB-O2B
28	J6	203	PUB	CAB-CBB-CGB-O1B
28	L6	202	PUB	CAB-CBB-CGB-O1B
28	N6	203	PUB	CAB-CBB-CGB-O1B
28	P6	203	PUB	CAB-CBB-CGB-O1B
28	P6	203	PUB	CAB-CBB-CGB-O2B
28	R6	203	PUB	CAB-CBB-CGB-O1B
28	R6	203	PUB	CAB-CBB-CGB-O2B
28	T6	203	PUB	CAB-CBB-CGB-O1B
28	T6	203	PUB	CAB-CBB-CGB-O2B
28	V6	203	PUB	CAB-CBB-CGB-O1B
28	V6	203	PUB	CAB-CBB-CGB-O2B
28	X6	203	PUB	CAB-CBB-CGB-O1B
28	X6	203	PUB	CAB-CBB-CGB-O2B
28	Z6	203	PUB	CAB-CBB-CGB-O1B
28	Z6	203	PUB	CAB-CBB-CGB-O2B
28	a6	203	PUB	CAB-CBB-CGB-O1B
28	a6	203	PUB	CAB-CBB-CGB-O2B
28	b6	203	PUB	CAB-CBB-CGB-O1B
28	b6	203	PUB	CAB-CBB-CGB-O2B
28	c6	1004	PUB	CAB-CBB-CGB-O1B
28	c6	1004	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	d6	203	PUB	CAB-CBB-CGB-O1B
28	d6	203	PUB	CAB-CBB-CGB-O2B
28	e6	203	PUB	CAB-CBB-CGB-O1B
28	e6	203	PUB	CAB-CBB-CGB-O2B
28	l6	203	PUB	CAB-CBB-CGB-O1B
28	l6	203	PUB	CAB-CBB-CGB-O2B
28	n6	203	PUB	CAB-CBB-CGB-O1B
28	n6	203	PUB	CAB-CBB-CGB-O2B
28	p6	203	PUB	CAB-CBB-CGB-O1B
28	p6	203	PUB	CAB-CBB-CGB-O2B
28	r6	203	PUB	CAB-CBB-CGB-O1B
28	r6	203	PUB	CAB-CBB-CGB-O2B
28	t6	203	PUB	CAB-CBB-CGB-O1B
28	t6	203	PUB	CAB-CBB-CGB-O2B
28	u6	203	PUB	CAB-CBB-CGB-O1B
28	u6	203	PUB	CAB-CBB-CGB-O2B
28	v6	203	PUB	CAB-CBB-CGB-O1B
28	x6	203	PUB	CAB-CBB-CGB-O1B
28	x6	203	PUB	CAB-CBB-CGB-O2B
28	y6	204	PUB	CAB-CBB-CGB-O1B
28	y6	204	PUB	CAB-CBB-CGB-O2B
28	z6	203	PUB	CAB-CBB-CGB-O1B
28	z6	203	PUB	CAB-CBB-CGB-O2B
28	n8	202	PUB	CAB-CBB-CGB-O1B
28	n8	202	PUB	CAB-CBB-CGB-O2B
28	o8	203	PUB	CAB-CBB-CGB-O1B
28	o8	203	PUB	CAB-CBB-CGB-O2B
28	p8	203	PUB	CAB-CBB-CGB-O1B
28	p8	203	PUB	CAB-CBB-CGB-O2B
28	B7	202	PUB	CAB-CBB-CGB-O1B
28	B7	202	PUB	CAB-CBB-CGB-O2B
28	D7	203	PUB	CAB-CBB-CGB-O1B
28	D7	203	PUB	CAB-CBB-CGB-O2B
28	F7	202	PUB	CAB-CBB-CGB-O1B
28	F7	202	PUB	CAB-CBB-CGB-O2B
28	H7	203	PUB	CAB-CBB-CGB-O1B
28	H7	203	PUB	CAB-CBB-CGB-O2B
28	J7	202	PUB	CAB-CBB-CGB-O1B
28	J7	202	PUB	CAB-CBB-CGB-O2B
28	L7	202	PUB	CAB-CBB-CGB-O1B
28	L7	202	PUB	CAB-CBB-CGB-O2B
28	N7	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	P7	203	PUB	CAB-CBB-CGB-O1B
28	R7	203	PUB	CAB-CBB-CGB-O1B
28	R7	203	PUB	CAB-CBB-CGB-O2B
28	T7	203	PUB	CAB-CBB-CGB-O1B
28	T7	203	PUB	CAB-CBB-CGB-O2B
28	V7	203	PUB	CAB-CBB-CGB-O1B
28	V7	203	PUB	CAB-CBB-CGB-O2B
28	X7	203	PUB	CAB-CBB-CGB-O1B
28	X7	203	PUB	CAB-CBB-CGB-O2B
28	Z7	203	PUB	CAB-CBB-CGB-O1B
28	Z7	203	PUB	CAB-CBB-CGB-O2B
28	a7	203	PUB	CAB-CBB-CGB-O1B
28	a7	203	PUB	CAB-CBB-CGB-O2B
28	b7	202	PUB	CAB-CBB-CGB-O1B
28	b7	202	PUB	CAB-CBB-CGB-O2B
28	c7	203	PUB	CAB-CBB-CGB-O1B
28	c7	203	PUB	CAB-CBB-CGB-O2B
28	d7	203	PUB	CAB-CBB-CGB-O1B
28	d7	203	PUB	CAB-CBB-CGB-O2B
28	e7	203	PUB	CAB-CBB-CGB-O1B
28	e7	203	PUB	CAB-CBB-CGB-O2B
28	l7	203	PUB	CAB-CBB-CGB-O1B
28	l7	203	PUB	CAB-CBB-CGB-O2B
28	n7	203	PUB	CAB-CBB-CGB-O1B
28	n7	203	PUB	CAB-CBB-CGB-O2B
28	p7	202	PUB	CAB-CBB-CGB-O1B
28	p7	202	PUB	CAB-CBB-CGB-O2B
28	r7	203	PUB	CAB-CBB-CGB-O1B
28	r7	203	PUB	CAB-CBB-CGB-O2B
28	s7	203	PUB	CAB-CBB-CGB-O1B
28	s7	203	PUB	CAB-CBB-CGB-O2B
28	t7	203	PUB	CAB-CBB-CGB-O1B
28	v7	203	PUB	CAB-CBB-CGB-O1B
28	v7	203	PUB	CAB-CBB-CGB-O2B
28	x7	203	PUB	CAB-CBB-CGB-O1B
28	x7	203	PUB	CAB-CBB-CGB-O2B
28	y7	203	PUB	CAB-CBB-CGB-O1B
28	y7	203	PUB	CAB-CBB-CGB-O2B
28	z7	203	PUB	CAB-CBB-CGB-O1B
28	z7	203	PUB	CAB-CBB-CGB-O2B
28	b8	1005	PUB	CAB-CBB-CGB-O1B
28	b8	1005	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	b8	1006	PUB	CAB-CBB-CGB-O1B
28	b8	1006	PUB	CAB-CBB-CGB-O2B
28	c8	304	PUB	CAB-CBB-CGB-O1B
28	c8	304	PUB	CAB-CBB-CGB-O2B
28	c8	305	PUB	CAB-CBB-CGB-O1B
28	c8	305	PUB	CAB-CBB-CGB-O2B
28	d8	304	PUB	CAB-CBB-CGB-O1B
28	d8	304	PUB	CAB-CBB-CGB-O2B
28	e8	304	PUB	CAB-CBB-CGB-O1B
28	e8	304	PUB	CAB-CBB-CGB-O2B
28	e8	305	PUB	CAB-CBB-CGB-O1B
28	e8	305	PUB	CAB-CBB-CGB-O2B
28	b9	406	PUB	CAB-CBB-CGB-O1B
28	b9	406	PUB	CAB-CBB-CGB-O2B
28	b9	407	PUB	CAB-CBB-CGB-O1B
28	b9	407	PUB	CAB-CBB-CGB-O2B
28	c9	304	PUB	CAB-CBB-CGB-O1B
28	c9	305	PUB	CAB-CBB-CGB-O1B
28	c9	305	PUB	CAB-CBB-CGB-O2B
28	d9	305	PUB	CAB-CBB-CGB-O1B
28	d9	305	PUB	CAB-CBB-CGB-O2B
28	e9	305	PUB	CAB-CBB-CGB-O1B
28	e9	305	PUB	CAB-CBB-CGB-O2B
28	e9	306	PUB	CAB-CBB-CGB-O1B
28	e9	306	PUB	CAB-CBB-CGB-O2B
28	w8	203	PUB	CAB-CBB-CGB-O1B
28	w8	203	PUB	CAB-CBB-CGB-O2B
28	y8	203	PUB	CAB-CBB-CGB-O1B
28	y8	203	PUB	CAB-CBB-CGB-O2B
28	A8	203	PUB	CAB-CBB-CGB-O1B
28	A8	203	PUB	CAB-CBB-CGB-O2B
28	C8	203	PUB	CAB-CBB-CGB-O1B
28	C8	203	PUB	CAB-CBB-CGB-O2B
28	E8	203	PUB	CAB-CBB-CGB-O1B
28	E8	203	PUB	CAB-CBB-CGB-O2B
28	G8	203	PUB	CAB-CBB-CGB-O1B
28	G8	203	PUB	CAB-CBB-CGB-O2B
28	I8	203	PUB	CAB-CBB-CGB-O1B
28	K8	203	PUB	CAB-CBB-CGB-O1B
28	K8	203	PUB	CAB-CBB-CGB-O2B
28	M8	203	PUB	CAB-CBB-CGB-O1B
28	M8	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	O8	203	PUB	CAB-CBB-CGB-O1B
28	O8	203	PUB	CAB-CBB-CGB-O2B
28	Q8	203	PUB	CAB-CBB-CGB-O1B
28	Q8	203	PUB	CAB-CBB-CGB-O2B
28	T8	304	PUB	CAB-CBB-CGB-O1B
28	T8	304	PUB	CAB-CBB-CGB-O2B
28	T8	305	PUB	CAB-CBB-CGB-O1B
28	T8	305	PUB	CAB-CBB-CGB-O2B
28	U8	1005	PUB	CAB-CBB-CGB-O1B
28	U8	1005	PUB	CAB-CBB-CGB-O2B
28	U8	1006	PUB	CAB-CBB-CGB-O1B
28	U8	1006	PUB	CAB-CBB-CGB-O2B
28	n9	202	PUB	CAB-CBB-CGB-O1B
28	n9	202	PUB	CAB-CBB-CGB-O2B
28	p9	203	PUB	CAB-CBB-CGB-O1B
28	p9	203	PUB	CAB-CBB-CGB-O2B
28	r9	203	PUB	CAB-CBB-CGB-O1B
28	r9	203	PUB	CAB-CBB-CGB-O2B
28	t9	203	PUB	CAB-CBB-CGB-O1B
28	t9	203	PUB	CAB-CBB-CGB-O2B
28	v9	203	PUB	CAB-CBB-CGB-O1B
28	v9	203	PUB	CAB-CBB-CGB-O2B
28	x9	203	PUB	CAB-CBB-CGB-O1B
28	x9	203	PUB	CAB-CBB-CGB-O2B
28	z9	203	PUB	CAB-CBB-CGB-O1B
28	z9	203	PUB	CAB-CBB-CGB-O2B
28	B9	203	PUB	CAB-CBB-CGB-O1B
28	B9	203	PUB	CAB-CBB-CGB-O2B
28	D9	203	PUB	CAB-CBB-CGB-O1B
28	D9	203	PUB	CAB-CBB-CGB-O2B
28	F9	203	PUB	CAB-CBB-CGB-O1B
28	F9	203	PUB	CAB-CBB-CGB-O2B
28	H9	203	PUB	CAB-CBB-CGB-O1B
28	H9	203	PUB	CAB-CBB-CGB-O2B
28	J9	203	PUB	CAB-CBB-CGB-O1B
28	J9	203	PUB	CAB-CBB-CGB-O2B
28	L9	203	PUB	CAB-CBB-CGB-O1B
28	L9	203	PUB	CAB-CBB-CGB-O2B
28	N9	203	PUB	CAB-CBB-CGB-O1B
28	N9	203	PUB	CAB-CBB-CGB-O2B
28	P9	203	PUB	CAB-CBB-CGB-O1B
28	P9	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	R9	203	PUB	CAB-CBB-CGB-O1B
28	R9	203	PUB	CAB-CBB-CGB-O2B
28	T9	203	PUB	CAB-CBB-CGB-O1B
28	T9	203	PUB	CAB-CBB-CGB-O2B
28	V9	203	PUB	CAB-CBB-CGB-O1B
28	V9	203	PUB	CAB-CBB-CGB-O2B
28	Y9	304	PUB	CAB-CBB-CGB-O1B
28	Y9	304	PUB	CAB-CBB-CGB-O2B
28	Y9	305	PUB	CAB-CBB-CGB-O1B
28	Y9	305	PUB	CAB-CBB-CGB-O2B
28	Z9	1005	PUB	CAB-CBB-CGB-O1B
28	Z9	1005	PUB	CAB-CBB-CGB-O2B
28	Z9	1006	PUB	CAB-CBB-CGB-O1B
28	Z9	1006	PUB	CAB-CBB-CGB-O2B
28	an	202	PUB	CAB-CBB-CGB-O1B
28	an	202	PUB	CAB-CBB-CGB-O2B
28	ap	203	PUB	CAB-CBB-CGB-O1B
28	ap	203	PUB	CAB-CBB-CGB-O2B
28	ar	203	PUB	CAB-CBB-CGB-O1B
28	ar	203	PUB	CAB-CBB-CGB-O2B
28	at	203	PUB	CAB-CBB-CGB-O1B
28	at	203	PUB	CAB-CBB-CGB-O2B
28	av	203	PUB	CAB-CBB-CGB-O1B
28	av	203	PUB	CAB-CBB-CGB-O2B
28	ax	202	PUB	CAB-CBB-CGB-O1B
28	ax	202	PUB	CAB-CBB-CGB-O2B
28	az	203	PUB	CAB-CBB-CGB-O1B
28	az	203	PUB	CAB-CBB-CGB-O2B
28	aB	203	PUB	CAB-CBB-CGB-O1B
28	aB	203	PUB	CAB-CBB-CGB-O2B
28	aD	203	PUB	CAB-CBB-CGB-O1B
28	aD	203	PUB	CAB-CBB-CGB-O2B
28	aF	203	PUB	CAB-CBB-CGB-O1B
28	aF	203	PUB	CAB-CBB-CGB-O2B
28	aH	203	PUB	CAB-CBB-CGB-O1B
28	aH	203	PUB	CAB-CBB-CGB-O2B
28	aJ	203	PUB	CAB-CBB-CGB-O1B
28	aJ	203	PUB	CAB-CBB-CGB-O2B
28	aL	203	PUB	CAB-CBB-CGB-O1B
28	aL	203	PUB	CAB-CBB-CGB-O2B
28	aN	203	PUB	CAB-CBB-CGB-O1B
28	aN	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	aP	203	PUB	CAB-CBB-CGB-O1B
28	aP	203	PUB	CAB-CBB-CGB-O2B
28	aR	203	PUB	CAB-CBB-CGB-O1B
28	aR	203	PUB	CAB-CBB-CGB-O2B
28	aT	203	PUB	CAB-CBB-CGB-O1B
28	aT	203	PUB	CAB-CBB-CGB-O2B
28	aV	203	PUB	CAB-CBB-CGB-O1B
28	aV	203	PUB	CAB-CBB-CGB-O2B
28	aY	404	PUB	CAB-CBB-CGB-O1B
28	aY	404	PUB	CAB-CBB-CGB-O2B
28	aY	405	PUB	CAB-CBB-CGB-O1B
28	aY	405	PUB	CAB-CBB-CGB-O2B
28	aZ	304	PUB	CAB-CBB-CGB-O1B
28	aZ	304	PUB	CAB-CBB-CGB-O2B
28	aZ	305	PUB	CAB-CBB-CGB-O1B
28	aZ	305	PUB	CAB-CBB-CGB-O2B
28	bn	202	PUB	CAB-CBB-CGB-O1B
28	bn	202	PUB	CAB-CBB-CGB-O2B
28	bo	202	PUB	CAB-CBB-CGB-O1B
28	bp	202	PUB	CAB-CBB-CGB-O1B
28	bq	203	PUB	CAB-CBB-CGB-O1B
28	bq	203	PUB	CAB-CBB-CGB-O2B
28	br	203	PUB	CAB-CBB-CGB-O1B
28	br	203	PUB	CAB-CBB-CGB-O2B
28	bs	1004	PUB	CAB-CBB-CGB-O1B
28	bs	1004	PUB	CAB-CBB-CGB-O2B
28	bz	203	PUB	CAB-CBB-CGB-O1B
28	bz	203	PUB	CAB-CBB-CGB-O2B
28	bB	203	PUB	CAB-CBB-CGB-O1B
28	bB	203	PUB	CAB-CBB-CGB-O2B
28	bD	203	PUB	CAB-CBB-CGB-O1B
28	bD	203	PUB	CAB-CBB-CGB-O2B
28	bF	203	PUB	CAB-CBB-CGB-O1B
28	bF	203	PUB	CAB-CBB-CGB-O2B
28	bH	203	PUB	CAB-CBB-CGB-O1B
28	bH	203	PUB	CAB-CBB-CGB-O2B
28	bJ	203	PUB	CAB-CBB-CGB-O1B
28	bL	203	PUB	CAB-CBB-CGB-O1B
28	bL	203	PUB	CAB-CBB-CGB-O2B
28	bN	203	PUB	CAB-CBB-CGB-O1B
28	bN	203	PUB	CAB-CBB-CGB-O2B
28	bP	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	bP	203	PUB	CAB-CBB-CGB-O2B
28	bR	202	PUB	CAB-CBB-CGB-O1B
28	bR	202	PUB	CAB-CBB-CGB-O2B
28	bT	202	PUB	CAB-CBB-CGB-O1B
28	bT	202	PUB	CAB-CBB-CGB-O2B
28	bV	203	PUB	CAB-CBB-CGB-O1B
28	bV	203	PUB	CAB-CBB-CGB-O2B
28	bY	1005	PUB	CAB-CBB-CGB-O1B
28	bY	1005	PUB	CAB-CBB-CGB-O2B
28	bY	1006	PUB	CAB-CBB-CGB-O1B
28	bY	1006	PUB	CAB-CBB-CGB-O2B
28	bZ	305	PUB	CAB-CBB-CGB-O1B
28	bZ	305	PUB	CAB-CBB-CGB-O2B
28	bZ	306	PUB	CAB-CBB-CGB-O1B
28	bZ	306	PUB	CAB-CBB-CGB-O2B
28	cn	202	PUB	CAB-CBB-CGB-O1B
28	cn	202	PUB	CAB-CBB-CGB-O2B
28	co	202	PUB	CAB-CBB-CGB-O1B
28	co	202	PUB	CAB-CBB-CGB-O2B
28	cp	203	PUB	CAB-CBB-CGB-O1B
28	cp	203	PUB	CAB-CBB-CGB-O2B
28	cq	203	PUB	CAB-CBB-CGB-O1B
28	cq	203	PUB	CAB-CBB-CGB-O2B
28	cr	203	PUB	CAB-CBB-CGB-O1B
28	cr	203	PUB	CAB-CBB-CGB-O2B
28	cs	203	PUB	CAB-CBB-CGB-O1B
28	cs	203	PUB	CAB-CBB-CGB-O2B
28	cz	203	PUB	CAB-CBB-CGB-O1B
28	cz	203	PUB	CAB-CBB-CGB-O2B
28	cB	203	PUB	CAB-CBB-CGB-O1B
28	cB	203	PUB	CAB-CBB-CGB-O2B
28	cE	203	PUB	CAB-CBB-CGB-O1B
28	cE	203	PUB	CAB-CBB-CGB-O2B
28	cF	202	PUB	CAB-CBB-CGB-O1B
28	cF	202	PUB	CAB-CBB-CGB-O2B
28	cH	202	PUB	CAB-CBB-CGB-O1B
28	cH	202	PUB	CAB-CBB-CGB-O2B
28	cJ	203	PUB	CAB-CBB-CGB-O1B
28	cJ	203	PUB	CAB-CBB-CGB-O2B
28	cL	203	PUB	CAB-CBB-CGB-O1B
28	cL	203	PUB	CAB-CBB-CGB-O2B
28	cM	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	cM	203	PUB	CAB-CBB-CGB-O2B
28	cN	202	PUB	CAB-CBB-CGB-O1B
28	cN	202	PUB	CAB-CBB-CGB-O2B
28	cO	203	PUB	CAB-CBB-CGB-O1B
28	cO	203	PUB	CAB-CBB-CGB-O2B
28	cP	203	PUB	CAB-CBB-CGB-O1B
28	cP	203	PUB	CAB-CBB-CGB-O2B
28	cQ	202	PUB	CAB-CBB-CGB-O1B
28	cQ	202	PUB	CAB-CBB-CGB-O2B
28	cR	203	PUB	CAB-CBB-CGB-O1B
28	cY	203	PUB	CAB-CBB-CGB-O1B
28	cY	203	PUB	CAB-CBB-CGB-O2B
28	dd	203	PUB	CAB-CBB-CGB-O1B
28	df	203	PUB	CAB-CBB-CGB-O1B
28	df	203	PUB	CAB-CBB-CGB-O2B
28	dh	203	PUB	CAB-CBB-CGB-O1B
28	dh	203	PUB	CAB-CBB-CGB-O2B
28	di	203	PUB	CAB-CBB-CGB-O1B
28	di	203	PUB	CAB-CBB-CGB-O2B
28	dj	203	PUB	CAB-CBB-CGB-O1B
28	dj	203	PUB	CAB-CBB-CGB-O2B
28	dl	203	PUB	CAB-CBB-CGB-O1B
28	dl	203	PUB	CAB-CBB-CGB-O2B
28	dn	203	PUB	CAB-CBB-CGB-O1B
28	dn	203	PUB	CAB-CBB-CGB-O2B
28	dp	203	PUB	CAB-CBB-CGB-O1B
28	dp	203	PUB	CAB-CBB-CGB-O2B
28	dr	203	PUB	CAB-CBB-CGB-O1B
28	dr	203	PUB	CAB-CBB-CGB-O2B
28	dt	203	PUB	CAB-CBB-CGB-O1B
28	dt	203	PUB	CAB-CBB-CGB-O2B
28	dv	202	PUB	CAB-CBB-CGB-O1B
28	dv	202	PUB	CAB-CBB-CGB-O2B
28	dw	405	PUB	CAB-CBB-CGB-O1B
28	dw	405	PUB	CAB-CBB-CGB-O2B
28	dw	406	PUB	CAB-CBB-CGB-O1B
28	dw	406	PUB	CAB-CBB-CGB-O2B
28	dx	406	PUB	CAB-CBB-CGB-O1B
28	dx	406	PUB	CAB-CBB-CGB-O2B
28	dx	407	PUB	CAB-CBB-CGB-O1B
28	dx	407	PUB	CAB-CBB-CGB-O2B
28	dB	202	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	dB	202	PUB	CAB-CBB-CGB-O2B
28	dD	203	PUB	CAB-CBB-CGB-O1B
28	dD	203	PUB	CAB-CBB-CGB-O2B
28	dF	203	PUB	CAB-CBB-CGB-O1B
28	dF	203	PUB	CAB-CBB-CGB-O2B
28	dH	203	PUB	CAB-CBB-CGB-O1B
28	dH	203	PUB	CAB-CBB-CGB-O2B
28	dK	203	PUB	CAB-CBB-CGB-O1B
28	dK	203	PUB	CAB-CBB-CGB-O2B
28	dL	203	PUB	CAB-CBB-CGB-O1B
28	dL	203	PUB	CAB-CBB-CGB-O2B
28	dN	203	PUB	CAB-CBB-CGB-O1B
28	dN	203	PUB	CAB-CBB-CGB-O2B
28	dP	203	PUB	CAB-CBB-CGB-O1B
28	dP	203	PUB	CAB-CBB-CGB-O2B
28	dR	203	PUB	CAB-CBB-CGB-O1B
28	dR	203	PUB	CAB-CBB-CGB-O2B
28	dT	203	PUB	CAB-CBB-CGB-O1B
28	dT	203	PUB	CAB-CBB-CGB-O2B
28	dV	203	PUB	CAB-CBB-CGB-O1B
28	dX	203	PUB	CAB-CBB-CGB-O1B
28	dY	203	PUB	CAB-CBB-CGB-O1B
28	dY	203	PUB	CAB-CBB-CGB-O2B
28	eb	202	PUB	CAB-CBB-CGB-O1B
28	eb	202	PUB	CAB-CBB-CGB-O2B
28	ec	203	PUB	CAB-CBB-CGB-O1B
28	ec	203	PUB	CAB-CBB-CGB-O2B
28	ee	203	PUB	CAB-CBB-CGB-O1B
28	ee	203	PUB	CAB-CBB-CGB-O2B
28	eg	203	PUB	CAB-CBB-CGB-O1B
28	eg	203	PUB	CAB-CBB-CGB-O2B
28	ei	203	PUB	CAB-CBB-CGB-O1B
28	ei	203	PUB	CAB-CBB-CGB-O2B
28	el	203	PUB	CAB-CBB-CGB-O1B
28	el	203	PUB	CAB-CBB-CGB-O2B
28	en	203	PUB	CAB-CBB-CGB-O1B
28	ep	203	PUB	CAB-CBB-CGB-O1B
28	ep	203	PUB	CAB-CBB-CGB-O2B
28	er	203	PUB	CAB-CBB-CGB-O1B
28	er	203	PUB	CAB-CBB-CGB-O2B
28	et	203	PUB	CAB-CBB-CGB-O1B
28	et	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	ev	203	PUB	CAB-CBB-CGB-O1B
28	ev	203	PUB	CAB-CBB-CGB-O2B
28	ey	1005	PUB	CAB-CBB-CGB-O1B
28	ey	1005	PUB	CAB-CBB-CGB-O2B
28	ey	1006	PUB	CAB-CBB-CGB-O1B
28	ey	1006	PUB	CAB-CBB-CGB-O2B
28	ez	1005	PUB	CAB-CBB-CGB-O1B
28	ez	1005	PUB	CAB-CBB-CGB-O2B
28	ez	1006	PUB	CAB-CBB-CGB-O1B
28	ez	1006	PUB	CAB-CBB-CGB-O2B
28	eB	204	PUB	CAB-CBB-CGB-O1B
28	eB	204	PUB	CAB-CBB-CGB-O2B
28	eD	203	PUB	CAB-CBB-CGB-O1B
28	eD	203	PUB	CAB-CBB-CGB-O2B
28	eF	203	PUB	CAB-CBB-CGB-O1B
28	eF	203	PUB	CAB-CBB-CGB-O2B
28	eH	203	PUB	CAB-CBB-CGB-O1B
28	eH	203	PUB	CAB-CBB-CGB-O2B
28	eJ	203	PUB	CAB-CBB-CGB-O1B
28	eJ	203	PUB	CAB-CBB-CGB-O2B
28	eL	203	PUB	CAB-CBB-CGB-O1B
28	eL	203	PUB	CAB-CBB-CGB-O2B
28	eN	203	PUB	CAB-CBB-CGB-O1B
28	eP	204	PUB	CAB-CBB-CGB-O1B
28	eP	204	PUB	CAB-CBB-CGB-O2B
28	eR	203	PUB	CAB-CBB-CGB-O1B
28	eR	203	PUB	CAB-CBB-CGB-O2B
28	eV	203	PUB	CAB-CBB-CGB-O1B
28	eV	203	PUB	CAB-CBB-CGB-O2B
28	eX	202	PUB	CAB-CBB-CGB-O1B
28	eX	202	PUB	CAB-CBB-CGB-O2B
28	eY	404	PUB	CAB-CBB-CGB-O1B
28	eY	404	PUB	CAB-CBB-CGB-O2B
28	eY	405	PUB	CAB-CBB-CGB-O1B
28	eY	405	PUB	CAB-CBB-CGB-O2B
28	eZ	403	PUB	CAB-CBB-CGB-O1B
28	eZ	403	PUB	CAB-CBB-CGB-O2B
28	eZ	404	PUB	CAB-CBB-CGB-O1B
28	eZ	404	PUB	CAB-CBB-CGB-O2B
28	lb	203	PUB	CAB-CBB-CGB-O1B
28	lb	203	PUB	CAB-CBB-CGB-O2B
28	ld	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	ld	203	PUB	CAB-CBB-CGB-O2B
28	lf	203	PUB	CAB-CBB-CGB-O1B
28	lf	203	PUB	CAB-CBB-CGB-O2B
28	lh	203	PUB	CAB-CBB-CGB-O1B
28	lh	203	PUB	CAB-CBB-CGB-O2B
28	lj	202	PUB	CAB-CBB-CGB-O1B
28	lj	202	PUB	CAB-CBB-CGB-O2B
28	ll	203	PUB	CAB-CBB-CGB-O1B
28	ll	203	PUB	CAB-CBB-CGB-O2B
28	ln	203	PUB	CAB-CBB-CGB-O1B
28	ln	203	PUB	CAB-CBB-CGB-O2B
28	lp	203	PUB	CAB-CBB-CGB-O1B
28	lp	203	PUB	CAB-CBB-CGB-O2B
28	lr	203	PUB	CAB-CBB-CGB-O1B
28	lr	203	PUB	CAB-CBB-CGB-O2B
28	lt	203	PUB	CAB-CBB-CGB-O1B
28	lt	203	PUB	CAB-CBB-CGB-O2B
28	lv	202	PUB	CAB-CBB-CGB-O1B
28	lv	202	PUB	CAB-CBB-CGB-O2B
28	lx	201	PUB	CAB-CBB-CGB-O1B
28	lx	201	PUB	CAB-CBB-CGB-O2B
28	ly	405	PUB	CAB-CBB-CGB-O1B
28	ly	405	PUB	CAB-CBB-CGB-O2B
28	ly	406	PUB	CAB-CBB-CGB-O1B
28	ly	406	PUB	CAB-CBB-CGB-O2B
28	lz	404	PUB	CAB-CBB-CGB-O1B
28	lz	404	PUB	CAB-CBB-CGB-O2B
28	lz	405	PUB	CAB-CBB-CGB-O1B
28	lz	405	PUB	CAB-CBB-CGB-O2B
28	fa	202	PUB	CAB-CBB-CGB-O1B
28	fa	202	PUB	CAB-CBB-CGB-O2B
28	fc	203	PUB	CAB-CBB-CGB-O1B
28	fc	203	PUB	CAB-CBB-CGB-O2B
28	ff	203	PUB	CAB-CBB-CGB-O1B
28	ff	203	PUB	CAB-CBB-CGB-O2B
28	fi	203	PUB	CAB-CBB-CGB-O1B
28	fj	203	PUB	CAB-CBB-CGB-O1B
28	fj	203	PUB	CAB-CBB-CGB-O2B
28	fm	203	PUB	CAB-CBB-CGB-O1B
28	fm	203	PUB	CAB-CBB-CGB-O2B
28	fo	203	PUB	CAB-CBB-CGB-O1B
28	fo	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	fq	203	PUB	CAB-CBB-CGB-O1B
28	fq	203	PUB	CAB-CBB-CGB-O2B
28	fs	203	PUB	CAB-CBB-CGB-O1B
28	fs	203	PUB	CAB-CBB-CGB-O2B
28	fu	202	PUB	CAB-CBB-CGB-O1B
28	fu	202	PUB	CAB-CBB-CGB-O2B
28	fw	203	PUB	CAB-CBB-CGB-O1B
28	fw	203	PUB	CAB-CBB-CGB-O2B
28	fy	202	PUB	CAB-CBB-CGB-O1B
28	fy	202	PUB	CAB-CBB-CGB-O2B
28	ga	203	PUB	CAB-CBB-CGB-O1B
28	ga	203	PUB	CAB-CBB-CGB-O2B
28	gd	202	PUB	CAB-CBB-CGB-O1B
28	gd	202	PUB	CAB-CBB-CGB-O2B
28	ge	203	PUB	CAB-CBB-CGB-O1B
28	ge	203	PUB	CAB-CBB-CGB-O2B
28	gg	203	PUB	CAB-CBB-CGB-O1B
28	gg	203	PUB	CAB-CBB-CGB-O2B
28	gi	203	PUB	CAB-CBB-CGB-O1B
28	gk	203	PUB	CAB-CBB-CGB-O1B
28	gk	203	PUB	CAB-CBB-CGB-O2B
28	gn	203	PUB	CAB-CBB-CGB-O1B
28	gn	203	PUB	CAB-CBB-CGB-O2B
28	gp	203	PUB	CAB-CBB-CGB-O1B
28	gp	203	PUB	CAB-CBB-CGB-O2B
28	gr	202	PUB	CAB-CBB-CGB-O1B
28	gr	202	PUB	CAB-CBB-CGB-O2B
28	gt	203	PUB	CAB-CBB-CGB-O1B
28	gt	203	PUB	CAB-CBB-CGB-O2B
28	gv	203	PUB	CAB-CBB-CGB-O1B
28	gv	203	PUB	CAB-CBB-CGB-O2B
28	gx	203	PUB	CAB-CBB-CGB-O1B
28	gx	203	PUB	CAB-CBB-CGB-O2B
28	gy	305	PUB	CAB-CBB-CGB-O1B
28	gy	305	PUB	CAB-CBB-CGB-O2B
28	gy	306	PUB	CAB-CBB-CGB-O1B
28	gy	306	PUB	CAB-CBB-CGB-O2B
28	gz	305	PUB	CAB-CBB-CGB-O1B
28	gz	305	PUB	CAB-CBB-CGB-O2B
28	gz	306	PUB	CAB-CBB-CGB-O1B
28	gz	306	PUB	CAB-CBB-CGB-O2B
28	hB	203	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	hB	203	PUB	CAB-CBB-CGB-O2B
28	hD	203	PUB	CAB-CBB-CGB-O1B
28	hD	203	PUB	CAB-CBB-CGB-O2B
28	hG	202	PUB	CAB-CBB-CGB-O1B
28	hG	202	PUB	CAB-CBB-CGB-O2B
28	hH	203	PUB	CAB-CBB-CGB-O1B
28	hH	203	PUB	CAB-CBB-CGB-O2B
28	hJ	203	PUB	CAB-CBB-CGB-O1B
28	hJ	203	PUB	CAB-CBB-CGB-O2B
28	hL	203	PUB	CAB-CBB-CGB-O1B
28	hL	203	PUB	CAB-CBB-CGB-O2B
28	hN	203	PUB	CAB-CBB-CGB-O1B
28	hN	203	PUB	CAB-CBB-CGB-O2B
28	hP	203	PUB	CAB-CBB-CGB-O1B
28	hP	203	PUB	CAB-CBB-CGB-O2B
28	hR	203	PUB	CAB-CBB-CGB-O1B
28	hR	203	PUB	CAB-CBB-CGB-O2B
28	hT	203	PUB	CAB-CBB-CGB-O1B
28	hT	203	PUB	CAB-CBB-CGB-O2B
28	hV	203	PUB	CAB-CBB-CGB-O1B
28	hV	203	PUB	CAB-CBB-CGB-O2B
28	hX	203	PUB	CAB-CBB-CGB-O1B
28	hX	203	PUB	CAB-CBB-CGB-O2B
28	hY	405	PUB	CAB-CBB-CGB-O1B
28	hY	405	PUB	CAB-CBB-CGB-O2B
28	hY	406	PUB	CAB-CBB-CGB-O1B
28	hY	406	PUB	CAB-CBB-CGB-O2B
28	hZ	404	PUB	CAB-CBB-CGB-O1B
28	hZ	404	PUB	CAB-CBB-CGB-O2B
28	hZ	405	PUB	CAB-CBB-CGB-O1B
28	hZ	405	PUB	CAB-CBB-CGB-O2B
28	iC	1003	PUB	CAB-CBB-CGB-O1B
28	iC	1003	PUB	CAB-CBB-CGB-O2B
28	iD	1003	PUB	CAB-CBB-CGB-O1B
28	iD	1003	PUB	CAB-CBB-CGB-O2B
28	iE	1003	PUB	CAB-CBB-CGB-O1B
28	iE	1003	PUB	CAB-CBB-CGB-O2B
28	iF	1003	PUB	CAB-CBB-CGB-O1B
28	iF	1003	PUB	CAB-CBB-CGB-O2B
28	iG	1002	PUB	CAB-CBB-CGB-O1B
28	iG	1002	PUB	CAB-CBB-CGB-O2B
28	iH	1002	PUB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
28	iH	1002	PUB	CAB-CBB-CGB-O2B
28	jI	1003	PUB	CAB-CBB-CGB-O1B
28	jI	1003	PUB	CAB-CBB-CGB-O2B
28	jJ	1003	PUB	CAB-CBB-CGB-O1B
28	jJ	1003	PUB	CAB-CBB-CGB-O2B
28	jK	1003	PUB	CAB-CBB-CGB-O1B
28	jK	1003	PUB	CAB-CBB-CGB-O2B
28	jL	1003	PUB	CAB-CBB-CGB-O2B
28	jM	1003	PUB	CAB-CBB-CGB-O1B
28	jM	1003	PUB	CAB-CBB-CGB-O2B
28	jN	1003	PUB	CAB-CBB-CGB-O1B
28	jN	1003	PUB	CAB-CBB-CGB-O2B
28	jO	1003	PUB	CAB-CBB-CGB-O1B
28	jO	1003	PUB	CAB-CBB-CGB-O2B
28	jP	1003	PUB	CAB-CBB-CGB-O1B
28	jP	1003	PUB	CAB-CBB-CGB-O2B
28	kQ	1003	PUB	CAB-CBB-CGB-O1B
28	kQ	1003	PUB	CAB-CBB-CGB-O2B
28	kR	1003	PUB	CAB-CBB-CGB-O1B
28	kR	1003	PUB	CAB-CBB-CGB-O2B
28	kS	1003	PUB	CAB-CBB-CGB-O1B
28	kS	1003	PUB	CAB-CBB-CGB-O2B
28	kT	1003	PUB	CAB-CBB-CGB-O1B
28	kT	1003	PUB	CAB-CBB-CGB-O2B
28	kU	1003	PUB	CAB-CBB-CGB-O1B
28	kU	1003	PUB	CAB-CBB-CGB-O2B
28	kV	1003	PUB	CAB-CBB-CGB-O1B
28	kV	1003	PUB	CAB-CBB-CGB-O2B
28	kW	1003	PUB	CAB-CBB-CGB-O1B
28	kW	1003	PUB	CAB-CBB-CGB-O2B
28	kX	1003	PUB	CAB-CBB-CGB-O1B
28	kX	1003	PUB	CAB-CBB-CGB-O2B
28	N2	203	PUB	CAB-CBB-CGB-O2B
28	d3	303	PUB	CAB-CBB-CGB-O2B
28	34	1006	PUB	CAB-CBB-CGB-O1B
28	r4	202	PUB	CAB-CBB-CGB-O2B
28	r5	203	PUB	CAB-CBB-CGB-O2B
28	B6	203	PUB	CAB-CBB-CGB-O2B
28	J6	203	PUB	CAB-CBB-CGB-O2B
28	L6	202	PUB	CAB-CBB-CGB-O2B
28	N6	203	PUB	CAB-CBB-CGB-O2B
28	v6	203	PUB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
28	N7	203	PUB	CAB-CBB-CGB-O2B
28	P7	203	PUB	CAB-CBB-CGB-O2B
28	t7	203	PUB	CAB-CBB-CGB-O2B
28	c9	304	PUB	CAB-CBB-CGB-O2B
28	I8	203	PUB	CAB-CBB-CGB-O2B
28	bo	202	PUB	CAB-CBB-CGB-O2B
28	bp	202	PUB	CAB-CBB-CGB-O2B
28	bJ	203	PUB	CAB-CBB-CGB-O2B
28	cR	203	PUB	CAB-CBB-CGB-O2B
28	dd	203	PUB	CAB-CBB-CGB-O2B
28	dV	203	PUB	CAB-CBB-CGB-O2B
28	dX	203	PUB	CAB-CBB-CGB-O2B
28	en	203	PUB	CAB-CBB-CGB-O2B
28	eN	203	PUB	CAB-CBB-CGB-O2B
28	eT	203	PUB	CAB-CBB-CGB-O1B
28	eT	203	PUB	CAB-CBB-CGB-O2B
28	fi	203	PUB	CAB-CBB-CGB-O2B
28	gi	203	PUB	CAB-CBB-CGB-O2B
28	jL	1003	PUB	CAB-CBB-CGB-O1B
29	D2	303	PVN	C51-C52-C53-O55
29	d3	302	PVN	C51-C52-C53-O55
29	44	303	PVN	C51-C52-C53-O54
29	Z5	304	PVN	C51-C52-C53-O54
27	J1	201	CYC	CAD-CBD-CGD-O1D
27	M1	1001	CYC	CAD-CBD-CGD-O1D
27	Y1	201	CYC	CAD-CBD-CGD-O1D
27	t1	201	CYC	CAD-CBD-CGD-O1D
27	z1	201	CYC	CAD-CBD-CGD-O1D
27	a2	901	CYC	CAD-CBD-CGD-O1D
27	a2	902	CYC	CAD-CBD-CGD-O1D
27	b2	1001	CYC	CAD-CBD-CGD-O1D
26	f2	201	PEB	CAB-CBB-CGB-O1B
26	h2	201	PEB	CAB-CBB-CGB-O1B
26	q2	201	PEB	CAB-CBB-CGB-O1B
26	t2	201	PEB	CAB-CBB-CGB-O1B
26	v2	202	PEB	CAB-CBB-CGB-O1B
26	x2	201	PEB	CAB-CBB-CGB-O1B
26	B2	501	PEB	CAB-CBB-CGB-O1B
26	D2	301	PEB	CAB-CBB-CGB-O1B
26	E2	1001	PEB	CAB-CBB-CGB-O1B
26	G2	202	PEB	CAB-CBB-CGB-O1B
26	N2	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	S2	201	PEB	CAB-CBB-CGB-O1B
26	X2	201	PEB	CAB-CBB-CGB-O1B
26	Y2	202	PEB	CAB-CBB-CGB-O1B
26	Z2	201	PEB	CAB-CBB-CGB-O1B
26	O3	1001	PEB	CAB-CBB-CGB-O1B
26	S3	201	PEB	CAB-CBB-CGB-O1B
26	X3	201	PEB	CAB-CBB-CGB-O1B
26	a3	1001	PEB	CAB-CBB-CGB-O1B
26	l3	201	PEB	CAB-CBB-CGB-O1B
26	u3	201	PEB	CAB-CBB-CGB-O1B
26	x3	201	PEB	CAB-CBB-CGB-O1B
26	B4	201	PEB	CAB-CBB-CGB-O1B
26	F4	202	PEB	CAB-CBB-CGB-O1B
26	G4	202	PEB	CAB-CBB-CGB-O1B
26	H4	201	PEB	CAB-CBB-CGB-O1B
26	M4	202	PEB	CAB-CBB-CGB-O1B
26	R4	202	PEB	CAB-CBB-CGB-O1B
26	S4	201	PEB	CAB-CBB-CGB-O1B
26	X4	201	PEB	CAB-CBB-CGB-O1B
26	j4	201	PEB	CAB-CBB-CGB-O1B
26	o4	201	PEB	CAB-CBB-CGB-O1B
26	C5	201	PEB	CAB-CBB-CGB-O1B
26	D5	201	PEB	CAB-CBB-CGB-O1B
26	K5	1001	PEB	CAB-CBB-CGB-O1B
26	T5	201	PEB	CAB-CBB-CGB-O1B
26	Z5	303	PEB	CAB-CBB-CGB-O1B
26	c5	202	PEB	CAB-CBB-CGB-O1B
26	j5	201	PEB	CAB-CBB-CGB-O1B
26	j5	202	PEB	CAB-CBB-CGB-O1B
26	n5	201	PEB	CAB-CBB-CGB-O1B
26	o5	201	PEB	CAB-CBB-CGB-O1B
26	q5	201	PEB	CAB-CBB-CGB-O1B
26	w5	201	PEB	CAB-CBB-CGB-O1B
26	x5	201	PEB	CAB-CBB-CGB-O1B
26	f8	202	PEB	CAB-CBB-CGB-O1B
26	j8	202	PEB	CAB-CBB-CGB-O1B
26	k8	202	PEB	CAB-CBB-CGB-O1B
26	l8	201	PEB	CAB-CBB-CGB-O1B
26	m8	202	PEB	CAB-CBB-CGB-O1B
26	A6	1002	PEB	CAB-CBB-CGB-O1B
26	C6	202	PEB	CAB-CBB-CGB-O1B
26	E6	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	K6	201	PEB	CAB-CBB-CGB-O1B
26	L6	201	PEB	CAB-CBB-CGB-O1B
26	M6	1002	PEB	CAB-CBB-CGB-O1B
26	S6	202	PEB	CAB-CBB-CGB-O1B
26	V6	201	PEB	CAB-CBB-CGB-O1B
26	W6	201	PEB	CAB-CBB-CGB-O1B
26	g6	201	PEB	CAB-CBB-CGB-O1B
26	g6	202	PEB	CAB-CBB-CGB-O1B
26	j6	201	PEB	CAB-CBB-CGB-O1B
26	k6	1002	PEB	CAB-CBB-CGB-O1B
26	o6	201	PEB	CAB-CBB-CGB-O1B
26	p6	201	PEB	CAB-CBB-CGB-O1B
26	r6	201	PEB	CAB-CBB-CGB-O1B
26	r6	202	PEB	CAB-CBB-CGB-O1B
26	t6	202	PEB	CAB-CBB-CGB-O1B
26	y6	201	PEB	CAB-CBB-CGB-O1B
26	p8	201	PEB	CAB-CBB-CGB-O1B
26	t8	201	PEB	CAB-CBB-CGB-O1B
26	C7	201	PEB	CAB-CBB-CGB-O1B
26	G7	201	PEB	CAB-CBB-CGB-O1B
26	H7	201	PEB	CAB-CBB-CGB-O1B
26	d7	201	PEB	CAB-CBB-CGB-O1B
26	f7	201	PEB	CAB-CBB-CGB-O1B
26	h7	201	PEB	CAB-CBB-CGB-O1B
26	n7	201	PEB	CAB-CBB-CGB-O1B
26	t7	201	PEB	CAB-CBB-CGB-O1B
26	a8	601	PEB	CAB-CBB-CGB-O1B
26	b8	1001	PEB	CAB-CBB-CGB-O1B
26	c8	302	PEB	CAB-CBB-CGB-O1B
26	a9	602	PEB	CAB-CBB-CGB-O1B
26	c9	301	PEB	CAB-CBB-CGB-O1B
26	z8	201	PEB	CAB-CBB-CGB-O1B
26	z8	202	PEB	CAB-CBB-CGB-O1B
26	B8	202	PEB	CAB-CBB-CGB-O1B
26	G8	202	PEB	CAB-CBB-CGB-O1B
26	H8	201	PEB	CAB-CBB-CGB-O1B
26	K8	201	PEB	CAB-CBB-CGB-O1B
26	M8	201	PEB	CAB-CBB-CGB-O1B
26	W8	201	PEB	CAB-CBB-CGB-O1B
26	Y8	201	PEB	CAB-CBB-CGB-O1B
26	f9	201	PEB	CAB-CBB-CGB-O1B
26	j9	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	t9	202	PEB	CAB-CBB-CGB-O1B
26	u9	202	PEB	CAB-CBB-CGB-O1B
26	A9	201	PEB	CAB-CBB-CGB-O1B
26	H9	201	PEB	CAB-CBB-CGB-O1B
26	M9	201	PEB	CAB-CBB-CGB-O1B
26	O9	201	PEB	CAB-CBB-CGB-O1B
26	U9	201	PEB	CAB-CBB-CGB-O1B
26	X9	401	PEB	CAB-CBB-CGB-O1B
26	ah	201	PEB	CAB-CBB-CGB-O1B
26	as	201	PEB	CAB-CBB-CGB-O1B
26	au	201	PEB	CAB-CBB-CGB-O1B
26	ay	1001	PEB	CAB-CBB-CGB-O1B
26	aB	202	PEB	CAB-CBB-CGB-O1B
26	aE	202	PEB	CAB-CBB-CGB-O1B
26	aF	204	PEB	CAB-CBB-CGB-O1B
26	aK	1001	PEB	CAB-CBB-CGB-O1B
26	aL	201	PEB	CAB-CBB-CGB-O1B
26	aN	204	PEB	CAB-CBB-CGB-O1B
26	aU	202	PEB	CAB-CBB-CGB-O1B
26	aV	202	PEB	CAB-CBB-CGB-O1B
26	aX	401	PEB	CAB-CBB-CGB-O1B
26	aY	401	PEB	CAB-CBB-CGB-O1B
26	aZ	302	PEB	CAB-CBB-CGB-O1B
26	bf	201	PEB	CAB-CBB-CGB-O1B
26	bm	1001	PEB	CAB-CBB-CGB-O1B
26	br	201	PEB	CAB-CBB-CGB-O1B
26	bw	202	PEB	CAB-CBB-CGB-O1B
26	bx	202	PEB	CAB-CBB-CGB-O1B
26	bB	201	PEB	CAB-CBB-CGB-O1B
26	bC	201	PEB	CAB-CBB-CGB-O1B
26	bJ	201	PEB	CAB-CBB-CGB-O1B
26	bN	201	PEB	CAB-CBB-CGB-O1B
26	ce	201	PEB	CAB-CBB-CGB-O1B
26	cg	201	PEB	CAB-CBB-CGB-O1B
26	cr	201	PEB	CAB-CBB-CGB-O1B
26	cs	201	PEB	CAB-CBB-CGB-O1B
26	cu	201	PEB	CAB-CBB-CGB-O1B
26	cD	201	PEB	CAB-CBB-CGB-O1B
26	cI	201	PEB	CAB-CBB-CGB-O1B
26	cM	202	PEB	CAB-CBB-CGB-O1B
26	cO	202	PEB	CAB-CBB-CGB-O1B
26	cP	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	cQ	201	PEB	CAB-CBB-CGB-O1B
26	cR	201	PEB	CAB-CBB-CGB-O1B
26	cV	201	PEB	CAB-CBB-CGB-O1B
26	cZ	201	PEB	CAB-CBB-CGB-O1B
26	da	1001	PEB	CAB-CBB-CGB-O1B
26	dn	202	PEB	CAB-CBB-CGB-O1B
26	dr	201	PEB	CAB-CBB-CGB-O1B
26	dr	202	PEB	CAB-CBB-CGB-O1B
26	ds	201	PEB	CAB-CBB-CGB-O1B
26	dw	401	PEB	CAB-CBB-CGB-O1B
26	dx	403	PEB	CAB-CBB-CGB-O1B
26	dB	201	PEB	CAB-CBB-CGB-O1B
26	dD	201	PEB	CAB-CBB-CGB-O1B
26	dG	202	PEB	CAB-CBB-CGB-O1B
26	dH	201	PEB	CAB-CBB-CGB-O1B
26	dJ	201	PEB	CAB-CBB-CGB-O1B
26	dK	201	PEB	CAB-CBB-CGB-O1B
26	dM	1002	PEB	CAB-CBB-CGB-O1B
26	dP	201	PEB	CAB-CBB-CGB-O1B
26	dV	201	PEB	CAB-CBB-CGB-O1B
26	dZ	1001	PEB	CAB-CBB-CGB-O1B
26	ea	201	PEB	CAB-CBB-CGB-O1B
26	ej	202	PEB	CAB-CBB-CGB-O1B
26	ew	301	PEB	CAB-CBB-CGB-O1B
26	eA	1001	PEB	CAB-CBB-CGB-O1B
26	eC	202	PEB	CAB-CBB-CGB-O1B
26	eD	201	PEB	CAB-CBB-CGB-O1B
26	eH	201	PEB	CAB-CBB-CGB-O1B
26	eI	202	PEB	CAB-CBB-CGB-O1B
26	eR	201	PEB	CAB-CBB-CGB-O1B
26	eZ	401	PEB	CAB-CBB-CGB-O1B
26	le	201	PEB	CAB-CBB-CGB-O1B
26	ll	201	PEB	CAB-CBB-CGB-O1B
26	ly	401	PEB	CAB-CBB-CGB-O1B
26	ly	403	PEB	CAB-CBB-CGB-O1B
26	lz	402	PEB	CAB-CBB-CGB-O1B
26	fm	201	PEB	CAB-CBB-CGB-O1B
26	fn	1001	PEB	CAB-CBB-CGB-O1B
26	ft	201	PEB	CAB-CBB-CGB-O1B
26	gc	201	PEB	CAB-CBB-CGB-O1B
26	gk	201	PEB	CAB-CBB-CGB-O1B
26	gp	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	gs	201	PEB	CAB-CBB-CGB-O1B
26	gv	201	PEB	CAB-CBB-CGB-O1B
26	gx	201	PEB	CAB-CBB-CGB-O1B
26	hF	201	PEB	CAB-CBB-CGB-O1B
26	hH	201	PEB	CAB-CBB-CGB-O1B
26	hN	201	PEB	CAB-CBB-CGB-O1B
26	hO	201	PEB	CAB-CBB-CGB-O1B
26	hP	201	PEB	CAB-CBB-CGB-O1B
26	hY	401	PEB	CAB-CBB-CGB-O1B
26	iE	1001	PEB	CAB-CBB-CGB-O1B
26	iH	1001	PEB	CAB-CBB-CGB-O1B
26	jM	1001	PEB	CAB-CBB-CGB-O1B
26	jO	1001	PEB	CAB-CBB-CGB-O1B
26	kS	1001	PEB	CAB-CBB-CGB-O1B
26	kW	1001	PEB	CAB-CBB-CGB-O1B
27	H1	201	CYC	CAD-CBD-CGD-O1D
27	S1	201	CYC	CAD-CBD-CGD-O1D
27	S1	202	CYC	CAD-CBD-CGD-O1D
27	c1	201	CYC	CAD-CBD-CGD-O1D
27	h1	201	CYC	CAD-CBD-CGD-O1D
27	j1	201	CYC	CAD-CBD-CGD-O1D
27	p1	201	CYC	CAD-CBD-CGD-O1D
27	r1	201	CYC	CAD-CBD-CGD-O1D
27	v1	201	CYC	CAD-CBD-CGD-O1D
29	aZ	303	PVN	C61-C62-C63-O65
29	bZ	304	PVN	C61-C62-C63-O65
29	aY	403	PVN	C2-C3-C31-C32
29	bY	1004	PVN	C2-C3-C31-C32
26	g2	201	PEB	CAB-CBB-CGB-O1B
26	i2	201	PEB	CAB-CBB-CGB-O1B
26	k2	201	PEB	CAB-CBB-CGB-O1B
26	o2	1002	PEB	CAB-CBB-CGB-O1B
26	r2	201	PEB	CAB-CBB-CGB-O1B
26	M2	201	PEB	CAB-CBB-CGB-O1B
26	O2	201	PEB	CAB-CBB-CGB-O1B
26	R2	202	PEB	CAB-CBB-CGB-O1B
26	C3	1001	PEB	CAB-CBB-CGB-O1B
26	F3	201	PEB	CAB-CBB-CGB-O1B
26	G3	201	PEB	CAB-CBB-CGB-O1B
26	L3	201	PEB	CAB-CBB-CGB-O1B
26	N3	201	PEB	CAB-CBB-CGB-O1B
26	Q3	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	V3	201	PEB	CAB-CBB-CGB-O1B
26	e3	1001	PEB	CAB-CBB-CGB-O1B
26	f3	201	PEB	CAB-CBB-CGB-O1B
26	g3	201	PEB	CAB-CBB-CGB-O1B
26	i3	201	PEB	CAB-CBB-CGB-O1B
26	k3	201	PEB	CAB-CBB-CGB-O1B
26	m3	201	PEB	CAB-CBB-CGB-O1B
26	o3	201	PEB	CAB-CBB-CGB-O1B
26	t3	201	PEB	CAB-CBB-CGB-O1B
26	y3	201	PEB	CAB-CBB-CGB-O1B
26	A4	201	PEB	CAB-CBB-CGB-O1B
26	E4	202	PEB	CAB-CBB-CGB-O1B
26	H4	202	PEB	CAB-CBB-CGB-O1B
26	I4	202	PEB	CAB-CBB-CGB-O1B
26	J4	202	PEB	CAB-CBB-CGB-O1B
26	L4	201	PEB	CAB-CBB-CGB-O1B
26	O4	1001	PEB	CAB-CBB-CGB-O1B
26	U4	202	PEB	CAB-CBB-CGB-O1B
26	X4	202	PEB	CAB-CBB-CGB-O1B
26	Y4	202	PEB	CAB-CBB-CGB-O1B
26	34	1007	PEB	CAB-CBB-CGB-O1B
26	a4	201	PEB	CAB-CBB-CGB-O1B
26	f4	201	PEB	CAB-CBB-CGB-O1B
26	g4	201	PEB	CAB-CBB-CGB-O1B
26	i4	201	PEB	CAB-CBB-CGB-O1B
26	l4	201	PEB	CAB-CBB-CGB-O1B
26	m4	1001	PEB	CAB-CBB-CGB-O1B
26	q4	201	PEB	CAB-CBB-CGB-O1B
26	q4	202	PEB	CAB-CBB-CGB-O1B
26	t4	202	PEB	CAB-CBB-CGB-O1B
26	w4	201	PEB	CAB-CBB-CGB-O1B
26	z4	201	PEB	CAB-CBB-CGB-O1B
26	z4	202	PEB	CAB-CBB-CGB-O1B
26	A5	201	PEB	CAB-CBB-CGB-O1B
26	B5	201	PEB	CAB-CBB-CGB-O1B
26	E5	201	PEB	CAB-CBB-CGB-O1B
26	H5	201	PEB	CAB-CBB-CGB-O1B
26	I5	201	PEB	CAB-CBB-CGB-O1B
26	L5	201	PEB	CAB-CBB-CGB-O1B
26	N5	201	PEB	CAB-CBB-CGB-O1B
26	X5	401	PEB	CAB-CBB-CGB-O1B
26	Y5	1001	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	b5	1001	PEB	CAB-CBB-CGB-O1B
26	h5	201	PEB	CAB-CBB-CGB-O1B
26	y5	1001	PEB	CAB-CBB-CGB-O1B
26	z5	201	PEB	CAB-CBB-CGB-O1B
26	j8	201	PEB	CAB-CBB-CGB-O1B
26	k8	203	PEB	CAB-CBB-CGB-O1B
26	l8	202	PEB	CAB-CBB-CGB-O1B
26	m8	201	PEB	CAB-CBB-CGB-O1B
26	E6	201	PEB	CAB-CBB-CGB-O1B
26	I6	202	PEB	CAB-CBB-CGB-O1B
26	O6	202	PEB	CAB-CBB-CGB-O1B
26	P6	201	PEB	CAB-CBB-CGB-O1B
26	a6	201	PEB	CAB-CBB-CGB-O1B
26	e6	201	PEB	CAB-CBB-CGB-O1B
26	h6	201	PEB	CAB-CBB-CGB-O1B
26	h6	202	PEB	CAB-CBB-CGB-O1B
26	l6	201	PEB	CAB-CBB-CGB-O1B
26	m6	202	PEB	CAB-CBB-CGB-O1B
26	q6	202	PEB	CAB-CBB-CGB-O1B
26	u6	201	PEB	CAB-CBB-CGB-O1B
26	v6	201	PEB	CAB-CBB-CGB-O1B
26	v6	202	PEB	CAB-CBB-CGB-O1B
26	x6	201	PEB	CAB-CBB-CGB-O1B
26	x6	202	PEB	CAB-CBB-CGB-O1B
26	s8	201	PEB	CAB-CBB-CGB-O1B
26	I7	201	PEB	CAB-CBB-CGB-O1B
26	S7	201	PEB	CAB-CBB-CGB-O1B
26	U7	201	PEB	CAB-CBB-CGB-O1B
26	V7	201	PEB	CAB-CBB-CGB-O1B
26	b7	201	PEB	CAB-CBB-CGB-O1B
26	c7	201	PEB	CAB-CBB-CGB-O1B
26	e7	201	PEB	CAB-CBB-CGB-O1B
26	g7	201	PEB	CAB-CBB-CGB-O1B
26	m7	201	PEB	CAB-CBB-CGB-O1B
26	r7	201	PEB	CAB-CBB-CGB-O1B
26	s7	201	PEB	CAB-CBB-CGB-O1B
26	u7	201	PEB	CAB-CBB-CGB-O1B
26	y7	201	PEB	CAB-CBB-CGB-O1B
26	b8	1003	PEB	CAB-CBB-CGB-O1B
26	d8	302	PEB	CAB-CBB-CGB-O1B
26	d9	301	PEB	CAB-CBB-CGB-O1B
26	v8	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	v8	202	PEB	CAB-CBB-CGB-O1B
26	x8	201	PEB	CAB-CBB-CGB-O1B
26	C8	201	PEB	CAB-CBB-CGB-O1B
26	D8	202	PEB	CAB-CBB-CGB-O1B
26	E8	201	PEB	CAB-CBB-CGB-O1B
26	G8	201	PEB	CAB-CBB-CGB-O1B
26	H8	202	PEB	CAB-CBB-CGB-O1B
26	I8	202	PEB	CAB-CBB-CGB-O1B
26	J8	201	PEB	CAB-CBB-CGB-O1B
26	P8	201	PEB	CAB-CBB-CGB-O1B
26	T8	302	PEB	CAB-CBB-CGB-O1B
26	U8	1001	PEB	CAB-CBB-CGB-O1B
26	U8	1002	PEB	CAB-CBB-CGB-O1B
26	U8	1003	PEB	CAB-CBB-CGB-O1B
26	W8	202	PEB	CAB-CBB-CGB-O1B
26	Y8	202	PEB	CAB-CBB-CGB-O1B
26	g9	201	PEB	CAB-CBB-CGB-O1B
26	h9	201	PEB	CAB-CBB-CGB-O1B
26	h9	202	PEB	CAB-CBB-CGB-O1B
26	o9	201	PEB	CAB-CBB-CGB-O1B
26	p9	201	PEB	CAB-CBB-CGB-O1B
26	q9	201	PEB	CAB-CBB-CGB-O1B
26	q9	202	PEB	CAB-CBB-CGB-O1B
26	r9	202	PEB	CAB-CBB-CGB-O1B
26	s9	202	PEB	CAB-CBB-CGB-O1B
26	t9	201	PEB	CAB-CBB-CGB-O1B
26	u9	201	PEB	CAB-CBB-CGB-O1B
26	w9	202	PEB	CAB-CBB-CGB-O1B
26	x9	202	PEB	CAB-CBB-CGB-O1B
26	y9	1001	PEB	CAB-CBB-CGB-O1B
26	z9	202	PEB	CAB-CBB-CGB-O1B
26	D9	201	PEB	CAB-CBB-CGB-O1B
26	E9	201	PEB	CAB-CBB-CGB-O1B
26	I9	201	PEB	CAB-CBB-CGB-O1B
26	Q9	201	PEB	CAB-CBB-CGB-O1B
26	S9	201	PEB	CAB-CBB-CGB-O1B
26	V9	201	PEB	CAB-CBB-CGB-O1B
26	Y9	302	PEB	CAB-CBB-CGB-O1B
26	Z9	1001	PEB	CAB-CBB-CGB-O1B
26	ac	201	PEB	CAB-CBB-CGB-O1B
26	ag	201	PEB	CAB-CBB-CGB-O1B
26	ai	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	am	1001	PEB	CAB-CBB-CGB-O1B
26	ap	201	PEB	CAB-CBB-CGB-O1B
26	av	201	PEB	CAB-CBB-CGB-O1B
26	aF	201	PEB	CAB-CBB-CGB-O1B
26	aI	201	PEB	CAB-CBB-CGB-O1B
26	aI	202	PEB	CAB-CBB-CGB-O1B
26	aL	202	PEB	CAB-CBB-CGB-O1B
26	aM	201	PEB	CAB-CBB-CGB-O1B
26	aP	202	PEB	CAB-CBB-CGB-O1B
26	aS	201	PEB	CAB-CBB-CGB-O1B
26	aU	201	PEB	CAB-CBB-CGB-O1B
26	bb	201	PEB	CAB-CBB-CGB-O1B
26	be	201	PEB	CAB-CBB-CGB-O1B
26	bg	201	PEB	CAB-CBB-CGB-O1B
26	bh	202	PEB	CAB-CBB-CGB-O1B
26	bj	201	PEB	CAB-CBB-CGB-O1B
26	bj	202	PEB	CAB-CBB-CGB-O1B
26	bl	202	PEB	CAB-CBB-CGB-O1B
26	bo	201	PEB	CAB-CBB-CGB-O1B
26	bp	201	PEB	CAB-CBB-CGB-O1B
26	bs	1003	PEB	CAB-CBB-CGB-O1B
26	bt	201	PEB	CAB-CBB-CGB-O1B
26	bu	201	PEB	CAB-CBB-CGB-O1B
26	bw	201	PEB	CAB-CBB-CGB-O1B
26	bx	201	PEB	CAB-CBB-CGB-O1B
26	by	1001	PEB	CAB-CBB-CGB-O1B
26	bz	201	PEB	CAB-CBB-CGB-O1B
26	bz	202	PEB	CAB-CBB-CGB-O1B
26	bE	201	PEB	CAB-CBB-CGB-O1B
26	bG	201	PEB	CAB-CBB-CGB-O1B
26	bU	201	PEB	CAB-CBB-CGB-O1B
26	bX	402	PEB	CAB-CBB-CGB-O1B
26	bY	1003	PEB	CAB-CBB-CGB-O1B
26	cd	201	PEB	CAB-CBB-CGB-O1B
26	ch	201	PEB	CAB-CBB-CGB-O1B
26	cl	201	PEB	CAB-CBB-CGB-O1B
26	cp	201	PEB	CAB-CBB-CGB-O1B
26	ct	201	PEB	CAB-CBB-CGB-O1B
26	cB	201	PEB	CAB-CBB-CGB-O1B
26	cG	201	PEB	CAB-CBB-CGB-O1B
26	cL	201	PEB	CAB-CBB-CGB-O1B
26	cR	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	cS	202	PEB	CAB-CBB-CGB-O1B
26	cT	1002	PEB	CAB-CBB-CGB-O1B
26	cU	201	PEB	CAB-CBB-CGB-O1B
26	cV	202	PEB	CAB-CBB-CGB-O1B
26	cV	203	PEB	CAB-CBB-CGB-O1B
26	cW	202	PEB	CAB-CBB-CGB-O1B
26	cY	201	PEB	CAB-CBB-CGB-O1B
26	dg	201	PEB	CAB-CBB-CGB-O1B
26	dk	1002	PEB	CAB-CBB-CGB-O1B
26	dm	202	PEB	CAB-CBB-CGB-O1B
26	dn	201	PEB	CAB-CBB-CGB-O1B
26	do	202	PEB	CAB-CBB-CGB-O1B
26	dp	201	PEB	CAB-CBB-CGB-O1B
26	dq	201	PEB	CAB-CBB-CGB-O1B
26	du	202	PEB	CAB-CBB-CGB-O1B
26	du	203	PEB	CAB-CBB-CGB-O1B
26	dv	201	PEB	CAB-CBB-CGB-O1B
26	dA	201	PEB	CAB-CBB-CGB-O1B
26	dC	202	PEB	CAB-CBB-CGB-O1B
26	dD	202	PEB	CAB-CBB-CGB-O1B
26	dM	1001	PEB	CAB-CBB-CGB-O1B
26	dN	201	PEB	CAB-CBB-CGB-O1B
26	dN	202	PEB	CAB-CBB-CGB-O1B
26	dQ	201	PEB	CAB-CBB-CGB-O1B
26	dR	202	PEB	CAB-CBB-CGB-O1B
26	dT	201	PEB	CAB-CBB-CGB-O1B
26	ed	202	PEB	CAB-CBB-CGB-O1B
26	ef	201	PEB	CAB-CBB-CGB-O1B
26	eo	202	PEB	CAB-CBB-CGB-O1B
26	ep	201	PEB	CAB-CBB-CGB-O1B
26	eq	202	PEB	CAB-CBB-CGB-O1B
26	es	201	PEB	CAB-CBB-CGB-O1B
26	ey	1002	PEB	CAB-CBB-CGB-O1B
26	ez	1002	PEB	CAB-CBB-CGB-O1B
26	ez	1003	PEB	CAB-CBB-CGB-O1B
26	eC	201	PEB	CAB-CBB-CGB-O1B
26	eF	201	PEB	CAB-CBB-CGB-O1B
26	eF	202	PEB	CAB-CBB-CGB-O1B
26	eG	201	PEB	CAB-CBB-CGB-O1B
26	eH	202	PEB	CAB-CBB-CGB-O1B
26	eO	201	PEB	CAB-CBB-CGB-O1B
26	eS	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	eS	202	PEB	CAB-CBB-CGB-O1B
26	eT	201	PEB	CAB-CBB-CGB-O1B
26	eT	202	PEB	CAB-CBB-CGB-O1B
26	eV	201	PEB	CAB-CBB-CGB-O1B
26	eY	402	PEB	CAB-CBB-CGB-O1B
26	lf	201	PEB	CAB-CBB-CGB-O1B
26	ln	201	PEB	CAB-CBB-CGB-O1B
26	lz	401	PEB	CAB-CBB-CGB-O1B
26	fd	301	PEB	CAB-CBB-CGB-O1B
26	fh	1001	PEB	CAB-CBB-CGB-O1B
26	fk	201	PEB	CAB-CBB-CGB-O1B
26	fl	201	PEB	CAB-CBB-CGB-O1B
26	fo	201	PEB	CAB-CBB-CGB-O1B
26	fq	201	PEB	CAB-CBB-CGB-O1B
26	fs	201	PEB	CAB-CBB-CGB-O1B
26	fv	201	PEB	CAB-CBB-CGB-O1B
26	ge	201	PEB	CAB-CBB-CGB-O1B
26	gf	201	PEB	CAB-CBB-CGB-O1B
26	gg	201	PEB	CAB-CBB-CGB-O1B
26	gh	201	PEB	CAB-CBB-CGB-O1B
26	gi	201	PEB	CAB-CBB-CGB-O1B
26	gj	201	PEB	CAB-CBB-CGB-O1B
26	gy	303	PEB	CAB-CBB-CGB-O1B
26	hJ	201	PEB	CAB-CBB-CGB-O1B
26	hK	201	PEB	CAB-CBB-CGB-O1B
26	hL	201	PEB	CAB-CBB-CGB-O1B
26	hR	201	PEB	CAB-CBB-CGB-O1B
26	hS	201	PEB	CAB-CBB-CGB-O1B
26	hT	201	PEB	CAB-CBB-CGB-O1B
26	hY	403	PEB	CAB-CBB-CGB-O1B
26	iB	1001	PEB	CAB-CBB-CGB-O1B
26	iF	1001	PEB	CAB-CBB-CGB-O1B
26	jI	1001	PEB	CAB-CBB-CGB-O1B
26	kQ	1001	PEB	CAB-CBB-CGB-O1B
26	kV	1001	PEB	CAB-CBB-CGB-O1B
26	e2	202	PEB	CAB-CBB-CGB-O1B
26	n2	201	PEB	CAB-CBB-CGB-O1B
26	p2	201	PEB	CAB-CBB-CGB-O1B
26	w2	202	PEB	CAB-CBB-CGB-O1B
26	y2	202	PEB	CAB-CBB-CGB-O1B
26	z2	201	PEB	CAB-CBB-CGB-O1B
26	G2	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	J2	201	PEB	CAB-CBB-CGB-O1B
26	K2	202	PEB	CAB-CBB-CGB-O1B
26	T2	201	PEB	CAB-CBB-CGB-O1B
26	B3	201	PEB	CAB-CBB-CGB-O1B
26	H3	201	PEB	CAB-CBB-CGB-O1B
26	I3	201	PEB	CAB-CBB-CGB-O1B
26	Z3	201	PEB	CAB-CBB-CGB-O1B
26	p3	201	PEB	CAB-CBB-CGB-O1B
26	r3	201	PEB	CAB-CBB-CGB-O1B
26	F4	201	PEB	CAB-CBB-CGB-O1B
26	J4	201	PEB	CAB-CBB-CGB-O1B
26	S4	202	PEB	CAB-CBB-CGB-O1B
26	Z4	201	PEB	CAB-CBB-CGB-O1B
26	44	301	PEB	CAB-CBB-CGB-O1B
26	d4	201	PEB	CAB-CBB-CGB-O1B
26	t4	201	PEB	CAB-CBB-CGB-O1B
26	G5	201	PEB	CAB-CBB-CGB-O1B
26	V5	201	PEB	CAB-CBB-CGB-O1B
26	a5	201	PEB	CAB-CBB-CGB-O1B
26	i5	201	PEB	CAB-CBB-CGB-O1B
26	l5	201	PEB	CAB-CBB-CGB-O1B
26	r5	201	PEB	CAB-CBB-CGB-O1B
26	t5	201	PEB	CAB-CBB-CGB-O1B
26	g8	201	PEB	CAB-CBB-CGB-O1B
26	A6	1001	PEB	CAB-CBB-CGB-O1B
26	F6	201	PEB	CAB-CBB-CGB-O1B
26	Q6	201	PEB	CAB-CBB-CGB-O1B
26	R6	201	PEB	CAB-CBB-CGB-O1B
26	W6	202	PEB	CAB-CBB-CGB-O1B
26	X6	201	PEB	CAB-CBB-CGB-O1B
26	i6	201	PEB	CAB-CBB-CGB-O1B
26	M7	1002	PEB	CAB-CBB-CGB-O1B
26	N7	201	PEB	CAB-CBB-CGB-O1B
26	O7	201	PEB	CAB-CBB-CGB-O1B
26	R7	201	PEB	CAB-CBB-CGB-O1B
26	T7	201	PEB	CAB-CBB-CGB-O1B
26	Y7	1001	PEB	CAB-CBB-CGB-O1B
26	a7	201	PEB	CAB-CBB-CGB-O1B
26	z7	201	PEB	CAB-CBB-CGB-O1B
26	e8	301	PEB	CAB-CBB-CGB-O1B
26	e8	302	PEB	CAB-CBB-CGB-O1B
26	a9	601	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	b9	401	PEB	CAB-CBB-CGB-O1B
26	x8	202	PEB	CAB-CBB-CGB-O1B
26	E8	202	PEB	CAB-CBB-CGB-O1B
26	I8	201	PEB	CAB-CBB-CGB-O1B
26	L8	201	PEB	CAB-CBB-CGB-O1B
26	L8	202	PEB	CAB-CBB-CGB-O1B
26	N8	201	PEB	CAB-CBB-CGB-O1B
26	Q8	201	PEB	CAB-CBB-CGB-O1B
26	T8	301	PEB	CAB-CBB-CGB-O1B
26	k9	201	PEB	CAB-CBB-CGB-O1B
26	C9	201	PEB	CAB-CBB-CGB-O1B
26	J9	201	PEB	CAB-CBB-CGB-O1B
26	Z9	1003	PEB	CAB-CBB-CGB-O1B
26	aa	1001	PEB	CAB-CBB-CGB-O1B
26	ad	201	PEB	CAB-CBB-CGB-O1B
26	al	201	PEB	CAB-CBB-CGB-O1B
26	aq	201	PEB	CAB-CBB-CGB-O1B
26	ar	201	PEB	CAB-CBB-CGB-O1B
26	at	201	PEB	CAB-CBB-CGB-O1B
26	aA	202	PEB	CAB-CBB-CGB-O1B
26	aC	202	PEB	CAB-CBB-CGB-O1B
26	aH	202	PEB	CAB-CBB-CGB-O1B
26	aY	402	PEB	CAB-CBB-CGB-O1B
26	bd	201	PEB	CAB-CBB-CGB-O1B
26	bt	202	PEB	CAB-CBB-CGB-O1B
26	bA	201	PEB	CAB-CBB-CGB-O1B
26	bD	201	PEB	CAB-CBB-CGB-O1B
26	bF	201	PEB	CAB-CBB-CGB-O1B
26	bI	201	PEB	CAB-CBB-CGB-O1B
26	bQ	201	PEB	CAB-CBB-CGB-O1B
26	bZ	301	PEB	CAB-CBB-CGB-O1B
26	cA	201	PEB	CAB-CBB-CGB-O1B
26	cK	201	PEB	CAB-CBB-CGB-O1B
26	cO	201	PEB	CAB-CBB-CGB-O1B
26	cW	201	PEB	CAB-CBB-CGB-O1B
26	dc	201	PEB	CAB-CBB-CGB-O1B
26	dc	203	PEB	CAB-CBB-CGB-O1B
26	dh	201	PEB	CAB-CBB-CGB-O1B
26	do	201	PEB	CAB-CBB-CGB-O1B
26	dG	201	PEB	CAB-CBB-CGB-O1B
26	dO	201	PEB	CAB-CBB-CGB-O1B
26	dO	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	dS	201	PEB	CAB-CBB-CGB-O1B
26	dT	202	PEB	CAB-CBB-CGB-O1B
26	dU	201	PEB	CAB-CBB-CGB-O1B
26	dW	201	PEB	CAB-CBB-CGB-O1B
26	dW	202	PEB	CAB-CBB-CGB-O1B
26	dX	202	PEB	CAB-CBB-CGB-O1B
26	eo	201	PEB	CAB-CBB-CGB-O1B
26	eq	201	PEB	CAB-CBB-CGB-O1B
26	ez	1001	PEB	CAB-CBB-CGB-O1B
26	eE	202	PEB	CAB-CBB-CGB-O1B
26	eK	201	PEB	CAB-CBB-CGB-O1B
26	eK	202	PEB	CAB-CBB-CGB-O1B
26	eM	1001	PEB	CAB-CBB-CGB-O1B
26	eN	201	PEB	CAB-CBB-CGB-O1B
26	eO	202	PEB	CAB-CBB-CGB-O1B
26	eP	202	PEB	CAB-CBB-CGB-O1B
26	eQ	201	PEB	CAB-CBB-CGB-O1B
26	eQ	202	PEB	CAB-CBB-CGB-O1B
26	eU	202	PEB	CAB-CBB-CGB-O1B
26	li	201	PEB	CAB-CBB-CGB-O1B
26	lp	201	PEB	CAB-CBB-CGB-O1B
26	lu	201	PEB	CAB-CBB-CGB-O1B
26	fd	303	PEB	CAB-CBB-CGB-O1B
26	fi	201	PEB	CAB-CBB-CGB-O1B
26	fj	201	PEB	CAB-CBB-CGB-O1B
26	fp	201	PEB	CAB-CBB-CGB-O1B
26	gm	1001	PEB	CAB-CBB-CGB-O1B
26	gw	201	PEB	CAB-CBB-CGB-O1B
26	gz	303	PEB	CAB-CBB-CGB-O1B
26	hT	204	PEB	CAB-CBB-CGB-O1B
26	jJ	1001	PEB	CAB-CBB-CGB-O1B
26	jK	1001	PEB	CAB-CBB-CGB-O1B
26	jP	1001	PEB	CAB-CBB-CGB-O1B
26	kT	1001	PEB	CAB-CBB-CGB-O1B
26	kX	1001	PEB	CAB-CBB-CGB-O1B
29	e8	303	PVN	C51-C52-C53-O54
29	e9	304	PVN	C51-C52-C53-O54
29	T8	303	PVN	C61-C62-C63-O65
29	Y9	303	PVN	C61-C62-C63-O65
29	ey	1004	PVN	C61-C62-C63-O65
26	e2	201	PEB	CAB-CBB-CGB-O1B
26	g2	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	i2	202	PEB	CAB-CBB-CGB-O1B
26	j2	201	PEB	CAB-CBB-CGB-O1B
26	k2	202	PEB	CAB-CBB-CGB-O1B
26	l2	201	PEB	CAB-CBB-CGB-O1B
26	m2	201	PEB	CAB-CBB-CGB-O1B
26	m2	202	PEB	CAB-CBB-CGB-O1B
26	o2	1001	PEB	CAB-CBB-CGB-O1B
26	q2	202	PEB	CAB-CBB-CGB-O1B
26	r2	202	PEB	CAB-CBB-CGB-O1B
26	s2	201	PEB	CAB-CBB-CGB-O1B
26	s2	202	PEB	CAB-CBB-CGB-O1B
26	t2	202	PEB	CAB-CBB-CGB-O1B
26	u2	201	PEB	CAB-CBB-CGB-O1B
26	u2	202	PEB	CAB-CBB-CGB-O1B
26	v2	201	PEB	CAB-CBB-CGB-O1B
26	w2	201	PEB	CAB-CBB-CGB-O1B
26	w2	203	PEB	CAB-CBB-CGB-O1B
26	y2	201	PEB	CAB-CBB-CGB-O1B
26	z2	202	PEB	CAB-CBB-CGB-O1B
26	A2	1002	PEB	CAB-CBB-CGB-O1B
26	B2	502	PEB	CAB-CBB-CGB-O1B
26	C2	301	PEB	CAB-CBB-CGB-O1B
26	C2	302	PEB	CAB-CBB-CGB-O1B
26	D2	302	PEB	CAB-CBB-CGB-O1B
26	F2	201	PEB	CAB-CBB-CGB-O1B
26	F2	202	PEB	CAB-CBB-CGB-O1B
26	I2	201	PEB	CAB-CBB-CGB-O1B
26	I2	202	PEB	CAB-CBB-CGB-O1B
26	K2	201	PEB	CAB-CBB-CGB-O1B
26	L2	201	PEB	CAB-CBB-CGB-O1B
26	M2	202	PEB	CAB-CBB-CGB-O1B
26	O2	202	PEB	CAB-CBB-CGB-O1B
26	P2	201	PEB	CAB-CBB-CGB-O1B
26	Q2	1001	PEB	CAB-CBB-CGB-O1B
26	U2	201	PEB	CAB-CBB-CGB-O1B
26	V2	201	PEB	CAB-CBB-CGB-O1B
26	W2	201	PEB	CAB-CBB-CGB-O1B
26	W2	202	PEB	CAB-CBB-CGB-O1B
26	Y2	201	PEB	CAB-CBB-CGB-O1B
26	A3	201	PEB	CAB-CBB-CGB-O1B
26	D3	201	PEB	CAB-CBB-CGB-O1B
26	E3	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	J3	201	PEB	CAB-CBB-CGB-O1B
26	K3	201	PEB	CAB-CBB-CGB-O1B
26	M3	201	PEB	CAB-CBB-CGB-O1B
26	P3	201	PEB	CAB-CBB-CGB-O1B
26	R3	201	PEB	CAB-CBB-CGB-O1B
26	S3	203	PEB	CAB-CBB-CGB-O1B
26	T3	201	PEB	CAB-CBB-CGB-O1B
26	U3	201	PEB	CAB-CBB-CGB-O1B
26	W3	201	PEB	CAB-CBB-CGB-O1B
26	Y3	201	PEB	CAB-CBB-CGB-O1B
26	a3	1003	PEB	CAB-CBB-CGB-O1B
26	b3	501	PEB	CAB-CBB-CGB-O1B
26	b3	502	PEB	CAB-CBB-CGB-O1B
26	c3	302	PEB	CAB-CBB-CGB-O1B
26	n3	201	PEB	CAB-CBB-CGB-O1B
26	q3	1001	PEB	CAB-CBB-CGB-O1B
26	s3	201	PEB	CAB-CBB-CGB-O1B
26	v3	201	PEB	CAB-CBB-CGB-O1B
26	w3	201	PEB	CAB-CBB-CGB-O1B
26	z3	201	PEB	CAB-CBB-CGB-O1B
26	C4	1001	PEB	CAB-CBB-CGB-O1B
26	D4	201	PEB	CAB-CBB-CGB-O1B
26	E4	201	PEB	CAB-CBB-CGB-O1B
26	G4	201	PEB	CAB-CBB-CGB-O1B
26	I4	201	PEB	CAB-CBB-CGB-O1B
26	K4	201	PEB	CAB-CBB-CGB-O1B
26	K4	202	PEB	CAB-CBB-CGB-O1B
26	L4	202	PEB	CAB-CBB-CGB-O1B
26	M4	201	PEB	CAB-CBB-CGB-O1B
26	N4	201	PEB	CAB-CBB-CGB-O1B
26	O4	1002	PEB	CAB-CBB-CGB-O1B
26	P4	201	PEB	CAB-CBB-CGB-O1B
26	P4	202	PEB	CAB-CBB-CGB-O1B
26	Q4	201	PEB	CAB-CBB-CGB-O1B
26	Q4	202	PEB	CAB-CBB-CGB-O1B
26	Q4	203	PEB	CAB-CBB-CGB-O1B
26	R4	201	PEB	CAB-CBB-CGB-O1B
26	T4	201	PEB	CAB-CBB-CGB-O1B
26	U4	201	PEB	CAB-CBB-CGB-O1B
26	V4	201	PEB	CAB-CBB-CGB-O1B
26	V4	202	PEB	CAB-CBB-CGB-O1B
26	W4	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	W4	202	PEB	CAB-CBB-CGB-O1B
26	Y4	201	PEB	CAB-CBB-CGB-O1B
26	Z4	202	PEB	CAB-CBB-CGB-O1B
26	24	401	PEB	CAB-CBB-CGB-O1B
26	34	1003	PEB	CAB-CBB-CGB-O1B
26	44	302	PEB	CAB-CBB-CGB-O1B
26	b4	1001	PEB	CAB-CBB-CGB-O1B
26	c4	202	PEB	CAB-CBB-CGB-O1B
26	e4	201	PEB	CAB-CBB-CGB-O1B
26	h4	202	PEB	CAB-CBB-CGB-O1B
26	k4	201	PEB	CAB-CBB-CGB-O1B
26	n4	201	PEB	CAB-CBB-CGB-O1B
26	o4	202	PEB	CAB-CBB-CGB-O1B
26	p4	201	PEB	CAB-CBB-CGB-O1B
26	s4	201	PEB	CAB-CBB-CGB-O1B
26	u4	201	PEB	CAB-CBB-CGB-O1B
26	u4	202	PEB	CAB-CBB-CGB-O1B
26	v4	201	PEB	CAB-CBB-CGB-O1B
26	x4	201	PEB	CAB-CBB-CGB-O1B
26	y4	1001	PEB	CAB-CBB-CGB-O1B
26	y4	1002	PEB	CAB-CBB-CGB-O1B
26	F5	201	PEB	CAB-CBB-CGB-O1B
26	J5	201	PEB	CAB-CBB-CGB-O1B
26	M5	201	PEB	CAB-CBB-CGB-O1B
26	O5	201	PEB	CAB-CBB-CGB-O1B
26	Q5	201	PEB	CAB-CBB-CGB-O1B
26	R5	201	PEB	CAB-CBB-CGB-O1B
26	S5	201	PEB	CAB-CBB-CGB-O1B
26	U5	201	PEB	CAB-CBB-CGB-O1B
26	W5	301	PEB	CAB-CBB-CGB-O1B
26	Y5	1003	PEB	CAB-CBB-CGB-O1B
26	Z5	301	PEB	CAB-CBB-CGB-O1B
26	d5	201	PEB	CAB-CBB-CGB-O1B
26	e5	201	PEB	CAB-CBB-CGB-O1B
26	g5	201	PEB	CAB-CBB-CGB-O1B
26	k5	201	PEB	CAB-CBB-CGB-O1B
26	l5	202	PEB	CAB-CBB-CGB-O1B
26	m5	1001	PEB	CAB-CBB-CGB-O1B
26	s5	201	PEB	CAB-CBB-CGB-O1B
26	u5	201	PEB	CAB-CBB-CGB-O1B
26	v5	201	PEB	CAB-CBB-CGB-O1B
26	f8	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	h8	201	PEB	CAB-CBB-CGB-O1B
26	i8	201	PEB	CAB-CBB-CGB-O1B
26	k8	201	PEB	CAB-CBB-CGB-O1B
26	B6	201	PEB	CAB-CBB-CGB-O1B
26	C6	201	PEB	CAB-CBB-CGB-O1B
26	D6	201	PEB	CAB-CBB-CGB-O1B
26	F6	202	PEB	CAB-CBB-CGB-O1B
26	G6	201	PEB	CAB-CBB-CGB-O1B
26	H6	202	PEB	CAB-CBB-CGB-O1B
26	I6	201	PEB	CAB-CBB-CGB-O1B
26	J6	201	PEB	CAB-CBB-CGB-O1B
26	K6	202	PEB	CAB-CBB-CGB-O1B
26	M6	1001	PEB	CAB-CBB-CGB-O1B
26	N6	201	PEB	CAB-CBB-CGB-O1B
26	O6	201	PEB	CAB-CBB-CGB-O1B
26	P6	202	PEB	CAB-CBB-CGB-O1B
26	Q6	202	PEB	CAB-CBB-CGB-O1B
26	S6	201	PEB	CAB-CBB-CGB-O1B
26	T6	201	PEB	CAB-CBB-CGB-O1B
26	T6	202	PEB	CAB-CBB-CGB-O1B
26	U6	201	PEB	CAB-CBB-CGB-O1B
26	Y6	201	PEB	CAB-CBB-CGB-O1B
26	Z6	201	PEB	CAB-CBB-CGB-O1B
26	Z6	202	PEB	CAB-CBB-CGB-O1B
26	b6	201	PEB	CAB-CBB-CGB-O1B
26	b6	202	PEB	CAB-CBB-CGB-O1B
26	c6	1001	PEB	CAB-CBB-CGB-O1B
26	c6	1002	PEB	CAB-CBB-CGB-O1B
26	c6	1003	PEB	CAB-CBB-CGB-O1B
26	d6	201	PEB	CAB-CBB-CGB-O1B
26	f6	201	PEB	CAB-CBB-CGB-O1B
26	i6	202	PEB	CAB-CBB-CGB-O1B
26	j6	202	PEB	CAB-CBB-CGB-O1B
26	k6	1001	PEB	CAB-CBB-CGB-O1B
26	l6	202	PEB	CAB-CBB-CGB-O1B
26	m6	201	PEB	CAB-CBB-CGB-O1B
26	o6	202	PEB	CAB-CBB-CGB-O1B
26	q6	201	PEB	CAB-CBB-CGB-O1B
26	s6	201	PEB	CAB-CBB-CGB-O1B
26	s6	202	PEB	CAB-CBB-CGB-O1B
26	u6	202	PEB	CAB-CBB-CGB-O1B
26	w6	1001	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	w6	1002	PEB	CAB-CBB-CGB-O1B
26	y6	202	PEB	CAB-CBB-CGB-O1B
26	y6	203	PEB	CAB-CBB-CGB-O1B
26	z6	201	PEB	CAB-CBB-CGB-O1B
26	z6	202	PEB	CAB-CBB-CGB-O1B
26	o8	202	PEB	CAB-CBB-CGB-O1B
26	q8	201	PEB	CAB-CBB-CGB-O1B
26	r8	201	PEB	CAB-CBB-CGB-O1B
26	u8	201	PEB	CAB-CBB-CGB-O1B
26	D7	201	PEB	CAB-CBB-CGB-O1B
26	E7	201	PEB	CAB-CBB-CGB-O1B
26	K7	201	PEB	CAB-CBB-CGB-O1B
26	M7	1001	PEB	CAB-CBB-CGB-O1B
26	P7	201	PEB	CAB-CBB-CGB-O1B
26	Q7	201	PEB	CAB-CBB-CGB-O1B
26	W7	201	PEB	CAB-CBB-CGB-O1B
26	X7	201	PEB	CAB-CBB-CGB-O1B
26	Z7	201	PEB	CAB-CBB-CGB-O1B
26	i7	201	PEB	CAB-CBB-CGB-O1B
26	j7	201	PEB	CAB-CBB-CGB-O1B
26	k7	1001	PEB	CAB-CBB-CGB-O1B
26	l7	201	PEB	CAB-CBB-CGB-O1B
26	o7	201	PEB	CAB-CBB-CGB-O1B
26	q7	201	PEB	CAB-CBB-CGB-O1B
26	v7	201	PEB	CAB-CBB-CGB-O1B
26	w7	1001	PEB	CAB-CBB-CGB-O1B
26	x7	201	PEB	CAB-CBB-CGB-O1B
26	a8	602	PEB	CAB-CBB-CGB-O1B
26	b8	1002	PEB	CAB-CBB-CGB-O1B
26	a9	603	PEB	CAB-CBB-CGB-O1B
26	b9	402	PEB	CAB-CBB-CGB-O1B
26	b9	403	PEB	CAB-CBB-CGB-O1B
26	b9	404	PEB	CAB-CBB-CGB-O1B
26	c9	302	PEB	CAB-CBB-CGB-O1B
26	d9	302	PEB	CAB-CBB-CGB-O1B
26	d9	303	PEB	CAB-CBB-CGB-O1B
26	e9	301	PEB	CAB-CBB-CGB-O1B
26	e9	302	PEB	CAB-CBB-CGB-O1B
26	e9	303	PEB	CAB-CBB-CGB-O1B
26	w8	201	PEB	CAB-CBB-CGB-O1B
26	w8	202	PEB	CAB-CBB-CGB-O1B
26	y8	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	A8	201	PEB	CAB-CBB-CGB-O1B
26	A8	202	PEB	CAB-CBB-CGB-O1B
26	B8	201	PEB	CAB-CBB-CGB-O1B
26	D8	201	PEB	CAB-CBB-CGB-O1B
26	F8	1001	PEB	CAB-CBB-CGB-O1B
26	F8	1002	PEB	CAB-CBB-CGB-O1B
26	J8	202	PEB	CAB-CBB-CGB-O1B
26	K8	202	PEB	CAB-CBB-CGB-O1B
26	M8	202	PEB	CAB-CBB-CGB-O1B
26	N8	202	PEB	CAB-CBB-CGB-O1B
26	O8	201	PEB	CAB-CBB-CGB-O1B
26	O8	202	PEB	CAB-CBB-CGB-O1B
26	P8	202	PEB	CAB-CBB-CGB-O1B
26	Q8	202	PEB	CAB-CBB-CGB-O1B
26	S8	401	PEB	CAB-CBB-CGB-O1B
26	V8	1001	PEB	CAB-CBB-CGB-O1B
26	X8	201	PEB	CAB-CBB-CGB-O1B
26	Z8	201	PEB	CAB-CBB-CGB-O1B
26	f9	202	PEB	CAB-CBB-CGB-O1B
26	i9	201	PEB	CAB-CBB-CGB-O1B
26	j9	202	PEB	CAB-CBB-CGB-O1B
26	l9	201	PEB	CAB-CBB-CGB-O1B
26	l9	202	PEB	CAB-CBB-CGB-O1B
26	m9	1001	PEB	CAB-CBB-CGB-O1B
26	n9	201	PEB	CAB-CBB-CGB-O1B
26	p9	202	PEB	CAB-CBB-CGB-O1B
26	r9	201	PEB	CAB-CBB-CGB-O1B
26	s9	201	PEB	CAB-CBB-CGB-O1B
26	v9	201	PEB	CAB-CBB-CGB-O1B
26	w9	201	PEB	CAB-CBB-CGB-O1B
26	x9	201	PEB	CAB-CBB-CGB-O1B
26	y9	1002	PEB	CAB-CBB-CGB-O1B
26	z9	201	PEB	CAB-CBB-CGB-O1B
26	B9	201	PEB	CAB-CBB-CGB-O1B
26	F9	201	PEB	CAB-CBB-CGB-O1B
26	G9	201	PEB	CAB-CBB-CGB-O1B
26	K9	1001	PEB	CAB-CBB-CGB-O1B
26	L9	201	PEB	CAB-CBB-CGB-O1B
26	N9	201	PEB	CAB-CBB-CGB-O1B
26	P9	201	PEB	CAB-CBB-CGB-O1B
26	R9	201	PEB	CAB-CBB-CGB-O1B
26	T9	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	Z9	1007	PEB	CAB-CBB-CGB-O1B
26	ab	201	PEB	CAB-CBB-CGB-O1B
26	ae	201	PEB	CAB-CBB-CGB-O1B
26	af	201	PEB	CAB-CBB-CGB-O1B
26	aj	201	PEB	CAB-CBB-CGB-O1B
26	ak	201	PEB	CAB-CBB-CGB-O1B
26	ao	201	PEB	CAB-CBB-CGB-O1B
26	aw	201	PEB	CAB-CBB-CGB-O1B
26	az	201	PEB	CAB-CBB-CGB-O1B
26	aA	201	PEB	CAB-CBB-CGB-O1B
26	aB	201	PEB	CAB-CBB-CGB-O1B
26	aC	201	PEB	CAB-CBB-CGB-O1B
26	aD	201	PEB	CAB-CBB-CGB-O1B
26	aE	201	PEB	CAB-CBB-CGB-O1B
26	aG	201	PEB	CAB-CBB-CGB-O1B
26	aH	201	PEB	CAB-CBB-CGB-O1B
26	aJ	201	PEB	CAB-CBB-CGB-O1B
26	aJ	202	PEB	CAB-CBB-CGB-O1B
26	aK	1002	PEB	CAB-CBB-CGB-O1B
26	aM	202	PEB	CAB-CBB-CGB-O1B
26	aN	201	PEB	CAB-CBB-CGB-O1B
26	aN	202	PEB	CAB-CBB-CGB-O1B
26	aO	201	PEB	CAB-CBB-CGB-O1B
26	aP	201	PEB	CAB-CBB-CGB-O1B
26	aQ	201	PEB	CAB-CBB-CGB-O1B
26	aQ	202	PEB	CAB-CBB-CGB-O1B
26	aR	201	PEB	CAB-CBB-CGB-O1B
26	aR	202	PEB	CAB-CBB-CGB-O1B
26	aS	202	PEB	CAB-CBB-CGB-O1B
26	aT	201	PEB	CAB-CBB-CGB-O1B
26	aT	202	PEB	CAB-CBB-CGB-O1B
26	aV	201	PEB	CAB-CBB-CGB-O1B
26	aW	301	PEB	CAB-CBB-CGB-O1B
26	aW	302	PEB	CAB-CBB-CGB-O1B
26	aX	402	PEB	CAB-CBB-CGB-O1B
26	aY	406	PEB	CAB-CBB-CGB-O1B
26	aZ	301	PEB	CAB-CBB-CGB-O1B
26	ba	1001	PEB	CAB-CBB-CGB-O1B
26	bc	201	PEB	CAB-CBB-CGB-O1B
26	bd	202	PEB	CAB-CBB-CGB-O1B
26	bh	201	PEB	CAB-CBB-CGB-O1B
26	bi	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	bk	201	PEB	CAB-CBB-CGB-O1B
26	bl	201	PEB	CAB-CBB-CGB-O1B
26	bm	1002	PEB	CAB-CBB-CGB-O1B
26	bn	201	PEB	CAB-CBB-CGB-O1B
26	bq	201	PEB	CAB-CBB-CGB-O1B
26	bq	202	PEB	CAB-CBB-CGB-O1B
26	br	202	PEB	CAB-CBB-CGB-O1B
26	bs	1001	PEB	CAB-CBB-CGB-O1B
26	bs	1002	PEB	CAB-CBB-CGB-O1B
26	bu	202	PEB	CAB-CBB-CGB-O1B
26	bv	201	PEB	CAB-CBB-CGB-O1B
26	bv	202	PEB	CAB-CBB-CGB-O1B
26	by	1002	PEB	CAB-CBB-CGB-O1B
26	bH	201	PEB	CAB-CBB-CGB-O1B
26	bK	1001	PEB	CAB-CBB-CGB-O1B
26	bL	201	PEB	CAB-CBB-CGB-O1B
26	bM	201	PEB	CAB-CBB-CGB-O1B
26	bO	201	PEB	CAB-CBB-CGB-O1B
26	bP	201	PEB	CAB-CBB-CGB-O1B
26	bR	201	PEB	CAB-CBB-CGB-O1B
26	bS	201	PEB	CAB-CBB-CGB-O1B
26	bV	201	PEB	CAB-CBB-CGB-O1B
26	bW	301	PEB	CAB-CBB-CGB-O1B
26	bX	401	PEB	CAB-CBB-CGB-O1B
26	bY	1001	PEB	CAB-CBB-CGB-O1B
26	bZ	303	PEB	CAB-CBB-CGB-O1B
26	ca	1001	PEB	CAB-CBB-CGB-O1B
26	cb	201	PEB	CAB-CBB-CGB-O1B
26	cc	201	PEB	CAB-CBB-CGB-O1B
26	ci	201	PEB	CAB-CBB-CGB-O1B
26	cj	201	PEB	CAB-CBB-CGB-O1B
26	ck	201	PEB	CAB-CBB-CGB-O1B
26	cm	1001	PEB	CAB-CBB-CGB-O1B
26	cq	201	PEB	CAB-CBB-CGB-O1B
26	cv	201	PEB	CAB-CBB-CGB-O1B
26	cw	201	PEB	CAB-CBB-CGB-O1B
26	cx	201	PEB	CAB-CBB-CGB-O1B
26	cy	1001	PEB	CAB-CBB-CGB-O1B
26	cz	201	PEB	CAB-CBB-CGB-O1B
26	cC	1001	PEB	CAB-CBB-CGB-O1B
26	cC	1003	PEB	CAB-CBB-CGB-O1B
26	cE	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	cJ	201	PEB	CAB-CBB-CGB-O1B
26	cM	201	PEB	CAB-CBB-CGB-O1B
26	cN	201	PEB	CAB-CBB-CGB-O1B
26	cP	201	PEB	CAB-CBB-CGB-O1B
26	cS	201	PEB	CAB-CBB-CGB-O1B
26	cT	1001	PEB	CAB-CBB-CGB-O1B
26	cU	202	PEB	CAB-CBB-CGB-O1B
26	cX	201	PEB	CAB-CBB-CGB-O1B
26	cX	202	PEB	CAB-CBB-CGB-O1B
26	db	201	PEB	CAB-CBB-CGB-O1B
26	dd	201	PEB	CAB-CBB-CGB-O1B
26	de	201	PEB	CAB-CBB-CGB-O1B
26	df	201	PEB	CAB-CBB-CGB-O1B
26	di	201	PEB	CAB-CBB-CGB-O1B
26	dj	201	PEB	CAB-CBB-CGB-O1B
26	dk	1001	PEB	CAB-CBB-CGB-O1B
26	dl	201	PEB	CAB-CBB-CGB-O1B
26	dm	201	PEB	CAB-CBB-CGB-O1B
26	dp	202	PEB	CAB-CBB-CGB-O1B
26	dq	202	PEB	CAB-CBB-CGB-O1B
26	ds	202	PEB	CAB-CBB-CGB-O1B
26	dt	201	PEB	CAB-CBB-CGB-O1B
26	dt	202	PEB	CAB-CBB-CGB-O1B
26	du	201	PEB	CAB-CBB-CGB-O1B
26	dw	402	PEB	CAB-CBB-CGB-O1B
26	dw	403	PEB	CAB-CBB-CGB-O1B
26	dx	401	PEB	CAB-CBB-CGB-O1B
26	dx	402	PEB	CAB-CBB-CGB-O1B
26	dx	404	PEB	CAB-CBB-CGB-O1B
26	dy	401	PEB	CAB-CBB-CGB-O1B
26	dz	401	PEB	CAB-CBB-CGB-O1B
26	dz	402	PEB	CAB-CBB-CGB-O1B
26	dA	202	PEB	CAB-CBB-CGB-O1B
26	dC	201	PEB	CAB-CBB-CGB-O1B
26	dE	201	PEB	CAB-CBB-CGB-O1B
26	dF	201	PEB	CAB-CBB-CGB-O1B
26	dF	202	PEB	CAB-CBB-CGB-O1B
26	dH	202	PEB	CAB-CBB-CGB-O1B
26	dI	1001	PEB	CAB-CBB-CGB-O1B
26	dI	1002	PEB	CAB-CBB-CGB-O1B
26	dK	202	PEB	CAB-CBB-CGB-O1B
26	dL	201	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	dP	202	PEB	CAB-CBB-CGB-O1B
26	dQ	202	PEB	CAB-CBB-CGB-O1B
26	dR	201	PEB	CAB-CBB-CGB-O1B
26	dX	201	PEB	CAB-CBB-CGB-O1B
26	dY	201	PEB	CAB-CBB-CGB-O1B
26	ea	202	PEB	CAB-CBB-CGB-O1B
26	eb	201	PEB	CAB-CBB-CGB-O1B
26	ed	201	PEB	CAB-CBB-CGB-O1B
26	ee	201	PEB	CAB-CBB-CGB-O1B
26	eg	201	PEB	CAB-CBB-CGB-O1B
26	eh	201	PEB	CAB-CBB-CGB-O1B
26	ej	201	PEB	CAB-CBB-CGB-O1B
26	ek	1001	PEB	CAB-CBB-CGB-O1B
26	el	201	PEB	CAB-CBB-CGB-O1B
26	em	201	PEB	CAB-CBB-CGB-O1B
26	en	201	PEB	CAB-CBB-CGB-O1B
26	er	201	PEB	CAB-CBB-CGB-O1B
26	es	202	PEB	CAB-CBB-CGB-O1B
26	eu	201	PEB	CAB-CBB-CGB-O1B
26	ey	1003	PEB	CAB-CBB-CGB-O1B
26	eB	202	PEB	CAB-CBB-CGB-O1B
26	eD	202	PEB	CAB-CBB-CGB-O1B
26	eE	201	PEB	CAB-CBB-CGB-O1B
26	eG	202	PEB	CAB-CBB-CGB-O1B
26	eI	201	PEB	CAB-CBB-CGB-O1B
26	eJ	201	PEB	CAB-CBB-CGB-O1B
26	eM	1002	PEB	CAB-CBB-CGB-O1B
26	eP	203	PEB	CAB-CBB-CGB-O1B
26	eR	202	PEB	CAB-CBB-CGB-O1B
26	eU	201	PEB	CAB-CBB-CGB-O1B
26	eW	201	PEB	CAB-CBB-CGB-O1B
26	eW	202	PEB	CAB-CBB-CGB-O1B
26	la	1001	PEB	CAB-CBB-CGB-O1B
26	la	1002	PEB	CAB-CBB-CGB-O1B
26	lb	201	PEB	CAB-CBB-CGB-O1B
26	lb	202	PEB	CAB-CBB-CGB-O1B
26	lc	201	PEB	CAB-CBB-CGB-O1B
26	li	202	PEB	CAB-CBB-CGB-O1B
26	lk	201	PEB	CAB-CBB-CGB-O1B
26	lm	1001	PEB	CAB-CBB-CGB-O1B
26	lq	201	PEB	CAB-CBB-CGB-O1B
26	lq	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	lr	201	PEB	CAB-CBB-CGB-O1B
26	ls	201	PEB	CAB-CBB-CGB-O1B
26	lt	201	PEB	CAB-CBB-CGB-O1B
26	lv	201	PEB	CAB-CBB-CGB-O1B
26	ly	402	PEB	CAB-CBB-CGB-O1B
26	fa	201	PEB	CAB-CBB-CGB-O1B
26	fb	201	PEB	CAB-CBB-CGB-O1B
26	fc	201	PEB	CAB-CBB-CGB-O1B
26	fd	302	PEB	CAB-CBB-CGB-O1B
26	fe	201	PEB	CAB-CBB-CGB-O1B
26	ff	201	PEB	CAB-CBB-CGB-O1B
26	ff	204	PEB	CAB-CBB-CGB-O1B
26	fr	201	PEB	CAB-CBB-CGB-O1B
26	fw	201	PEB	CAB-CBB-CGB-O1B
26	fx	201	PEB	CAB-CBB-CGB-O1B
26	ga	201	PEB	CAB-CBB-CGB-O1B
26	gb	1001	PEB	CAB-CBB-CGB-O1B
26	gl	201	PEB	CAB-CBB-CGB-O1B
26	gn	201	PEB	CAB-CBB-CGB-O1B
26	go	201	PEB	CAB-CBB-CGB-O1B
26	gq	201	PEB	CAB-CBB-CGB-O1B
26	gt	201	PEB	CAB-CBB-CGB-O1B
26	gu	201	PEB	CAB-CBB-CGB-O1B
26	gy	301	PEB	CAB-CBB-CGB-O1B
26	gz	301	PEB	CAB-CBB-CGB-O1B
26	hA	201	PEB	CAB-CBB-CGB-O1B
26	hB	201	PEB	CAB-CBB-CGB-O1B
26	hC	201	PEB	CAB-CBB-CGB-O1B
26	hD	201	PEB	CAB-CBB-CGB-O1B
26	hE	1001	PEB	CAB-CBB-CGB-O1B
26	hI	201	PEB	CAB-CBB-CGB-O1B
26	hM	1001	PEB	CAB-CBB-CGB-O1B
26	hQ	201	PEB	CAB-CBB-CGB-O1B
26	hV	201	PEB	CAB-CBB-CGB-O1B
26	hW	201	PEB	CAB-CBB-CGB-O1B
26	hX	201	PEB	CAB-CBB-CGB-O1B
26	hZ	402	PEB	CAB-CBB-CGB-O1B
26	iA	1001	PEB	CAB-CBB-CGB-O1B
26	iC	1001	PEB	CAB-CBB-CGB-O1B
26	iD	1001	PEB	CAB-CBB-CGB-O1B
26	iG	1001	PEB	CAB-CBB-CGB-O1B
26	jL	1001	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	jN	1001	PEB	CAB-CBB-CGB-O1B
26	kR	1001	PEB	CAB-CBB-CGB-O1B
26	kU	1001	PEB	CAB-CBB-CGB-O1B
29	b8	1004	PVN	C51-C52-C53-O55
29	b9	405	PVN	C51-C52-C53-O55
29	aZ	303	PVN	C61-C62-C63-O64
29	bZ	304	PVN	C61-C62-C63-O64
26	g2	201	PEB	CAB-CBB-CGB-O2B
26	i2	202	PEB	CAB-CBB-CGB-O2B
26	j2	201	PEB	CAB-CBB-CGB-O2B
26	k2	201	PEB	CAB-CBB-CGB-O2B
26	k2	202	PEB	CAB-CBB-CGB-O2B
26	m2	201	PEB	CAB-CBB-CGB-O2B
26	s2	201	PEB	CAB-CBB-CGB-O2B
26	s2	202	PEB	CAB-CBB-CGB-O2B
26	v2	201	PEB	CAB-CBB-CGB-O2B
26	B2	501	PEB	CAB-CBB-CGB-O2B
26	B2	502	PEB	CAB-CBB-CGB-O2B
26	C2	302	PEB	CAB-CBB-CGB-O2B
26	K2	202	PEB	CAB-CBB-CGB-O2B
26	O2	201	PEB	CAB-CBB-CGB-O2B
26	R2	202	PEB	CAB-CBB-CGB-O2B
26	S2	201	PEB	CAB-CBB-CGB-O2B
26	T2	201	PEB	CAB-CBB-CGB-O2B
26	U2	201	PEB	CAB-CBB-CGB-O2B
26	Y2	202	PEB	CAB-CBB-CGB-O2B
26	Z2	201	PEB	CAB-CBB-CGB-O2B
26	F3	201	PEB	CAB-CBB-CGB-O2B
26	H3	201	PEB	CAB-CBB-CGB-O2B
26	R3	201	PEB	CAB-CBB-CGB-O2B
26	U3	201	PEB	CAB-CBB-CGB-O2B
26	W3	201	PEB	CAB-CBB-CGB-O2B
26	a3	1001	PEB	CAB-CBB-CGB-O2B
26	c3	302	PEB	CAB-CBB-CGB-O2B
26	k3	201	PEB	CAB-CBB-CGB-O2B
26	m3	201	PEB	CAB-CBB-CGB-O2B
26	n3	201	PEB	CAB-CBB-CGB-O2B
26	v3	201	PEB	CAB-CBB-CGB-O2B
26	A4	201	PEB	CAB-CBB-CGB-O2B
26	D4	201	PEB	CAB-CBB-CGB-O2B
26	E4	201	PEB	CAB-CBB-CGB-O2B
26	G4	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	H4	202	PEB	CAB-CBB-CGB-O2B
26	M4	202	PEB	CAB-CBB-CGB-O2B
26	Q4	201	PEB	CAB-CBB-CGB-O2B
26	R4	201	PEB	CAB-CBB-CGB-O2B
26	V4	201	PEB	CAB-CBB-CGB-O2B
26	W4	201	PEB	CAB-CBB-CGB-O2B
26	W4	202	PEB	CAB-CBB-CGB-O2B
26	Z4	202	PEB	CAB-CBB-CGB-O2B
26	24	401	PEB	CAB-CBB-CGB-O2B
26	34	1003	PEB	CAB-CBB-CGB-O2B
26	44	302	PEB	CAB-CBB-CGB-O2B
26	c4	202	PEB	CAB-CBB-CGB-O2B
26	f4	201	PEB	CAB-CBB-CGB-O2B
26	k4	201	PEB	CAB-CBB-CGB-O2B
26	u4	201	PEB	CAB-CBB-CGB-O2B
26	v4	201	PEB	CAB-CBB-CGB-O2B
26	w4	201	PEB	CAB-CBB-CGB-O2B
26	C5	201	PEB	CAB-CBB-CGB-O2B
26	D5	201	PEB	CAB-CBB-CGB-O2B
26	Q5	201	PEB	CAB-CBB-CGB-O2B
26	Y5	1003	PEB	CAB-CBB-CGB-O2B
26	Z5	303	PEB	CAB-CBB-CGB-O2B
26	a5	201	PEB	CAB-CBB-CGB-O2B
26	e5	201	PEB	CAB-CBB-CGB-O2B
26	i5	201	PEB	CAB-CBB-CGB-O2B
26	j5	202	PEB	CAB-CBB-CGB-O2B
26	k5	201	PEB	CAB-CBB-CGB-O2B
26	l5	201	PEB	CAB-CBB-CGB-O2B
26	m5	1001	PEB	CAB-CBB-CGB-O2B
26	n5	201	PEB	CAB-CBB-CGB-O2B
26	w5	201	PEB	CAB-CBB-CGB-O2B
26	x5	201	PEB	CAB-CBB-CGB-O2B
26	f8	201	PEB	CAB-CBB-CGB-O2B
26	l8	201	PEB	CAB-CBB-CGB-O2B
26	A6	1002	PEB	CAB-CBB-CGB-O2B
26	C6	201	PEB	CAB-CBB-CGB-O2B
26	C6	202	PEB	CAB-CBB-CGB-O2B
26	F6	201	PEB	CAB-CBB-CGB-O2B
26	I6	201	PEB	CAB-CBB-CGB-O2B
26	L6	201	PEB	CAB-CBB-CGB-O2B
26	N6	201	PEB	CAB-CBB-CGB-O2B
26	R6	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	Z6	201	PEB	CAB-CBB-CGB-O2B
26	Z6	202	PEB	CAB-CBB-CGB-O2B
26	b6	202	PEB	CAB-CBB-CGB-O2B
26	c6	1002	PEB	CAB-CBB-CGB-O2B
26	i6	201	PEB	CAB-CBB-CGB-O2B
26	o6	202	PEB	CAB-CBB-CGB-O2B
26	s6	201	PEB	CAB-CBB-CGB-O2B
26	x6	202	PEB	CAB-CBB-CGB-O2B
26	z6	201	PEB	CAB-CBB-CGB-O2B
26	q8	201	PEB	CAB-CBB-CGB-O2B
26	r8	201	PEB	CAB-CBB-CGB-O2B
26	G7	201	PEB	CAB-CBB-CGB-O2B
26	H7	201	PEB	CAB-CBB-CGB-O2B
26	M7	1001	PEB	CAB-CBB-CGB-O2B
26	U7	201	PEB	CAB-CBB-CGB-O2B
26	V7	201	PEB	CAB-CBB-CGB-O2B
26	W7	201	PEB	CAB-CBB-CGB-O2B
26	X7	201	PEB	CAB-CBB-CGB-O2B
26	Z7	201	PEB	CAB-CBB-CGB-O2B
26	b7	201	PEB	CAB-CBB-CGB-O2B
26	g7	201	PEB	CAB-CBB-CGB-O2B
26	j7	201	PEB	CAB-CBB-CGB-O2B
26	s7	201	PEB	CAB-CBB-CGB-O2B
26	w7	1001	PEB	CAB-CBB-CGB-O2B
26	a8	601	PEB	CAB-CBB-CGB-O2B
26	b8	1003	PEB	CAB-CBB-CGB-O2B
26	d8	302	PEB	CAB-CBB-CGB-O2B
26	a9	602	PEB	CAB-CBB-CGB-O2B
26	b9	402	PEB	CAB-CBB-CGB-O2B
26	d9	301	PEB	CAB-CBB-CGB-O2B
26	e9	303	PEB	CAB-CBB-CGB-O2B
26	F8	1002	PEB	CAB-CBB-CGB-O2B
26	G8	202	PEB	CAB-CBB-CGB-O2B
26	H8	201	PEB	CAB-CBB-CGB-O2B
26	H8	202	PEB	CAB-CBB-CGB-O2B
26	J8	202	PEB	CAB-CBB-CGB-O2B
26	O8	201	PEB	CAB-CBB-CGB-O2B
26	P8	201	PEB	CAB-CBB-CGB-O2B
26	Q8	201	PEB	CAB-CBB-CGB-O2B
26	T8	302	PEB	CAB-CBB-CGB-O2B
26	W8	201	PEB	CAB-CBB-CGB-O2B
26	f9	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	f9	202	PEB	CAB-CBB-CGB-O2B
26	l9	201	PEB	CAB-CBB-CGB-O2B
26	n9	201	PEB	CAB-CBB-CGB-O2B
26	p9	201	PEB	CAB-CBB-CGB-O2B
26	p9	202	PEB	CAB-CBB-CGB-O2B
26	u9	201	PEB	CAB-CBB-CGB-O2B
26	v9	201	PEB	CAB-CBB-CGB-O2B
26	x9	201	PEB	CAB-CBB-CGB-O2B
26	x9	202	PEB	CAB-CBB-CGB-O2B
26	z9	202	PEB	CAB-CBB-CGB-O2B
26	G9	201	PEB	CAB-CBB-CGB-O2B
26	H9	201	PEB	CAB-CBB-CGB-O2B
26	K9	1001	PEB	CAB-CBB-CGB-O2B
26	P9	201	PEB	CAB-CBB-CGB-O2B
26	Z9	1007	PEB	CAB-CBB-CGB-O2B
26	aa	1001	PEB	CAB-CBB-CGB-O2B
26	ab	201	PEB	CAB-CBB-CGB-O2B
26	ad	201	PEB	CAB-CBB-CGB-O2B
26	af	201	PEB	CAB-CBB-CGB-O2B
26	aj	201	PEB	CAB-CBB-CGB-O2B
26	ak	201	PEB	CAB-CBB-CGB-O2B
26	ap	201	PEB	CAB-CBB-CGB-O2B
26	aq	201	PEB	CAB-CBB-CGB-O2B
26	az	201	PEB	CAB-CBB-CGB-O2B
26	aA	201	PEB	CAB-CBB-CGB-O2B
26	aA	202	PEB	CAB-CBB-CGB-O2B
26	aE	202	PEB	CAB-CBB-CGB-O2B
26	aI	202	PEB	CAB-CBB-CGB-O2B
26	aN	202	PEB	CAB-CBB-CGB-O2B
26	aP	202	PEB	CAB-CBB-CGB-O2B
26	aQ	202	PEB	CAB-CBB-CGB-O2B
26	aT	201	PEB	CAB-CBB-CGB-O2B
26	aV	201	PEB	CAB-CBB-CGB-O2B
26	aX	401	PEB	CAB-CBB-CGB-O2B
26	aY	402	PEB	CAB-CBB-CGB-O2B
26	aY	406	PEB	CAB-CBB-CGB-O2B
26	aZ	302	PEB	CAB-CBB-CGB-O2B
26	bc	201	PEB	CAB-CBB-CGB-O2B
26	bd	201	PEB	CAB-CBB-CGB-O2B
26	bm	1001	PEB	CAB-CBB-CGB-O2B
26	bm	1002	PEB	CAB-CBB-CGB-O2B
26	bn	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	bs	1002	PEB	CAB-CBB-CGB-O2B
26	bu	201	PEB	CAB-CBB-CGB-O2B
26	bx	201	PEB	CAB-CBB-CGB-O2B
26	by	1002	PEB	CAB-CBB-CGB-O2B
26	bz	202	PEB	CAB-CBB-CGB-O2B
26	bD	201	PEB	CAB-CBB-CGB-O2B
26	bR	201	PEB	CAB-CBB-CGB-O2B
26	bS	201	PEB	CAB-CBB-CGB-O2B
26	bV	201	PEB	CAB-CBB-CGB-O2B
26	bZ	301	PEB	CAB-CBB-CGB-O2B
26	cb	201	PEB	CAB-CBB-CGB-O2B
26	cj	201	PEB	CAB-CBB-CGB-O2B
26	cl	201	PEB	CAB-CBB-CGB-O2B
26	cu	201	PEB	CAB-CBB-CGB-O2B
26	cv	201	PEB	CAB-CBB-CGB-O2B
26	cx	201	PEB	CAB-CBB-CGB-O2B
26	cy	1001	PEB	CAB-CBB-CGB-O2B
26	cC	1001	PEB	CAB-CBB-CGB-O2B
26	cI	201	PEB	CAB-CBB-CGB-O2B
26	cK	201	PEB	CAB-CBB-CGB-O2B
26	cM	201	PEB	CAB-CBB-CGB-O2B
26	cO	202	PEB	CAB-CBB-CGB-O2B
26	cU	201	PEB	CAB-CBB-CGB-O2B
26	cW	201	PEB	CAB-CBB-CGB-O2B
26	cW	202	PEB	CAB-CBB-CGB-O2B
26	cX	201	PEB	CAB-CBB-CGB-O2B
26	db	201	PEB	CAB-CBB-CGB-O2B
26	dc	201	PEB	CAB-CBB-CGB-O2B
26	df	201	PEB	CAB-CBB-CGB-O2B
26	dg	201	PEB	CAB-CBB-CGB-O2B
26	dm	202	PEB	CAB-CBB-CGB-O2B
26	dn	202	PEB	CAB-CBB-CGB-O2B
26	do	201	PEB	CAB-CBB-CGB-O2B
26	dp	201	PEB	CAB-CBB-CGB-O2B
26	dq	201	PEB	CAB-CBB-CGB-O2B
26	dt	202	PEB	CAB-CBB-CGB-O2B
26	dv	201	PEB	CAB-CBB-CGB-O2B
26	dw	402	PEB	CAB-CBB-CGB-O2B
26	dx	401	PEB	CAB-CBB-CGB-O2B
26	dx	403	PEB	CAB-CBB-CGB-O2B
26	dA	201	PEB	CAB-CBB-CGB-O2B
26	dB	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	dC	201	PEB	CAB-CBB-CGB-O2B
26	dF	201	PEB	CAB-CBB-CGB-O2B
26	dF	202	PEB	CAB-CBB-CGB-O2B
26	dH	201	PEB	CAB-CBB-CGB-O2B
26	dJ	201	PEB	CAB-CBB-CGB-O2B
26	dM	1001	PEB	CAB-CBB-CGB-O2B
26	dM	1002	PEB	CAB-CBB-CGB-O2B
26	dQ	201	PEB	CAB-CBB-CGB-O2B
26	dR	202	PEB	CAB-CBB-CGB-O2B
26	dT	201	PEB	CAB-CBB-CGB-O2B
26	dU	201	PEB	CAB-CBB-CGB-O2B
26	dW	201	PEB	CAB-CBB-CGB-O2B
26	dW	202	PEB	CAB-CBB-CGB-O2B
26	dX	202	PEB	CAB-CBB-CGB-O2B
26	dZ	1001	PEB	CAB-CBB-CGB-O2B
26	eb	201	PEB	CAB-CBB-CGB-O2B
26	ek	1001	PEB	CAB-CBB-CGB-O2B
26	em	201	PEB	CAB-CBB-CGB-O2B
26	en	201	PEB	CAB-CBB-CGB-O2B
26	eF	202	PEB	CAB-CBB-CGB-O2B
26	eJ	201	PEB	CAB-CBB-CGB-O2B
26	eM	1002	PEB	CAB-CBB-CGB-O2B
26	eR	202	PEB	CAB-CBB-CGB-O2B
26	eS	202	PEB	CAB-CBB-CGB-O2B
26	eT	202	PEB	CAB-CBB-CGB-O2B
26	eU	201	PEB	CAB-CBB-CGB-O2B
26	eW	201	PEB	CAB-CBB-CGB-O2B
26	eW	202	PEB	CAB-CBB-CGB-O2B
26	la	1001	PEB	CAB-CBB-CGB-O2B
26	la	1002	PEB	CAB-CBB-CGB-O2B
26	lf	201	PEB	CAB-CBB-CGB-O2B
26	li	202	PEB	CAB-CBB-CGB-O2B
26	lr	201	PEB	CAB-CBB-CGB-O2B
26	ls	201	PEB	CAB-CBB-CGB-O2B
26	lu	201	PEB	CAB-CBB-CGB-O2B
26	lv	201	PEB	CAB-CBB-CGB-O2B
26	ly	402	PEB	CAB-CBB-CGB-O2B
26	fc	201	PEB	CAB-CBB-CGB-O2B
26	fd	302	PEB	CAB-CBB-CGB-O2B
26	ff	204	PEB	CAB-CBB-CGB-O2B
26	fm	201	PEB	CAB-CBB-CGB-O2B
26	fx	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	gb	1001	PEB	CAB-CBB-CGB-O2B
26	ge	201	PEB	CAB-CBB-CGB-O2B
26	gf	201	PEB	CAB-CBB-CGB-O2B
26	gh	201	PEB	CAB-CBB-CGB-O2B
26	gn	201	PEB	CAB-CBB-CGB-O2B
26	go	201	PEB	CAB-CBB-CGB-O2B
26	gq	201	PEB	CAB-CBB-CGB-O2B
26	hB	201	PEB	CAB-CBB-CGB-O2B
26	hD	201	PEB	CAB-CBB-CGB-O2B
26	hE	1001	PEB	CAB-CBB-CGB-O2B
26	hO	201	PEB	CAB-CBB-CGB-O2B
26	hS	201	PEB	CAB-CBB-CGB-O2B
26	hT	201	PEB	CAB-CBB-CGB-O2B
26	hW	201	PEB	CAB-CBB-CGB-O2B
26	iG	1001	PEB	CAB-CBB-CGB-O2B
26	jL	1001	PEB	CAB-CBB-CGB-O2B
26	kS	1001	PEB	CAB-CBB-CGB-O2B
26	kU	1001	PEB	CAB-CBB-CGB-O2B
26	kW	1001	PEB	CAB-CBB-CGB-O2B
26	e2	201	PEB	CAB-CBB-CGB-O2B
26	e2	202	PEB	CAB-CBB-CGB-O2B
26	f2	201	PEB	CAB-CBB-CGB-O2B
26	g2	202	PEB	CAB-CBB-CGB-O2B
26	h2	201	PEB	CAB-CBB-CGB-O2B
26	i2	201	PEB	CAB-CBB-CGB-O2B
26	l2	201	PEB	CAB-CBB-CGB-O2B
26	m2	202	PEB	CAB-CBB-CGB-O2B
26	n2	201	PEB	CAB-CBB-CGB-O2B
26	o2	1001	PEB	CAB-CBB-CGB-O2B
26	o2	1002	PEB	CAB-CBB-CGB-O2B
26	p2	201	PEB	CAB-CBB-CGB-O2B
26	q2	201	PEB	CAB-CBB-CGB-O2B
26	q2	202	PEB	CAB-CBB-CGB-O2B
26	r2	201	PEB	CAB-CBB-CGB-O2B
26	r2	202	PEB	CAB-CBB-CGB-O2B
26	t2	201	PEB	CAB-CBB-CGB-O2B
26	t2	202	PEB	CAB-CBB-CGB-O2B
26	u2	201	PEB	CAB-CBB-CGB-O2B
26	u2	202	PEB	CAB-CBB-CGB-O2B
26	v2	202	PEB	CAB-CBB-CGB-O2B
26	w2	201	PEB	CAB-CBB-CGB-O2B
26	w2	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	w2	203	PEB	CAB-CBB-CGB-O2B
26	x2	201	PEB	CAB-CBB-CGB-O2B
26	y2	201	PEB	CAB-CBB-CGB-O2B
26	y2	202	PEB	CAB-CBB-CGB-O2B
26	z2	201	PEB	CAB-CBB-CGB-O2B
26	z2	202	PEB	CAB-CBB-CGB-O2B
26	A2	1002	PEB	CAB-CBB-CGB-O2B
26	C2	301	PEB	CAB-CBB-CGB-O2B
26	D2	301	PEB	CAB-CBB-CGB-O2B
26	D2	302	PEB	CAB-CBB-CGB-O2B
26	E2	1001	PEB	CAB-CBB-CGB-O2B
26	F2	201	PEB	CAB-CBB-CGB-O2B
26	F2	202	PEB	CAB-CBB-CGB-O2B
26	G2	201	PEB	CAB-CBB-CGB-O2B
26	G2	202	PEB	CAB-CBB-CGB-O2B
26	I2	201	PEB	CAB-CBB-CGB-O2B
26	I2	202	PEB	CAB-CBB-CGB-O2B
26	J2	201	PEB	CAB-CBB-CGB-O2B
26	K2	201	PEB	CAB-CBB-CGB-O2B
26	L2	201	PEB	CAB-CBB-CGB-O2B
26	M2	201	PEB	CAB-CBB-CGB-O2B
26	M2	202	PEB	CAB-CBB-CGB-O2B
26	N2	202	PEB	CAB-CBB-CGB-O2B
26	O2	202	PEB	CAB-CBB-CGB-O2B
26	P2	201	PEB	CAB-CBB-CGB-O2B
26	Q2	1001	PEB	CAB-CBB-CGB-O2B
26	V2	201	PEB	CAB-CBB-CGB-O2B
26	W2	201	PEB	CAB-CBB-CGB-O2B
26	W2	202	PEB	CAB-CBB-CGB-O2B
26	X2	201	PEB	CAB-CBB-CGB-O2B
26	Y2	201	PEB	CAB-CBB-CGB-O2B
26	A3	201	PEB	CAB-CBB-CGB-O2B
26	B3	201	PEB	CAB-CBB-CGB-O2B
26	C3	1001	PEB	CAB-CBB-CGB-O2B
26	D3	201	PEB	CAB-CBB-CGB-O2B
26	E3	201	PEB	CAB-CBB-CGB-O2B
26	G3	201	PEB	CAB-CBB-CGB-O2B
26	I3	201	PEB	CAB-CBB-CGB-O2B
26	J3	201	PEB	CAB-CBB-CGB-O2B
26	K3	201	PEB	CAB-CBB-CGB-O2B
26	L3	201	PEB	CAB-CBB-CGB-O2B
26	M3	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	N3	201	PEB	CAB-CBB-CGB-O2B
26	O3	1001	PEB	CAB-CBB-CGB-O2B
26	P3	201	PEB	CAB-CBB-CGB-O2B
26	Q3	201	PEB	CAB-CBB-CGB-O2B
26	S3	201	PEB	CAB-CBB-CGB-O2B
26	S3	203	PEB	CAB-CBB-CGB-O2B
26	T3	201	PEB	CAB-CBB-CGB-O2B
26	V3	201	PEB	CAB-CBB-CGB-O2B
26	X3	201	PEB	CAB-CBB-CGB-O2B
26	Y3	201	PEB	CAB-CBB-CGB-O2B
26	Z3	201	PEB	CAB-CBB-CGB-O2B
26	a3	1003	PEB	CAB-CBB-CGB-O2B
26	b3	501	PEB	CAB-CBB-CGB-O2B
26	b3	502	PEB	CAB-CBB-CGB-O2B
26	e3	1001	PEB	CAB-CBB-CGB-O2B
26	f3	201	PEB	CAB-CBB-CGB-O2B
26	g3	201	PEB	CAB-CBB-CGB-O2B
26	i3	201	PEB	CAB-CBB-CGB-O2B
26	l3	201	PEB	CAB-CBB-CGB-O2B
26	o3	201	PEB	CAB-CBB-CGB-O2B
26	p3	201	PEB	CAB-CBB-CGB-O2B
26	q3	1001	PEB	CAB-CBB-CGB-O2B
26	r3	201	PEB	CAB-CBB-CGB-O2B
26	s3	201	PEB	CAB-CBB-CGB-O2B
26	t3	201	PEB	CAB-CBB-CGB-O2B
26	u3	201	PEB	CAB-CBB-CGB-O2B
26	w3	201	PEB	CAB-CBB-CGB-O2B
26	x3	201	PEB	CAB-CBB-CGB-O2B
26	y3	201	PEB	CAB-CBB-CGB-O2B
26	z3	201	PEB	CAB-CBB-CGB-O2B
26	B4	201	PEB	CAB-CBB-CGB-O2B
26	C4	1001	PEB	CAB-CBB-CGB-O2B
26	E4	202	PEB	CAB-CBB-CGB-O2B
26	F4	201	PEB	CAB-CBB-CGB-O2B
26	F4	202	PEB	CAB-CBB-CGB-O2B
26	G4	202	PEB	CAB-CBB-CGB-O2B
26	H4	201	PEB	CAB-CBB-CGB-O2B
26	I4	201	PEB	CAB-CBB-CGB-O2B
26	I4	202	PEB	CAB-CBB-CGB-O2B
26	J4	201	PEB	CAB-CBB-CGB-O2B
26	J4	202	PEB	CAB-CBB-CGB-O2B
26	K4	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	K4	202	PEB	CAB-CBB-CGB-O2B
26	L4	201	PEB	CAB-CBB-CGB-O2B
26	L4	202	PEB	CAB-CBB-CGB-O2B
26	M4	201	PEB	CAB-CBB-CGB-O2B
26	N4	201	PEB	CAB-CBB-CGB-O2B
26	O4	1001	PEB	CAB-CBB-CGB-O2B
26	O4	1002	PEB	CAB-CBB-CGB-O2B
26	P4	201	PEB	CAB-CBB-CGB-O2B
26	P4	202	PEB	CAB-CBB-CGB-O2B
26	Q4	202	PEB	CAB-CBB-CGB-O2B
26	Q4	203	PEB	CAB-CBB-CGB-O2B
26	R4	202	PEB	CAB-CBB-CGB-O2B
26	S4	201	PEB	CAB-CBB-CGB-O2B
26	S4	202	PEB	CAB-CBB-CGB-O2B
26	T4	201	PEB	CAB-CBB-CGB-O2B
26	U4	201	PEB	CAB-CBB-CGB-O2B
26	U4	202	PEB	CAB-CBB-CGB-O2B
26	V4	202	PEB	CAB-CBB-CGB-O2B
26	X4	201	PEB	CAB-CBB-CGB-O2B
26	X4	202	PEB	CAB-CBB-CGB-O2B
26	Y4	201	PEB	CAB-CBB-CGB-O2B
26	Y4	202	PEB	CAB-CBB-CGB-O2B
26	Z4	201	PEB	CAB-CBB-CGB-O2B
26	34	1007	PEB	CAB-CBB-CGB-O2B
26	44	301	PEB	CAB-CBB-CGB-O2B
26	a4	201	PEB	CAB-CBB-CGB-O2B
26	b4	1001	PEB	CAB-CBB-CGB-O2B
26	d4	201	PEB	CAB-CBB-CGB-O2B
26	e4	201	PEB	CAB-CBB-CGB-O2B
26	g4	201	PEB	CAB-CBB-CGB-O2B
26	h4	202	PEB	CAB-CBB-CGB-O2B
26	i4	201	PEB	CAB-CBB-CGB-O2B
26	j4	201	PEB	CAB-CBB-CGB-O2B
26	l4	201	PEB	CAB-CBB-CGB-O2B
26	m4	1001	PEB	CAB-CBB-CGB-O2B
26	n4	201	PEB	CAB-CBB-CGB-O2B
26	o4	201	PEB	CAB-CBB-CGB-O2B
26	o4	202	PEB	CAB-CBB-CGB-O2B
26	p4	201	PEB	CAB-CBB-CGB-O2B
26	q4	201	PEB	CAB-CBB-CGB-O2B
26	q4	202	PEB	CAB-CBB-CGB-O2B
26	s4	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	t4	201	PEB	CAB-CBB-CGB-O2B
26	t4	202	PEB	CAB-CBB-CGB-O2B
26	u4	202	PEB	CAB-CBB-CGB-O2B
26	x4	201	PEB	CAB-CBB-CGB-O2B
26	y4	1001	PEB	CAB-CBB-CGB-O2B
26	y4	1002	PEB	CAB-CBB-CGB-O2B
26	z4	201	PEB	CAB-CBB-CGB-O2B
26	z4	202	PEB	CAB-CBB-CGB-O2B
26	A5	201	PEB	CAB-CBB-CGB-O2B
26	B5	201	PEB	CAB-CBB-CGB-O2B
26	E5	201	PEB	CAB-CBB-CGB-O2B
26	F5	201	PEB	CAB-CBB-CGB-O2B
26	G5	201	PEB	CAB-CBB-CGB-O2B
26	H5	201	PEB	CAB-CBB-CGB-O2B
26	I5	201	PEB	CAB-CBB-CGB-O2B
26	J5	201	PEB	CAB-CBB-CGB-O2B
26	K5	1001	PEB	CAB-CBB-CGB-O2B
26	L5	201	PEB	CAB-CBB-CGB-O2B
26	M5	201	PEB	CAB-CBB-CGB-O2B
26	N5	201	PEB	CAB-CBB-CGB-O2B
26	O5	201	PEB	CAB-CBB-CGB-O2B
26	R5	201	PEB	CAB-CBB-CGB-O2B
26	S5	201	PEB	CAB-CBB-CGB-O2B
26	T5	201	PEB	CAB-CBB-CGB-O2B
26	U5	201	PEB	CAB-CBB-CGB-O2B
26	V5	201	PEB	CAB-CBB-CGB-O2B
26	W5	301	PEB	CAB-CBB-CGB-O2B
26	X5	401	PEB	CAB-CBB-CGB-O2B
26	Y5	1001	PEB	CAB-CBB-CGB-O2B
26	Z5	301	PEB	CAB-CBB-CGB-O2B
26	b5	1001	PEB	CAB-CBB-CGB-O2B
26	c5	202	PEB	CAB-CBB-CGB-O2B
26	d5	201	PEB	CAB-CBB-CGB-O2B
26	g5	201	PEB	CAB-CBB-CGB-O2B
26	h5	201	PEB	CAB-CBB-CGB-O2B
26	j5	201	PEB	CAB-CBB-CGB-O2B
26	l5	202	PEB	CAB-CBB-CGB-O2B
26	o5	201	PEB	CAB-CBB-CGB-O2B
26	q5	201	PEB	CAB-CBB-CGB-O2B
26	r5	201	PEB	CAB-CBB-CGB-O2B
26	s5	201	PEB	CAB-CBB-CGB-O2B
26	t5	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	u5	201	PEB	CAB-CBB-CGB-O2B
26	v5	201	PEB	CAB-CBB-CGB-O2B
26	y5	1001	PEB	CAB-CBB-CGB-O2B
26	z5	201	PEB	CAB-CBB-CGB-O2B
26	f8	202	PEB	CAB-CBB-CGB-O2B
26	g8	201	PEB	CAB-CBB-CGB-O2B
26	h8	201	PEB	CAB-CBB-CGB-O2B
26	i8	201	PEB	CAB-CBB-CGB-O2B
26	j8	201	PEB	CAB-CBB-CGB-O2B
26	j8	202	PEB	CAB-CBB-CGB-O2B
26	k8	201	PEB	CAB-CBB-CGB-O2B
26	k8	202	PEB	CAB-CBB-CGB-O2B
26	k8	203	PEB	CAB-CBB-CGB-O2B
26	l8	202	PEB	CAB-CBB-CGB-O2B
26	m8	201	PEB	CAB-CBB-CGB-O2B
26	m8	202	PEB	CAB-CBB-CGB-O2B
26	A6	1001	PEB	CAB-CBB-CGB-O2B
26	B6	201	PEB	CAB-CBB-CGB-O2B
26	D6	201	PEB	CAB-CBB-CGB-O2B
26	E6	201	PEB	CAB-CBB-CGB-O2B
26	E6	202	PEB	CAB-CBB-CGB-O2B
26	F6	202	PEB	CAB-CBB-CGB-O2B
26	G6	201	PEB	CAB-CBB-CGB-O2B
26	H6	202	PEB	CAB-CBB-CGB-O2B
26	I6	202	PEB	CAB-CBB-CGB-O2B
26	J6	201	PEB	CAB-CBB-CGB-O2B
26	K6	201	PEB	CAB-CBB-CGB-O2B
26	K6	202	PEB	CAB-CBB-CGB-O2B
26	M6	1001	PEB	CAB-CBB-CGB-O2B
26	M6	1002	PEB	CAB-CBB-CGB-O2B
26	O6	201	PEB	CAB-CBB-CGB-O2B
26	O6	202	PEB	CAB-CBB-CGB-O2B
26	P6	201	PEB	CAB-CBB-CGB-O2B
26	P6	202	PEB	CAB-CBB-CGB-O2B
26	Q6	201	PEB	CAB-CBB-CGB-O2B
26	Q6	202	PEB	CAB-CBB-CGB-O2B
26	S6	201	PEB	CAB-CBB-CGB-O2B
26	S6	202	PEB	CAB-CBB-CGB-O2B
26	T6	201	PEB	CAB-CBB-CGB-O2B
26	T6	202	PEB	CAB-CBB-CGB-O2B
26	U6	201	PEB	CAB-CBB-CGB-O2B
26	V6	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	W6	201	PEB	CAB-CBB-CGB-O2B
26	W6	202	PEB	CAB-CBB-CGB-O2B
26	X6	201	PEB	CAB-CBB-CGB-O2B
26	Y6	201	PEB	CAB-CBB-CGB-O2B
26	a6	201	PEB	CAB-CBB-CGB-O2B
26	b6	201	PEB	CAB-CBB-CGB-O2B
26	c6	1001	PEB	CAB-CBB-CGB-O2B
26	c6	1003	PEB	CAB-CBB-CGB-O2B
26	d6	201	PEB	CAB-CBB-CGB-O2B
26	e6	201	PEB	CAB-CBB-CGB-O2B
26	f6	201	PEB	CAB-CBB-CGB-O2B
26	g6	201	PEB	CAB-CBB-CGB-O2B
26	g6	202	PEB	CAB-CBB-CGB-O2B
26	h6	201	PEB	CAB-CBB-CGB-O2B
26	h6	202	PEB	CAB-CBB-CGB-O2B
26	i6	202	PEB	CAB-CBB-CGB-O2B
26	j6	201	PEB	CAB-CBB-CGB-O2B
26	j6	202	PEB	CAB-CBB-CGB-O2B
26	k6	1001	PEB	CAB-CBB-CGB-O2B
26	k6	1002	PEB	CAB-CBB-CGB-O2B
26	l6	201	PEB	CAB-CBB-CGB-O2B
26	l6	202	PEB	CAB-CBB-CGB-O2B
26	m6	201	PEB	CAB-CBB-CGB-O2B
26	m6	202	PEB	CAB-CBB-CGB-O2B
26	o6	201	PEB	CAB-CBB-CGB-O2B
26	p6	201	PEB	CAB-CBB-CGB-O2B
26	q6	201	PEB	CAB-CBB-CGB-O2B
26	q6	202	PEB	CAB-CBB-CGB-O2B
26	r6	201	PEB	CAB-CBB-CGB-O2B
26	r6	202	PEB	CAB-CBB-CGB-O2B
26	s6	202	PEB	CAB-CBB-CGB-O2B
26	t6	202	PEB	CAB-CBB-CGB-O2B
26	u6	201	PEB	CAB-CBB-CGB-O2B
26	u6	202	PEB	CAB-CBB-CGB-O2B
26	v6	201	PEB	CAB-CBB-CGB-O2B
26	v6	202	PEB	CAB-CBB-CGB-O2B
26	w6	1001	PEB	CAB-CBB-CGB-O2B
26	w6	1002	PEB	CAB-CBB-CGB-O2B
26	x6	201	PEB	CAB-CBB-CGB-O2B
26	y6	201	PEB	CAB-CBB-CGB-O2B
26	y6	202	PEB	CAB-CBB-CGB-O2B
26	y6	203	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	z6	202	PEB	CAB-CBB-CGB-O2B
26	o8	202	PEB	CAB-CBB-CGB-O2B
26	p8	201	PEB	CAB-CBB-CGB-O2B
26	s8	201	PEB	CAB-CBB-CGB-O2B
26	t8	201	PEB	CAB-CBB-CGB-O2B
26	u8	201	PEB	CAB-CBB-CGB-O2B
26	C7	201	PEB	CAB-CBB-CGB-O2B
26	D7	201	PEB	CAB-CBB-CGB-O2B
26	E7	201	PEB	CAB-CBB-CGB-O2B
26	I7	201	PEB	CAB-CBB-CGB-O2B
26	K7	201	PEB	CAB-CBB-CGB-O2B
26	M7	1002	PEB	CAB-CBB-CGB-O2B
26	N7	201	PEB	CAB-CBB-CGB-O2B
26	O7	201	PEB	CAB-CBB-CGB-O2B
26	P7	201	PEB	CAB-CBB-CGB-O2B
26	Q7	201	PEB	CAB-CBB-CGB-O2B
26	R7	201	PEB	CAB-CBB-CGB-O2B
26	S7	201	PEB	CAB-CBB-CGB-O2B
26	T7	201	PEB	CAB-CBB-CGB-O2B
26	Y7	1001	PEB	CAB-CBB-CGB-O2B
26	a7	201	PEB	CAB-CBB-CGB-O2B
26	c7	201	PEB	CAB-CBB-CGB-O2B
26	d7	201	PEB	CAB-CBB-CGB-O2B
26	e7	201	PEB	CAB-CBB-CGB-O2B
26	f7	201	PEB	CAB-CBB-CGB-O2B
26	h7	201	PEB	CAB-CBB-CGB-O2B
26	i7	201	PEB	CAB-CBB-CGB-O2B
26	k7	1001	PEB	CAB-CBB-CGB-O2B
26	l7	201	PEB	CAB-CBB-CGB-O2B
26	m7	201	PEB	CAB-CBB-CGB-O2B
26	n7	201	PEB	CAB-CBB-CGB-O2B
26	o7	201	PEB	CAB-CBB-CGB-O2B
26	q7	201	PEB	CAB-CBB-CGB-O2B
26	r7	201	PEB	CAB-CBB-CGB-O2B
26	t7	201	PEB	CAB-CBB-CGB-O2B
26	u7	201	PEB	CAB-CBB-CGB-O2B
26	v7	201	PEB	CAB-CBB-CGB-O2B
26	x7	201	PEB	CAB-CBB-CGB-O2B
26	y7	201	PEB	CAB-CBB-CGB-O2B
26	z7	201	PEB	CAB-CBB-CGB-O2B
26	a8	602	PEB	CAB-CBB-CGB-O2B
26	b8	1001	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	b8	1002	PEB	CAB-CBB-CGB-O2B
26	c8	302	PEB	CAB-CBB-CGB-O2B
26	e8	301	PEB	CAB-CBB-CGB-O2B
26	e8	302	PEB	CAB-CBB-CGB-O2B
26	a9	601	PEB	CAB-CBB-CGB-O2B
26	a9	603	PEB	CAB-CBB-CGB-O2B
26	b9	401	PEB	CAB-CBB-CGB-O2B
26	b9	403	PEB	CAB-CBB-CGB-O2B
26	b9	404	PEB	CAB-CBB-CGB-O2B
26	c9	301	PEB	CAB-CBB-CGB-O2B
26	c9	302	PEB	CAB-CBB-CGB-O2B
26	d9	302	PEB	CAB-CBB-CGB-O2B
26	d9	303	PEB	CAB-CBB-CGB-O2B
26	e9	301	PEB	CAB-CBB-CGB-O2B
26	e9	302	PEB	CAB-CBB-CGB-O2B
26	v8	201	PEB	CAB-CBB-CGB-O2B
26	v8	202	PEB	CAB-CBB-CGB-O2B
26	w8	201	PEB	CAB-CBB-CGB-O2B
26	w8	202	PEB	CAB-CBB-CGB-O2B
26	x8	201	PEB	CAB-CBB-CGB-O2B
26	x8	202	PEB	CAB-CBB-CGB-O2B
26	y8	201	PEB	CAB-CBB-CGB-O2B
26	z8	201	PEB	CAB-CBB-CGB-O2B
26	z8	202	PEB	CAB-CBB-CGB-O2B
26	A8	201	PEB	CAB-CBB-CGB-O2B
26	A8	202	PEB	CAB-CBB-CGB-O2B
26	B8	201	PEB	CAB-CBB-CGB-O2B
26	B8	202	PEB	CAB-CBB-CGB-O2B
26	C8	201	PEB	CAB-CBB-CGB-O2B
26	D8	201	PEB	CAB-CBB-CGB-O2B
26	D8	202	PEB	CAB-CBB-CGB-O2B
26	E8	201	PEB	CAB-CBB-CGB-O2B
26	E8	202	PEB	CAB-CBB-CGB-O2B
26	F8	1001	PEB	CAB-CBB-CGB-O2B
26	G8	201	PEB	CAB-CBB-CGB-O2B
26	I8	201	PEB	CAB-CBB-CGB-O2B
26	I8	202	PEB	CAB-CBB-CGB-O2B
26	J8	201	PEB	CAB-CBB-CGB-O2B
26	K8	201	PEB	CAB-CBB-CGB-O2B
26	K8	202	PEB	CAB-CBB-CGB-O2B
26	L8	201	PEB	CAB-CBB-CGB-O2B
26	L8	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	M8	201	PEB	CAB-CBB-CGB-O2B
26	M8	202	PEB	CAB-CBB-CGB-O2B
26	N8	201	PEB	CAB-CBB-CGB-O2B
26	N8	202	PEB	CAB-CBB-CGB-O2B
26	O8	202	PEB	CAB-CBB-CGB-O2B
26	P8	202	PEB	CAB-CBB-CGB-O2B
26	Q8	202	PEB	CAB-CBB-CGB-O2B
26	S8	401	PEB	CAB-CBB-CGB-O2B
26	T8	301	PEB	CAB-CBB-CGB-O2B
26	U8	1001	PEB	CAB-CBB-CGB-O2B
26	U8	1002	PEB	CAB-CBB-CGB-O2B
26	U8	1003	PEB	CAB-CBB-CGB-O2B
26	V8	1001	PEB	CAB-CBB-CGB-O2B
26	W8	202	PEB	CAB-CBB-CGB-O2B
26	X8	201	PEB	CAB-CBB-CGB-O2B
26	Y8	201	PEB	CAB-CBB-CGB-O2B
26	Y8	202	PEB	CAB-CBB-CGB-O2B
26	Z8	201	PEB	CAB-CBB-CGB-O2B
26	g9	201	PEB	CAB-CBB-CGB-O2B
26	h9	201	PEB	CAB-CBB-CGB-O2B
26	h9	202	PEB	CAB-CBB-CGB-O2B
26	i9	201	PEB	CAB-CBB-CGB-O2B
26	j9	201	PEB	CAB-CBB-CGB-O2B
26	j9	202	PEB	CAB-CBB-CGB-O2B
26	k9	201	PEB	CAB-CBB-CGB-O2B
26	l9	202	PEB	CAB-CBB-CGB-O2B
26	m9	1001	PEB	CAB-CBB-CGB-O2B
26	o9	201	PEB	CAB-CBB-CGB-O2B
26	q9	201	PEB	CAB-CBB-CGB-O2B
26	q9	202	PEB	CAB-CBB-CGB-O2B
26	r9	201	PEB	CAB-CBB-CGB-O2B
26	r9	202	PEB	CAB-CBB-CGB-O2B
26	s9	201	PEB	CAB-CBB-CGB-O2B
26	s9	202	PEB	CAB-CBB-CGB-O2B
26	t9	201	PEB	CAB-CBB-CGB-O2B
26	t9	202	PEB	CAB-CBB-CGB-O2B
26	u9	202	PEB	CAB-CBB-CGB-O2B
26	w9	201	PEB	CAB-CBB-CGB-O2B
26	w9	202	PEB	CAB-CBB-CGB-O2B
26	y9	1001	PEB	CAB-CBB-CGB-O2B
26	y9	1002	PEB	CAB-CBB-CGB-O2B
26	z9	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	A9	201	PEB	CAB-CBB-CGB-O2B
26	B9	201	PEB	CAB-CBB-CGB-O2B
26	C9	201	PEB	CAB-CBB-CGB-O2B
26	D9	201	PEB	CAB-CBB-CGB-O2B
26	E9	201	PEB	CAB-CBB-CGB-O2B
26	F9	201	PEB	CAB-CBB-CGB-O2B
26	I9	201	PEB	CAB-CBB-CGB-O2B
26	J9	201	PEB	CAB-CBB-CGB-O2B
26	L9	201	PEB	CAB-CBB-CGB-O2B
26	M9	201	PEB	CAB-CBB-CGB-O2B
26	N9	201	PEB	CAB-CBB-CGB-O2B
26	O9	201	PEB	CAB-CBB-CGB-O2B
26	Q9	201	PEB	CAB-CBB-CGB-O2B
26	R9	201	PEB	CAB-CBB-CGB-O2B
26	S9	201	PEB	CAB-CBB-CGB-O2B
26	T9	201	PEB	CAB-CBB-CGB-O2B
26	U9	201	PEB	CAB-CBB-CGB-O2B
26	V9	201	PEB	CAB-CBB-CGB-O2B
26	X9	401	PEB	CAB-CBB-CGB-O2B
26	Y9	302	PEB	CAB-CBB-CGB-O2B
26	Z9	1001	PEB	CAB-CBB-CGB-O2B
26	Z9	1003	PEB	CAB-CBB-CGB-O2B
26	ac	201	PEB	CAB-CBB-CGB-O2B
26	ae	201	PEB	CAB-CBB-CGB-O2B
26	ag	201	PEB	CAB-CBB-CGB-O2B
26	ah	201	PEB	CAB-CBB-CGB-O2B
26	ai	201	PEB	CAB-CBB-CGB-O2B
26	al	201	PEB	CAB-CBB-CGB-O2B
26	am	1001	PEB	CAB-CBB-CGB-O2B
26	ao	201	PEB	CAB-CBB-CGB-O2B
26	ar	201	PEB	CAB-CBB-CGB-O2B
26	as	201	PEB	CAB-CBB-CGB-O2B
26	at	201	PEB	CAB-CBB-CGB-O2B
26	au	201	PEB	CAB-CBB-CGB-O2B
26	av	201	PEB	CAB-CBB-CGB-O2B
26	aw	201	PEB	CAB-CBB-CGB-O2B
26	ay	1001	PEB	CAB-CBB-CGB-O2B
26	aB	201	PEB	CAB-CBB-CGB-O2B
26	aB	202	PEB	CAB-CBB-CGB-O2B
26	aC	201	PEB	CAB-CBB-CGB-O2B
26	aC	202	PEB	CAB-CBB-CGB-O2B
26	aD	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	aE	201	PEB	CAB-CBB-CGB-O2B
26	aF	201	PEB	CAB-CBB-CGB-O2B
26	aF	204	PEB	CAB-CBB-CGB-O2B
26	aG	201	PEB	CAB-CBB-CGB-O2B
26	aH	201	PEB	CAB-CBB-CGB-O2B
26	aH	202	PEB	CAB-CBB-CGB-O2B
26	aI	201	PEB	CAB-CBB-CGB-O2B
26	aJ	201	PEB	CAB-CBB-CGB-O2B
26	aJ	202	PEB	CAB-CBB-CGB-O2B
26	aK	1001	PEB	CAB-CBB-CGB-O2B
26	aK	1002	PEB	CAB-CBB-CGB-O2B
26	aL	201	PEB	CAB-CBB-CGB-O2B
26	aL	202	PEB	CAB-CBB-CGB-O2B
26	aM	201	PEB	CAB-CBB-CGB-O2B
26	aM	202	PEB	CAB-CBB-CGB-O2B
26	aN	201	PEB	CAB-CBB-CGB-O2B
26	aN	204	PEB	CAB-CBB-CGB-O2B
26	aO	201	PEB	CAB-CBB-CGB-O2B
26	aP	201	PEB	CAB-CBB-CGB-O2B
26	aQ	201	PEB	CAB-CBB-CGB-O2B
26	aR	201	PEB	CAB-CBB-CGB-O2B
26	aR	202	PEB	CAB-CBB-CGB-O2B
26	aS	201	PEB	CAB-CBB-CGB-O2B
26	aS	202	PEB	CAB-CBB-CGB-O2B
26	aT	202	PEB	CAB-CBB-CGB-O2B
26	aU	201	PEB	CAB-CBB-CGB-O2B
26	aU	202	PEB	CAB-CBB-CGB-O2B
26	aV	202	PEB	CAB-CBB-CGB-O2B
26	aW	301	PEB	CAB-CBB-CGB-O2B
26	aW	302	PEB	CAB-CBB-CGB-O2B
26	aX	402	PEB	CAB-CBB-CGB-O2B
26	aY	401	PEB	CAB-CBB-CGB-O2B
26	aZ	301	PEB	CAB-CBB-CGB-O2B
26	ba	1001	PEB	CAB-CBB-CGB-O2B
26	bb	201	PEB	CAB-CBB-CGB-O2B
26	bd	202	PEB	CAB-CBB-CGB-O2B
26	be	201	PEB	CAB-CBB-CGB-O2B
26	bf	201	PEB	CAB-CBB-CGB-O2B
26	bg	201	PEB	CAB-CBB-CGB-O2B
26	bh	201	PEB	CAB-CBB-CGB-O2B
26	bh	202	PEB	CAB-CBB-CGB-O2B
26	bi	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	bj	201	PEB	CAB-CBB-CGB-O2B
26	bj	202	PEB	CAB-CBB-CGB-O2B
26	bk	201	PEB	CAB-CBB-CGB-O2B
26	bl	201	PEB	CAB-CBB-CGB-O2B
26	bl	202	PEB	CAB-CBB-CGB-O2B
26	bo	201	PEB	CAB-CBB-CGB-O2B
26	bp	201	PEB	CAB-CBB-CGB-O2B
26	bq	201	PEB	CAB-CBB-CGB-O2B
26	bq	202	PEB	CAB-CBB-CGB-O2B
26	br	201	PEB	CAB-CBB-CGB-O2B
26	br	202	PEB	CAB-CBB-CGB-O2B
26	bs	1001	PEB	CAB-CBB-CGB-O2B
26	bs	1003	PEB	CAB-CBB-CGB-O2B
26	bt	201	PEB	CAB-CBB-CGB-O2B
26	bt	202	PEB	CAB-CBB-CGB-O2B
26	bu	202	PEB	CAB-CBB-CGB-O2B
26	bv	201	PEB	CAB-CBB-CGB-O2B
26	bv	202	PEB	CAB-CBB-CGB-O2B
26	bw	201	PEB	CAB-CBB-CGB-O2B
26	bw	202	PEB	CAB-CBB-CGB-O2B
26	bx	202	PEB	CAB-CBB-CGB-O2B
26	by	1001	PEB	CAB-CBB-CGB-O2B
26	bz	201	PEB	CAB-CBB-CGB-O2B
26	bA	201	PEB	CAB-CBB-CGB-O2B
26	bB	201	PEB	CAB-CBB-CGB-O2B
26	bC	201	PEB	CAB-CBB-CGB-O2B
26	bE	201	PEB	CAB-CBB-CGB-O2B
26	bF	201	PEB	CAB-CBB-CGB-O2B
26	bG	201	PEB	CAB-CBB-CGB-O2B
26	bH	201	PEB	CAB-CBB-CGB-O2B
26	bI	201	PEB	CAB-CBB-CGB-O2B
26	bJ	201	PEB	CAB-CBB-CGB-O2B
26	bK	1001	PEB	CAB-CBB-CGB-O2B
26	bL	201	PEB	CAB-CBB-CGB-O2B
26	bM	201	PEB	CAB-CBB-CGB-O2B
26	bN	201	PEB	CAB-CBB-CGB-O2B
26	bO	201	PEB	CAB-CBB-CGB-O2B
26	bP	201	PEB	CAB-CBB-CGB-O2B
26	bQ	201	PEB	CAB-CBB-CGB-O2B
26	bU	201	PEB	CAB-CBB-CGB-O2B
26	bW	301	PEB	CAB-CBB-CGB-O2B
26	bX	401	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	bX	402	PEB	CAB-CBB-CGB-O2B
26	bY	1001	PEB	CAB-CBB-CGB-O2B
26	bY	1003	PEB	CAB-CBB-CGB-O2B
26	bZ	303	PEB	CAB-CBB-CGB-O2B
26	ca	1001	PEB	CAB-CBB-CGB-O2B
26	cc	201	PEB	CAB-CBB-CGB-O2B
26	cd	201	PEB	CAB-CBB-CGB-O2B
26	ce	201	PEB	CAB-CBB-CGB-O2B
26	cg	201	PEB	CAB-CBB-CGB-O2B
26	ch	201	PEB	CAB-CBB-CGB-O2B
26	ci	201	PEB	CAB-CBB-CGB-O2B
26	ck	201	PEB	CAB-CBB-CGB-O2B
26	cm	1001	PEB	CAB-CBB-CGB-O2B
26	cp	201	PEB	CAB-CBB-CGB-O2B
26	cq	201	PEB	CAB-CBB-CGB-O2B
26	cr	201	PEB	CAB-CBB-CGB-O2B
26	cs	201	PEB	CAB-CBB-CGB-O2B
26	ct	201	PEB	CAB-CBB-CGB-O2B
26	cw	201	PEB	CAB-CBB-CGB-O2B
26	cz	201	PEB	CAB-CBB-CGB-O2B
26	cA	201	PEB	CAB-CBB-CGB-O2B
26	cB	201	PEB	CAB-CBB-CGB-O2B
26	cC	1003	PEB	CAB-CBB-CGB-O2B
26	cD	201	PEB	CAB-CBB-CGB-O2B
26	cE	201	PEB	CAB-CBB-CGB-O2B
26	cG	201	PEB	CAB-CBB-CGB-O2B
26	cJ	201	PEB	CAB-CBB-CGB-O2B
26	cL	201	PEB	CAB-CBB-CGB-O2B
26	cM	202	PEB	CAB-CBB-CGB-O2B
26	cN	201	PEB	CAB-CBB-CGB-O2B
26	cO	201	PEB	CAB-CBB-CGB-O2B
26	cP	201	PEB	CAB-CBB-CGB-O2B
26	cP	202	PEB	CAB-CBB-CGB-O2B
26	cQ	201	PEB	CAB-CBB-CGB-O2B
26	cR	201	PEB	CAB-CBB-CGB-O2B
26	cR	202	PEB	CAB-CBB-CGB-O2B
26	cS	201	PEB	CAB-CBB-CGB-O2B
26	cS	202	PEB	CAB-CBB-CGB-O2B
26	cT	1001	PEB	CAB-CBB-CGB-O2B
26	cT	1002	PEB	CAB-CBB-CGB-O2B
26	cU	202	PEB	CAB-CBB-CGB-O2B
26	cV	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	cV	202	PEB	CAB-CBB-CGB-O2B
26	cV	203	PEB	CAB-CBB-CGB-O2B
26	cX	202	PEB	CAB-CBB-CGB-O2B
26	cY	201	PEB	CAB-CBB-CGB-O2B
26	cZ	201	PEB	CAB-CBB-CGB-O2B
26	da	1001	PEB	CAB-CBB-CGB-O2B
26	dc	203	PEB	CAB-CBB-CGB-O2B
26	dd	201	PEB	CAB-CBB-CGB-O2B
26	de	201	PEB	CAB-CBB-CGB-O2B
26	dh	201	PEB	CAB-CBB-CGB-O2B
26	di	201	PEB	CAB-CBB-CGB-O2B
26	dj	201	PEB	CAB-CBB-CGB-O2B
26	dk	1001	PEB	CAB-CBB-CGB-O2B
26	dk	1002	PEB	CAB-CBB-CGB-O2B
26	dl	201	PEB	CAB-CBB-CGB-O2B
26	dm	201	PEB	CAB-CBB-CGB-O2B
26	dn	201	PEB	CAB-CBB-CGB-O2B
26	do	202	PEB	CAB-CBB-CGB-O2B
26	dp	202	PEB	CAB-CBB-CGB-O2B
26	dq	202	PEB	CAB-CBB-CGB-O2B
26	dr	201	PEB	CAB-CBB-CGB-O2B
26	dr	202	PEB	CAB-CBB-CGB-O2B
26	ds	201	PEB	CAB-CBB-CGB-O2B
26	ds	202	PEB	CAB-CBB-CGB-O2B
26	dt	201	PEB	CAB-CBB-CGB-O2B
26	du	201	PEB	CAB-CBB-CGB-O2B
26	du	202	PEB	CAB-CBB-CGB-O2B
26	du	203	PEB	CAB-CBB-CGB-O2B
26	dw	401	PEB	CAB-CBB-CGB-O2B
26	dw	403	PEB	CAB-CBB-CGB-O2B
26	dx	402	PEB	CAB-CBB-CGB-O2B
26	dx	404	PEB	CAB-CBB-CGB-O2B
26	dy	401	PEB	CAB-CBB-CGB-O2B
26	dz	401	PEB	CAB-CBB-CGB-O2B
26	dz	402	PEB	CAB-CBB-CGB-O2B
26	dA	202	PEB	CAB-CBB-CGB-O2B
26	dC	202	PEB	CAB-CBB-CGB-O2B
26	dD	201	PEB	CAB-CBB-CGB-O2B
26	dD	202	PEB	CAB-CBB-CGB-O2B
26	dE	201	PEB	CAB-CBB-CGB-O2B
26	dG	201	PEB	CAB-CBB-CGB-O2B
26	dG	202	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	dH	202	PEB	CAB-CBB-CGB-O2B
26	dI	1001	PEB	CAB-CBB-CGB-O2B
26	dI	1002	PEB	CAB-CBB-CGB-O2B
26	dK	201	PEB	CAB-CBB-CGB-O2B
26	dK	202	PEB	CAB-CBB-CGB-O2B
26	dL	201	PEB	CAB-CBB-CGB-O2B
26	dN	201	PEB	CAB-CBB-CGB-O2B
26	dN	202	PEB	CAB-CBB-CGB-O2B
26	dO	201	PEB	CAB-CBB-CGB-O2B
26	dO	202	PEB	CAB-CBB-CGB-O2B
26	dP	201	PEB	CAB-CBB-CGB-O2B
26	dP	202	PEB	CAB-CBB-CGB-O2B
26	dQ	202	PEB	CAB-CBB-CGB-O2B
26	dR	201	PEB	CAB-CBB-CGB-O2B
26	dS	201	PEB	CAB-CBB-CGB-O2B
26	dT	202	PEB	CAB-CBB-CGB-O2B
26	dV	201	PEB	CAB-CBB-CGB-O2B
26	dX	201	PEB	CAB-CBB-CGB-O2B
26	dY	201	PEB	CAB-CBB-CGB-O2B
26	ea	201	PEB	CAB-CBB-CGB-O2B
26	ea	202	PEB	CAB-CBB-CGB-O2B
26	ed	201	PEB	CAB-CBB-CGB-O2B
26	ed	202	PEB	CAB-CBB-CGB-O2B
26	ee	201	PEB	CAB-CBB-CGB-O2B
26	ef	201	PEB	CAB-CBB-CGB-O2B
26	eg	201	PEB	CAB-CBB-CGB-O2B
26	eh	201	PEB	CAB-CBB-CGB-O2B
26	ej	201	PEB	CAB-CBB-CGB-O2B
26	ej	202	PEB	CAB-CBB-CGB-O2B
26	el	201	PEB	CAB-CBB-CGB-O2B
26	eo	201	PEB	CAB-CBB-CGB-O2B
26	eo	202	PEB	CAB-CBB-CGB-O2B
26	ep	201	PEB	CAB-CBB-CGB-O2B
26	eq	201	PEB	CAB-CBB-CGB-O2B
26	eq	202	PEB	CAB-CBB-CGB-O2B
26	er	201	PEB	CAB-CBB-CGB-O2B
26	es	201	PEB	CAB-CBB-CGB-O2B
26	es	202	PEB	CAB-CBB-CGB-O2B
26	eu	201	PEB	CAB-CBB-CGB-O2B
26	ew	301	PEB	CAB-CBB-CGB-O2B
26	ey	1002	PEB	CAB-CBB-CGB-O2B
26	ey	1003	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	ez	1001	PEB	CAB-CBB-CGB-O2B
26	ez	1002	PEB	CAB-CBB-CGB-O2B
26	ez	1003	PEB	CAB-CBB-CGB-O2B
26	eA	1001	PEB	CAB-CBB-CGB-O2B
26	eB	202	PEB	CAB-CBB-CGB-O2B
26	eC	201	PEB	CAB-CBB-CGB-O2B
26	eC	202	PEB	CAB-CBB-CGB-O2B
26	eD	201	PEB	CAB-CBB-CGB-O2B
26	eD	202	PEB	CAB-CBB-CGB-O2B
26	eE	201	PEB	CAB-CBB-CGB-O2B
26	eE	202	PEB	CAB-CBB-CGB-O2B
26	eF	201	PEB	CAB-CBB-CGB-O2B
26	eG	201	PEB	CAB-CBB-CGB-O2B
26	eG	202	PEB	CAB-CBB-CGB-O2B
26	eH	201	PEB	CAB-CBB-CGB-O2B
26	eH	202	PEB	CAB-CBB-CGB-O2B
26	eI	201	PEB	CAB-CBB-CGB-O2B
26	eI	202	PEB	CAB-CBB-CGB-O2B
26	eK	201	PEB	CAB-CBB-CGB-O2B
26	eK	202	PEB	CAB-CBB-CGB-O2B
26	eM	1001	PEB	CAB-CBB-CGB-O2B
26	eN	201	PEB	CAB-CBB-CGB-O2B
26	eO	201	PEB	CAB-CBB-CGB-O2B
26	eO	202	PEB	CAB-CBB-CGB-O2B
26	eP	202	PEB	CAB-CBB-CGB-O2B
26	eP	203	PEB	CAB-CBB-CGB-O2B
26	eQ	201	PEB	CAB-CBB-CGB-O2B
26	eQ	202	PEB	CAB-CBB-CGB-O2B
26	eR	201	PEB	CAB-CBB-CGB-O2B
26	eS	201	PEB	CAB-CBB-CGB-O2B
26	eT	201	PEB	CAB-CBB-CGB-O2B
26	eU	202	PEB	CAB-CBB-CGB-O2B
26	eV	201	PEB	CAB-CBB-CGB-O2B
26	eY	402	PEB	CAB-CBB-CGB-O2B
26	eZ	401	PEB	CAB-CBB-CGB-O2B
26	lb	201	PEB	CAB-CBB-CGB-O2B
26	lb	202	PEB	CAB-CBB-CGB-O2B
26	lc	201	PEB	CAB-CBB-CGB-O2B
26	le	201	PEB	CAB-CBB-CGB-O2B
26	li	201	PEB	CAB-CBB-CGB-O2B
26	lk	201	PEB	CAB-CBB-CGB-O2B
26	ll	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	lm	1001	PEB	CAB-CBB-CGB-O2B
26	ln	201	PEB	CAB-CBB-CGB-O2B
26	lp	201	PEB	CAB-CBB-CGB-O2B
26	lq	201	PEB	CAB-CBB-CGB-O2B
26	lq	202	PEB	CAB-CBB-CGB-O2B
26	lt	201	PEB	CAB-CBB-CGB-O2B
26	ly	401	PEB	CAB-CBB-CGB-O2B
26	ly	403	PEB	CAB-CBB-CGB-O2B
26	lz	401	PEB	CAB-CBB-CGB-O2B
26	lz	402	PEB	CAB-CBB-CGB-O2B
26	fa	201	PEB	CAB-CBB-CGB-O2B
26	fb	201	PEB	CAB-CBB-CGB-O2B
26	fd	301	PEB	CAB-CBB-CGB-O2B
26	fd	303	PEB	CAB-CBB-CGB-O2B
26	fe	201	PEB	CAB-CBB-CGB-O2B
26	ff	201	PEB	CAB-CBB-CGB-O2B
26	fh	1001	PEB	CAB-CBB-CGB-O2B
26	fi	201	PEB	CAB-CBB-CGB-O2B
26	fj	201	PEB	CAB-CBB-CGB-O2B
26	fk	201	PEB	CAB-CBB-CGB-O2B
26	fl	201	PEB	CAB-CBB-CGB-O2B
26	fn	1001	PEB	CAB-CBB-CGB-O2B
26	fo	201	PEB	CAB-CBB-CGB-O2B
26	fp	201	PEB	CAB-CBB-CGB-O2B
26	fq	201	PEB	CAB-CBB-CGB-O2B
26	fr	201	PEB	CAB-CBB-CGB-O2B
26	fs	201	PEB	CAB-CBB-CGB-O2B
26	ft	201	PEB	CAB-CBB-CGB-O2B
26	fv	201	PEB	CAB-CBB-CGB-O2B
26	fw	201	PEB	CAB-CBB-CGB-O2B
26	ga	201	PEB	CAB-CBB-CGB-O2B
26	gc	201	PEB	CAB-CBB-CGB-O2B
26	gg	201	PEB	CAB-CBB-CGB-O2B
26	gi	201	PEB	CAB-CBB-CGB-O2B
26	gj	201	PEB	CAB-CBB-CGB-O2B
26	gk	201	PEB	CAB-CBB-CGB-O2B
26	gl	201	PEB	CAB-CBB-CGB-O2B
26	gm	1001	PEB	CAB-CBB-CGB-O2B
26	gp	201	PEB	CAB-CBB-CGB-O2B
26	gs	201	PEB	CAB-CBB-CGB-O2B
26	gt	201	PEB	CAB-CBB-CGB-O2B
26	gu	201	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	gv	201	PEB	CAB-CBB-CGB-O2B
26	gw	201	PEB	CAB-CBB-CGB-O2B
26	gx	201	PEB	CAB-CBB-CGB-O2B
26	gy	301	PEB	CAB-CBB-CGB-O2B
26	gy	303	PEB	CAB-CBB-CGB-O2B
26	gz	301	PEB	CAB-CBB-CGB-O2B
26	gz	303	PEB	CAB-CBB-CGB-O2B
26	hA	201	PEB	CAB-CBB-CGB-O2B
26	hC	201	PEB	CAB-CBB-CGB-O2B
26	hF	201	PEB	CAB-CBB-CGB-O2B
26	hH	201	PEB	CAB-CBB-CGB-O2B
26	hI	201	PEB	CAB-CBB-CGB-O2B
26	hJ	201	PEB	CAB-CBB-CGB-O2B
26	hK	201	PEB	CAB-CBB-CGB-O2B
26	hL	201	PEB	CAB-CBB-CGB-O2B
26	hM	1001	PEB	CAB-CBB-CGB-O2B
26	hN	201	PEB	CAB-CBB-CGB-O2B
26	hP	201	PEB	CAB-CBB-CGB-O2B
26	hQ	201	PEB	CAB-CBB-CGB-O2B
26	hR	201	PEB	CAB-CBB-CGB-O2B
26	hT	204	PEB	CAB-CBB-CGB-O2B
26	hV	201	PEB	CAB-CBB-CGB-O2B
26	hX	201	PEB	CAB-CBB-CGB-O2B
26	hY	401	PEB	CAB-CBB-CGB-O2B
26	hY	403	PEB	CAB-CBB-CGB-O2B
26	hZ	402	PEB	CAB-CBB-CGB-O2B
26	iA	1001	PEB	CAB-CBB-CGB-O2B
26	iB	1001	PEB	CAB-CBB-CGB-O2B
26	iC	1001	PEB	CAB-CBB-CGB-O2B
26	iD	1001	PEB	CAB-CBB-CGB-O2B
26	iE	1001	PEB	CAB-CBB-CGB-O2B
26	iF	1001	PEB	CAB-CBB-CGB-O2B
26	iH	1001	PEB	CAB-CBB-CGB-O2B
26	jI	1001	PEB	CAB-CBB-CGB-O2B
26	jJ	1001	PEB	CAB-CBB-CGB-O2B
26	jK	1001	PEB	CAB-CBB-CGB-O2B
26	jM	1001	PEB	CAB-CBB-CGB-O2B
26	jN	1001	PEB	CAB-CBB-CGB-O2B
26	jO	1001	PEB	CAB-CBB-CGB-O2B
26	jP	1001	PEB	CAB-CBB-CGB-O2B
26	kQ	1001	PEB	CAB-CBB-CGB-O2B
26	kR	1001	PEB	CAB-CBB-CGB-O2B

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Mol	Chain	Res	Type	Atoms
26	kT	1001	PEB	CAB-CBB-CGB-O2B
26	kV	1001	PEB	CAB-CBB-CGB-O2B
26	kX	1001	PEB	CAB-CBB-CGB-O2B
29	b8	1004	PVN	C51-C52-C53-O54
29	b9	405	PVN	C51-C52-C53-O54
29	T8	303	PVN	C61-C62-C63-O64
29	Y9	303	PVN	C61-C62-C63-O64
29	ey	1004	PVN	C61-C62-C63-O64
29	lz	403	PVN	C4-C3-C31-C32
29	ly	404	PVN	C4-C3-C31-C32
29	34	1004	PVN	C51-C52-C53-O54
29	Y5	1004	PVN	C51-C52-C53-O54
29	hY	404	PVN	C51-C52-C53-O54
29	hZ	403	PVN	C51-C52-C53-O54
29	aY	403	PVN	C12-C61-C62-C63
29	bY	1004	PVN	C12-C61-C62-C63
29	ez	1004	PVN	C12-C61-C62-C63
29	D2	303	PVN	C51-C52-C53-O54
29	d3	302	PVN	C51-C52-C53-O54
29	dw	404	PVN	C3-C4-C5-C6
27	G1	1001	CYC	CAD-CBD-CGD-O2D
27	L1	201	CYC	CAD-CBD-CGD-O2D
27	O1	201	CYC	CAD-CBD-CGD-O2D
27	P1	201	CYC	CAD-CBD-CGD-O2D
27	Q1	201	CYC	CAD-CBD-CGD-O2D
27	R1	1001	CYC	CAD-CBD-CGD-O2D
27	U1	201	CYC	CAD-CBD-CGD-O2D
27	V1	201	CYC	CAD-CBD-CGD-O2D
27	a1	201	CYC	CAD-CBD-CGD-O2D
27	e1	201	CYC	CAD-CBD-CGD-O2D
27	f1	201	CYC	CAD-CBD-CGD-O2D
27	i1	1001	CYC	CAD-CBD-CGD-O2D
27	m1	201	CYC	CAD-CBD-CGD-O2D
27	n1	201	CYC	CAD-CBD-CGD-O2D
27	o1	1001	CYC	CAD-CBD-CGD-O2D
27	q1	201	CYC	CAD-CBD-CGD-O2D
27	s1	201	CYC	CAD-CBD-CGD-O2D
27	w1	201	CYC	CAD-CBD-CGD-O2D
27	y1	201	CYC	CAD-CBD-CGD-O2D
29	T8	303	PVN	C51-C52-C53-O54
29	Y9	303	PVN	C51-C52-C53-O54
27	I1	201	CYC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	K1	201	CYC	CAD-CBD-CGD-O2D
27	N1	201	CYC	CAD-CBD-CGD-O2D
27	W1	201	CYC	CAD-CBD-CGD-O2D
27	X1	201	CYC	CAD-CBD-CGD-O2D
27	Z1	201	CYC	CAD-CBD-CGD-O2D
27	b1	1001	CYC	CAD-CBD-CGD-O2D
27	d1	1001	CYC	CAD-CBD-CGD-O2D
27	g1	201	CYC	CAD-CBD-CGD-O2D
27	k1	201	CYC	CAD-CBD-CGD-O2D
27	u1	1001	CYC	CAD-CBD-CGD-O2D
27	d2	101	CYC	CAD-CBD-CGD-O2D
27	Z1	201	CYC	CAD-CBD-CGD-O1D
27	b1	1001	CYC	CAD-CBD-CGD-O1D
27	s1	201	CYC	CAD-CBD-CGD-O1D
29	aY	403	PVN	C51-C52-C53-O54
27	G1	1001	CYC	CAD-CBD-CGD-O1D
27	L1	201	CYC	CAD-CBD-CGD-O1D
27	O1	201	CYC	CAD-CBD-CGD-O1D
27	P1	201	CYC	CAD-CBD-CGD-O1D
27	Q1	201	CYC	CAD-CBD-CGD-O1D
27	R1	1001	CYC	CAD-CBD-CGD-O1D
27	V1	201	CYC	CAD-CBD-CGD-O1D
27	W1	201	CYC	CAD-CBD-CGD-O1D
27	X1	201	CYC	CAD-CBD-CGD-O1D
27	a1	201	CYC	CAD-CBD-CGD-O1D
27	d1	1001	CYC	CAD-CBD-CGD-O1D
27	e1	201	CYC	CAD-CBD-CGD-O1D
27	f1	201	CYC	CAD-CBD-CGD-O1D
27	g1	201	CYC	CAD-CBD-CGD-O1D
27	i1	1001	CYC	CAD-CBD-CGD-O1D
27	n1	201	CYC	CAD-CBD-CGD-O1D
27	o1	1001	CYC	CAD-CBD-CGD-O1D
27	q1	201	CYC	CAD-CBD-CGD-O1D
27	w1	201	CYC	CAD-CBD-CGD-O1D
27	y1	201	CYC	CAD-CBD-CGD-O1D
27	I1	201	CYC	CAD-CBD-CGD-O1D
27	K1	201	CYC	CAD-CBD-CGD-O1D
27	N1	201	CYC	CAD-CBD-CGD-O1D
27	U1	201	CYC	CAD-CBD-CGD-O1D
27	k1	201	CYC	CAD-CBD-CGD-O1D
27	m1	201	CYC	CAD-CBD-CGD-O1D
27	u1	1001	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
27	d2	101	CYC	CAD-CBD-CGD-O1D
26	F5	202	PEB	CAB-CBB-CGB-O1B
29	bY	1004	PVN	C51-C52-C53-O54
26	j2	202	PEB	CAB-CBB-CGB-O1B
26	l2	202	PEB	CAB-CBB-CGB-O1B
26	p2	202	PEB	CAB-CBB-CGB-O1B
26	A2	1003	PEB	CAB-CBB-CGB-O1B
26	T2	202	PEB	CAB-CBB-CGB-O1B
26	X2	202	PEB	CAB-CBB-CGB-O1B
26	B3	202	PEB	CAB-CBB-CGB-O1B
26	F3	202	PEB	CAB-CBB-CGB-O1B
26	J3	202	PEB	CAB-CBB-CGB-O1B
26	P3	202	PEB	CAB-CBB-CGB-O1B
26	V3	202	PEB	CAB-CBB-CGB-O1B
26	f3	202	PEB	CAB-CBB-CGB-O1B
26	i3	203	PEB	CAB-CBB-CGB-O1B
26	j3	201	PEB	CAB-CBB-CGB-O1B
26	p3	202	PEB	CAB-CBB-CGB-O1B
26	t3	202	PEB	CAB-CBB-CGB-O1B
26	x3	202	PEB	CAB-CBB-CGB-O1B
26	z3	202	PEB	CAB-CBB-CGB-O1B
26	B4	202	PEB	CAB-CBB-CGB-O1B
26	e4	202	PEB	CAB-CBB-CGB-O1B
26	g4	202	PEB	CAB-CBB-CGB-O1B
26	j4	202	PEB	CAB-CBB-CGB-O1B
26	l4	202	PEB	CAB-CBB-CGB-O1B
26	v4	202	PEB	CAB-CBB-CGB-O1B
26	A5	203	PEB	CAB-CBB-CGB-O1B
26	D5	202	PEB	CAB-CBB-CGB-O1B
26	L5	202	PEB	CAB-CBB-CGB-O1B
26	P5	201	PEB	CAB-CBB-CGB-O1B
26	p5	201	PEB	CAB-CBB-CGB-O1B
26	v5	202	PEB	CAB-CBB-CGB-O1B
26	z5	202	PEB	CAB-CBB-CGB-O1B
26	B6	202	PEB	CAB-CBB-CGB-O1B
26	J6	202	PEB	CAB-CBB-CGB-O1B
26	X6	202	PEB	CAB-CBB-CGB-O1B
26	p8	202	PEB	CAB-CBB-CGB-O1B
26	D7	202	PEB	CAB-CBB-CGB-O1B
26	H7	202	PEB	CAB-CBB-CGB-O1B
26	J7	201	PEB	CAB-CBB-CGB-O1B
26	N7	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	T7	202	PEB	CAB-CBB-CGB-O1B
26	V7	202	PEB	CAB-CBB-CGB-O1B
26	X7	202	PEB	CAB-CBB-CGB-O1B
26	Z7	202	PEB	CAB-CBB-CGB-O1B
26	c7	202	PEB	CAB-CBB-CGB-O1B
26	d7	202	PEB	CAB-CBB-CGB-O1B
26	e7	202	PEB	CAB-CBB-CGB-O1B
26	l7	202	PEB	CAB-CBB-CGB-O1B
26	p7	201	PEB	CAB-CBB-CGB-O1B
26	t7	202	PEB	CAB-CBB-CGB-O1B
26	v7	202	PEB	CAB-CBB-CGB-O1B
26	x7	202	PEB	CAB-CBB-CGB-O1B
26	y7	202	PEB	CAB-CBB-CGB-O1B
26	z7	202	PEB	CAB-CBB-CGB-O1B
26	J9	202	PEB	CAB-CBB-CGB-O1B
26	N9	202	PEB	CAB-CBB-CGB-O1B
26	P9	202	PEB	CAB-CBB-CGB-O1B
26	af	202	PEB	CAB-CBB-CGB-O1B
26	ah	202	PEB	CAB-CBB-CGB-O1B
26	av	202	PEB	CAB-CBB-CGB-O1B
26	az	202	PEB	CAB-CBB-CGB-O1B
26	bB	202	PEB	CAB-CBB-CGB-O1B
26	bF	202	PEB	CAB-CBB-CGB-O1B
26	bN	202	PEB	CAB-CBB-CGB-O1B
26	bP	202	PEB	CAB-CBB-CGB-O1B
26	bT	201	PEB	CAB-CBB-CGB-O1B
26	cb	202	PEB	CAB-CBB-CGB-O1B
26	cd	202	PEB	CAB-CBB-CGB-O1B
26	ch	202	PEB	CAB-CBB-CGB-O1B
26	cj	202	PEB	CAB-CBB-CGB-O1B
26	co	201	PEB	CAB-CBB-CGB-O1B
26	cs	202	PEB	CAB-CBB-CGB-O1B
26	cz	202	PEB	CAB-CBB-CGB-O1B
26	cB	202	PEB	CAB-CBB-CGB-O1B
26	cF	201	PEB	CAB-CBB-CGB-O1B
26	df	202	PEB	CAB-CBB-CGB-O1B
26	dh	202	PEB	CAB-CBB-CGB-O1B
26	dj	202	PEB	CAB-CBB-CGB-O1B
26	ec	202	PEB	CAB-CBB-CGB-O1B
26	ee	202	PEB	CAB-CBB-CGB-O1B
26	eg	202	PEB	CAB-CBB-CGB-O1B
26	ei	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	el	202	PEB	CAB-CBB-CGB-O1B
26	eJ	202	PEB	CAB-CBB-CGB-O1B
26	eL	202	PEB	CAB-CBB-CGB-O1B
26	eN	202	PEB	CAB-CBB-CGB-O1B
26	eX	201	PEB	CAB-CBB-CGB-O1B
26	ld	202	PEB	CAB-CBB-CGB-O1B
26	lh	202	PEB	CAB-CBB-CGB-O1B
26	ll	202	PEB	CAB-CBB-CGB-O1B
26	lo	203	PEB	CAB-CBB-CGB-O1B
26	lr	202	PEB	CAB-CBB-CGB-O1B
26	fc	202	PEB	CAB-CBB-CGB-O1B
26	ff	202	PEB	CAB-CBB-CGB-O1B
26	fi	202	PEB	CAB-CBB-CGB-O1B
26	fj	202	PEB	CAB-CBB-CGB-O1B
26	fq	202	PEB	CAB-CBB-CGB-O1B
26	fs	202	PEB	CAB-CBB-CGB-O1B
26	ga	202	PEB	CAB-CBB-CGB-O1B
26	ge	202	PEB	CAB-CBB-CGB-O1B
26	gi	202	PEB	CAB-CBB-CGB-O1B
26	gk	202	PEB	CAB-CBB-CGB-O1B
26	gv	202	PEB	CAB-CBB-CGB-O1B
26	gx	202	PEB	CAB-CBB-CGB-O1B
26	hB	202	PEB	CAB-CBB-CGB-O1B
26	hD	202	PEB	CAB-CBB-CGB-O1B
26	hH	202	PEB	CAB-CBB-CGB-O1B
26	hL	202	PEB	CAB-CBB-CGB-O1B
26	hP	202	PEB	CAB-CBB-CGB-O1B
26	hV	202	PEB	CAB-CBB-CGB-O1B
26	jJ	1002	PEB	CAB-CBB-CGB-O1B
26	jM	1002	PEB	CAB-CBB-CGB-O1B
26	jN	1002	PEB	CAB-CBB-CGB-O1B
26	jO	1002	PEB	CAB-CBB-CGB-O1B
26	kT	1002	PEB	CAB-CBB-CGB-O1B
29	C2	303	PVN	C12-C61-C62-C63
29	c3	303	PVN	C12-C61-C62-C63
29	44	303	PVN	C12-C61-C62-C63
29	Z5	304	PVN	C12-C61-C62-C63
26	A1	301	PEB	CAB-CBB-CGB-O1B
26	B1	301	PEB	CAB-CBB-CGB-O1B
26	f2	202	PEB	CAB-CBB-CGB-O1B
26	h2	202	PEB	CAB-CBB-CGB-O1B
26	n2	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	H2	201	PEB	CAB-CBB-CGB-O1B
26	L2	202	PEB	CAB-CBB-CGB-O1B
26	V2	202	PEB	CAB-CBB-CGB-O1B
26	Z2	202	PEB	CAB-CBB-CGB-O1B
26	D3	202	PEB	CAB-CBB-CGB-O1B
26	H3	202	PEB	CAB-CBB-CGB-O1B
26	L3	202	PEB	CAB-CBB-CGB-O1B
26	N3	202	PEB	CAB-CBB-CGB-O1B
26	R3	202	PEB	CAB-CBB-CGB-O1B
26	T3	202	PEB	CAB-CBB-CGB-O1B
26	W3	203	PEB	CAB-CBB-CGB-O1B
26	Z3	202	PEB	CAB-CBB-CGB-O1B
26	h3	201	PEB	CAB-CBB-CGB-O1B
26	n3	202	PEB	CAB-CBB-CGB-O1B
26	r3	202	PEB	CAB-CBB-CGB-O1B
26	v3	202	PEB	CAB-CBB-CGB-O1B
26	D4	202	PEB	CAB-CBB-CGB-O1B
26	34	1001	PEB	CAB-CBB-CGB-O1B
26	34	1002	PEB	CAB-CBB-CGB-O1B
26	n4	202	PEB	CAB-CBB-CGB-O1B
26	p4	202	PEB	CAB-CBB-CGB-O1B
26	r4	201	PEB	CAB-CBB-CGB-O1B
26	B5	202	PEB	CAB-CBB-CGB-O1B
26	J5	202	PEB	CAB-CBB-CGB-O1B
26	N5	202	PEB	CAB-CBB-CGB-O1B
26	R5	202	PEB	CAB-CBB-CGB-O1B
26	S5	203	PEB	CAB-CBB-CGB-O1B
26	V5	202	PEB	CAB-CBB-CGB-O1B
26	g5	202	PEB	CAB-CBB-CGB-O1B
26	m5	1003	PEB	CAB-CBB-CGB-O1B
26	n5	202	PEB	CAB-CBB-CGB-O1B
26	r5	202	PEB	CAB-CBB-CGB-O1B
26	t5	202	PEB	CAB-CBB-CGB-O1B
26	h8	202	PEB	CAB-CBB-CGB-O1B
26	R6	202	PEB	CAB-CBB-CGB-O1B
26	n6	202	PEB	CAB-CBB-CGB-O1B
26	n8	201	PEB	CAB-CBB-CGB-O1B
26	B7	201	PEB	CAB-CBB-CGB-O1B
26	F7	201	PEB	CAB-CBB-CGB-O1B
26	L7	201	PEB	CAB-CBB-CGB-O1B
26	P7	202	PEB	CAB-CBB-CGB-O1B
26	R7	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	Y7	1003	PEB	CAB-CBB-CGB-O1B
26	a7	202	PEB	CAB-CBB-CGB-O1B
26	n7	202	PEB	CAB-CBB-CGB-O1B
26	r7	202	PEB	CAB-CBB-CGB-O1B
26	y8	202	PEB	CAB-CBB-CGB-O1B
26	C8	202	PEB	CAB-CBB-CGB-O1B
26	v9	202	PEB	CAB-CBB-CGB-O1B
26	B9	202	PEB	CAB-CBB-CGB-O1B
26	D9	202	PEB	CAB-CBB-CGB-O1B
26	F9	202	PEB	CAB-CBB-CGB-O1B
26	H9	202	PEB	CAB-CBB-CGB-O1B
26	L9	202	PEB	CAB-CBB-CGB-O1B
26	R9	202	PEB	CAB-CBB-CGB-O1B
26	T9	202	PEB	CAB-CBB-CGB-O1B
26	V9	202	PEB	CAB-CBB-CGB-O1B
26	ab	202	PEB	CAB-CBB-CGB-O1B
26	ad	202	PEB	CAB-CBB-CGB-O1B
26	aj	202	PEB	CAB-CBB-CGB-O1B
26	al	202	PEB	CAB-CBB-CGB-O1B
26	an	201	PEB	CAB-CBB-CGB-O1B
26	ap	202	PEB	CAB-CBB-CGB-O1B
26	ar	202	PEB	CAB-CBB-CGB-O1B
26	at	202	PEB	CAB-CBB-CGB-O1B
26	ax	201	PEB	CAB-CBB-CGB-O1B
26	aD	202	PEB	CAB-CBB-CGB-O1B
26	aF	202	PEB	CAB-CBB-CGB-O1B
26	bD	202	PEB	CAB-CBB-CGB-O1B
26	bH	202	PEB	CAB-CBB-CGB-O1B
26	bJ	202	PEB	CAB-CBB-CGB-O1B
26	bL	202	PEB	CAB-CBB-CGB-O1B
26	bQ	203	PEB	CAB-CBB-CGB-O1B
26	bV	202	PEB	CAB-CBB-CGB-O1B
26	cf	201	PEB	CAB-CBB-CGB-O1B
26	cl	202	PEB	CAB-CBB-CGB-O1B
26	cn	201	PEB	CAB-CBB-CGB-O1B
26	cp	202	PEB	CAB-CBB-CGB-O1B
26	cq	202	PEB	CAB-CBB-CGB-O1B
26	cr	202	PEB	CAB-CBB-CGB-O1B
26	cE	202	PEB	CAB-CBB-CGB-O1B
26	cH	201	PEB	CAB-CBB-CGB-O1B
26	cJ	202	PEB	CAB-CBB-CGB-O1B
26	cL	202	PEB	CAB-CBB-CGB-O1B

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Mol	Chain	Res	Type	Atoms
26	cY	202	PEB	CAB-CBB-CGB-O1B
26	dd	202	PEB	CAB-CBB-CGB-O1B
26	di	202	PEB	CAB-CBB-CGB-O1B
26	dl	202	PEB	CAB-CBB-CGB-O1B
26	dL	202	PEB	CAB-CBB-CGB-O1B
26	dV	202	PEB	CAB-CBB-CGB-O1B
26	dY	202	PEB	CAB-CBB-CGB-O1B
26	ea	203	PEB	CAB-CBB-CGB-O1B
26	en	202	PEB	CAB-CBB-CGB-O1B
26	ep	202	PEB	CAB-CBB-CGB-O1B
26	er	202	PEB	CAB-CBB-CGB-O1B
26	et	202	PEB	CAB-CBB-CGB-O1B
26	ev	202	PEB	CAB-CBB-CGB-O1B
26	eB	203	PEB	CAB-CBB-CGB-O1B
26	eV	202	PEB	CAB-CBB-CGB-O1B
26	lf	202	PEB	CAB-CBB-CGB-O1B
26	li	203	PEB	CAB-CBB-CGB-O1B
26	ln	202	PEB	CAB-CBB-CGB-O1B
26	lp	202	PEB	CAB-CBB-CGB-O1B
26	lw	203	PEB	CAB-CBB-CGB-O1B
26	fg	201	PEB	CAB-CBB-CGB-O1B
26	fm	202	PEB	CAB-CBB-CGB-O1B
26	fo	202	PEB	CAB-CBB-CGB-O1B
26	fu	201	PEB	CAB-CBB-CGB-O1B
26	fw	202	PEB	CAB-CBB-CGB-O1B
26	fy	201	PEB	CAB-CBB-CGB-O1B
26	gd	201	PEB	CAB-CBB-CGB-O1B
26	gg	202	PEB	CAB-CBB-CGB-O1B
26	gn	202	PEB	CAB-CBB-CGB-O1B
26	gp	202	PEB	CAB-CBB-CGB-O1B
26	gr	201	PEB	CAB-CBB-CGB-O1B
26	gt	202	PEB	CAB-CBB-CGB-O1B
26	hG	201	PEB	CAB-CBB-CGB-O1B
26	hJ	202	PEB	CAB-CBB-CGB-O1B
26	hN	202	PEB	CAB-CBB-CGB-O1B
26	hR	202	PEB	CAB-CBB-CGB-O1B
26	hT	202	PEB	CAB-CBB-CGB-O1B
26	hX	202	PEB	CAB-CBB-CGB-O1B
26	iC	1002	PEB	CAB-CBB-CGB-O1B
26	iD	1002	PEB	CAB-CBB-CGB-O1B
26	iE	1002	PEB	CAB-CBB-CGB-O1B
26	jI	1002	PEB	CAB-CBB-CGB-O1B

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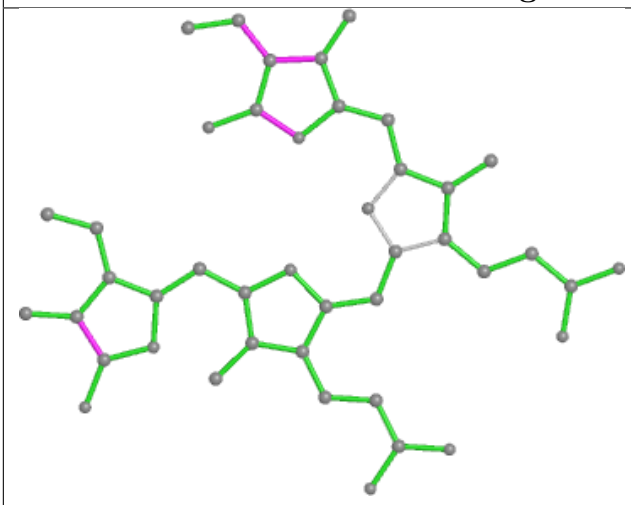
Mol	Chain	Res	Type	Atoms
26	jK	1002	PEB	CAB-CBB-CGB-O1B
26	jL	1002	PEB	CAB-CBB-CGB-O1B
26	jP	1002	PEB	CAB-CBB-CGB-O1B
26	kQ	1002	PEB	CAB-CBB-CGB-O1B
26	kR	1002	PEB	CAB-CBB-CGB-O1B
26	kS	1002	PEB	CAB-CBB-CGB-O1B
26	kU	1002	PEB	CAB-CBB-CGB-O1B
26	kV	1002	PEB	CAB-CBB-CGB-O1B
26	kW	1002	PEB	CAB-CBB-CGB-O1B
26	kX	1002	PEB	CAB-CBB-CGB-O1B

There are no ring outliers.

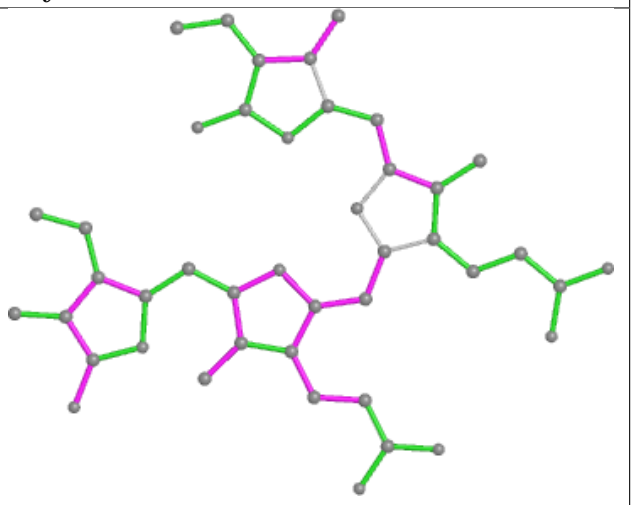
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

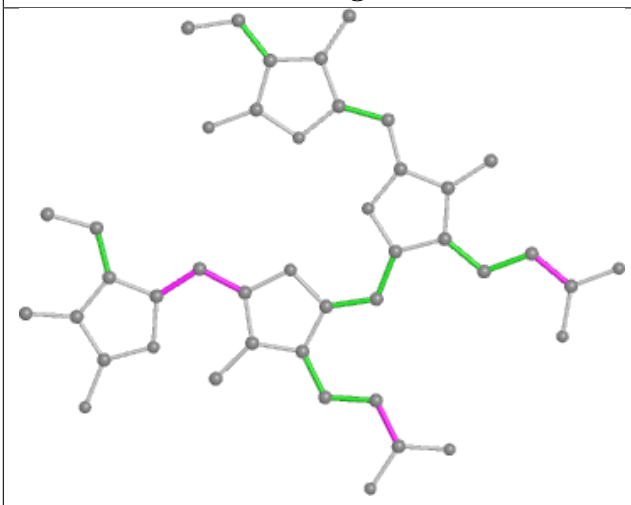
Ligand PEB y2 202



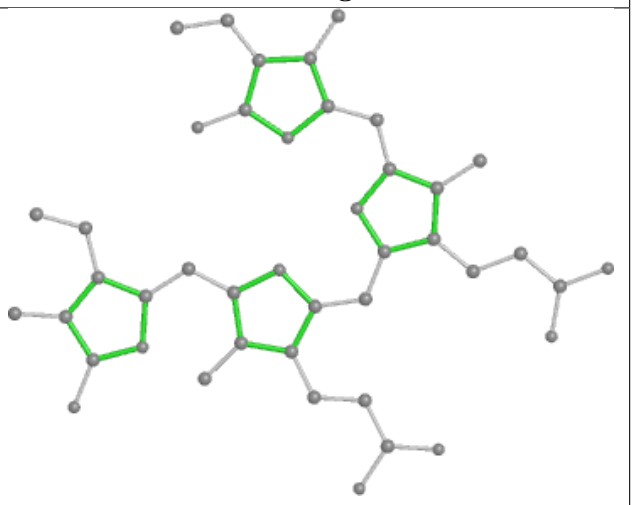
Bond lengths



Bond angles

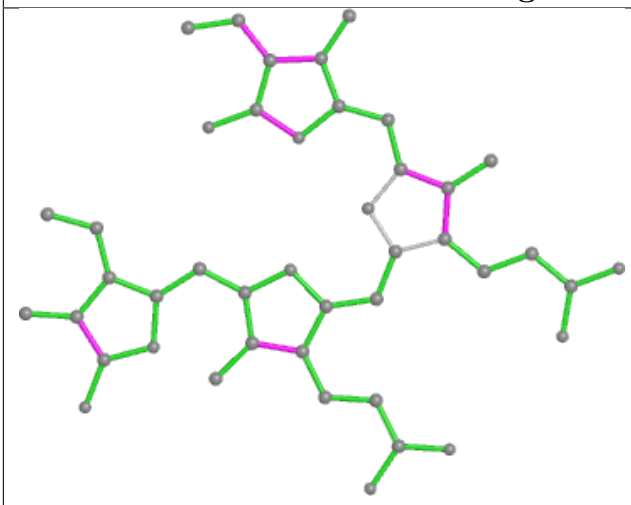


Torsions

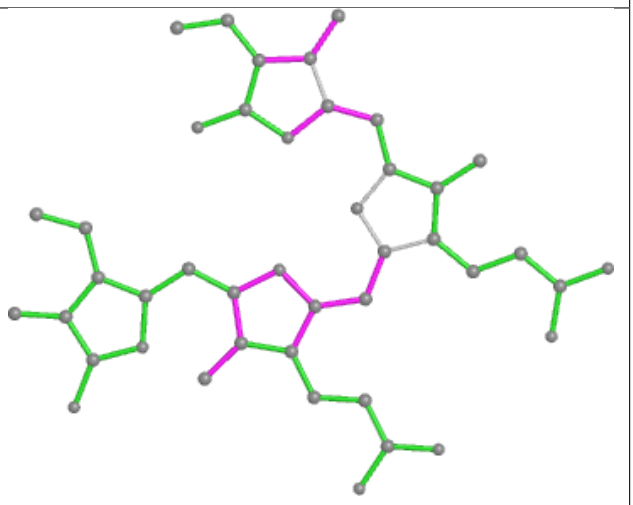


Rings

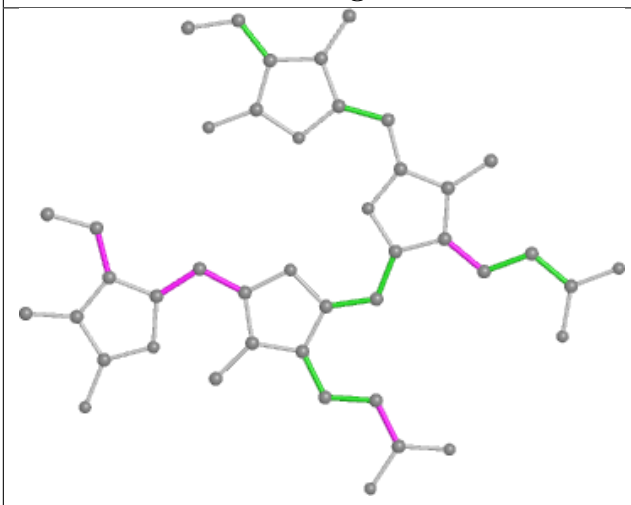
Ligand PEB L7 201



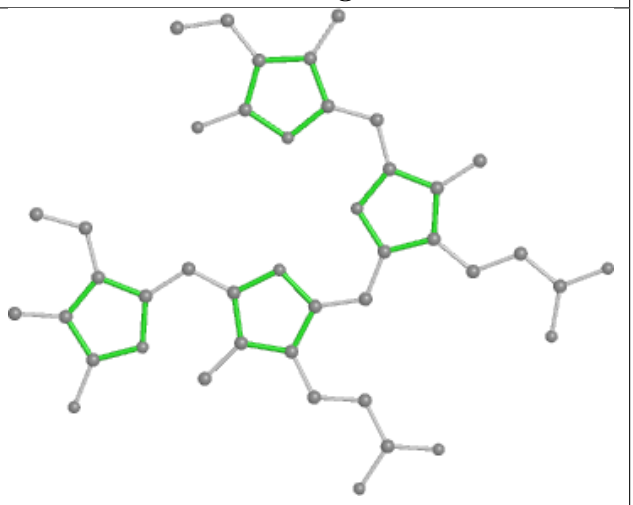
Bond lengths



Bond angles

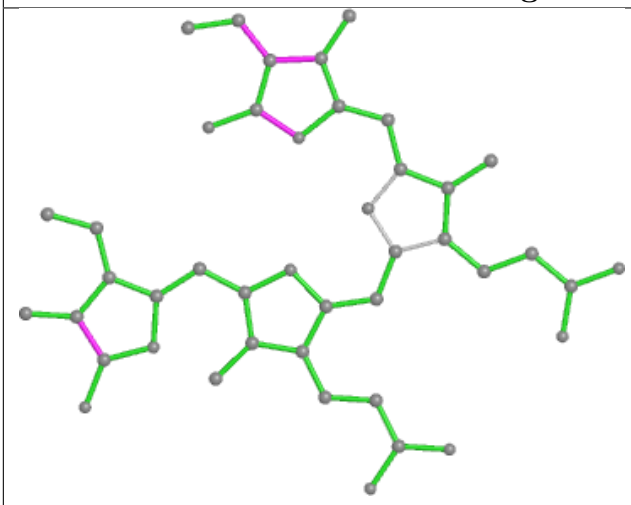


Torsions

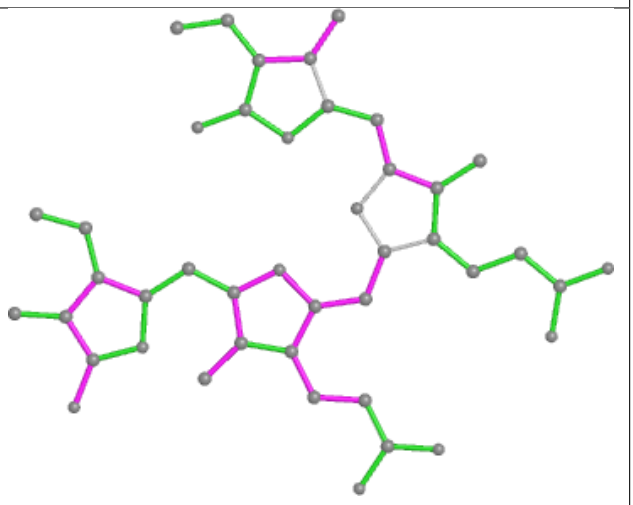


Rings

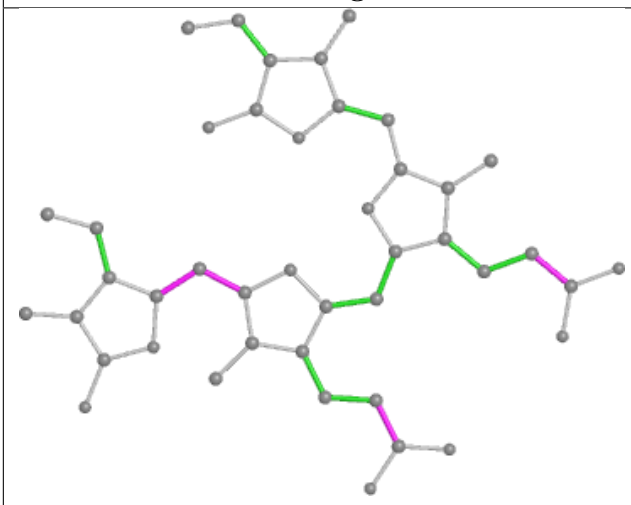
Ligand PEB ea 202



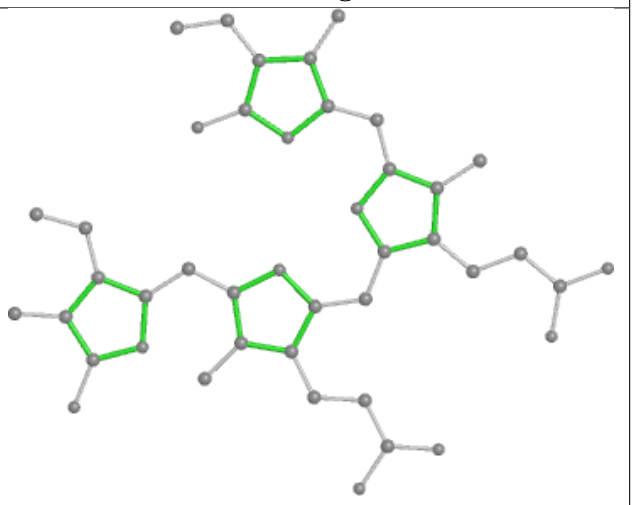
Bond lengths



Bond angles

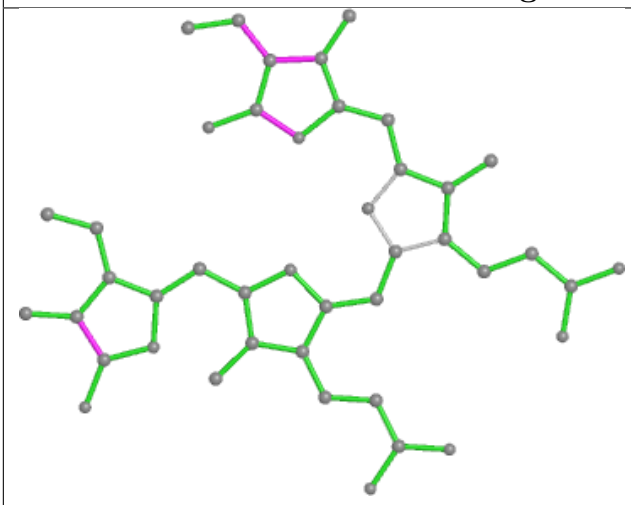


Torsions

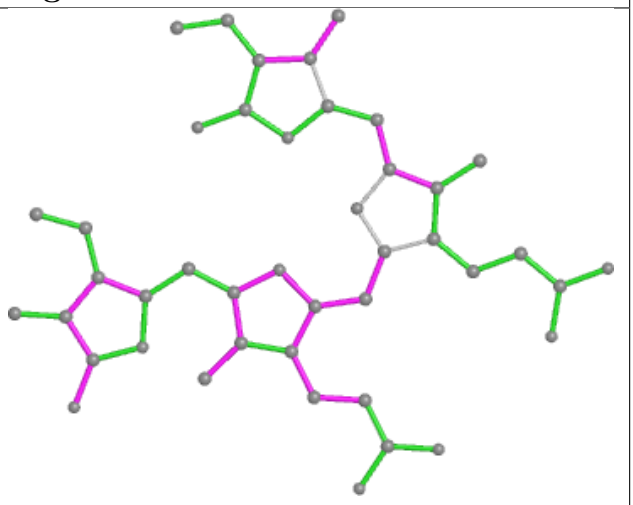


Rings

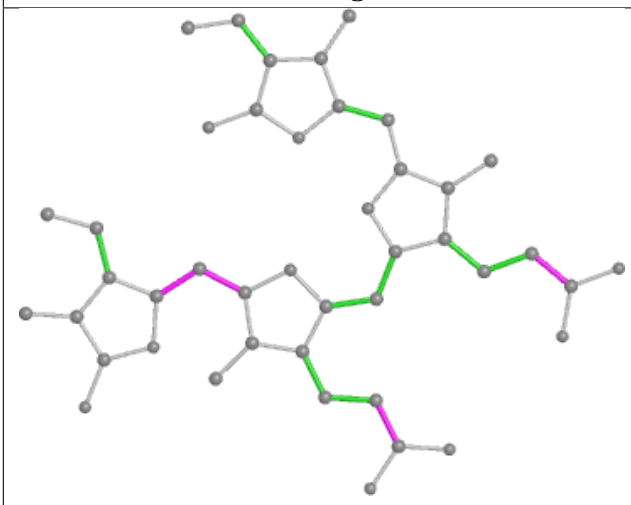
Ligand PEB g3 201



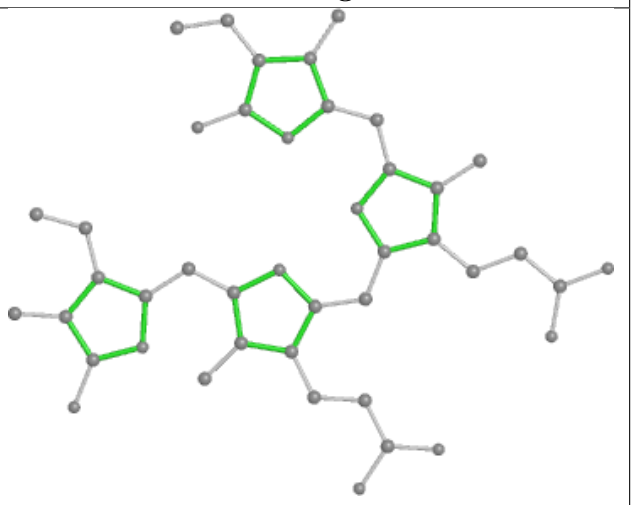
Bond lengths



Bond angles

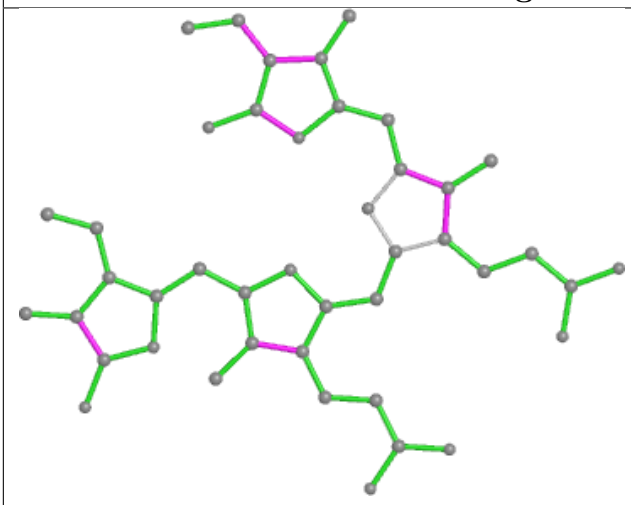


Torsions

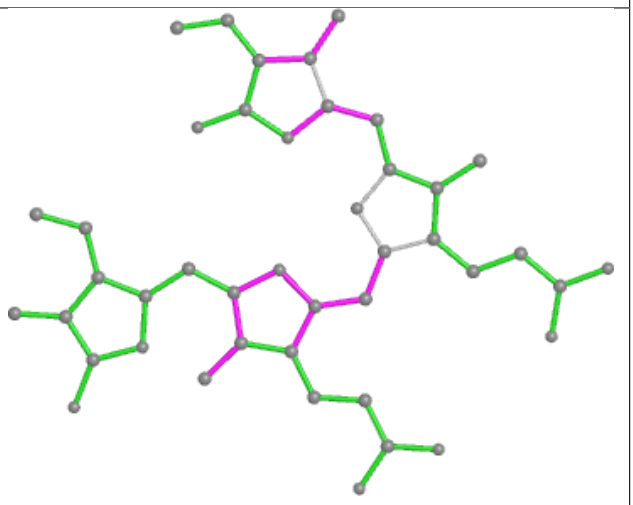


Rings

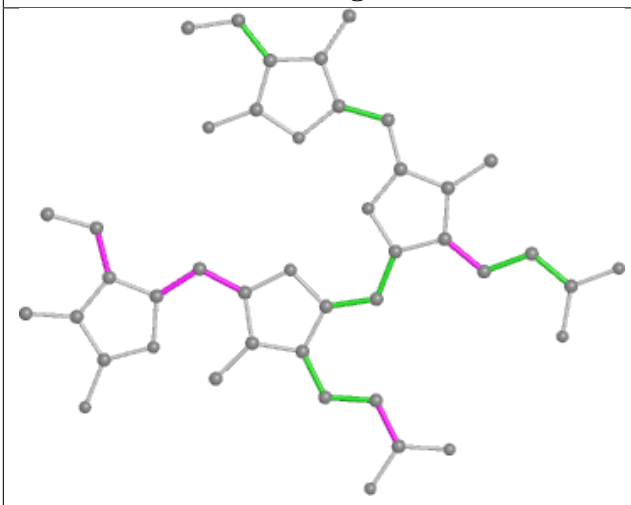
Ligand PEB V7 202



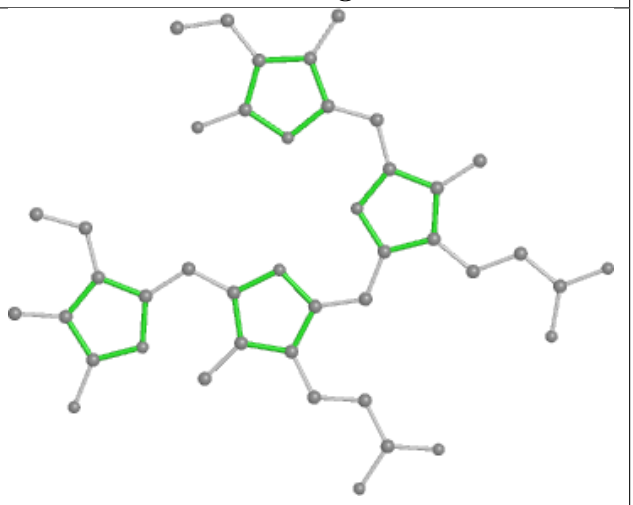
Bond lengths



Bond angles

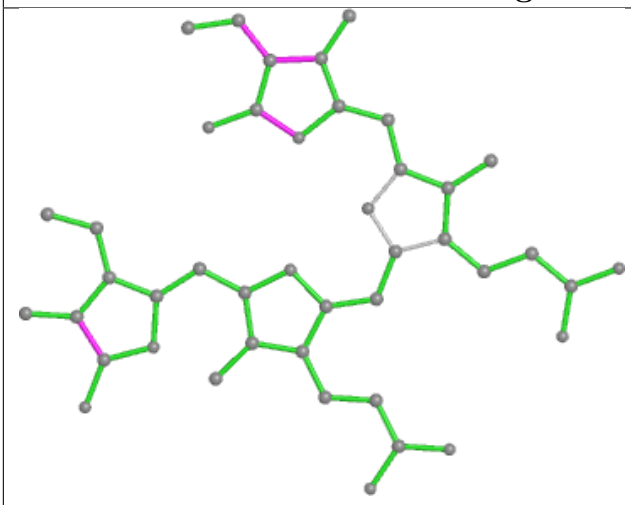


Torsions



Rings

Ligand PEB aD 201



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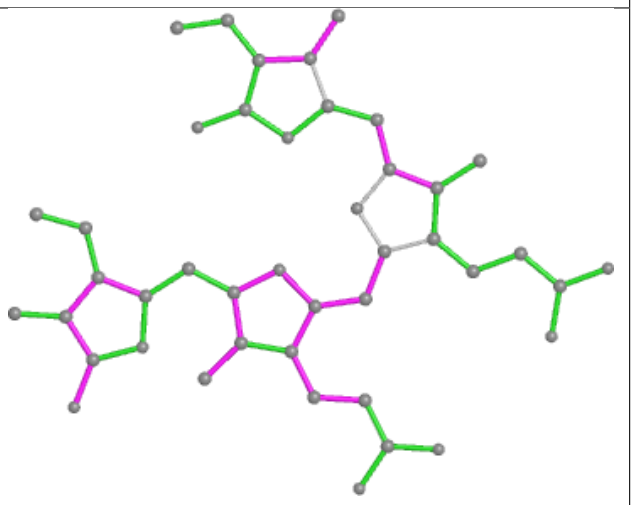

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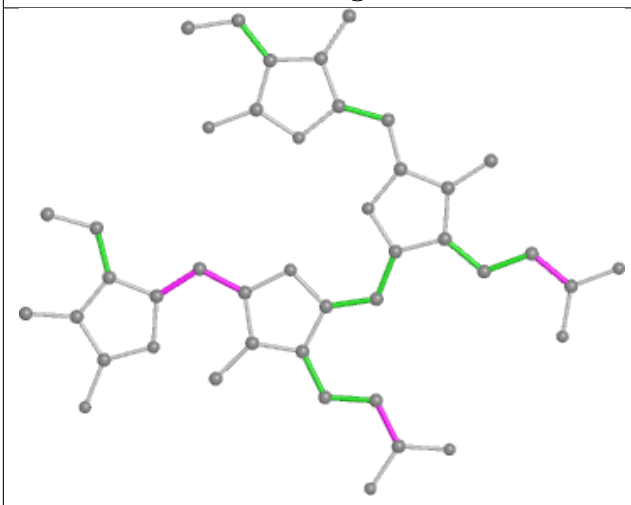
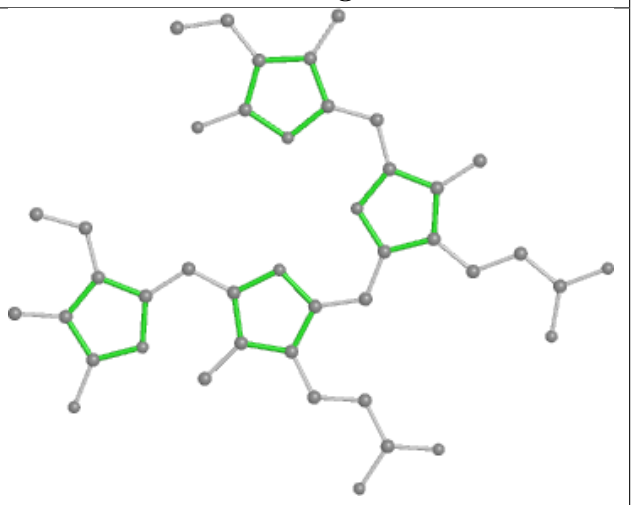
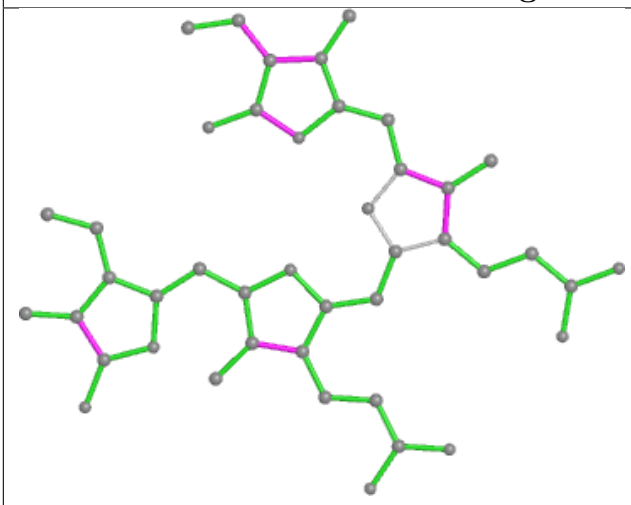


Torsions



Rings

Ligand PEB J3 202



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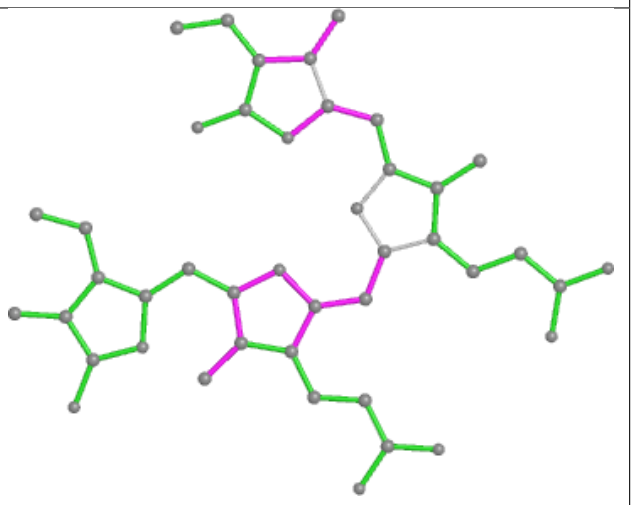

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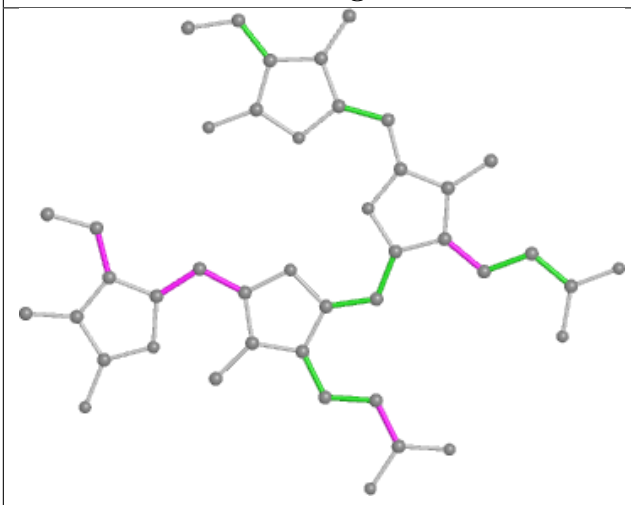

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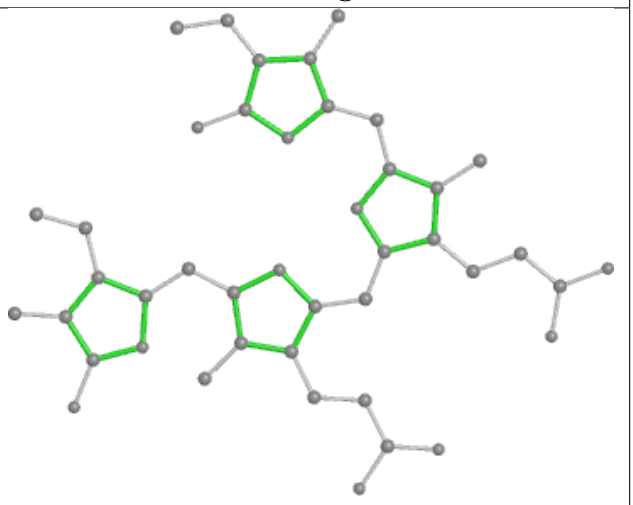
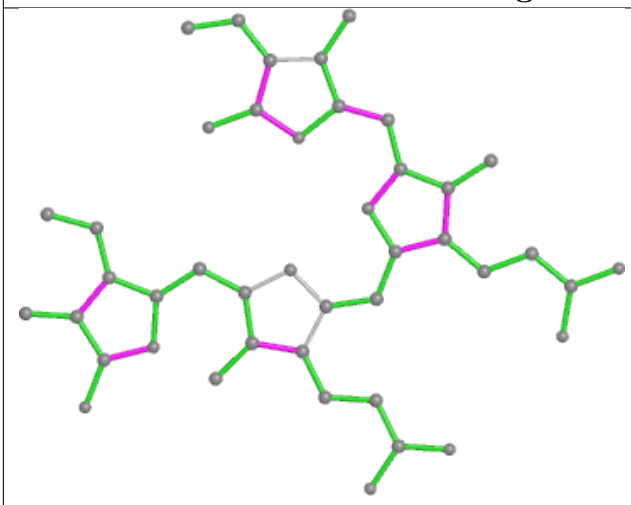


Rings

Ligand PUB Z7 203



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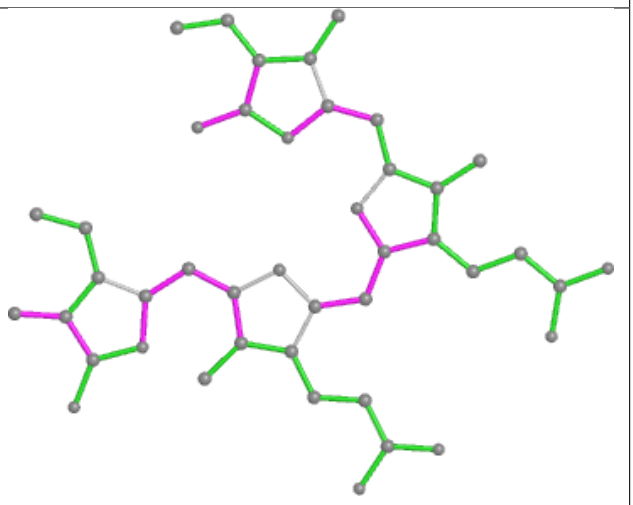

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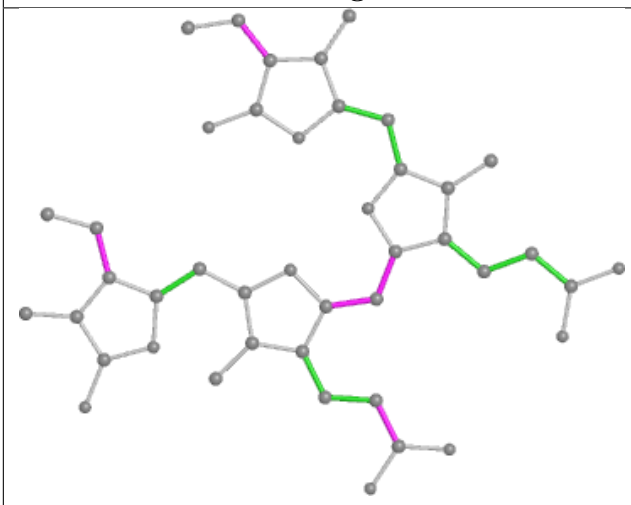

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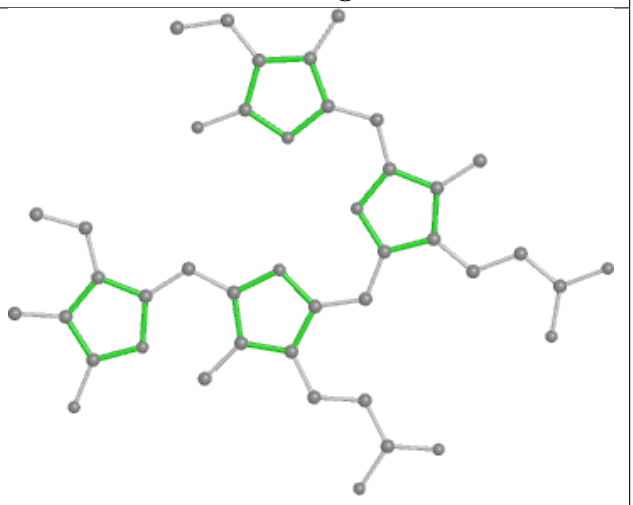

Rings

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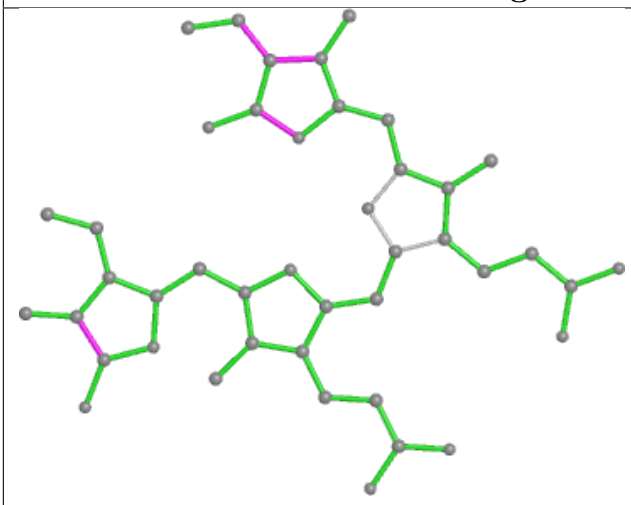

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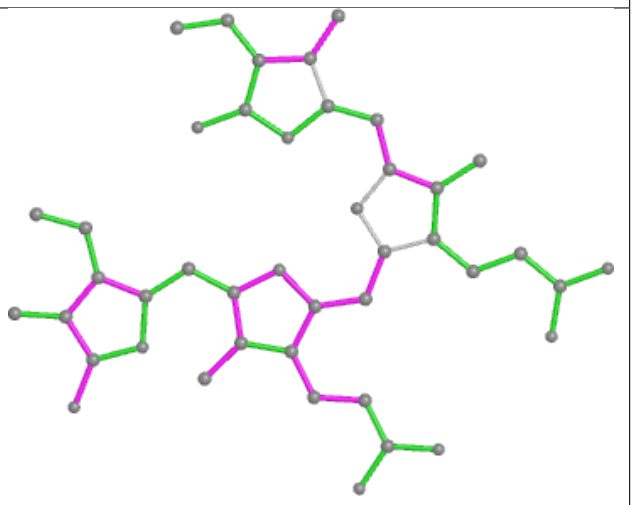

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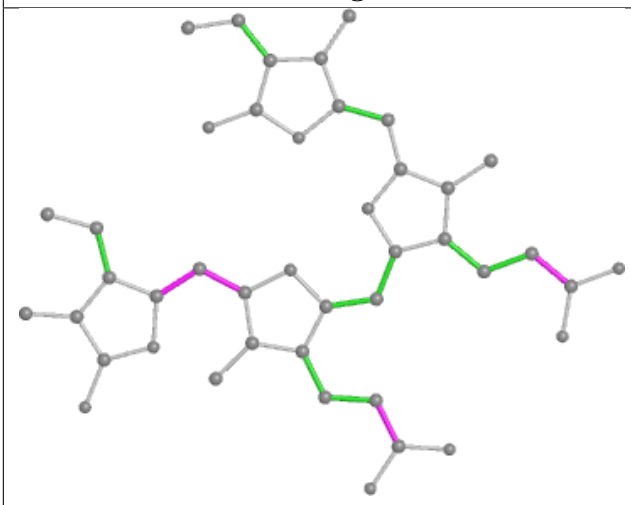

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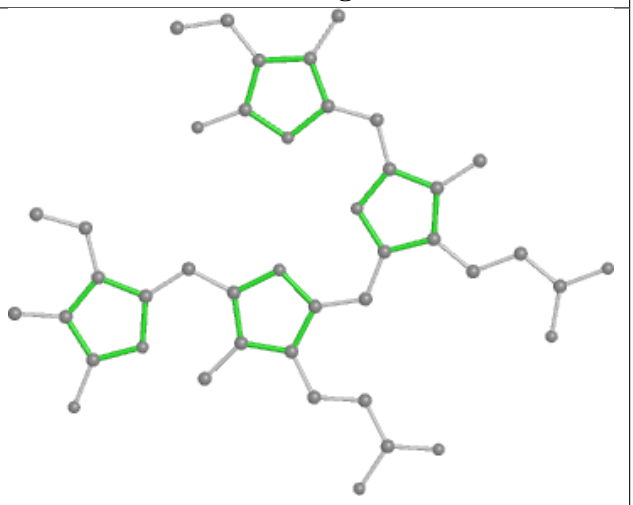

Rings

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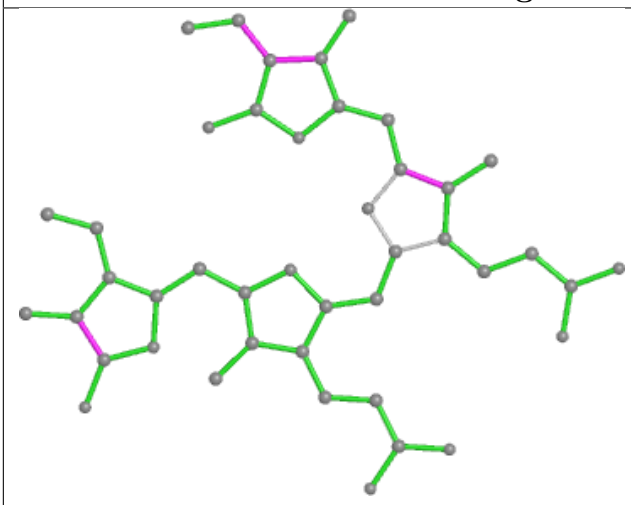

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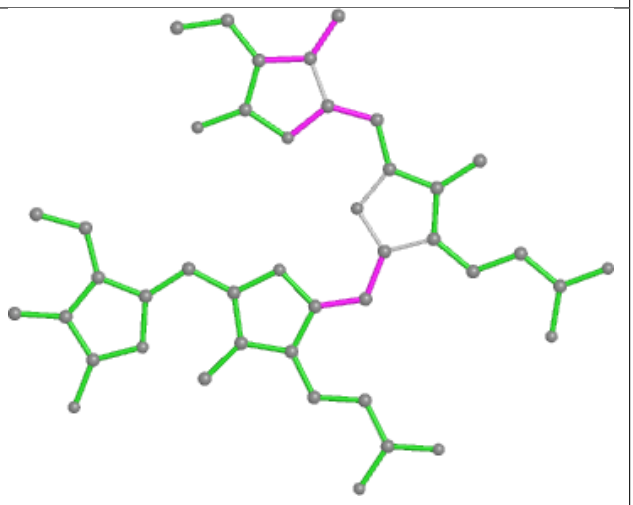

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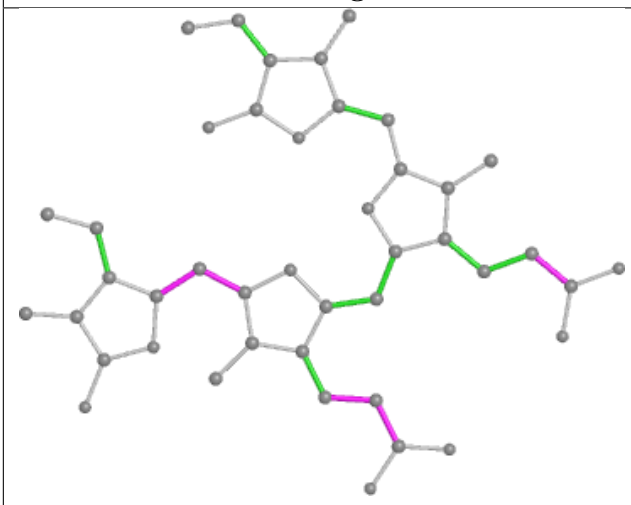

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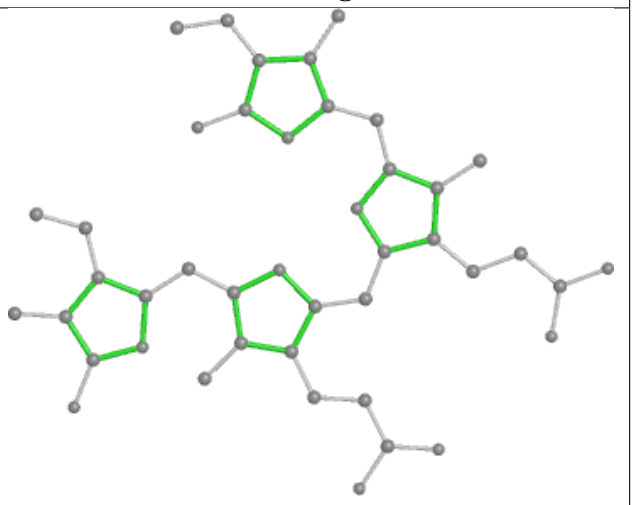

Rings

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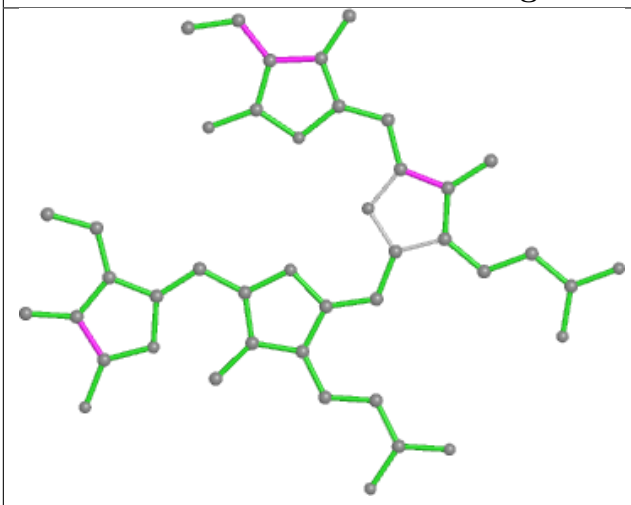

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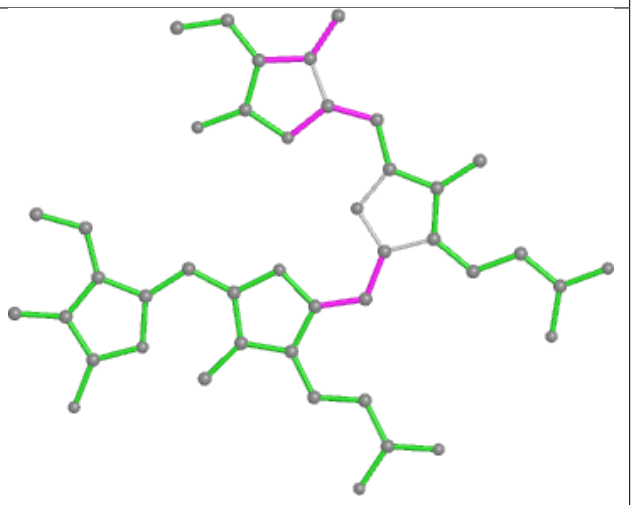

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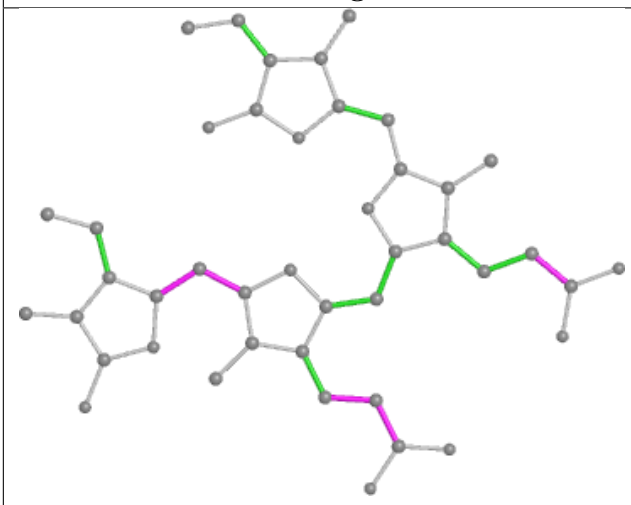

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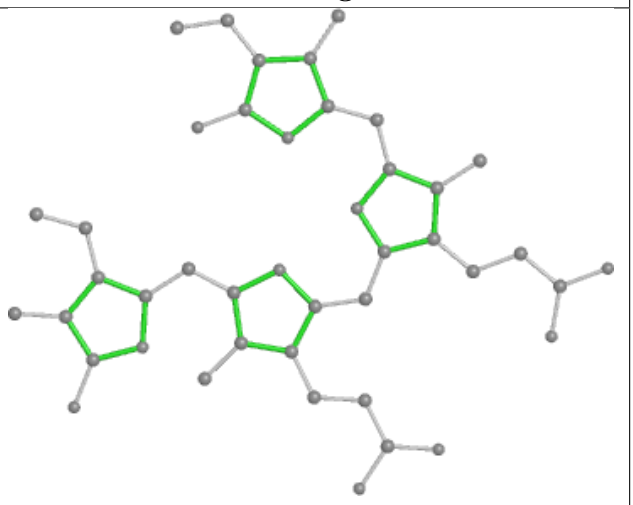

Rings

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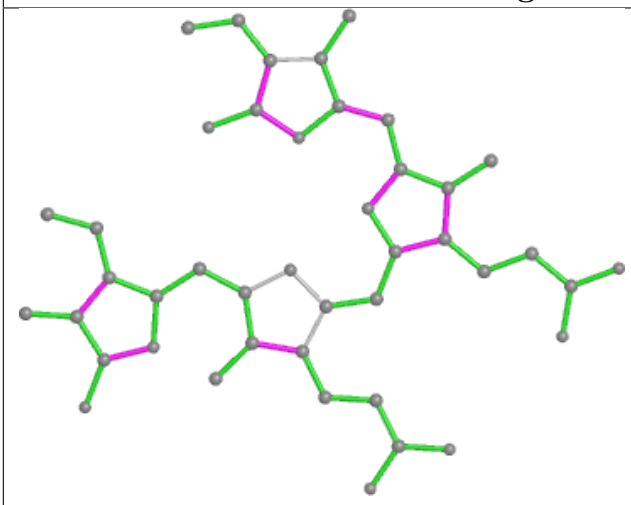

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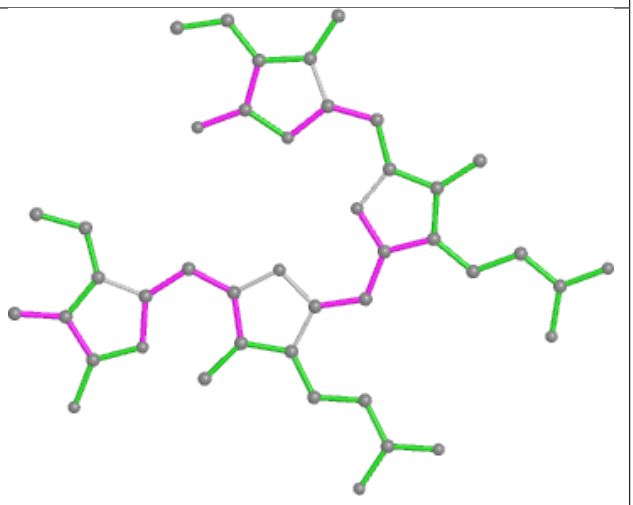

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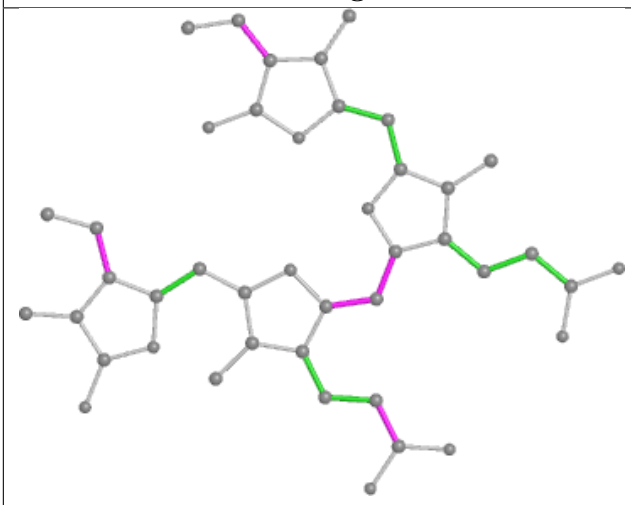

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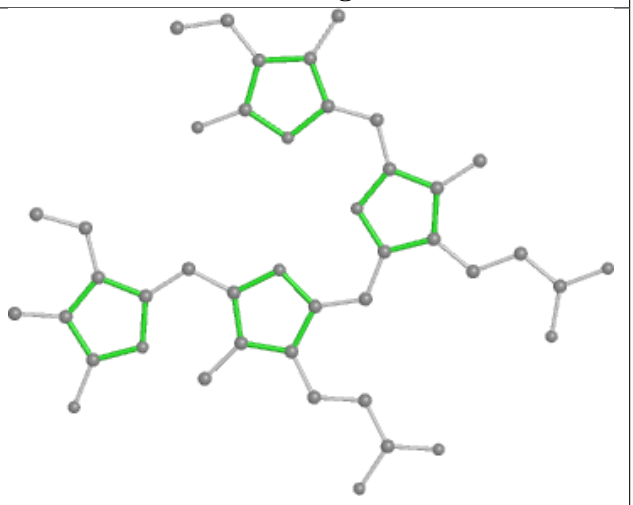

Rings

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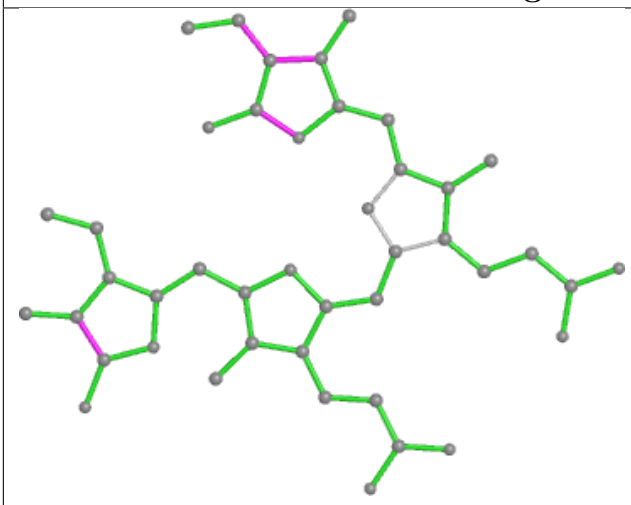

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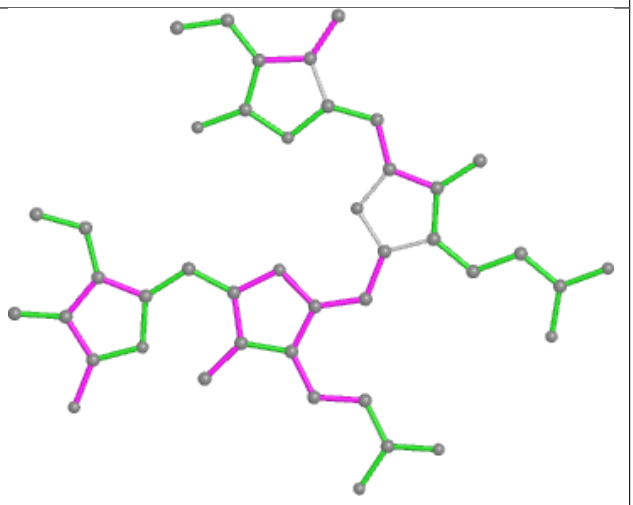

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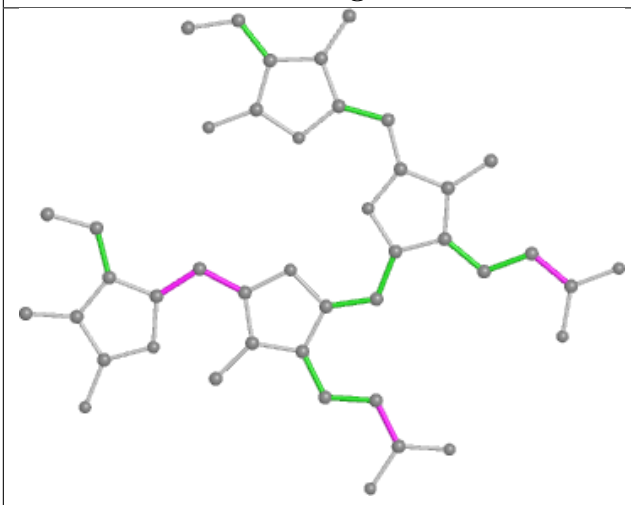

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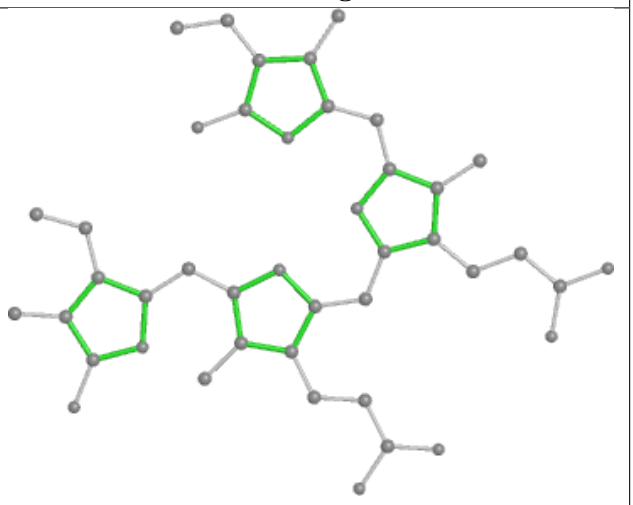

Rings

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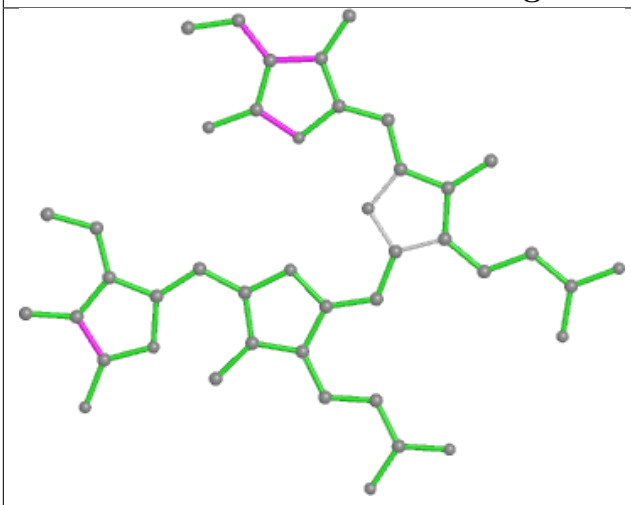

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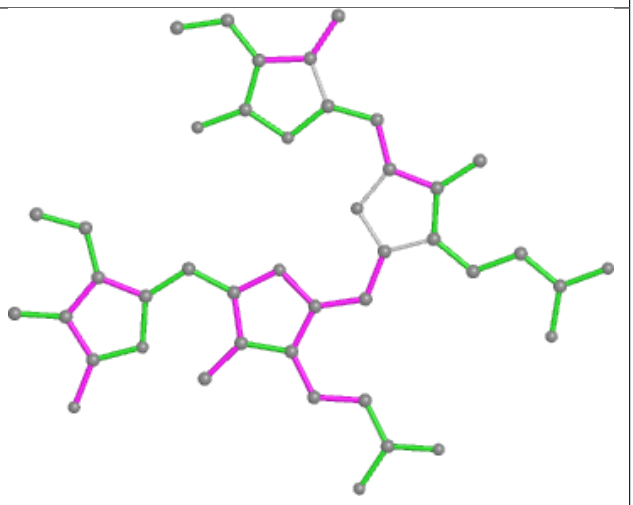

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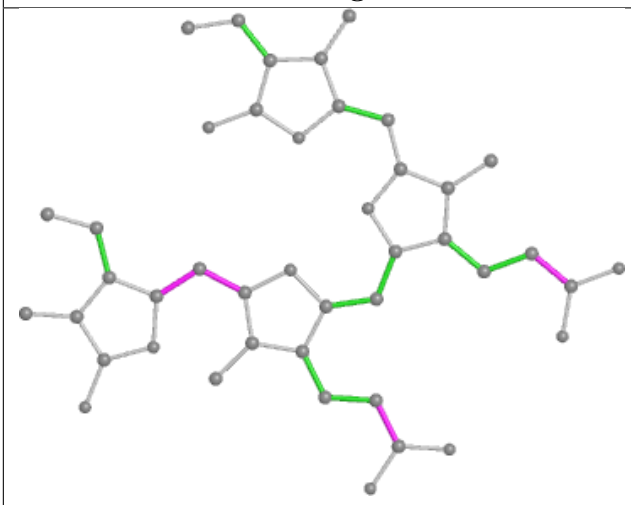

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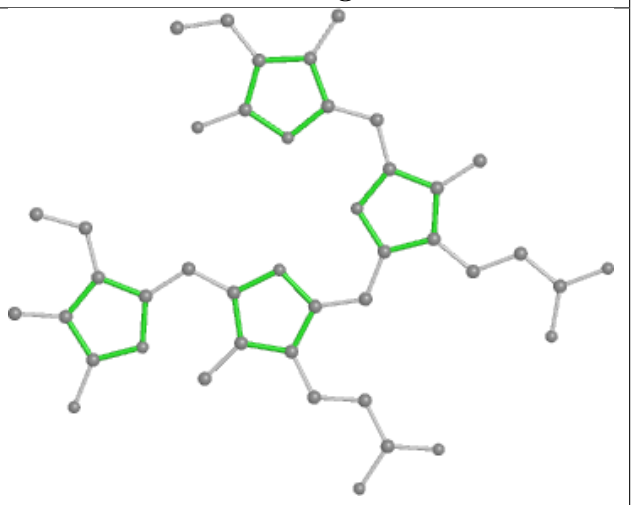

Rings

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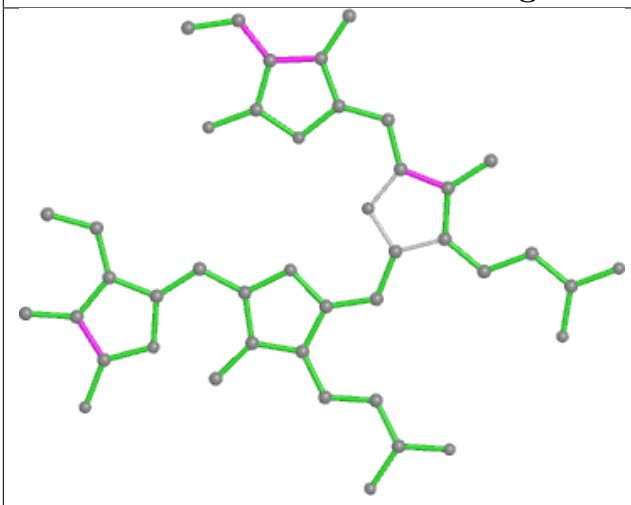

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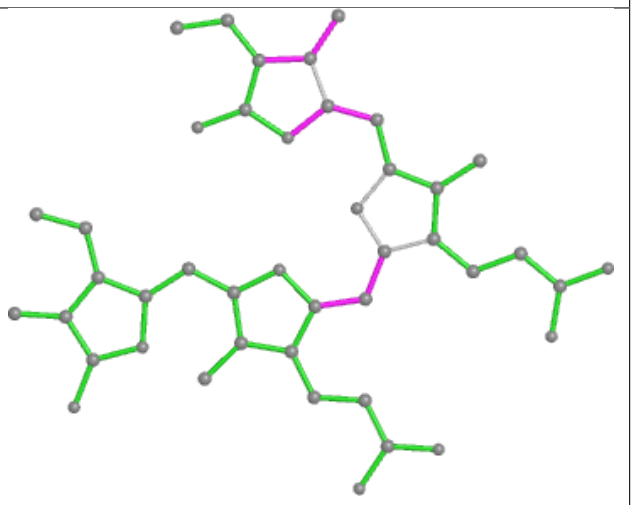

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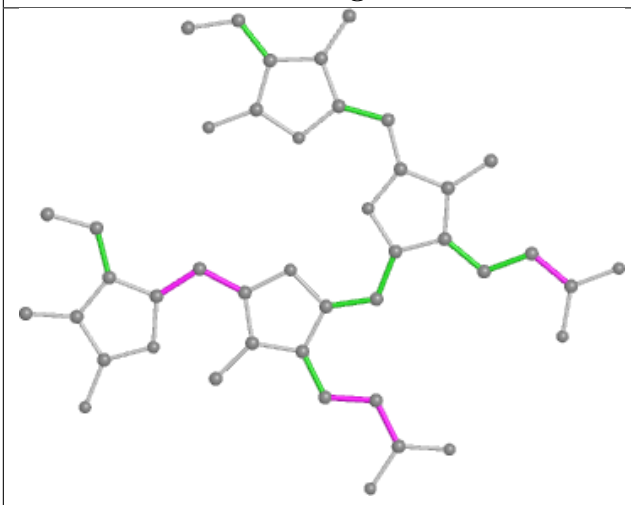

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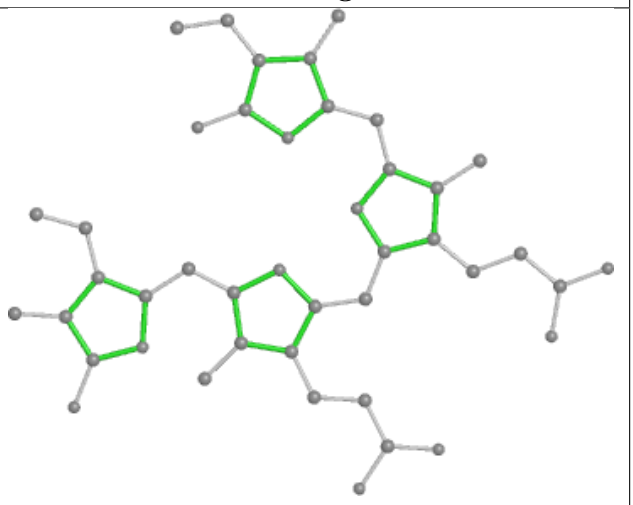
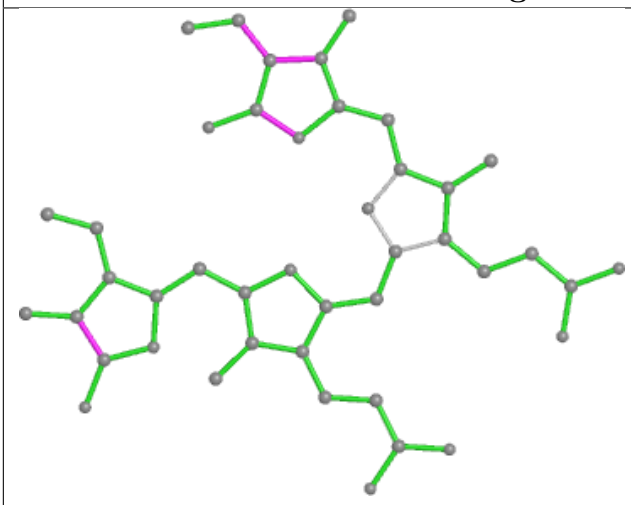


Rings

Ligand PEB kS 1001



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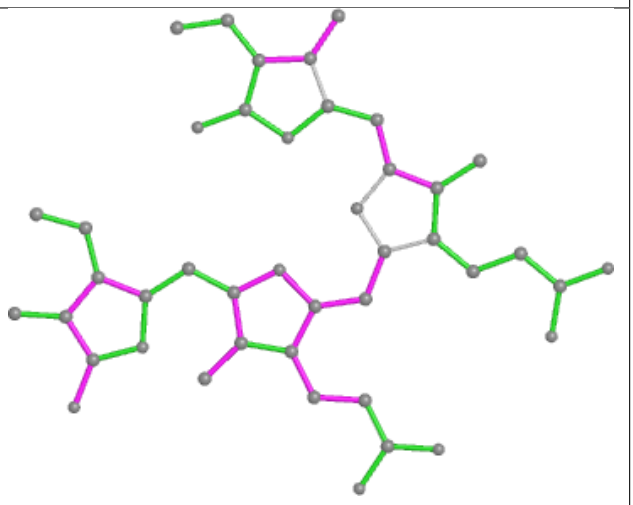

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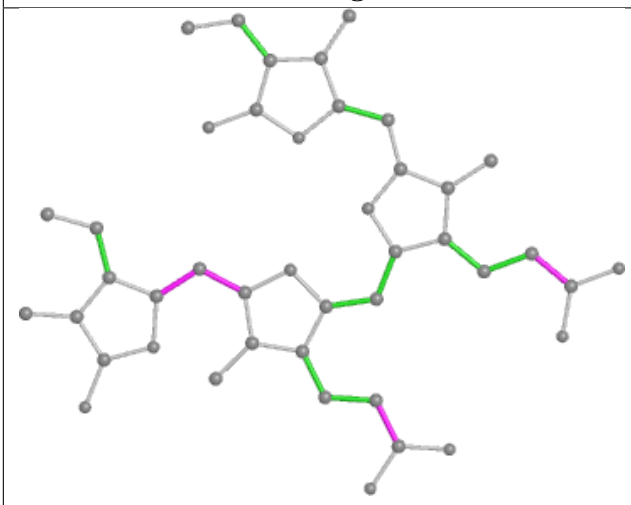

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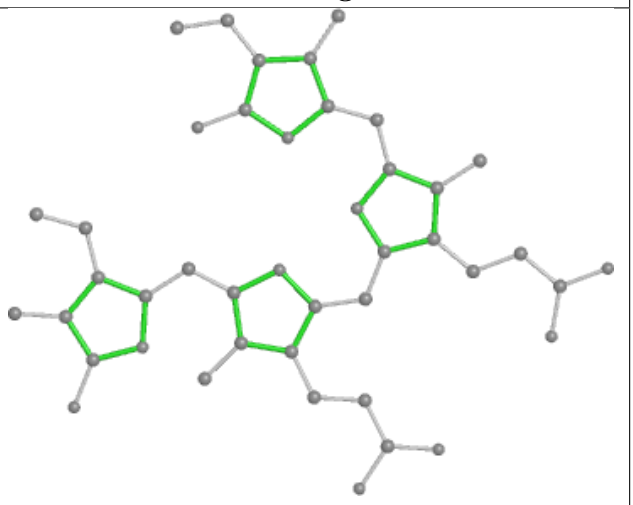
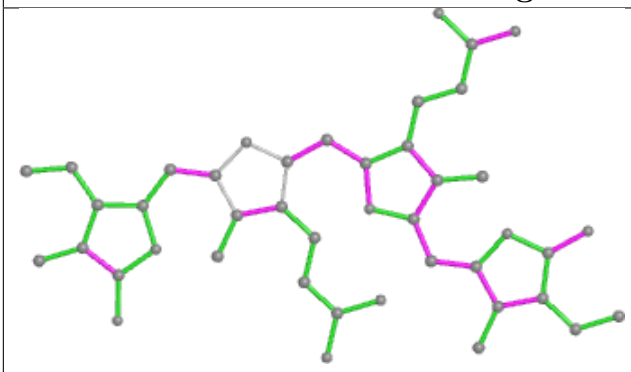


Rings

Ligand CYC n1 201



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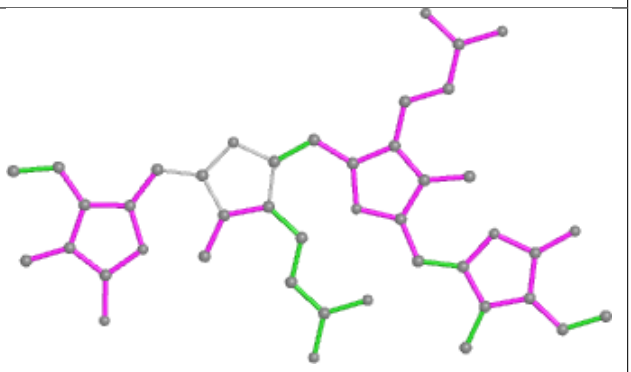

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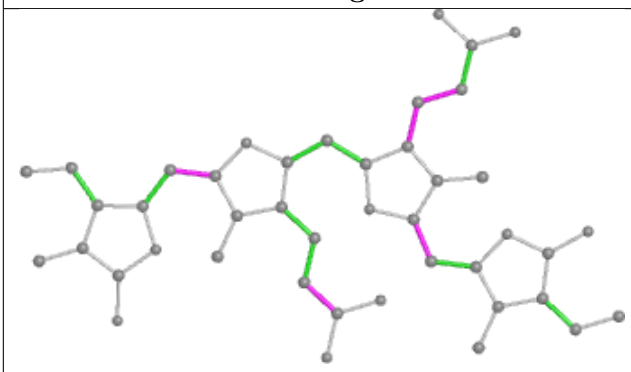

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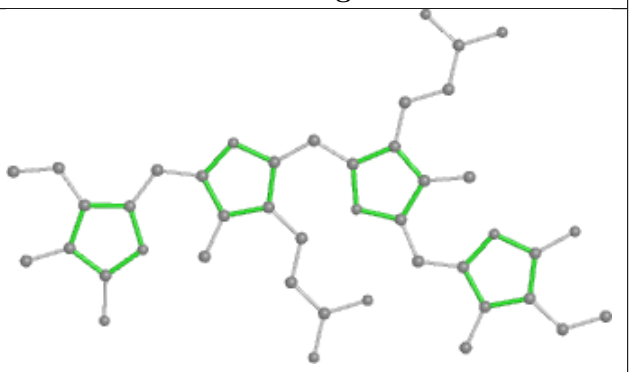

Rings

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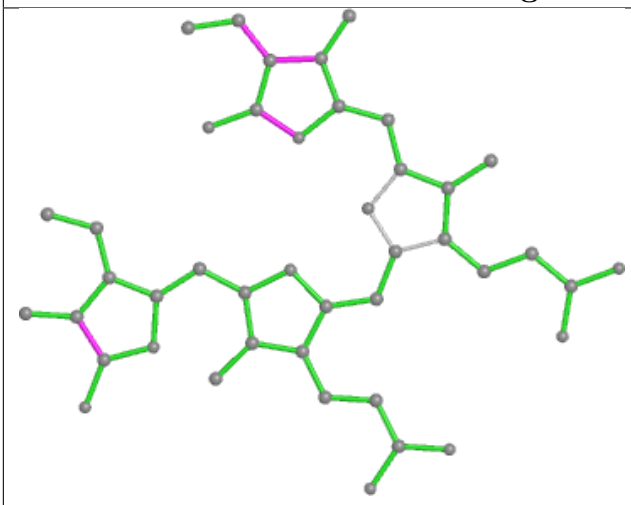

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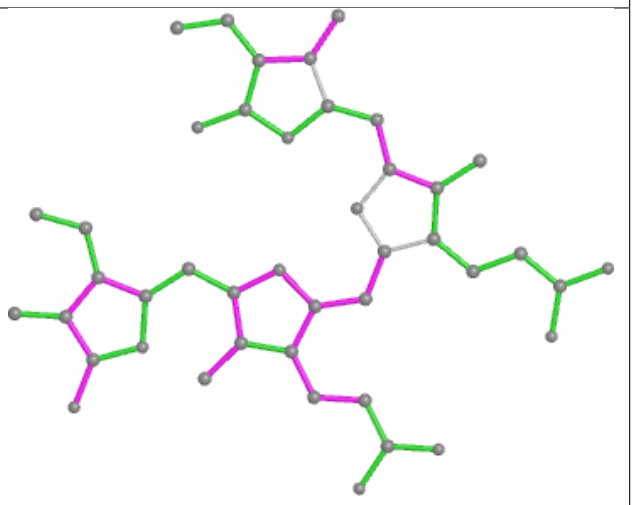

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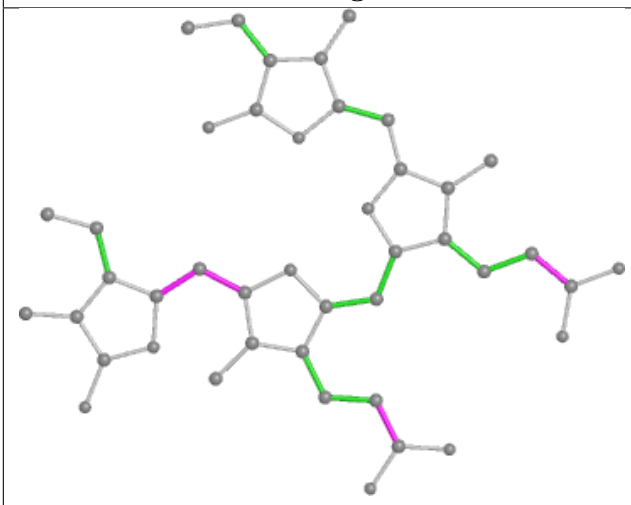

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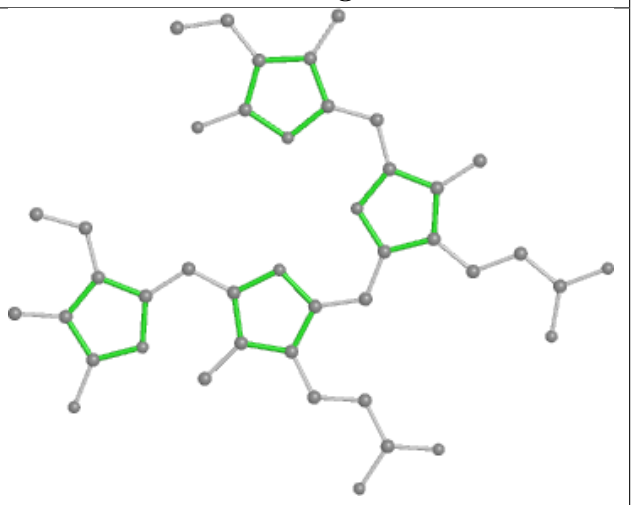

Rings

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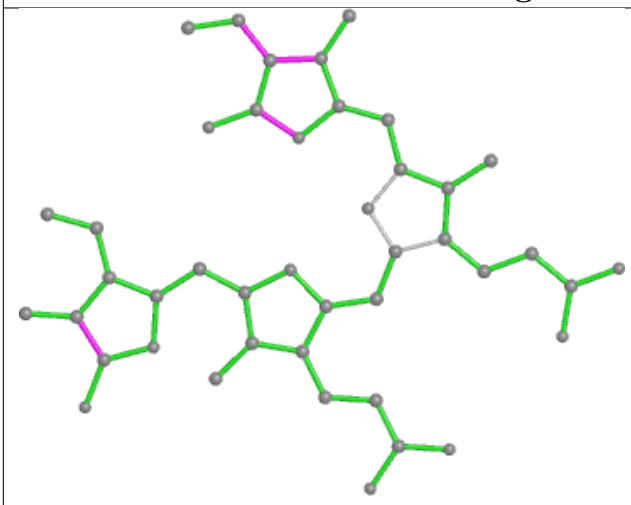

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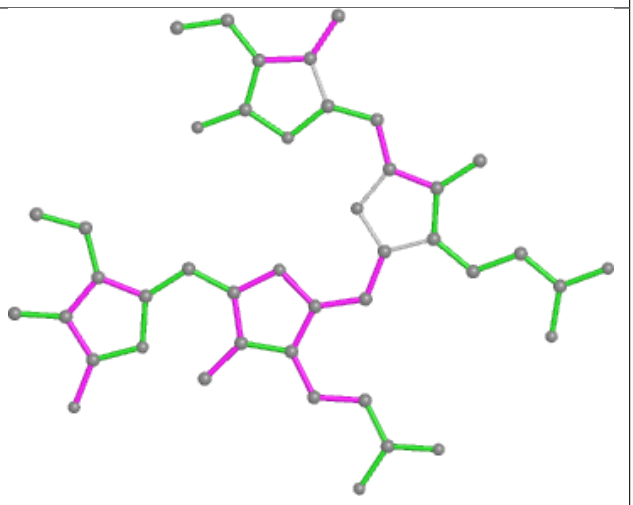
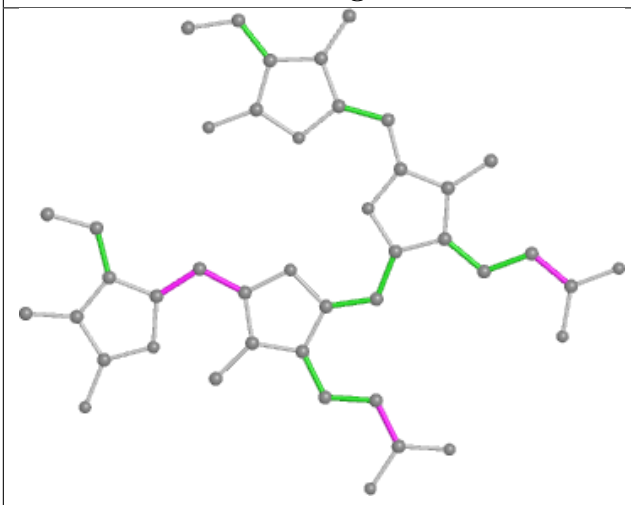
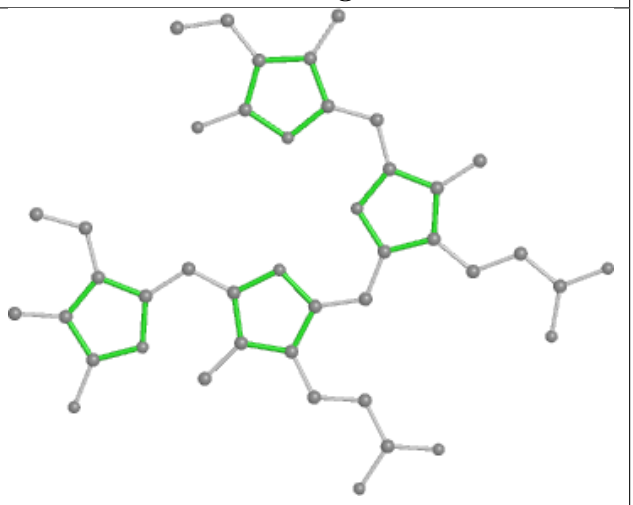


Bond angles

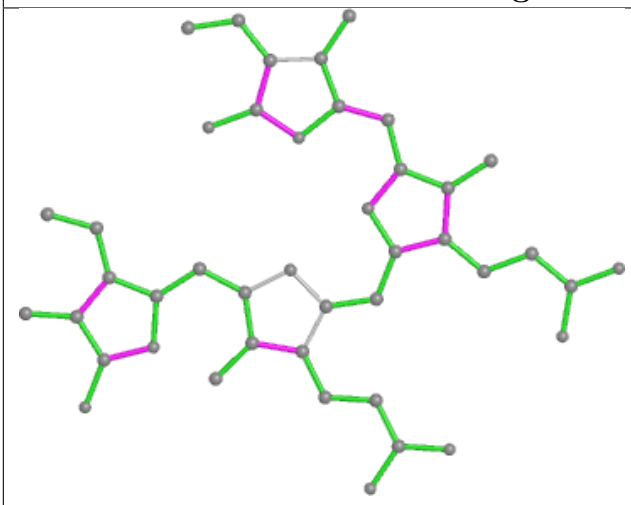


Torsions



Rings

Ligand PUB hX 203



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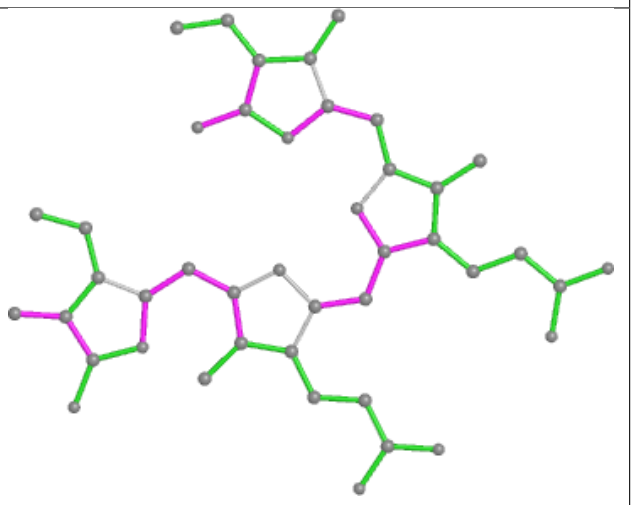

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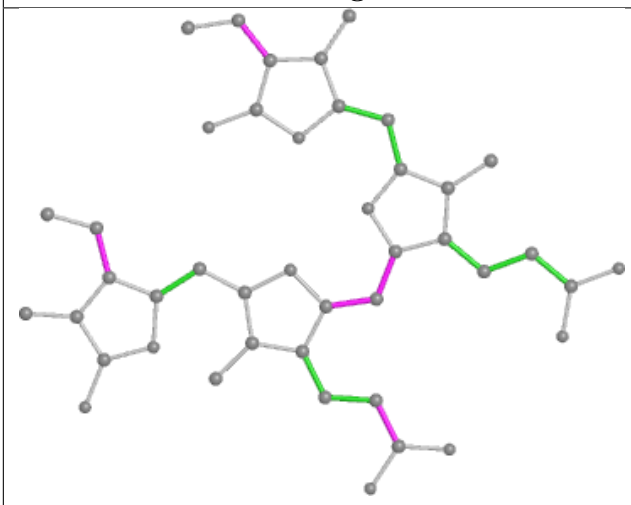

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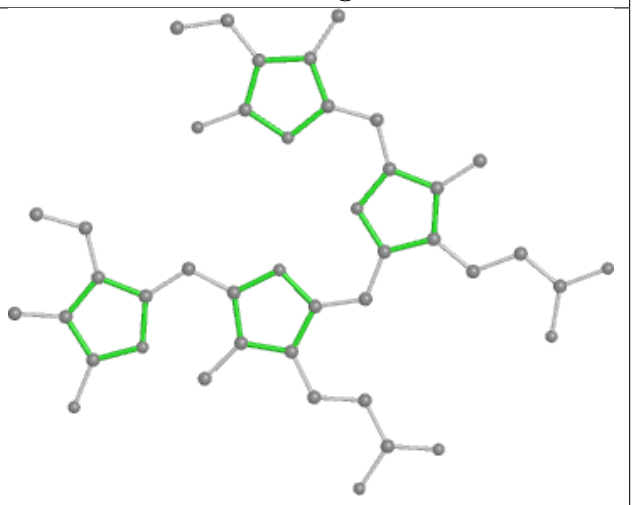
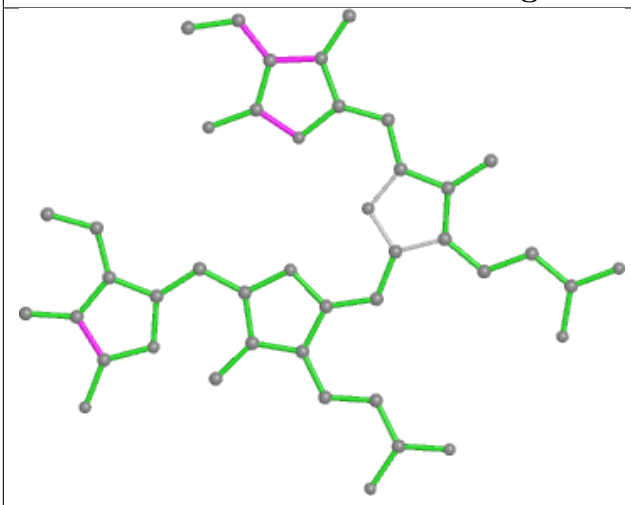


Rings

Ligand PEB ge 201



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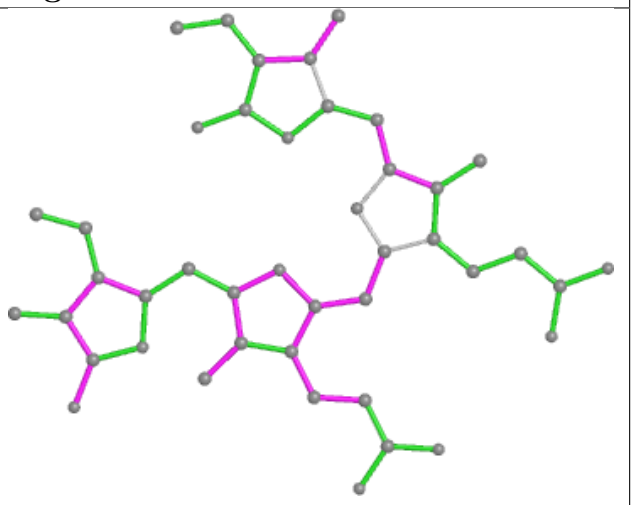

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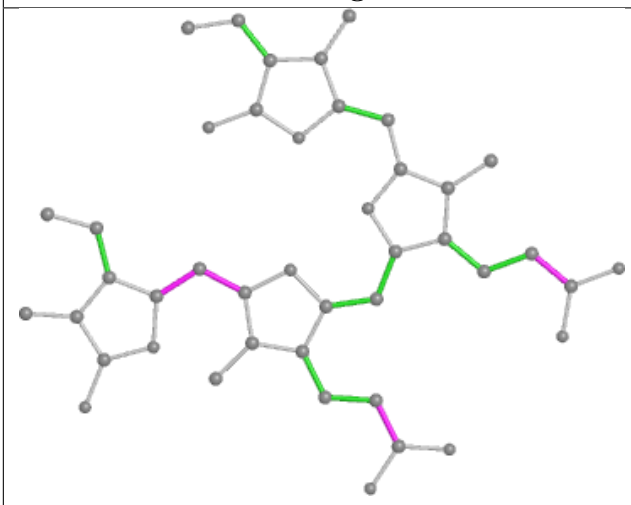

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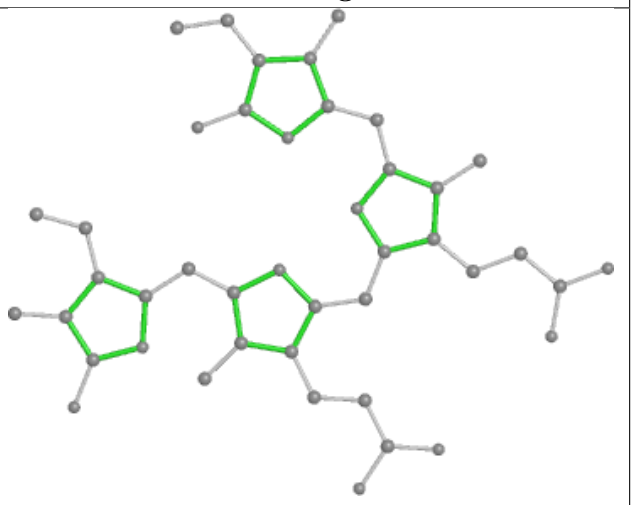
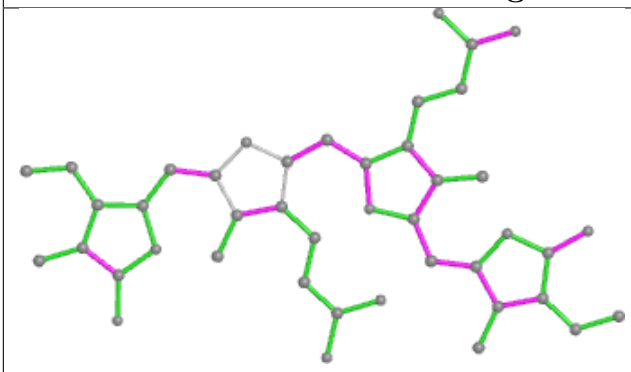


Rings

Ligand CYC u1 1001



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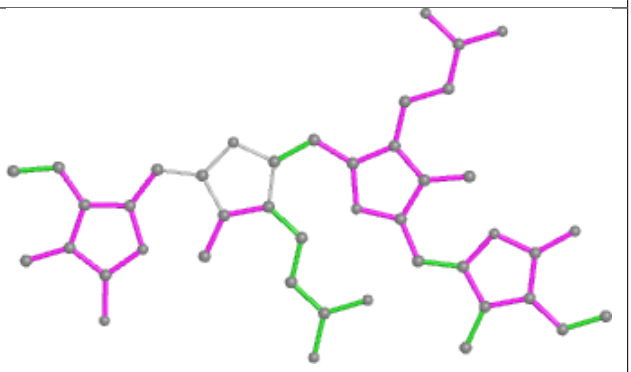

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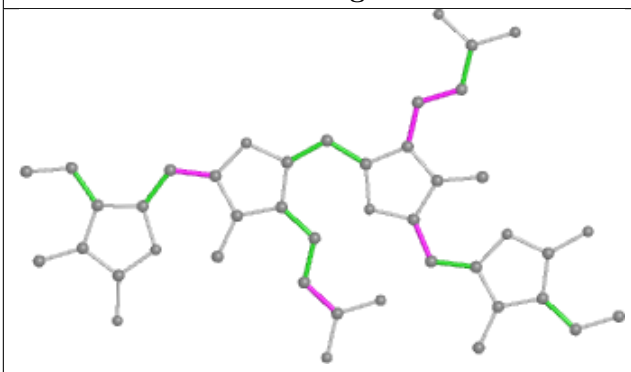

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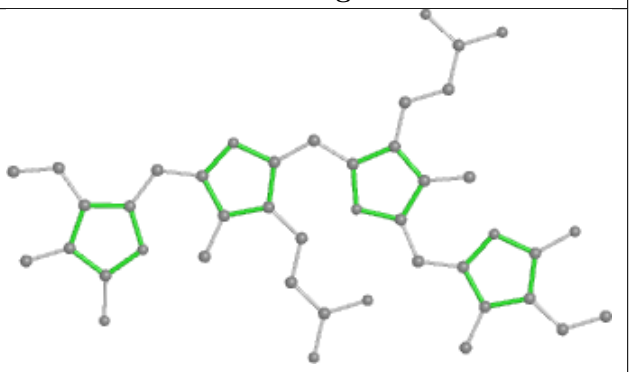
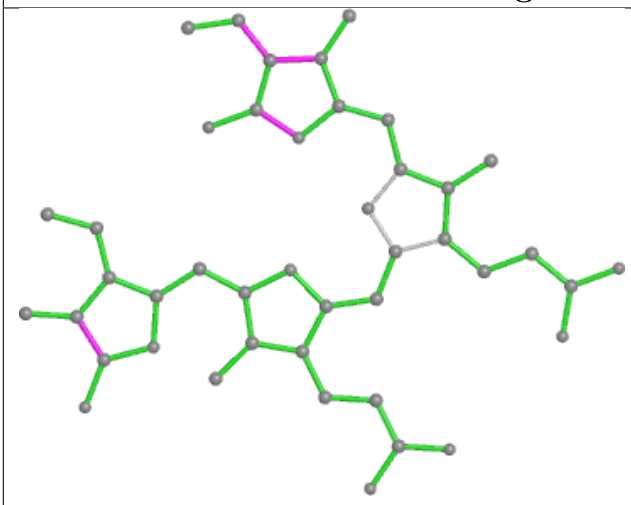


Rings

Ligand PEB eK 201



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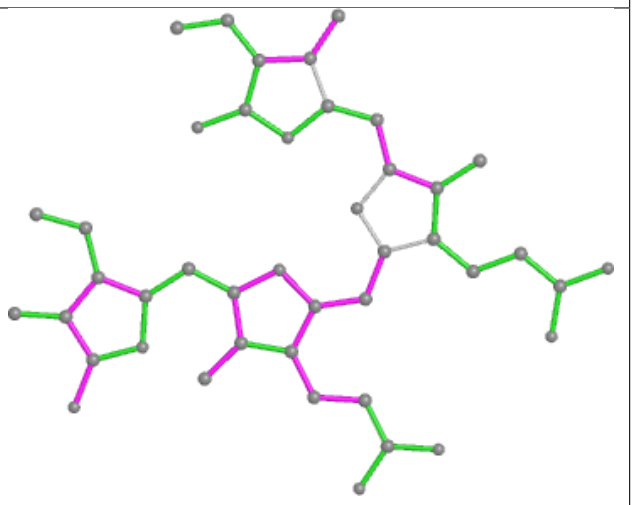

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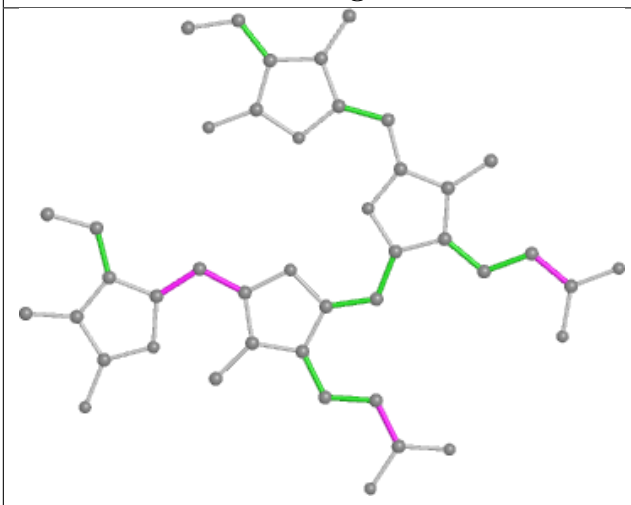

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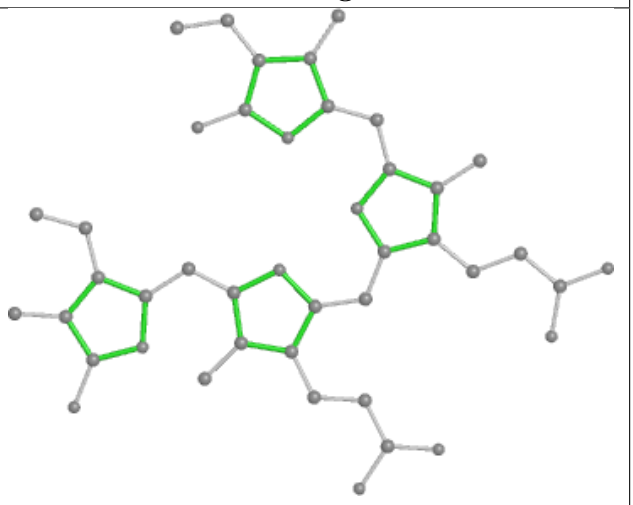

Rings

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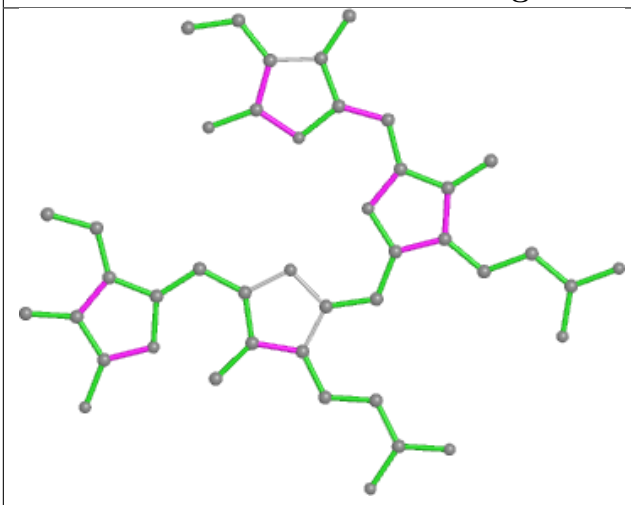

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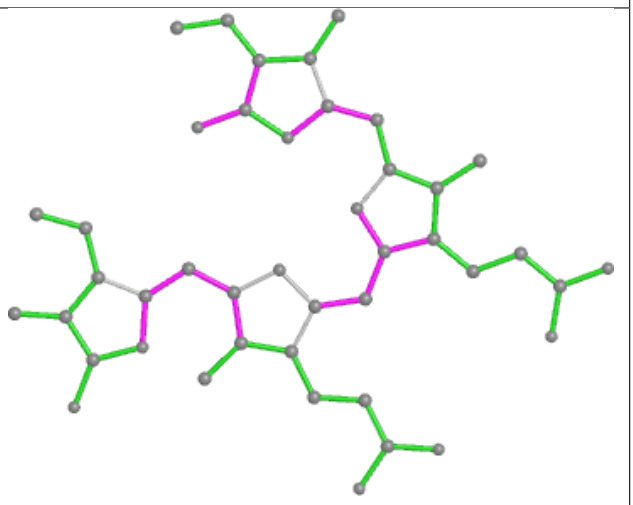

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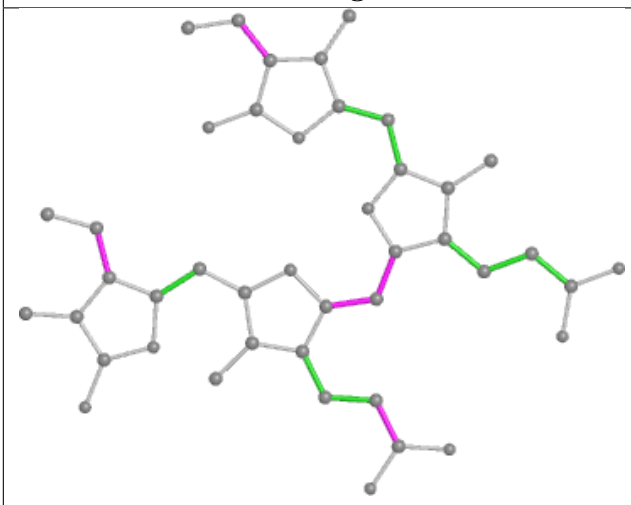

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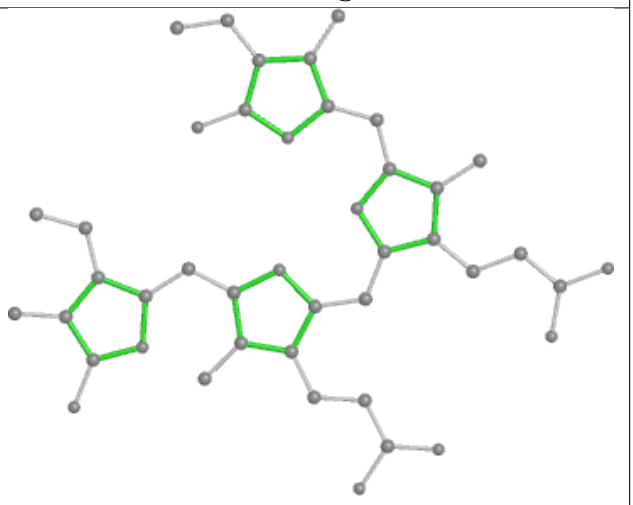
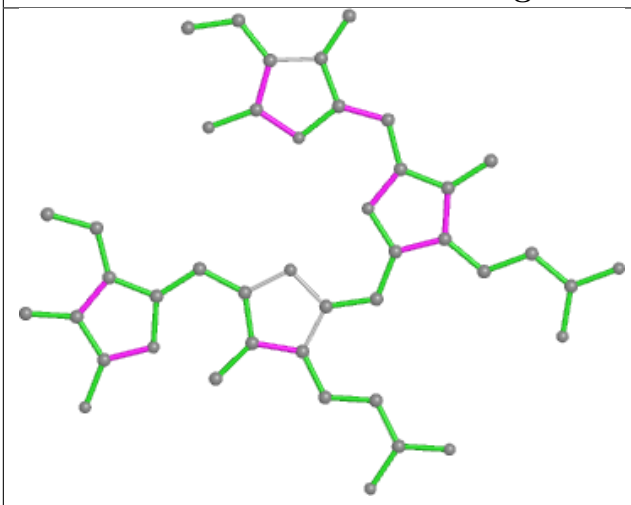


Rings

Ligand PUB eY 405



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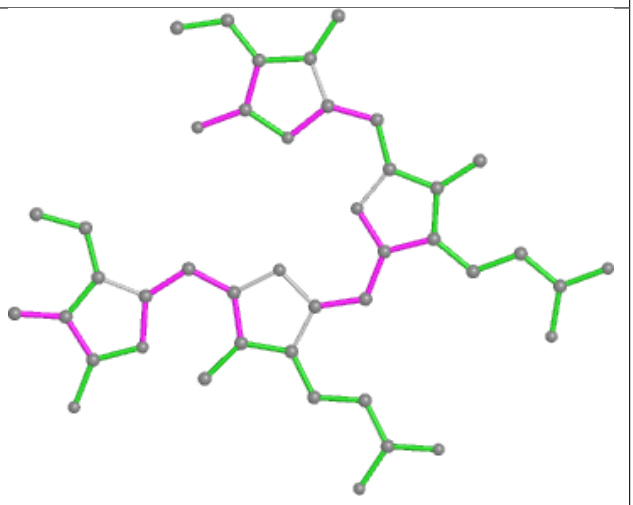

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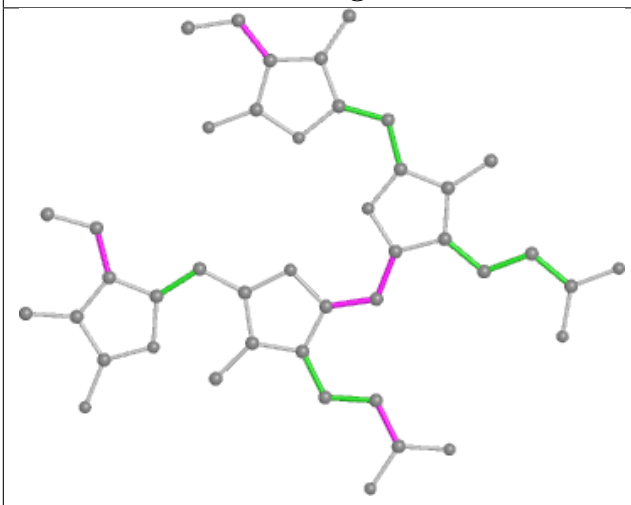

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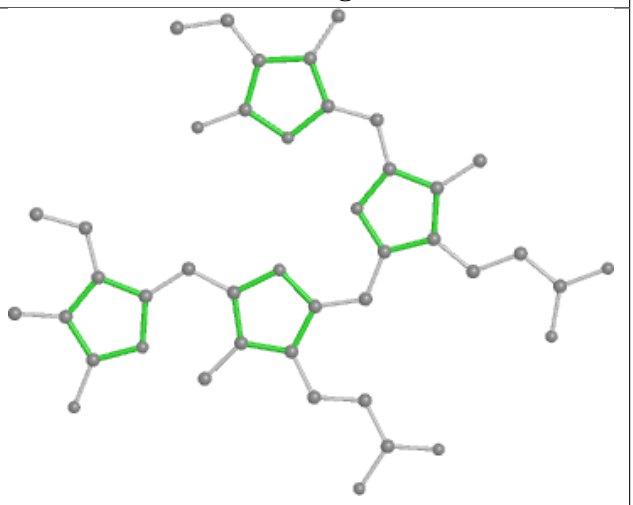
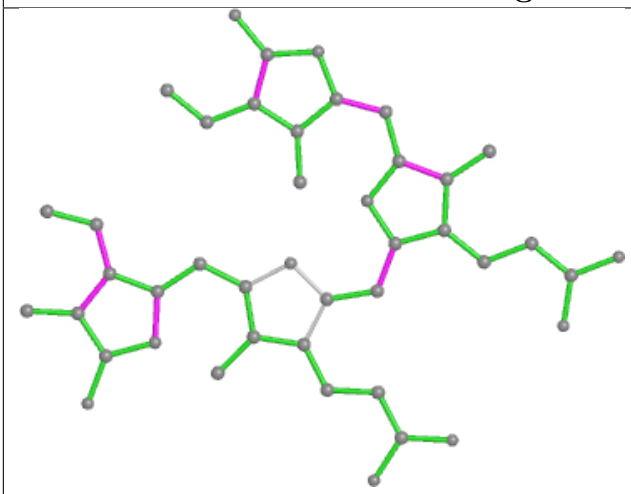


Rings

Ligand PVN dx 405



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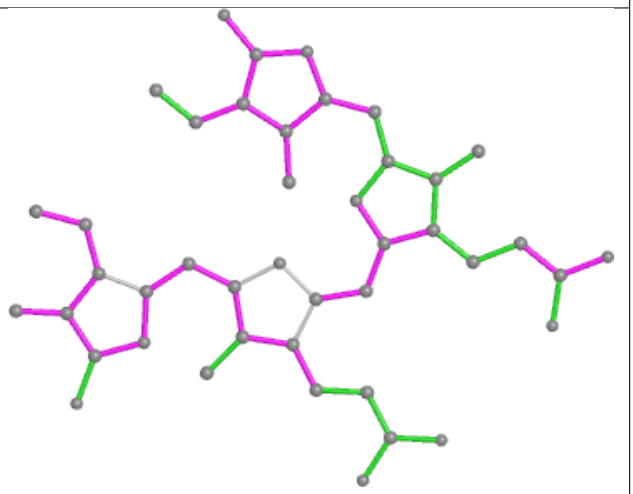

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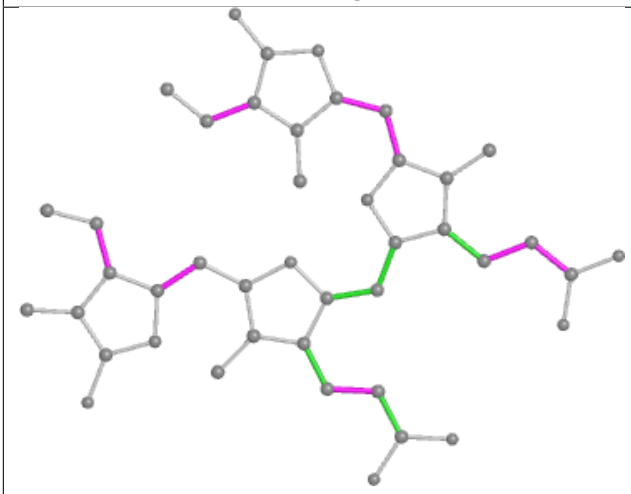

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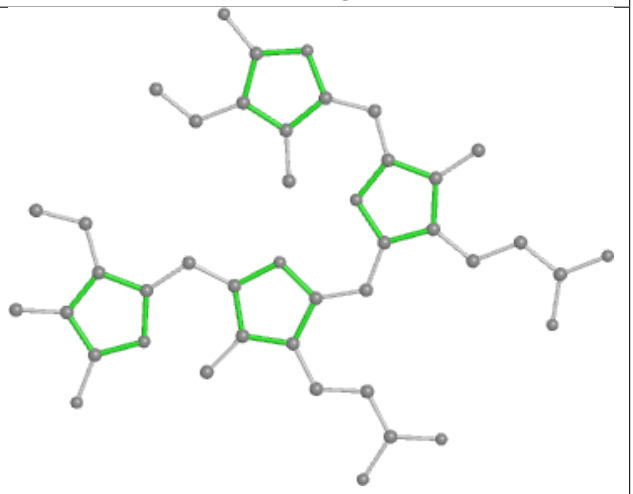
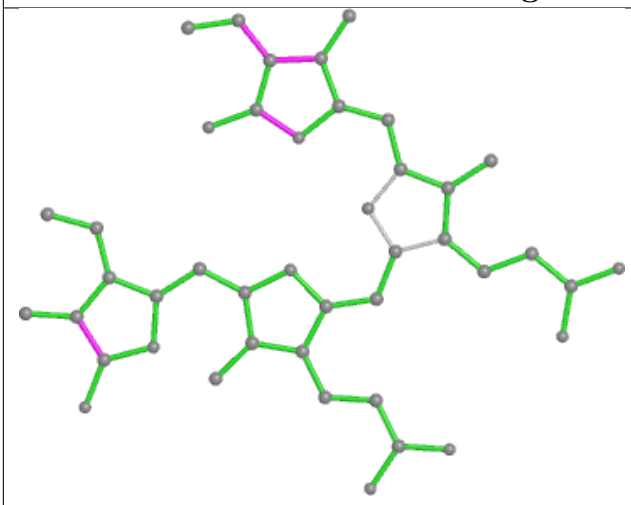


Rings

Ligand PEB r8 201



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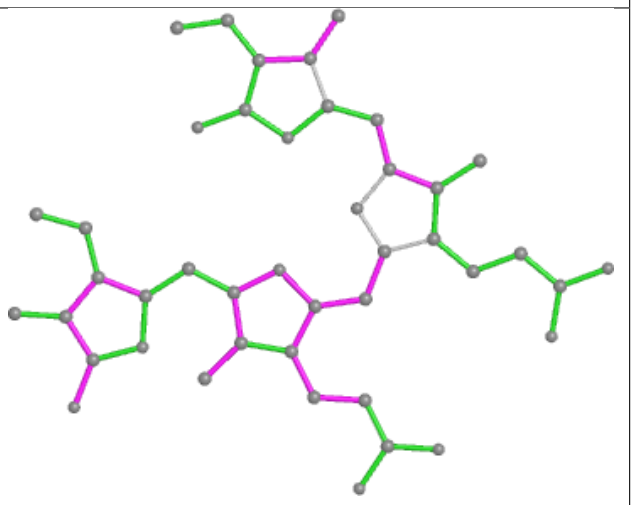

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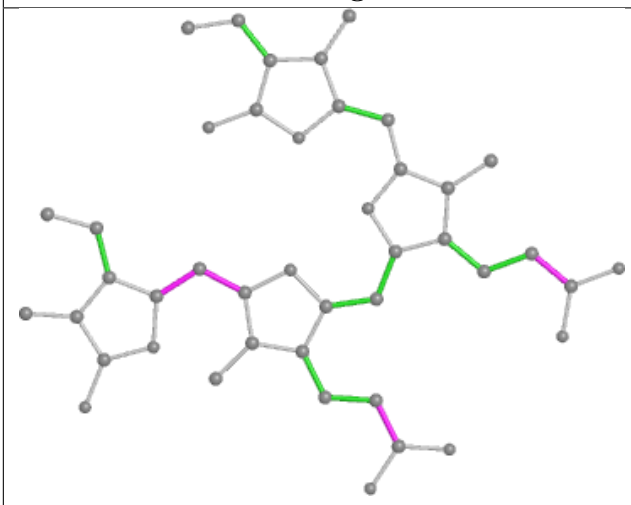

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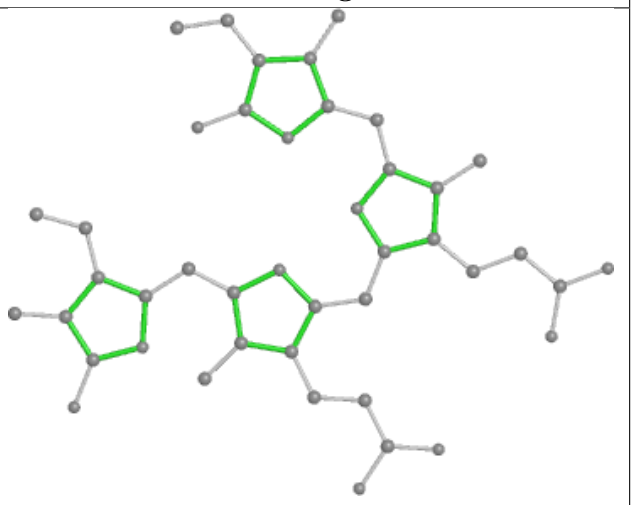

Rings

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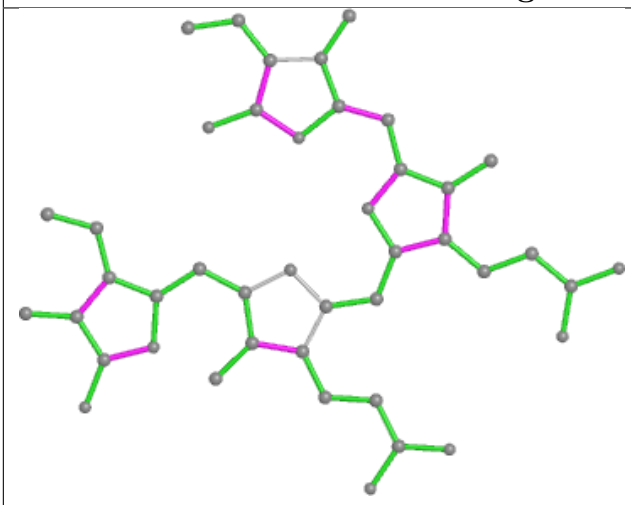

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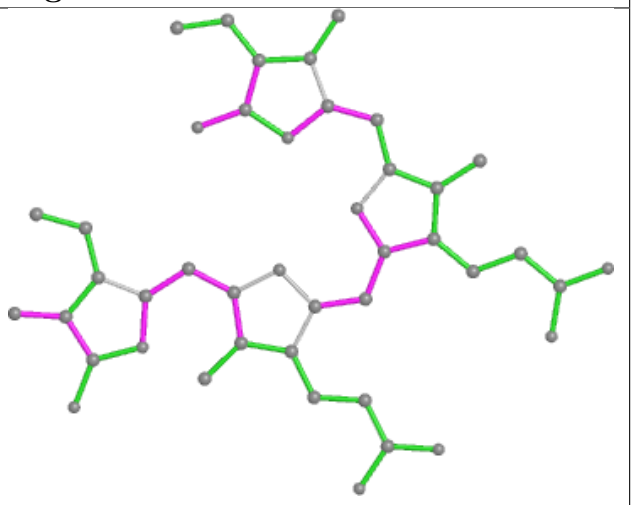

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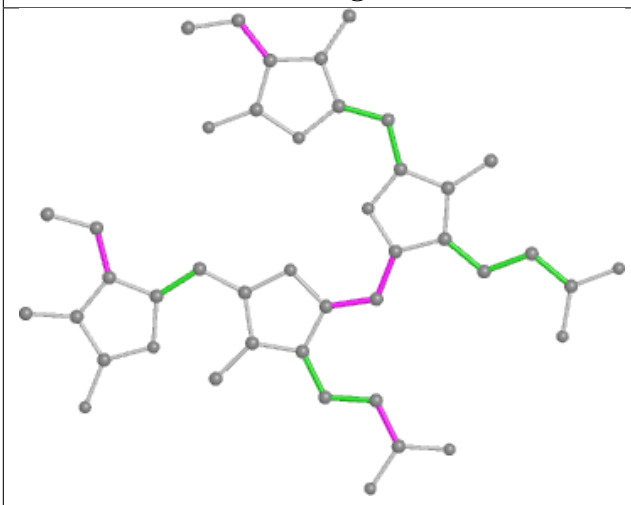

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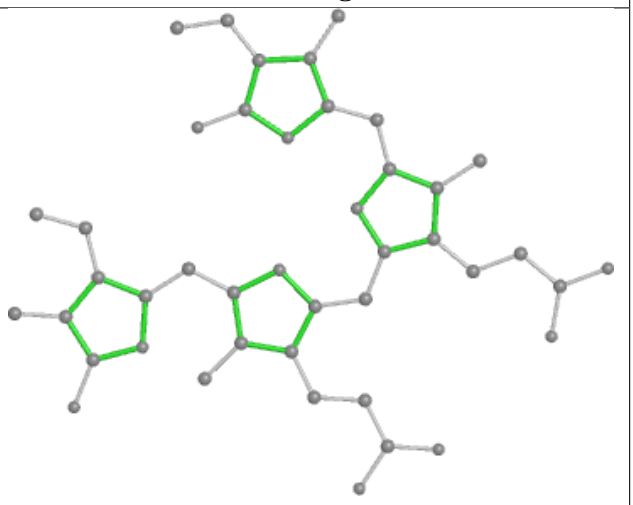
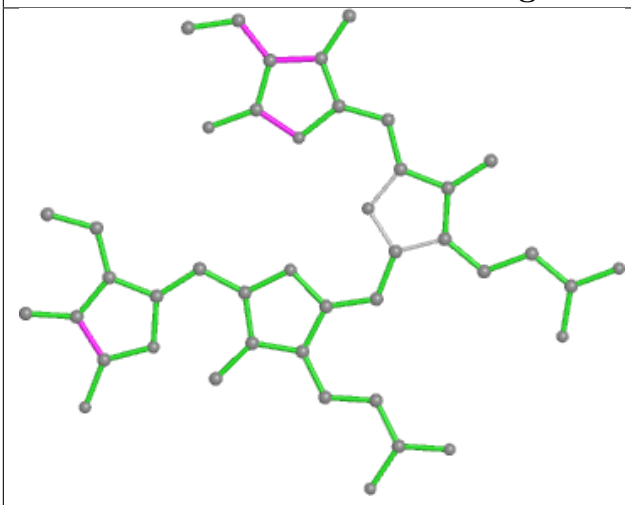


Rings

Ligand PEB h6 202



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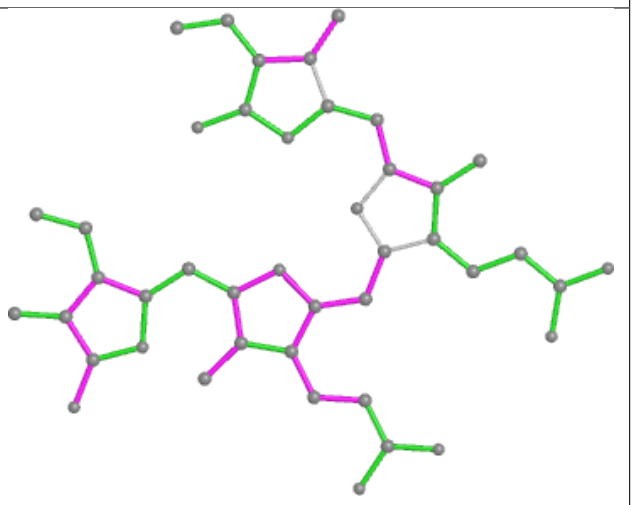

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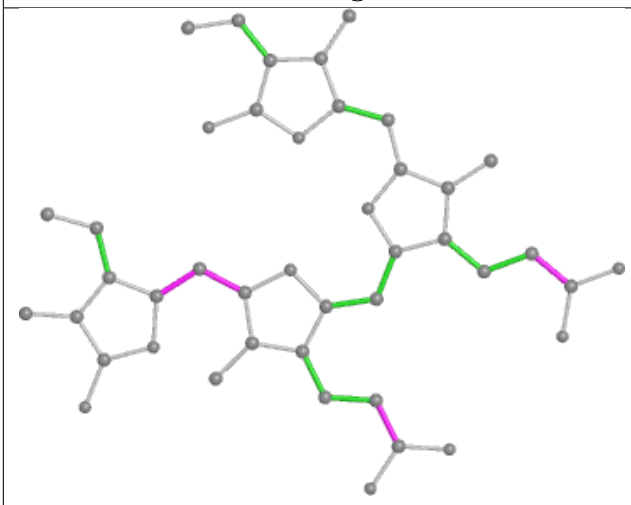

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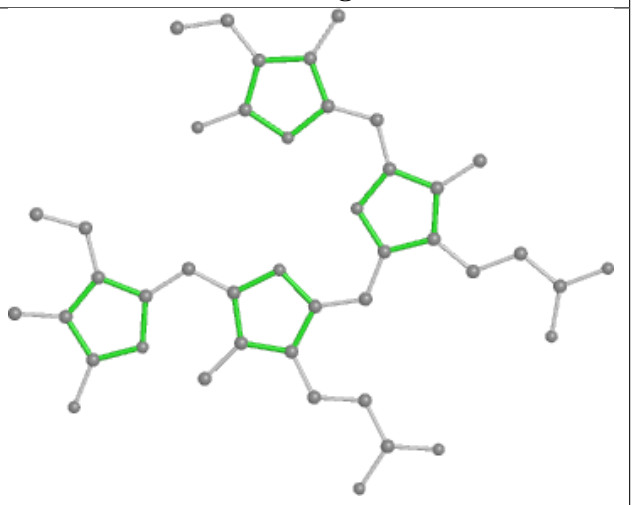
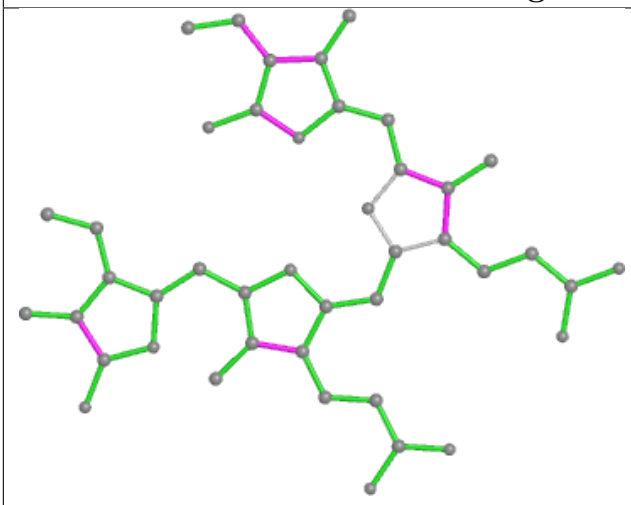


Rings

Ligand PEB li 203



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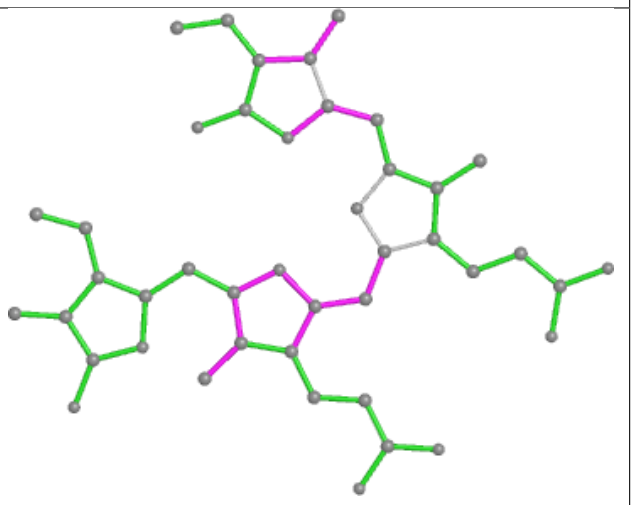

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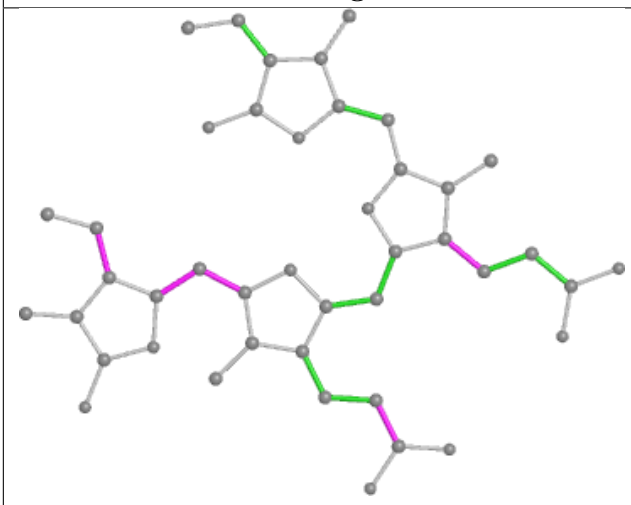

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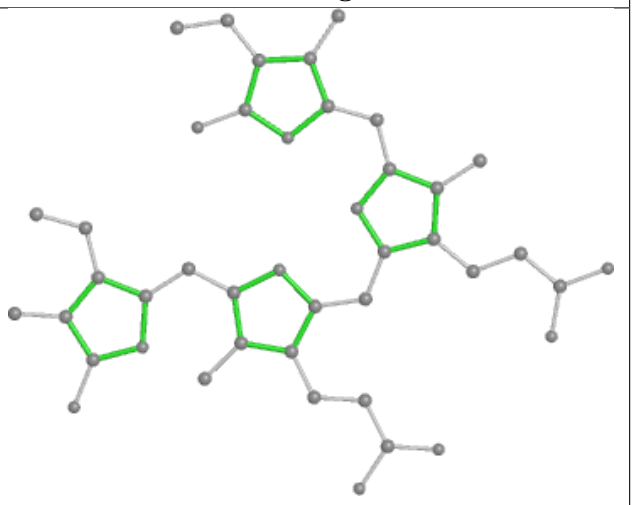
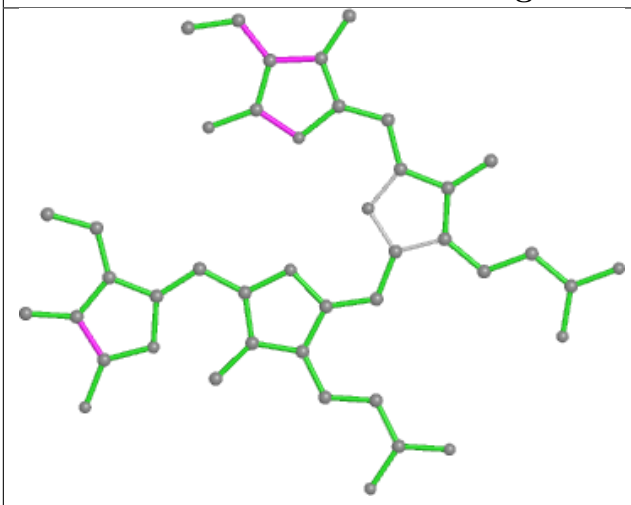


Rings

Ligand PEB Q4 201



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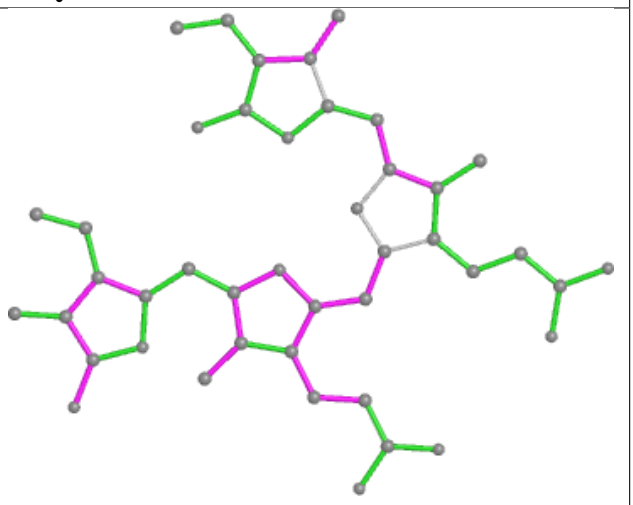

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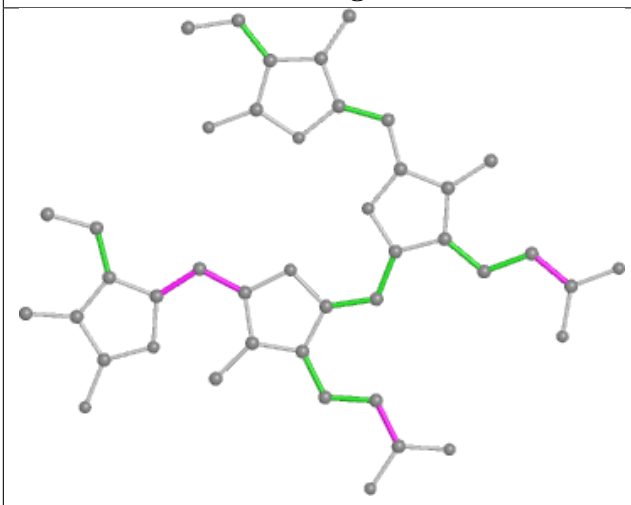

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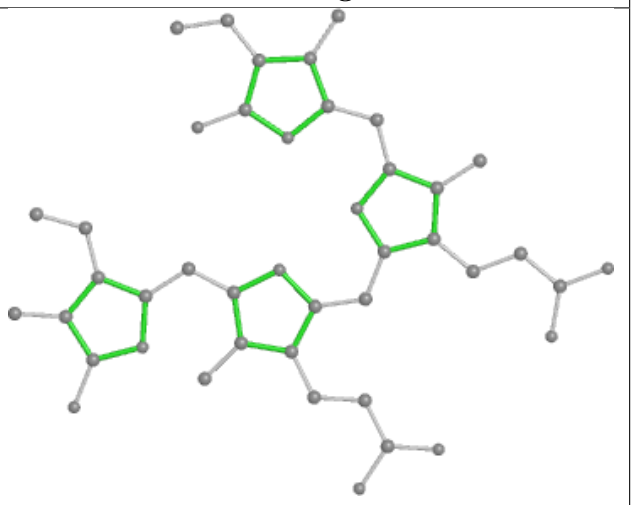
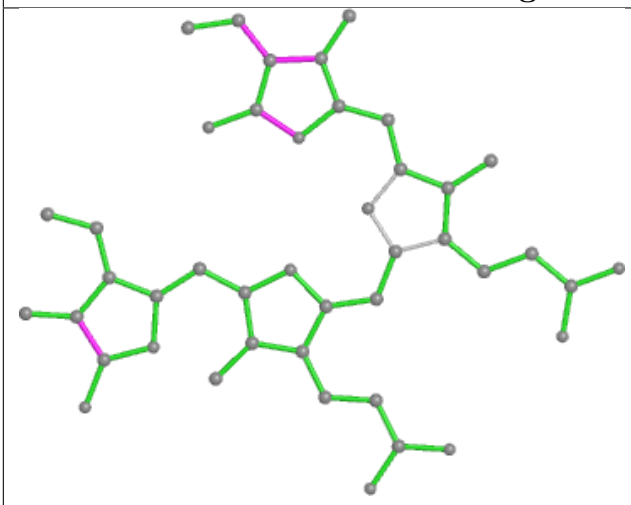


Rings

Ligand PEB cL 201



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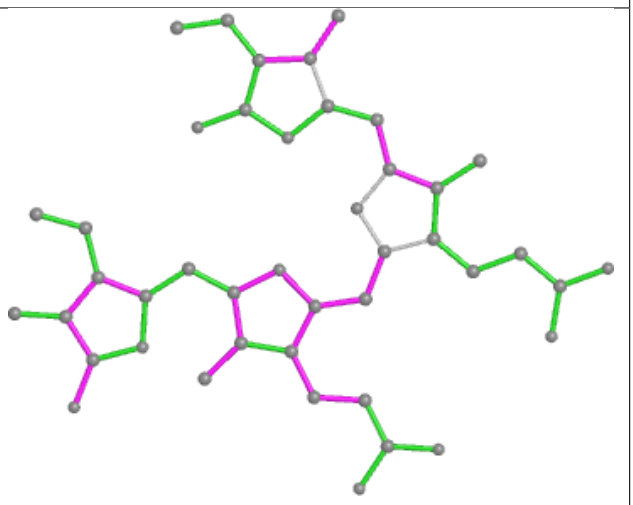

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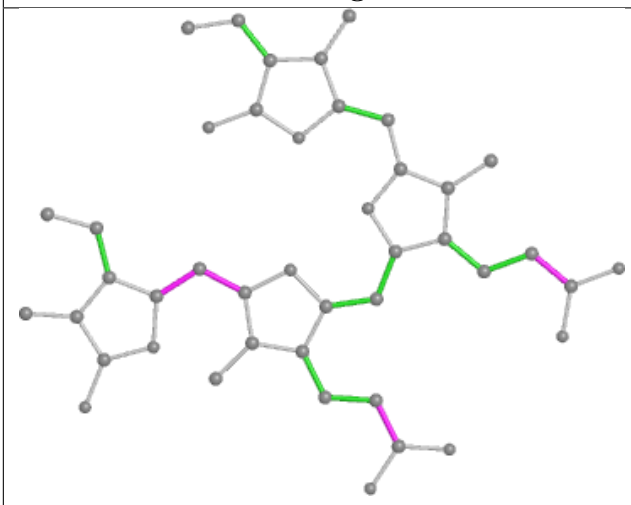
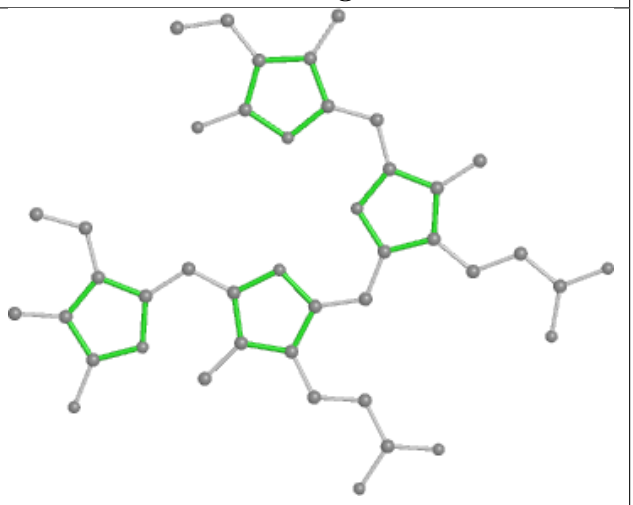
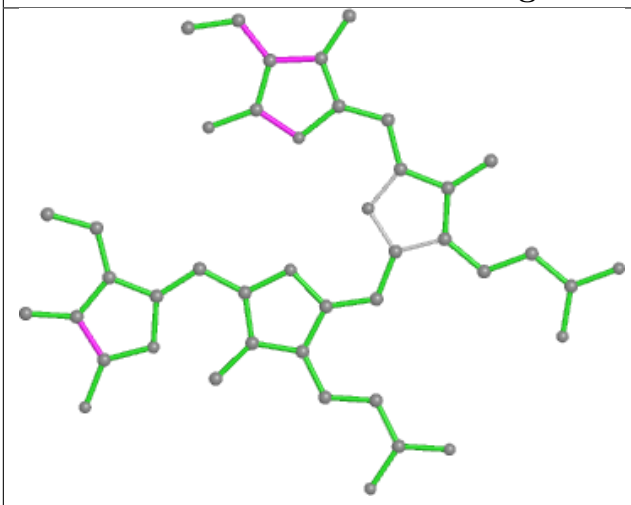


Torsions



Rings

Ligand PEB u4 202



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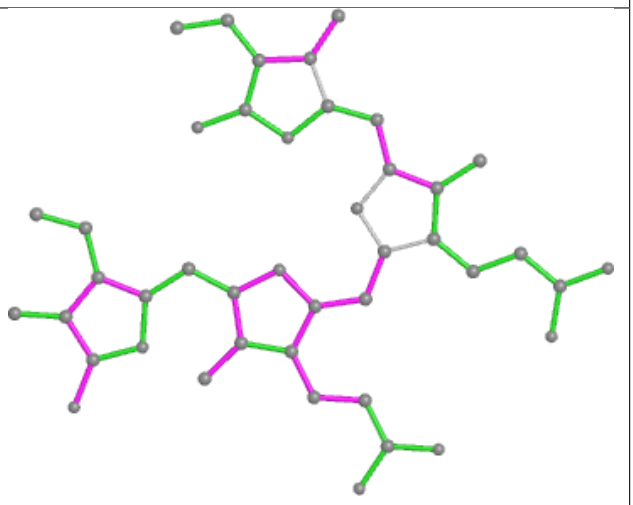
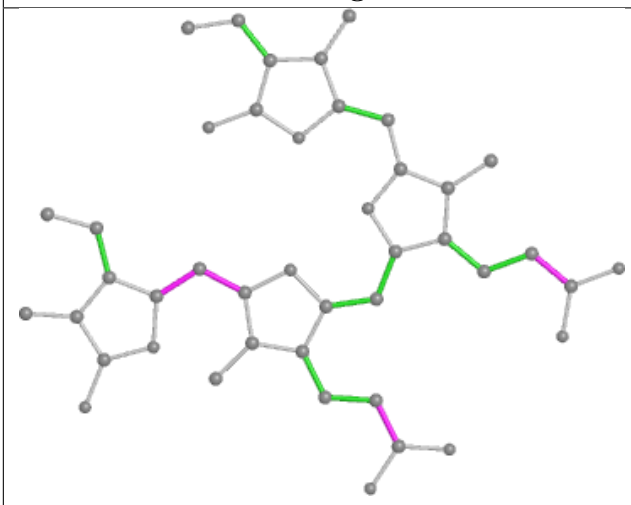


Bond angles



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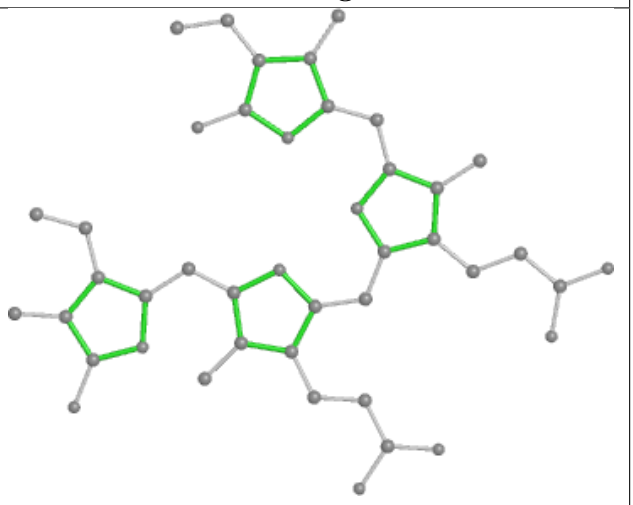
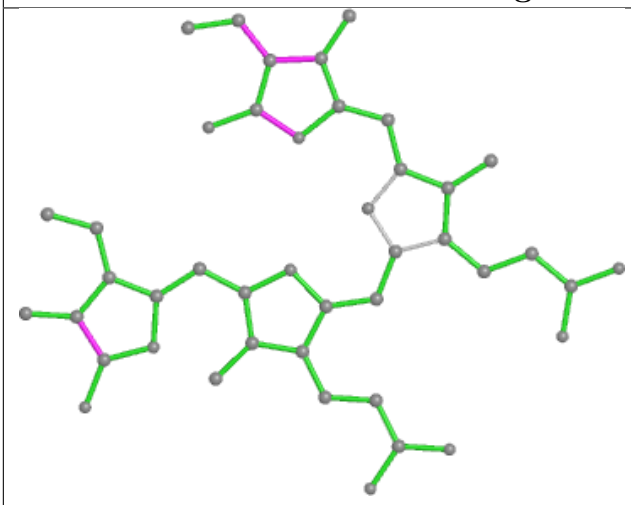


Rings

Ligand PEB dV 201



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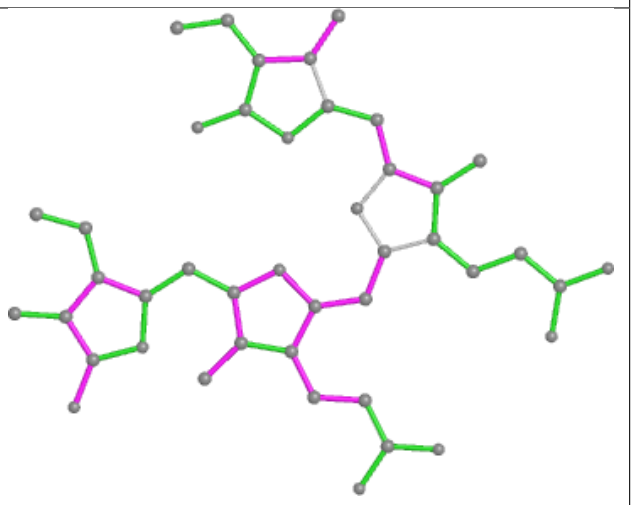

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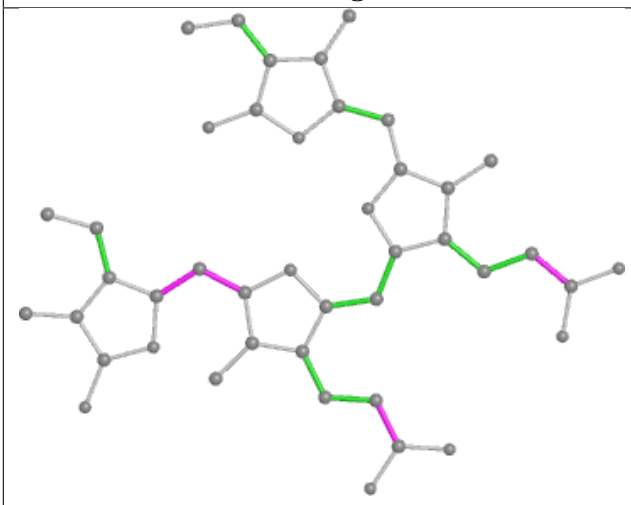

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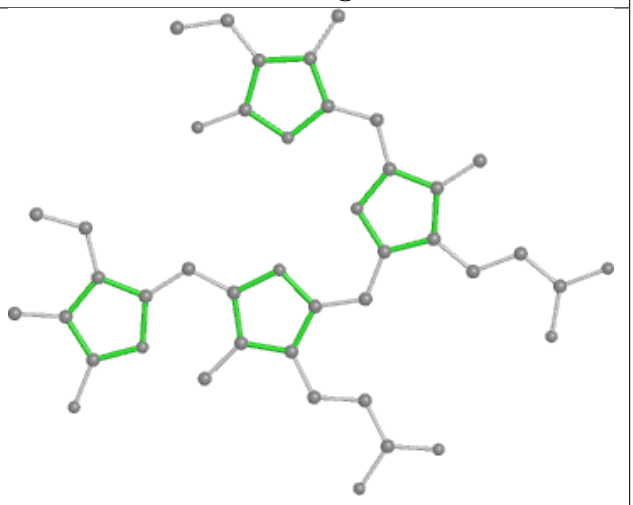
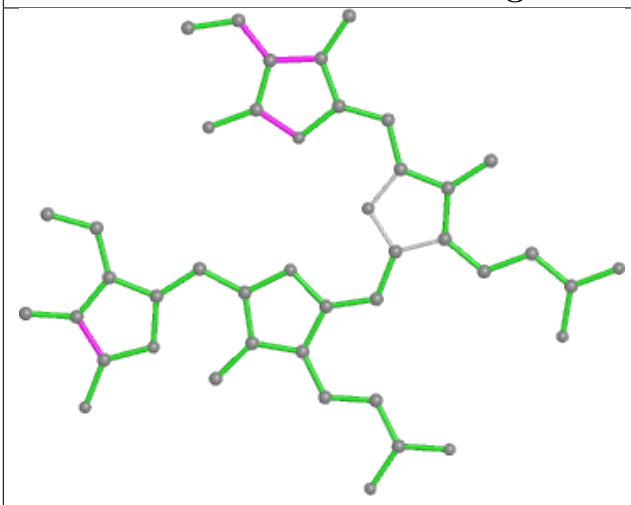


Rings

Ligand PEB jM 1001



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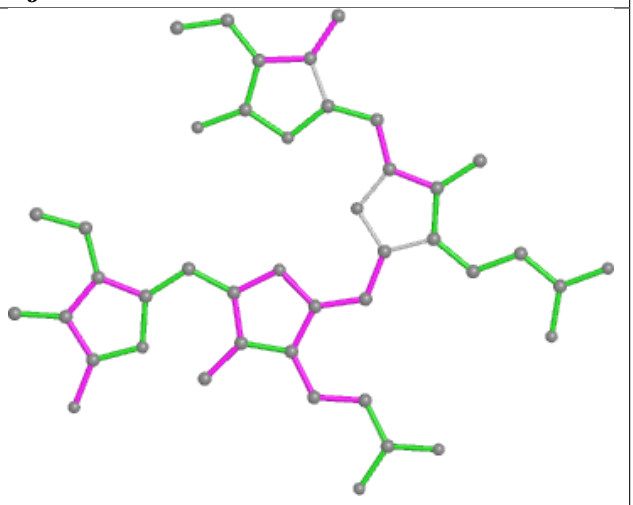

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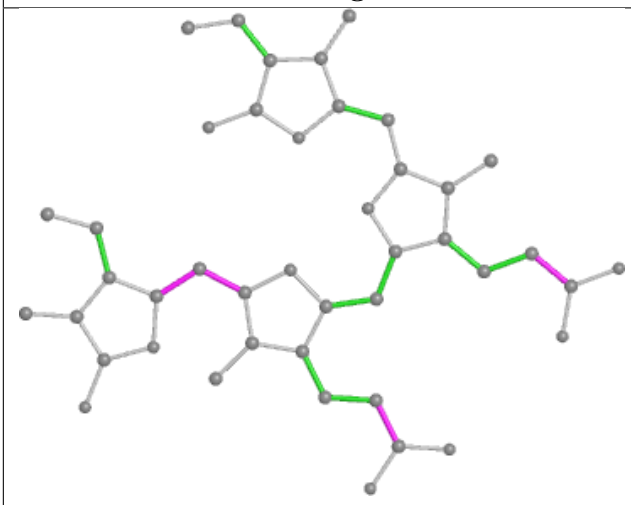

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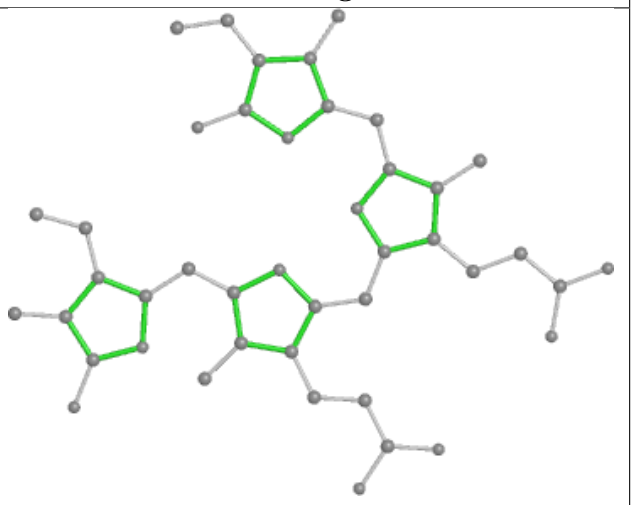
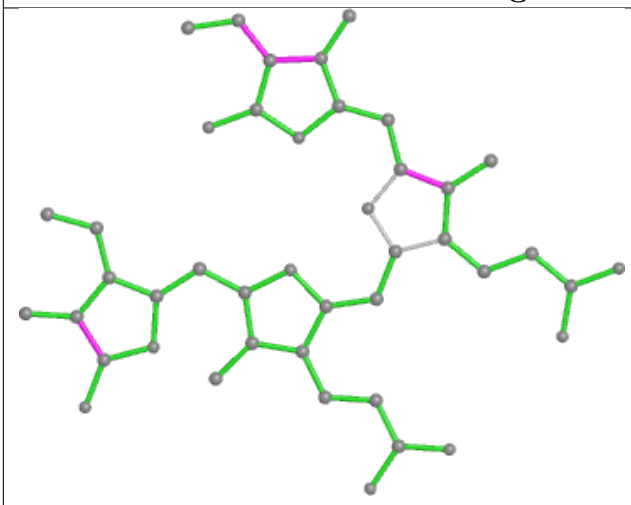


Rings

Ligand PEB gb 1002



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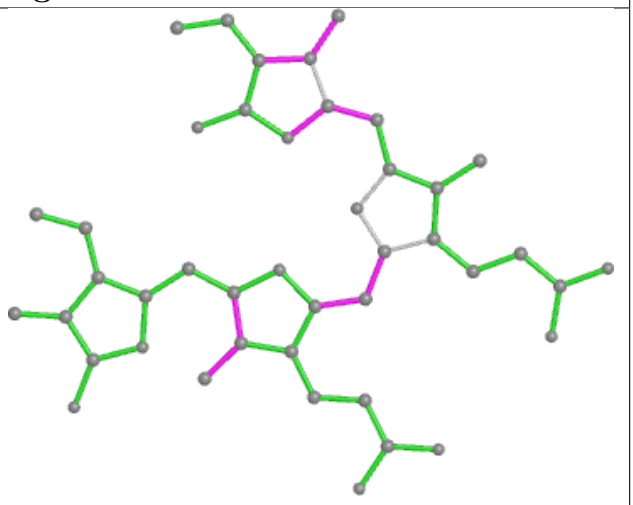

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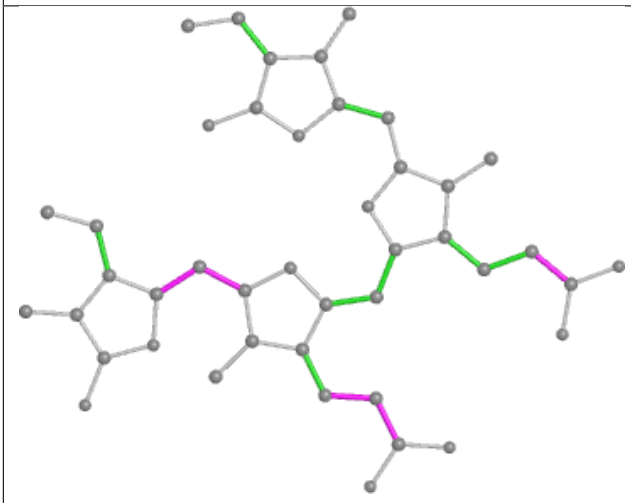

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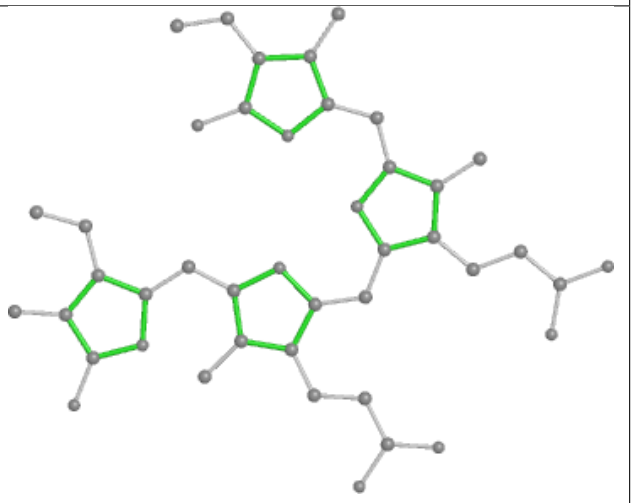
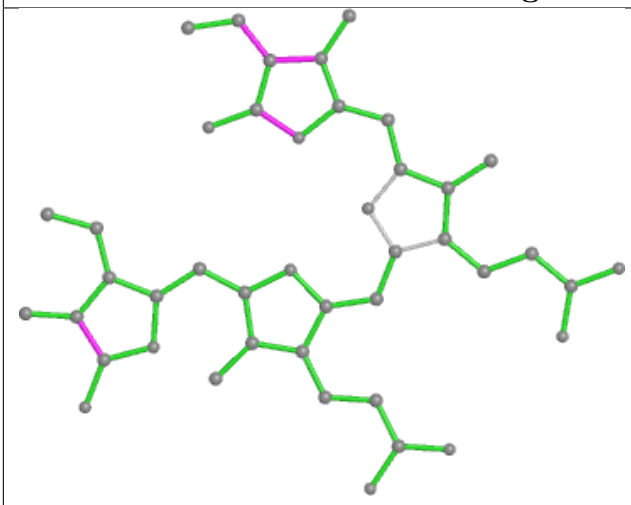


Rings

Ligand PEB t4 202



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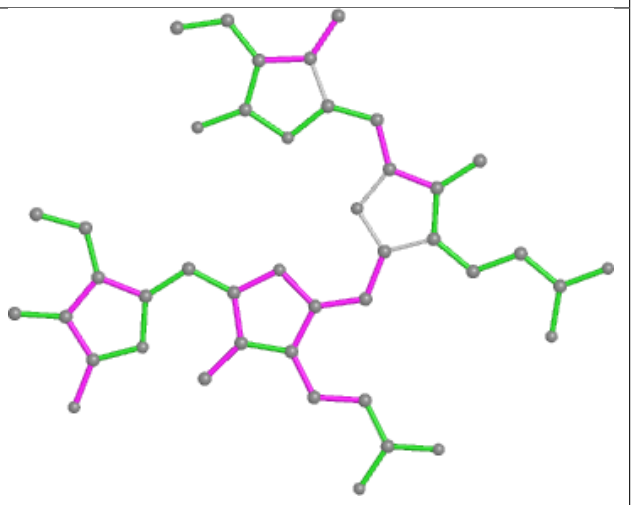

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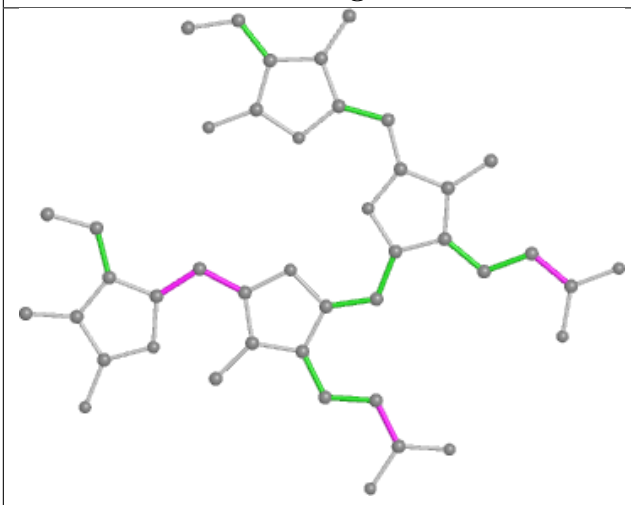

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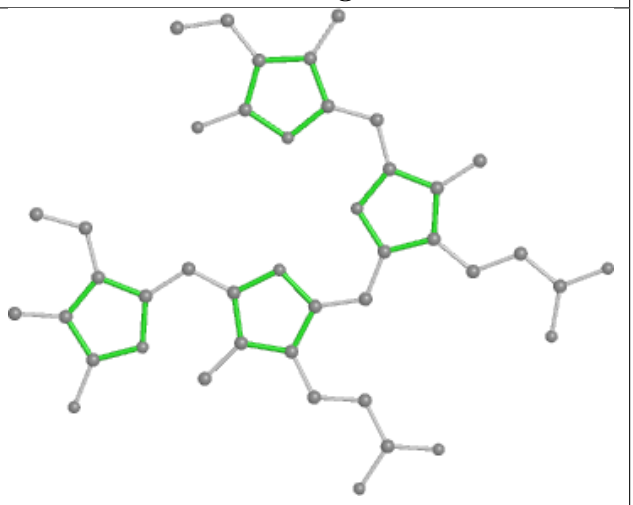

Rings

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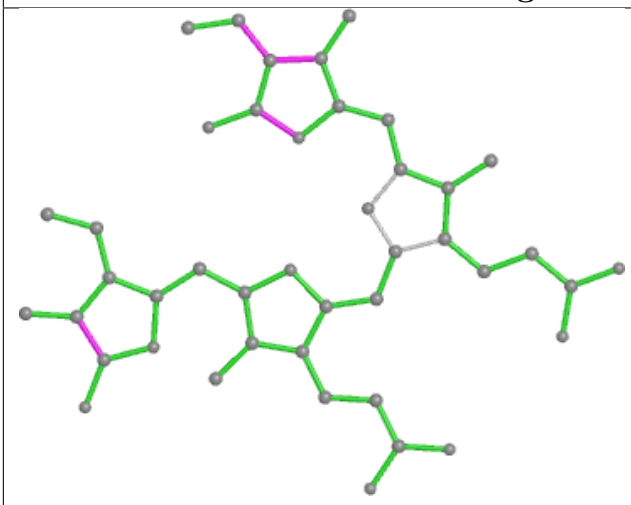

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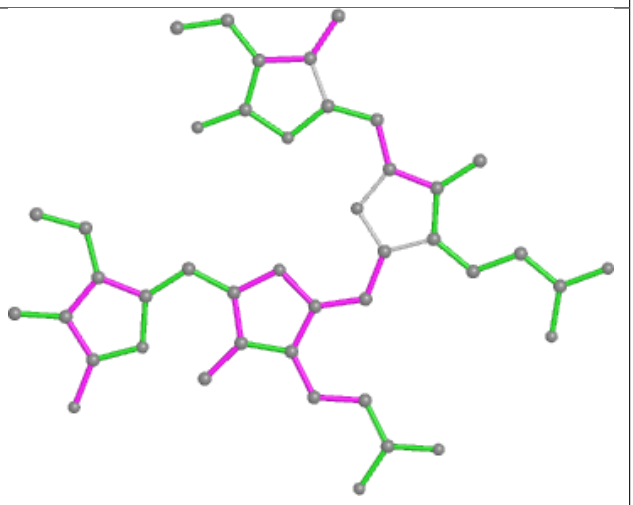

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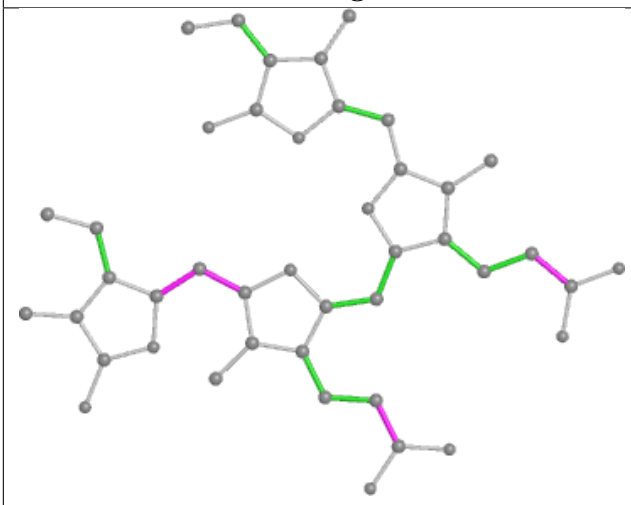

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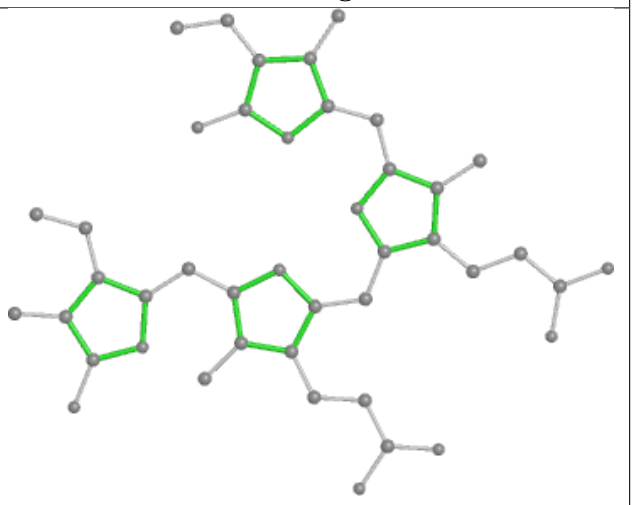
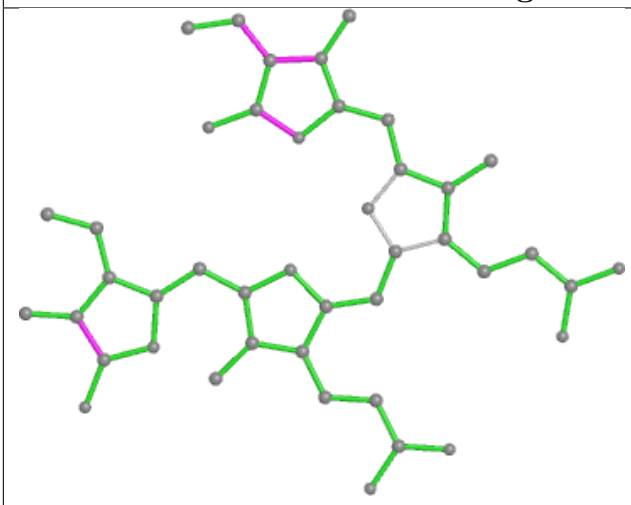


Rings

Ligand PEB T8 301



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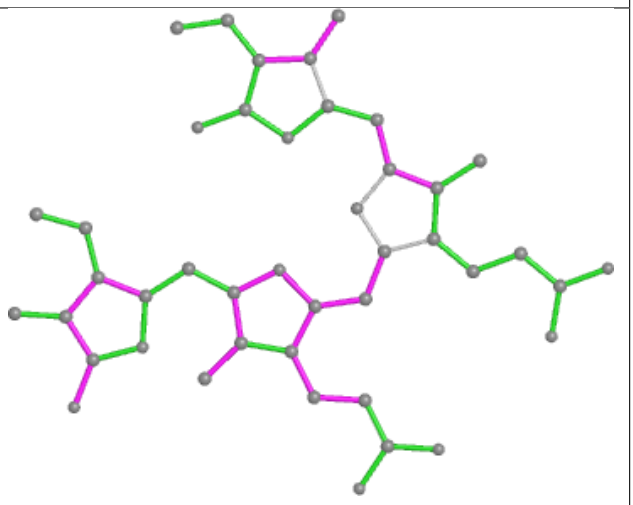

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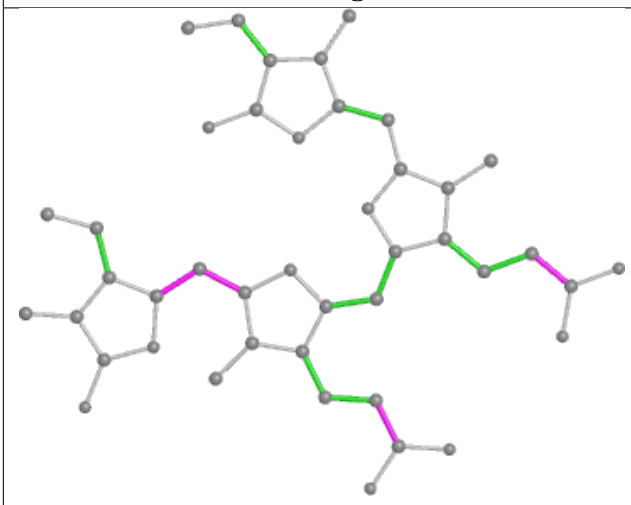

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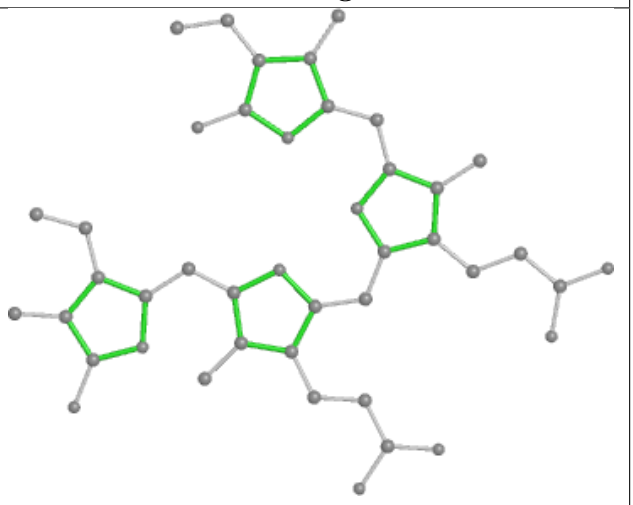

Rings

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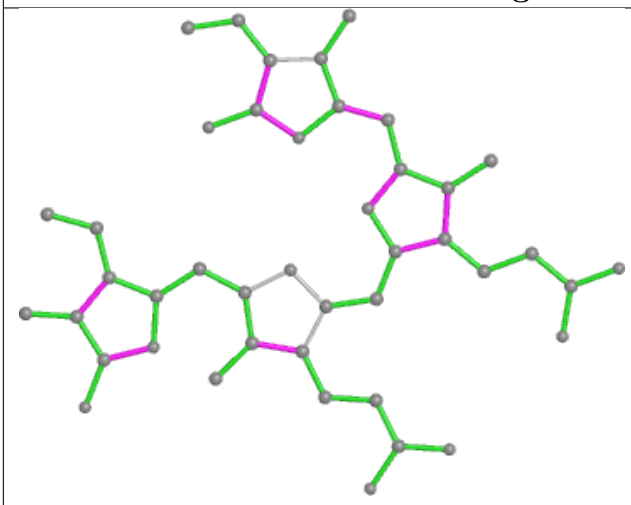

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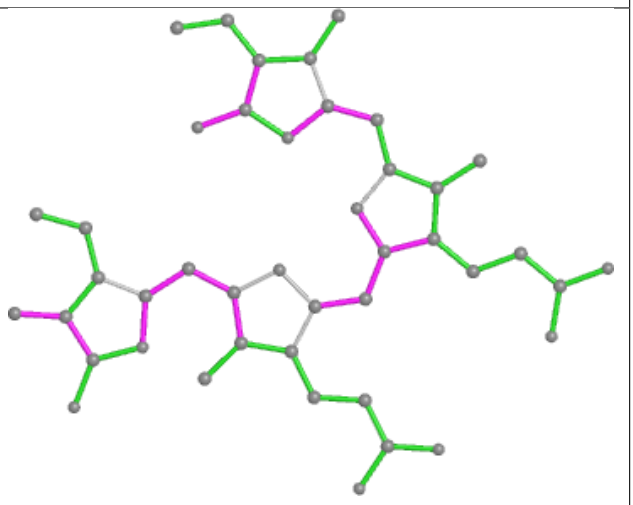

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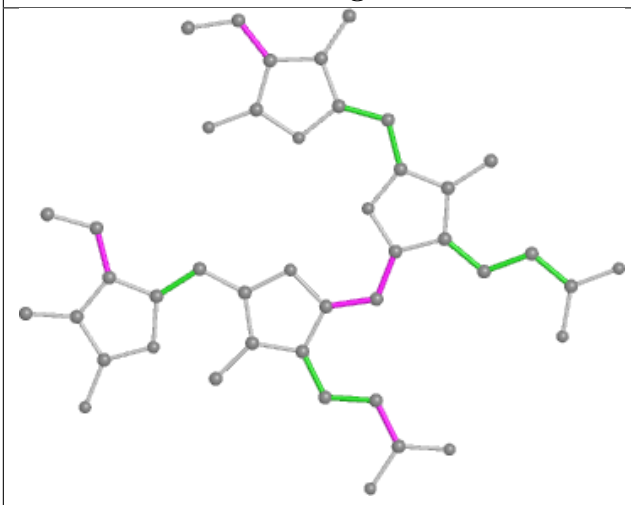

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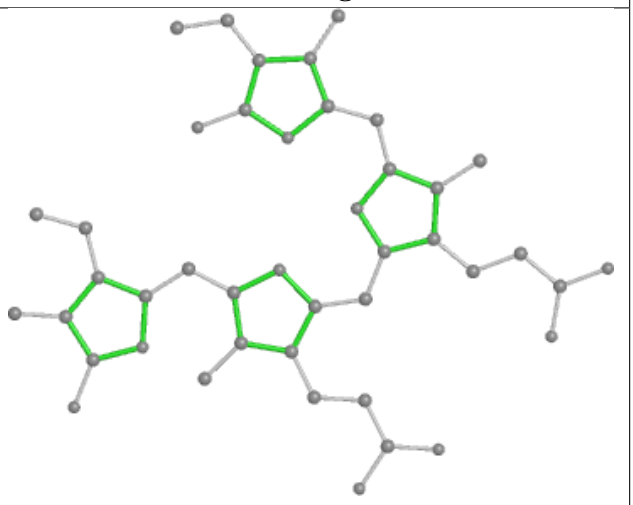

Rings

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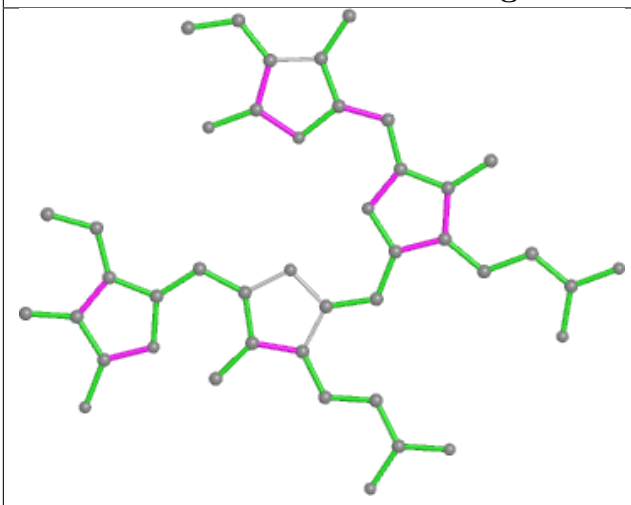

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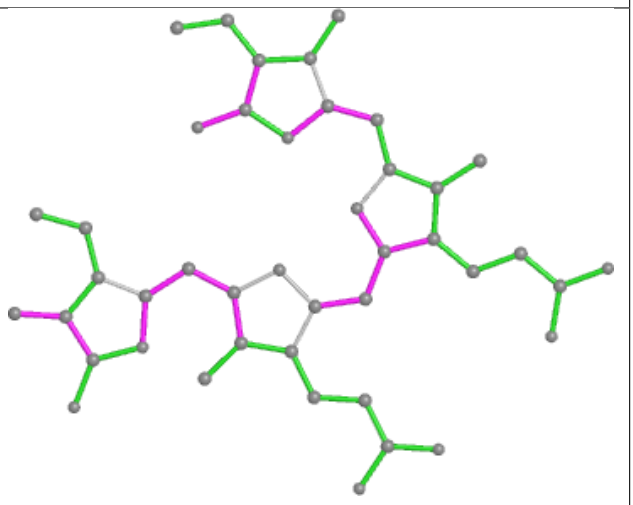

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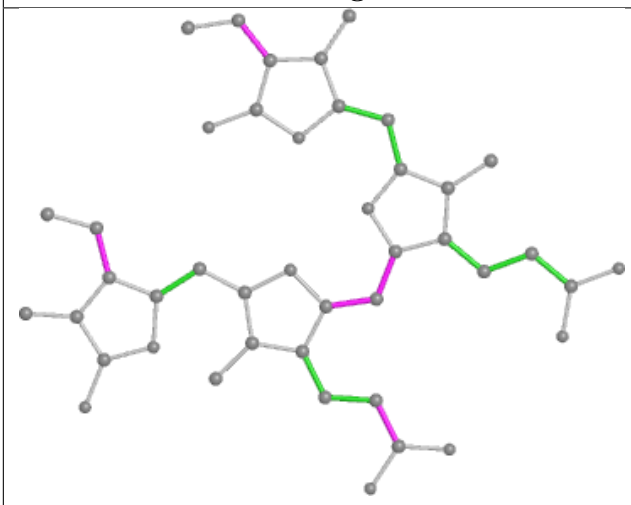

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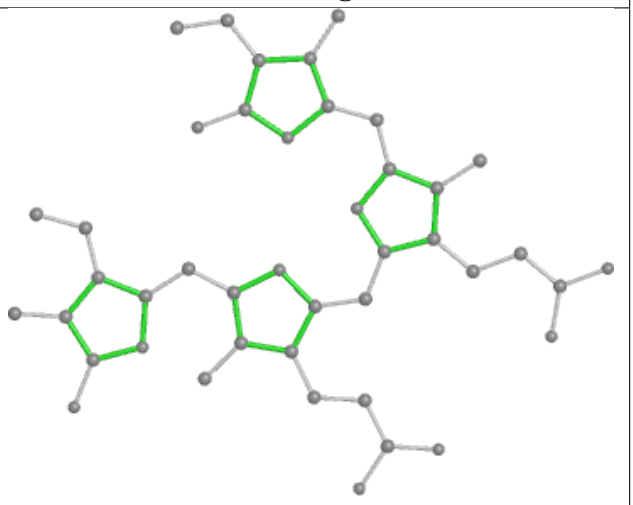

Rings

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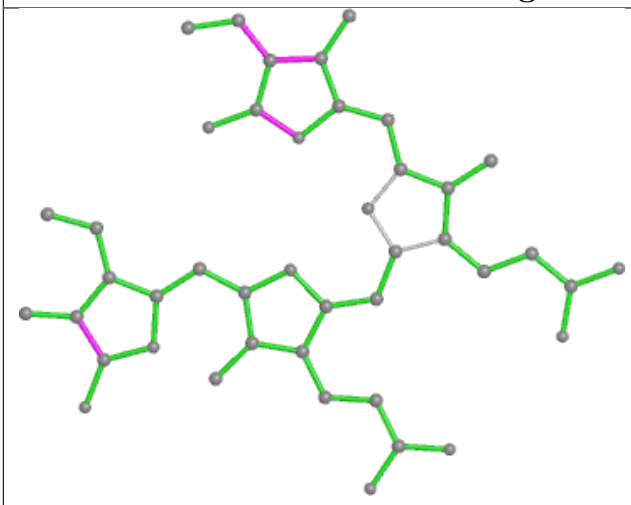

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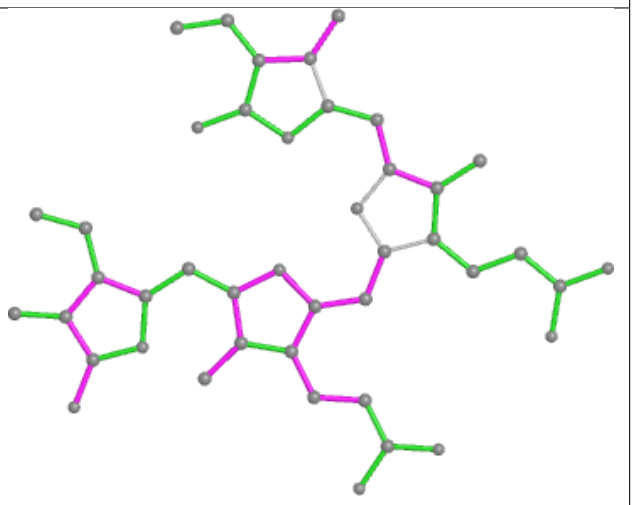

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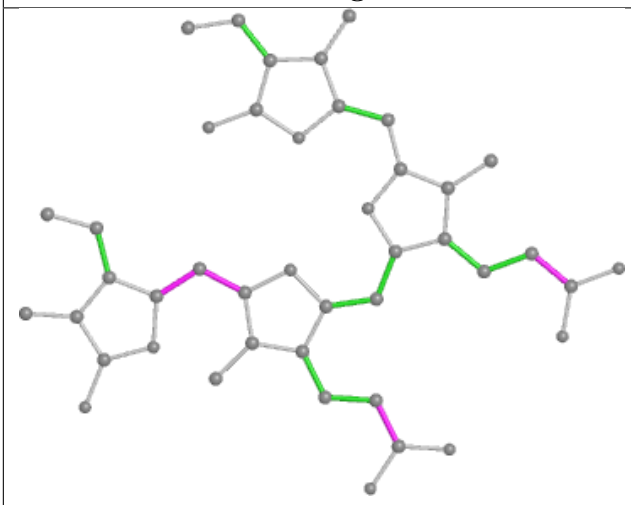

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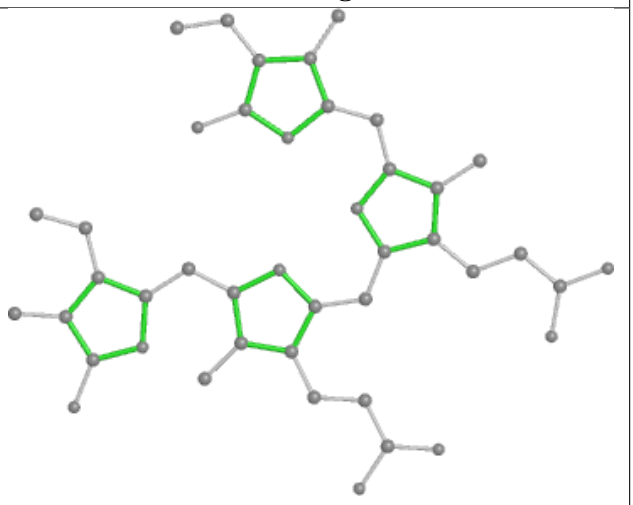

Rings

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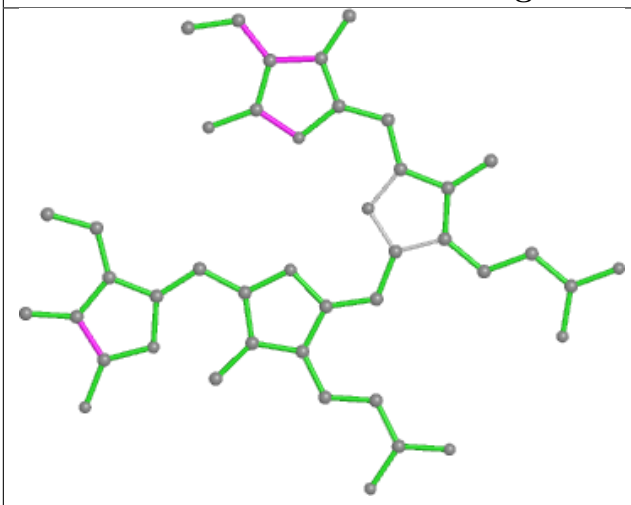

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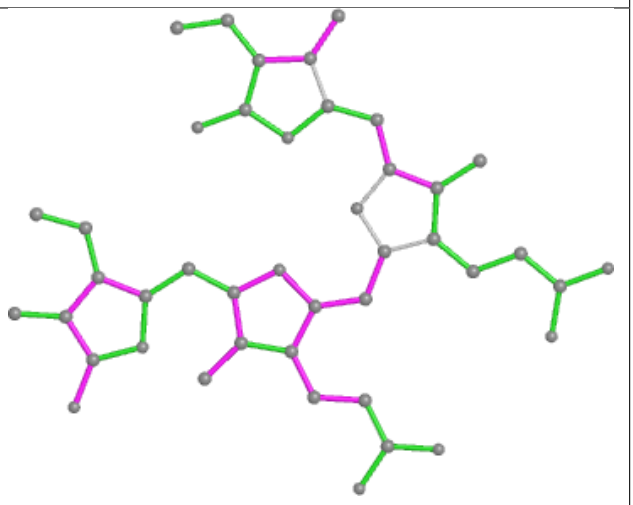

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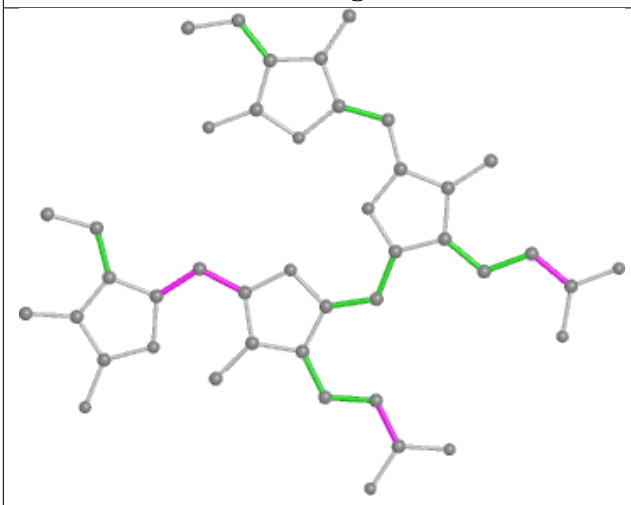

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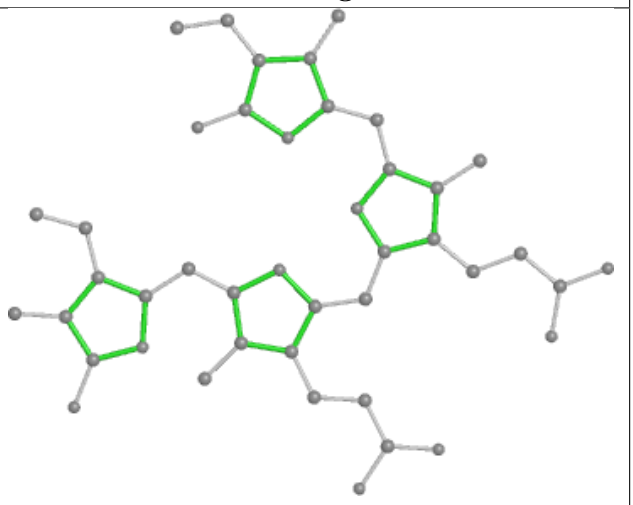
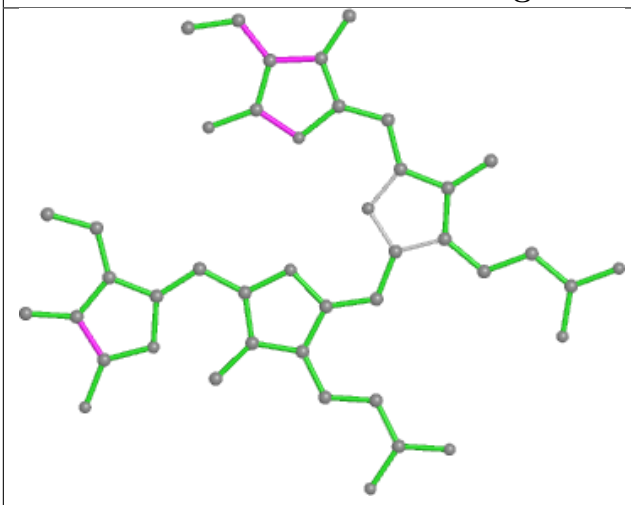


Rings

Ligand PEB bG 201



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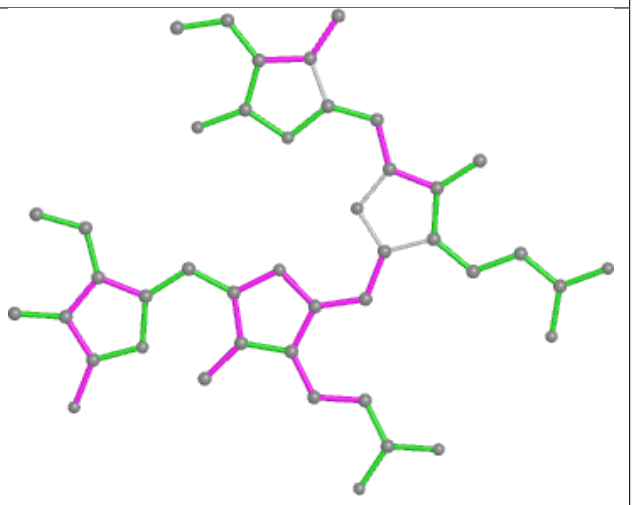

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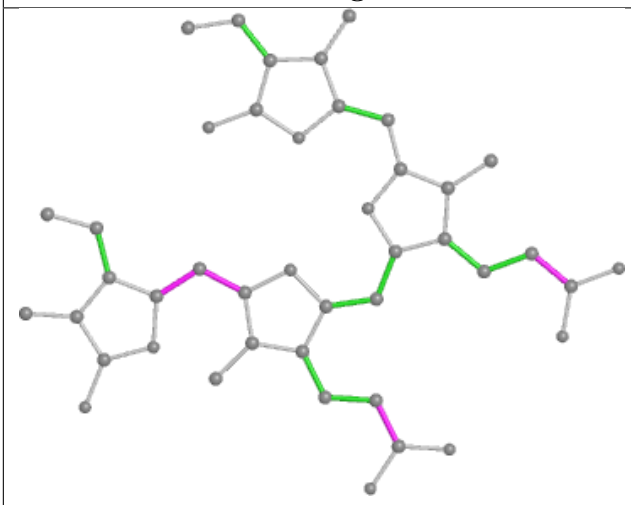

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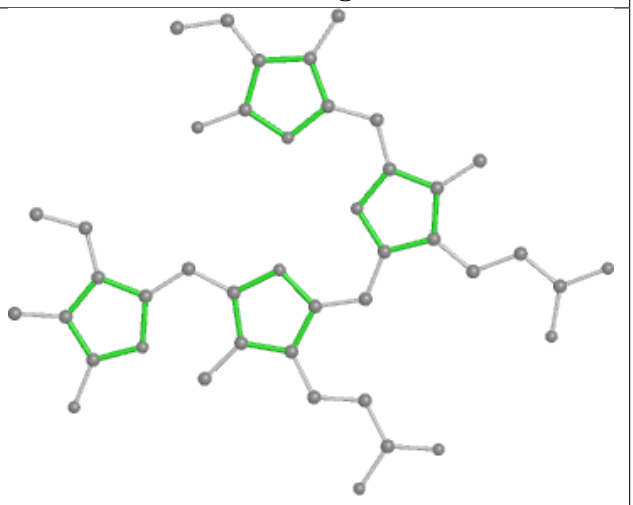
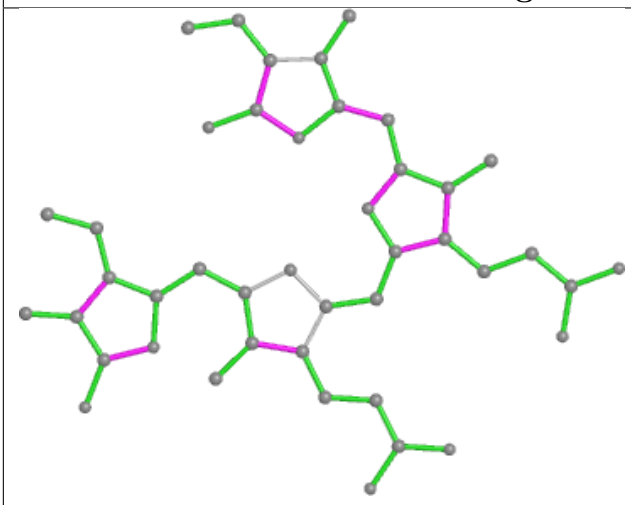


Rings

Ligand PUB dd 203



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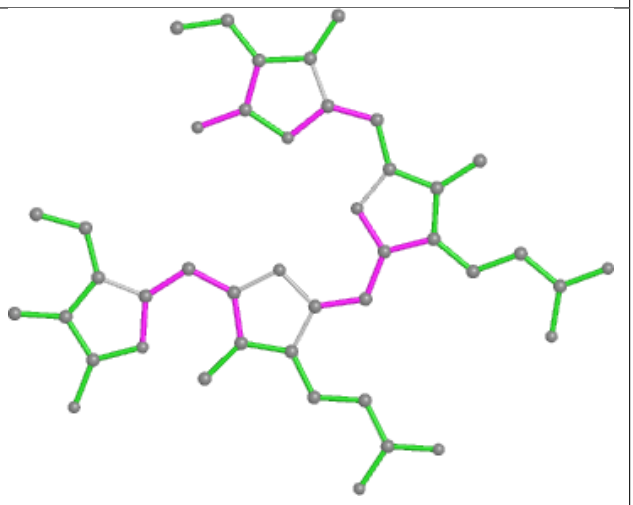

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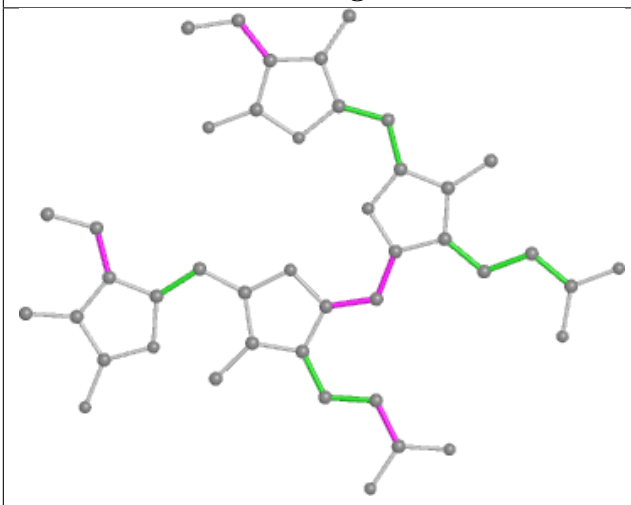

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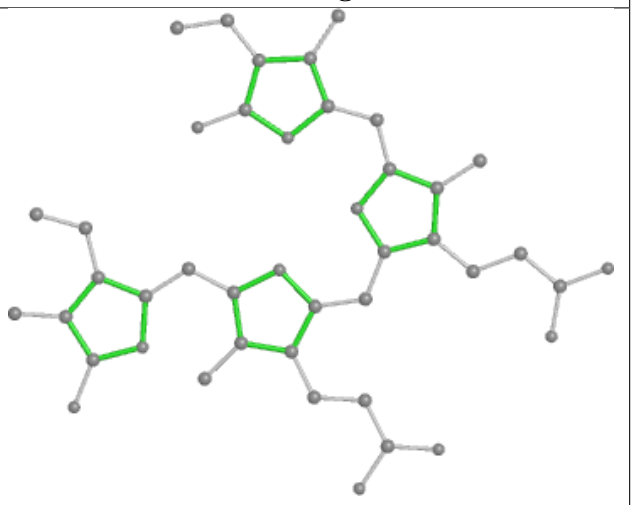
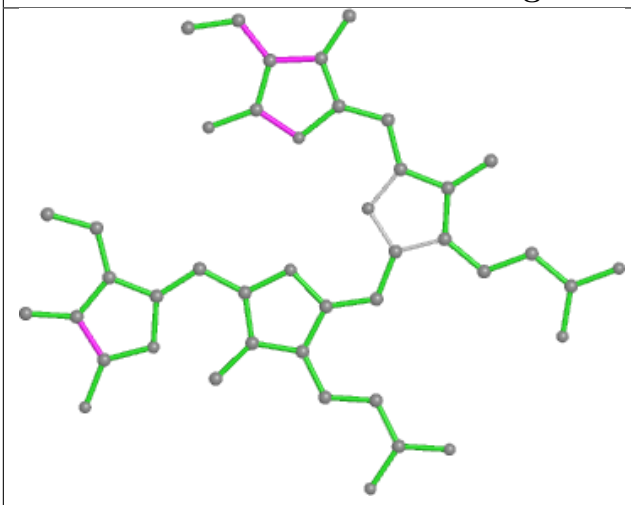


Rings

Ligand PEB j7 201



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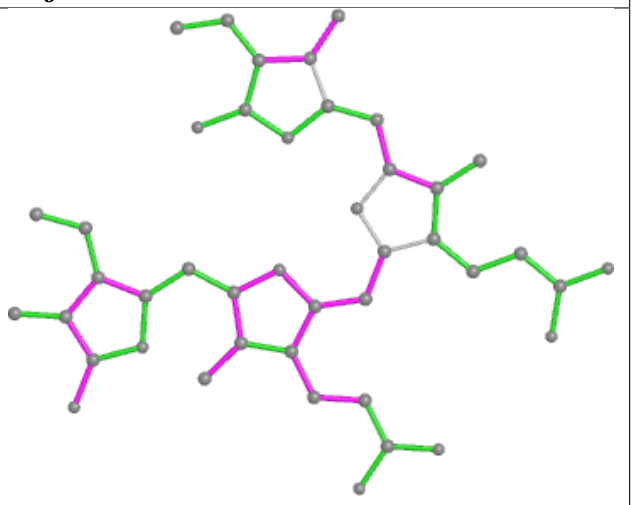

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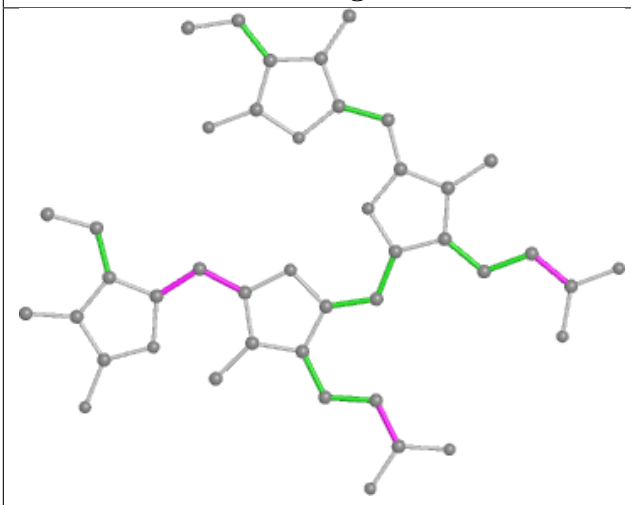
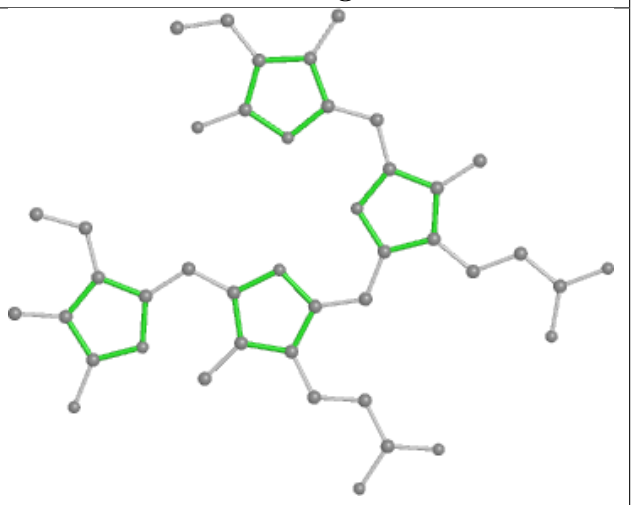
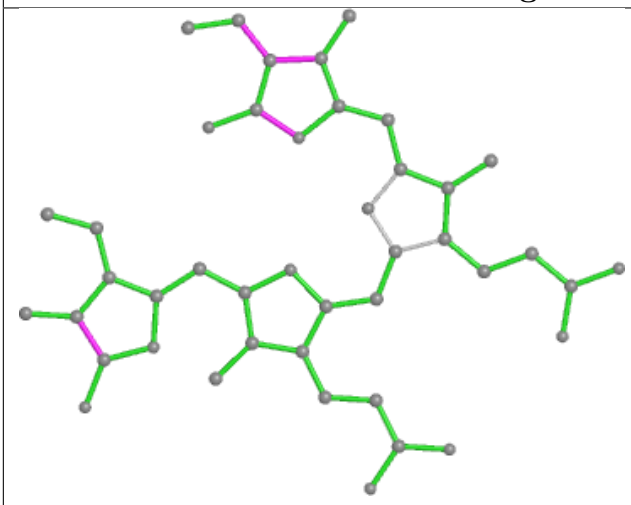


Torsions



Rings

Ligand PEB ak 201



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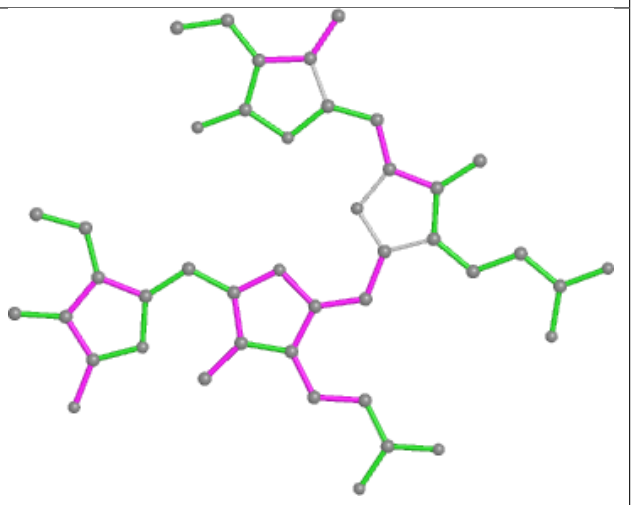

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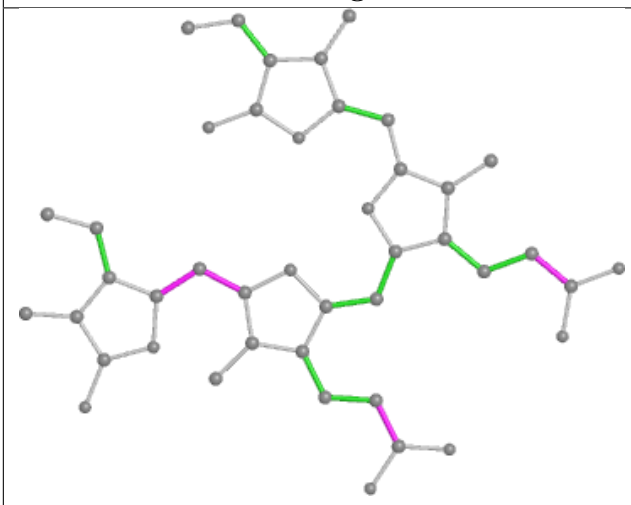

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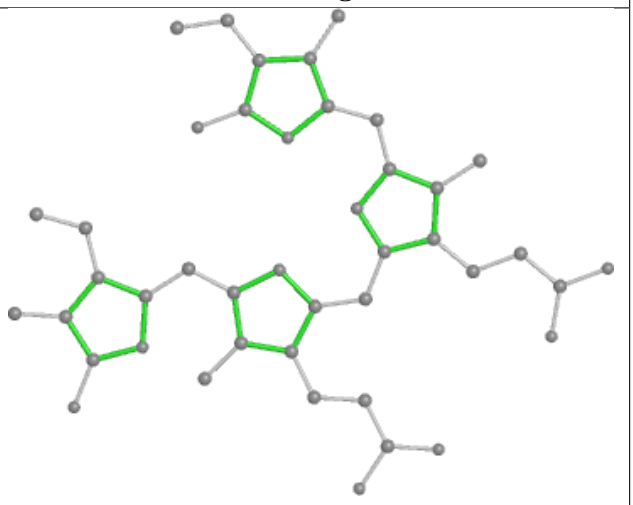
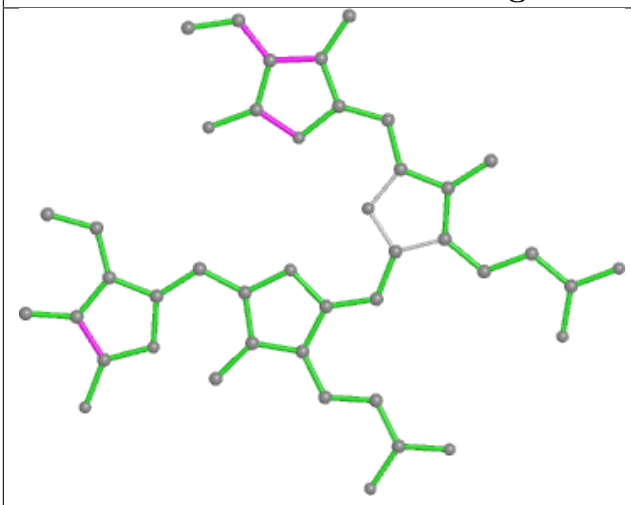


Rings

Ligand PEB F8 1002



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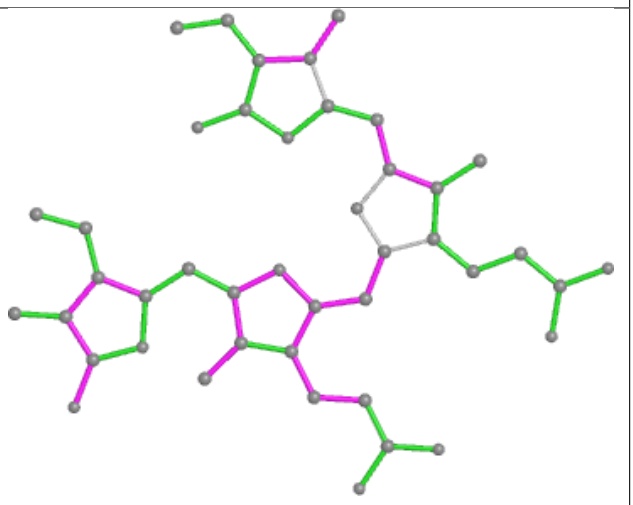

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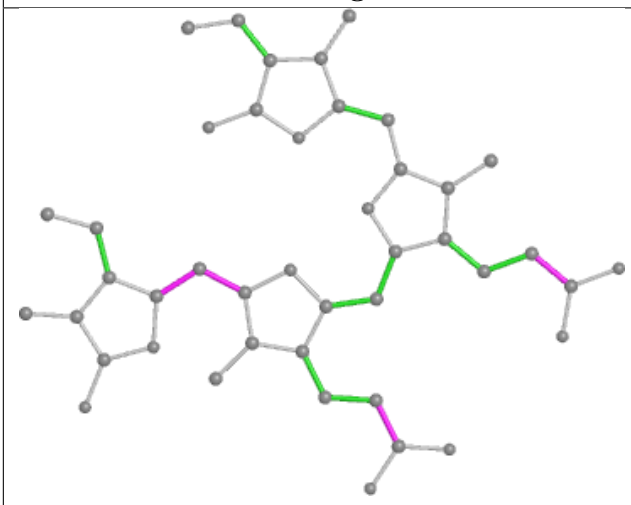

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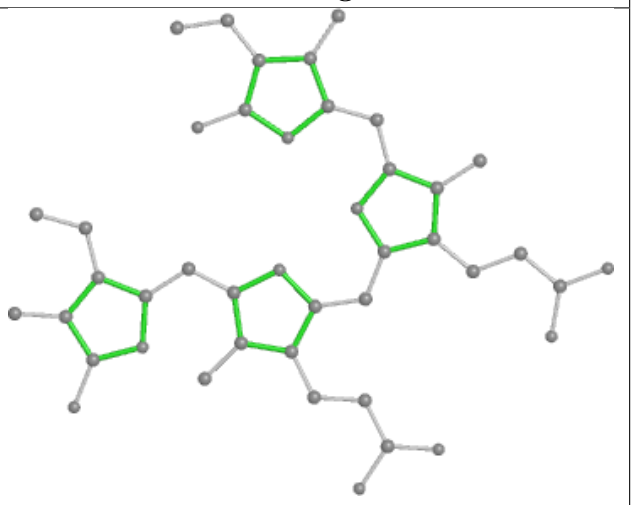

Rings

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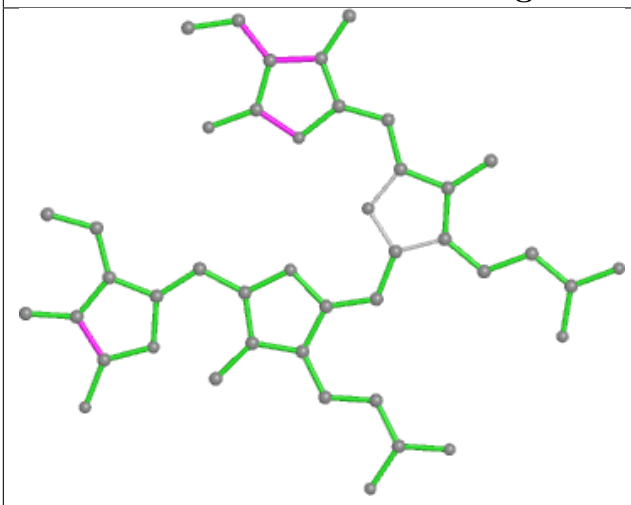

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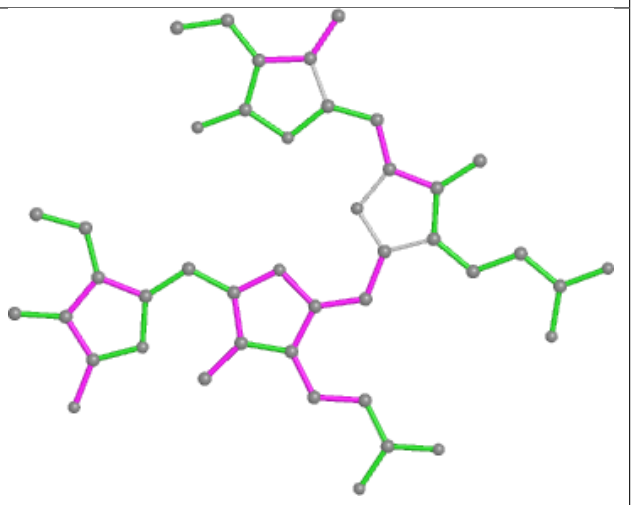

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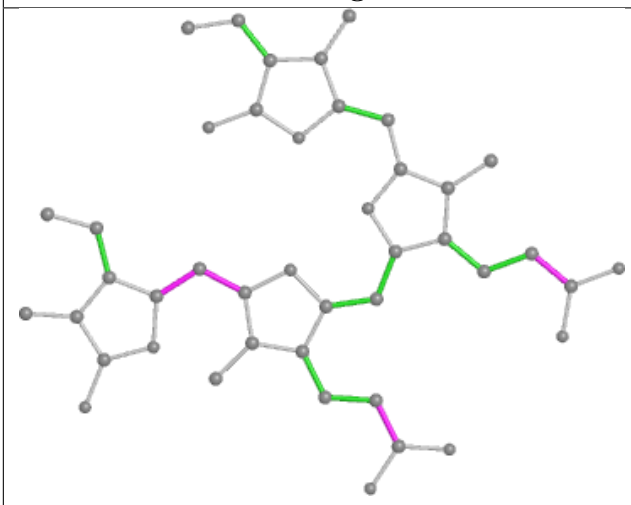

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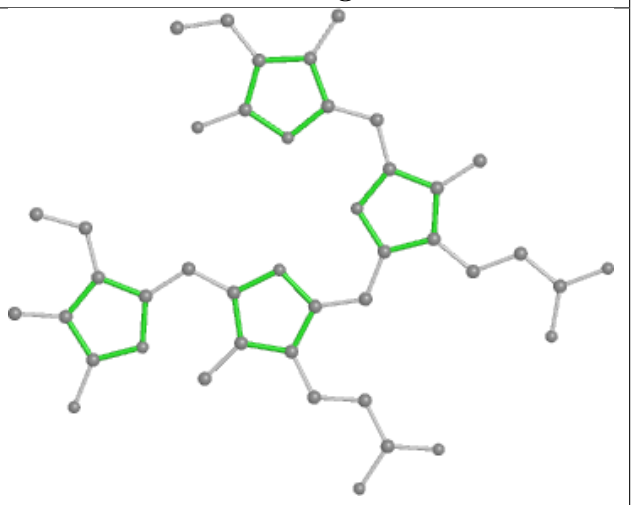
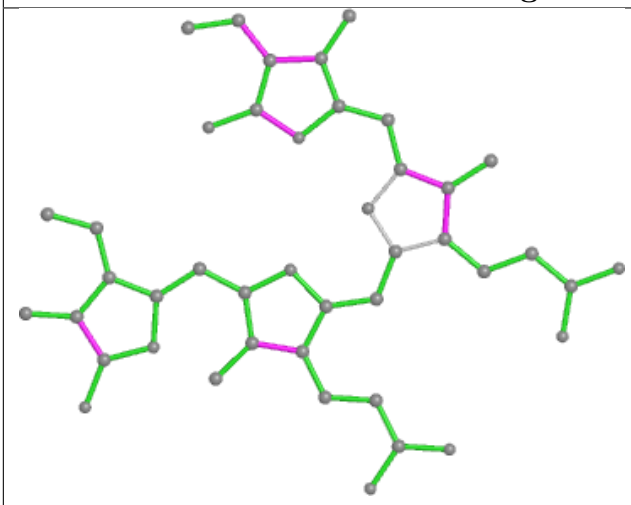


Rings

Ligand PEB eJ 202



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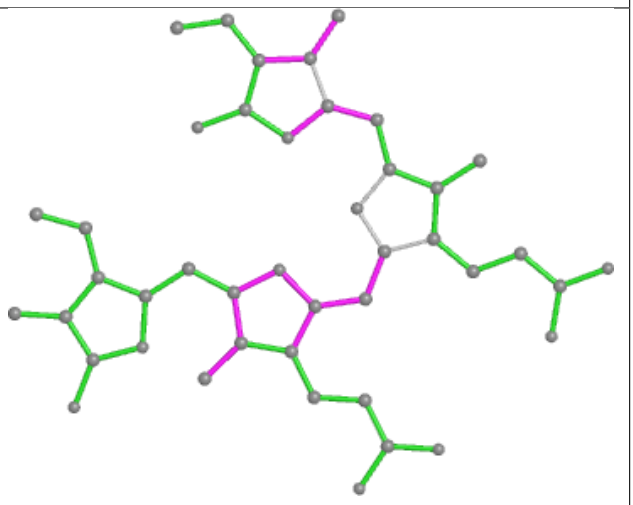

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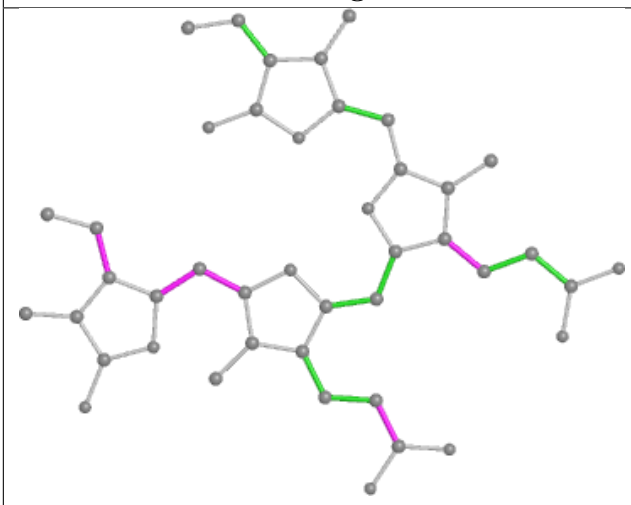

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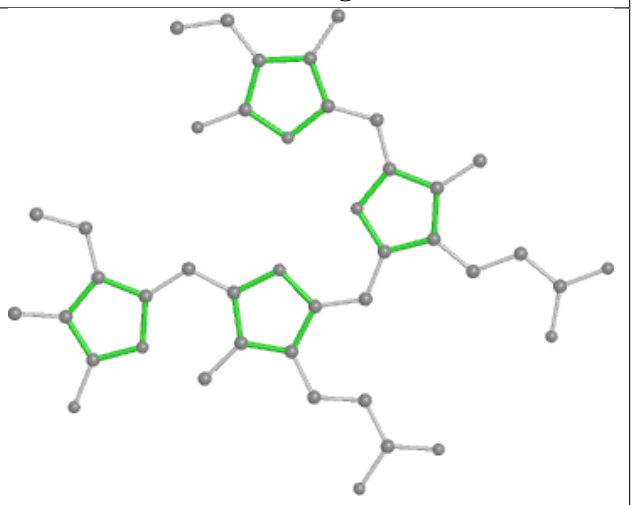
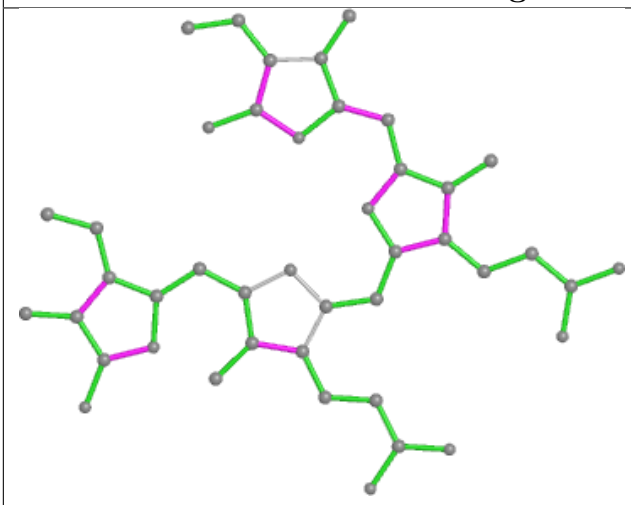


Rings

Ligand PUB a3 1006



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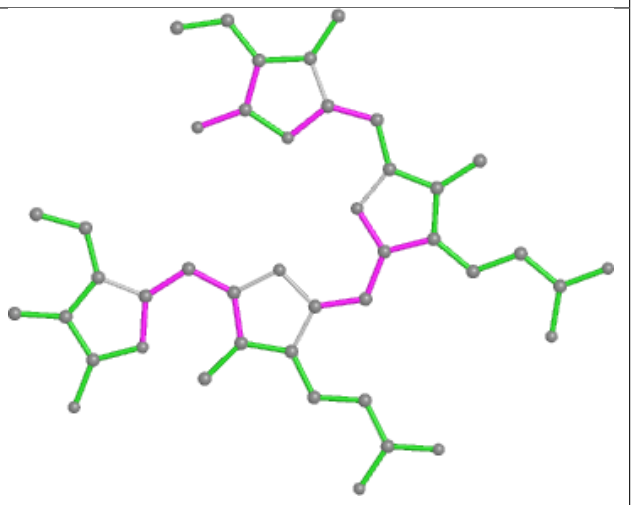

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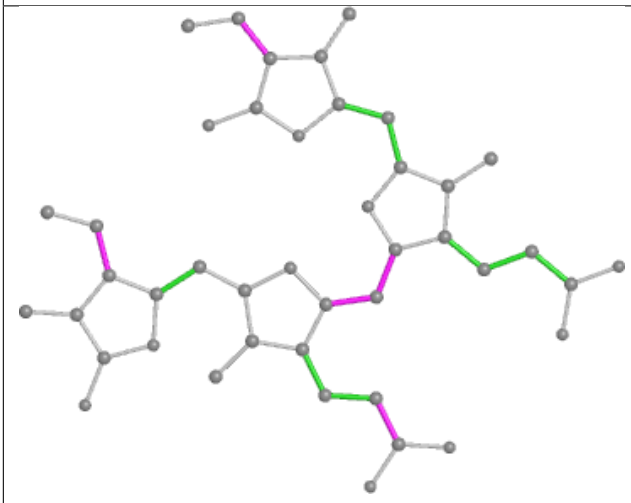

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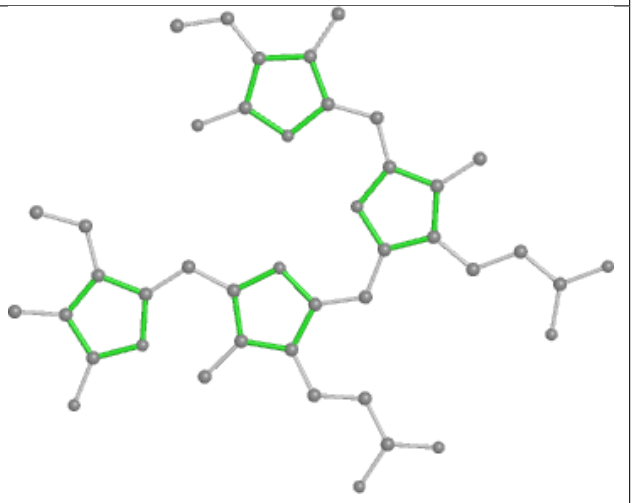

Rings

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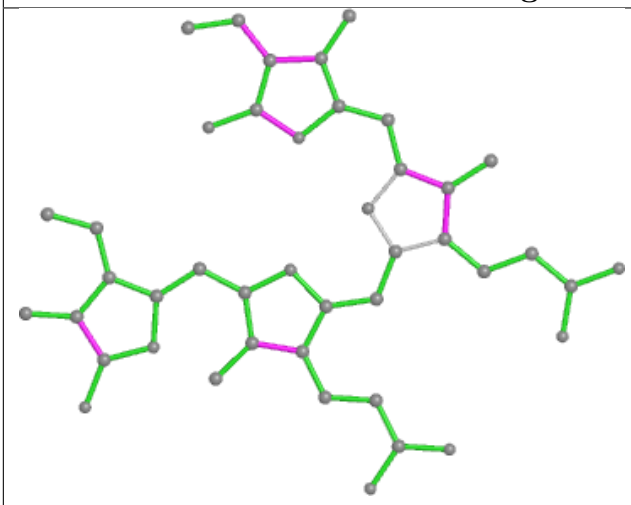

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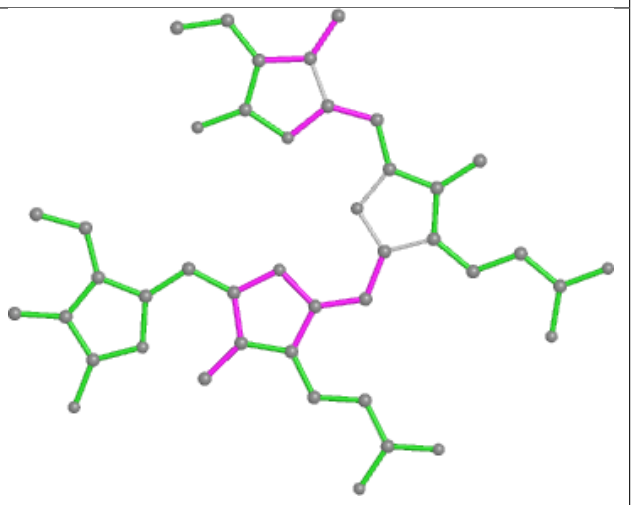

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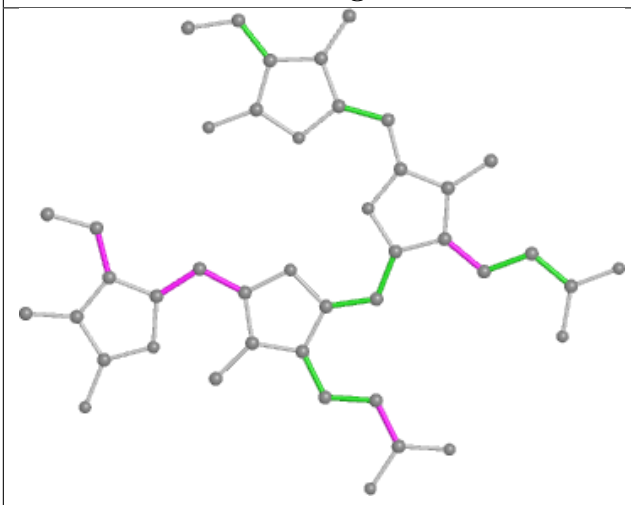

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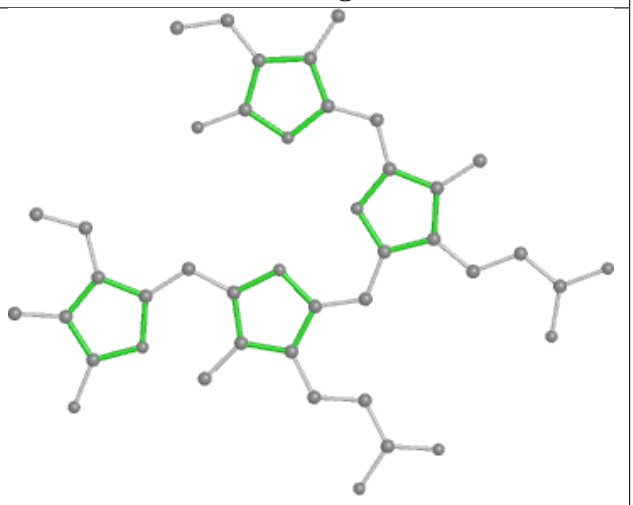

Rings

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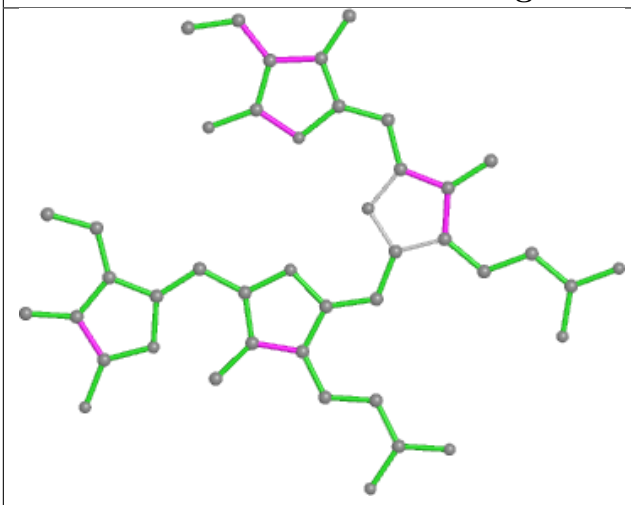

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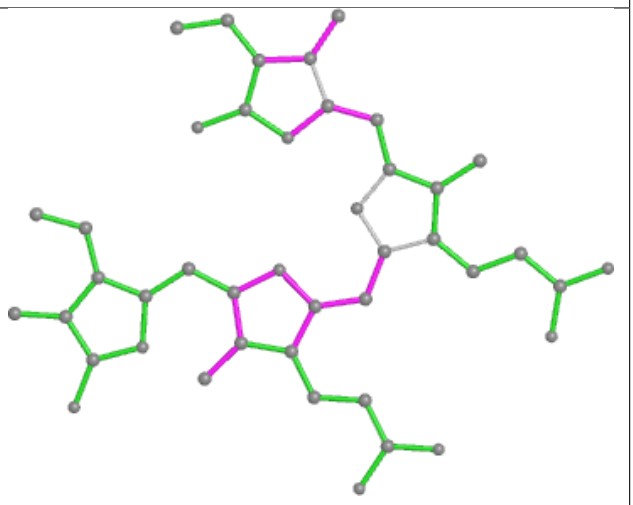

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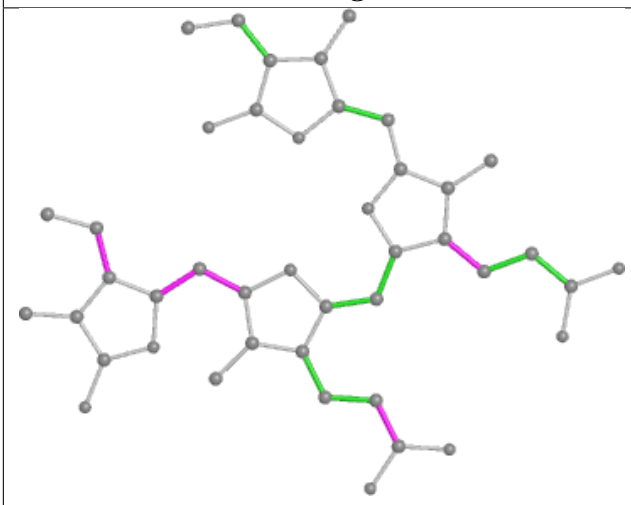

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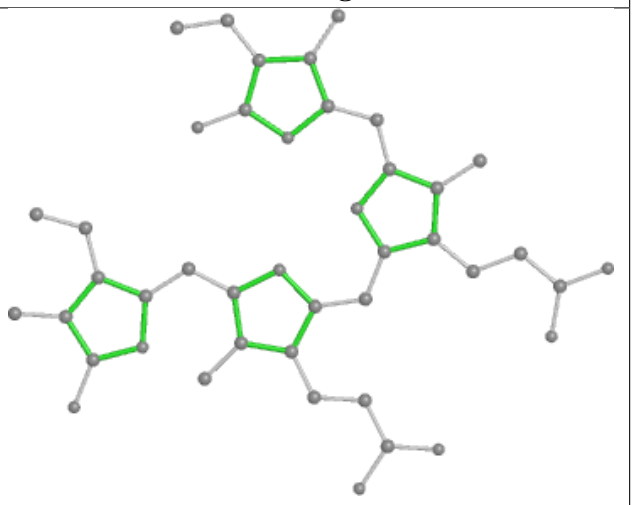

Rings

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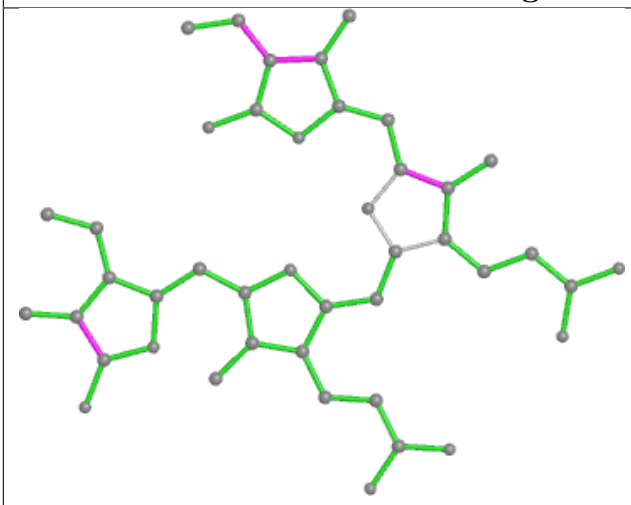

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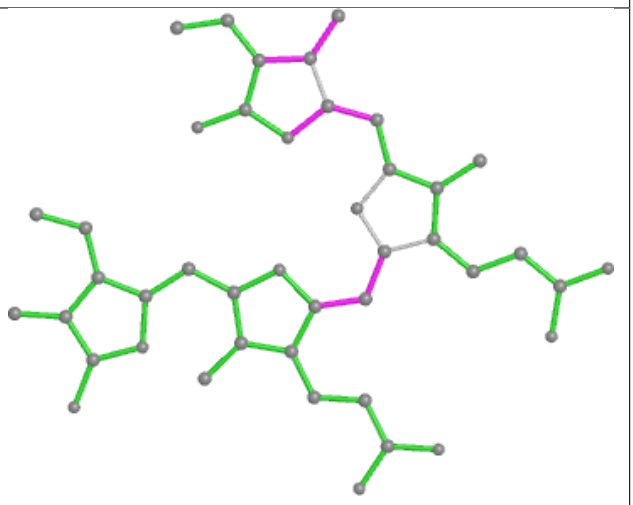

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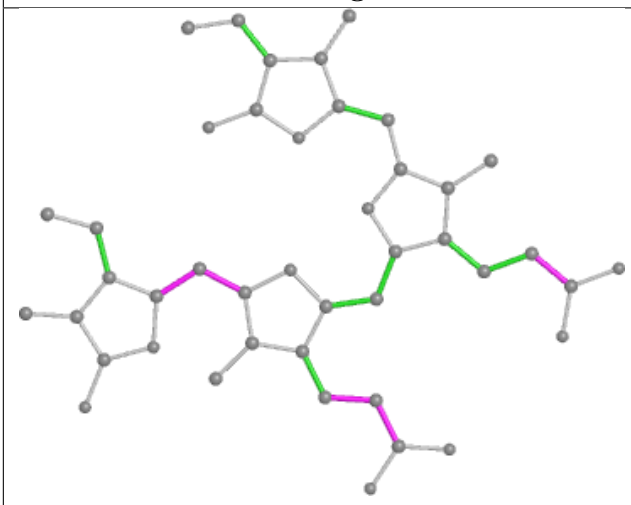

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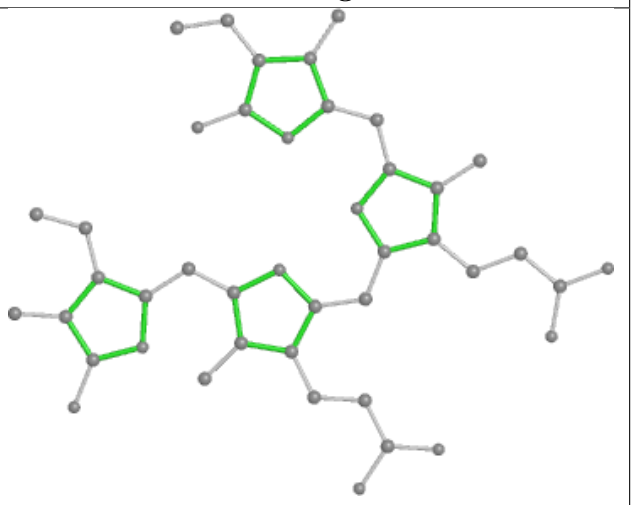

Rings

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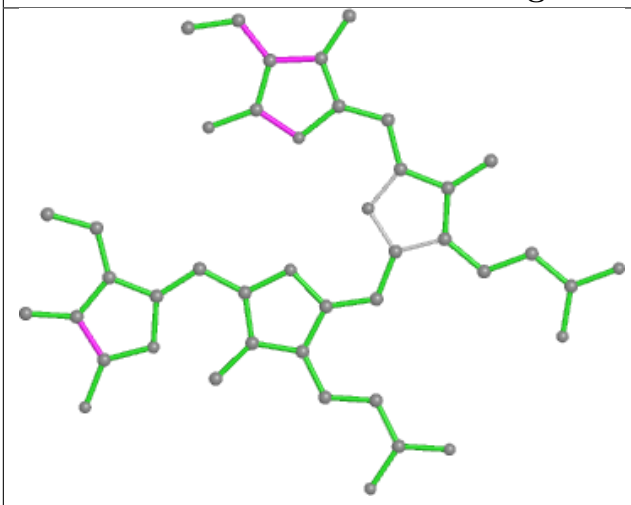

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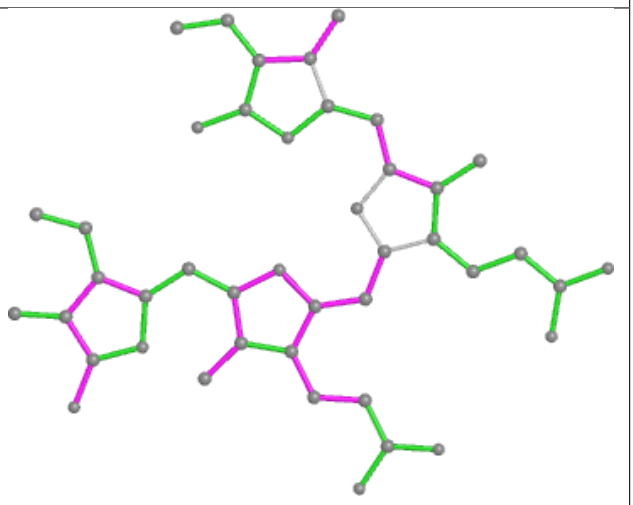

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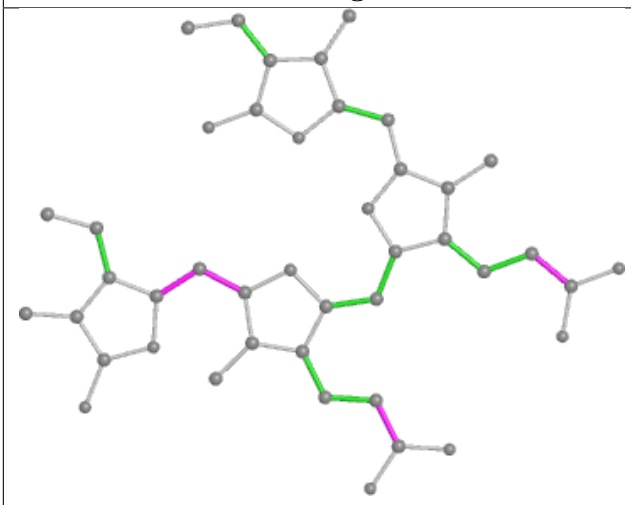

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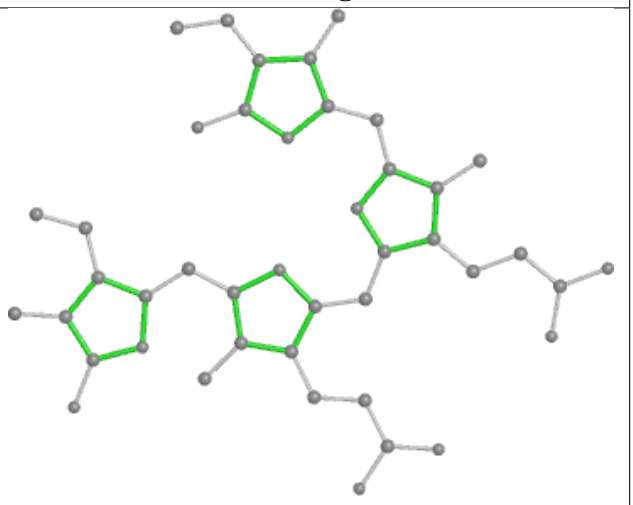

Rings

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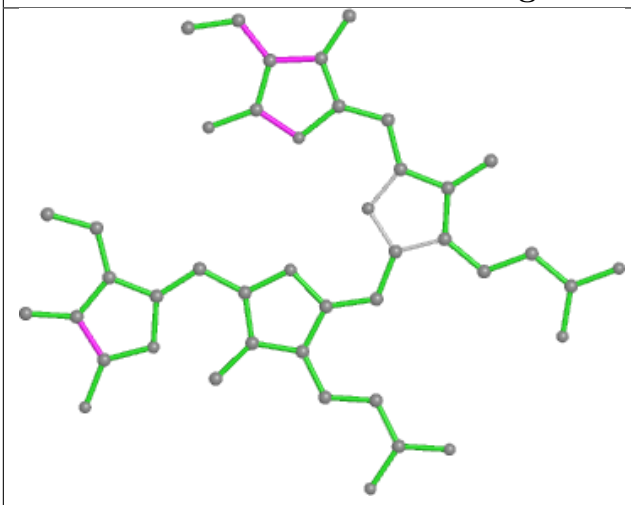

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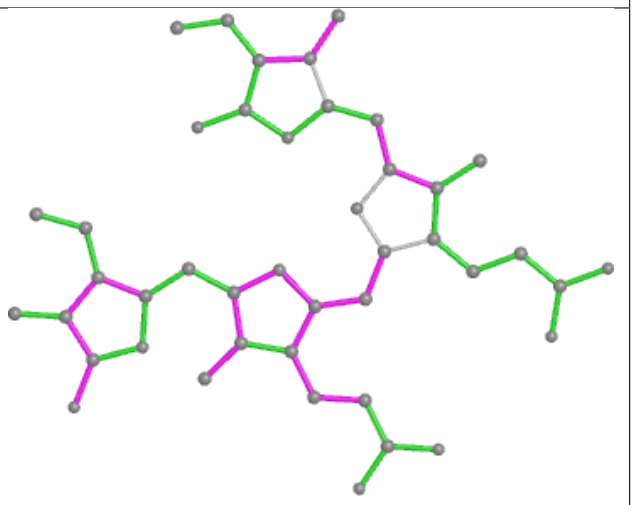

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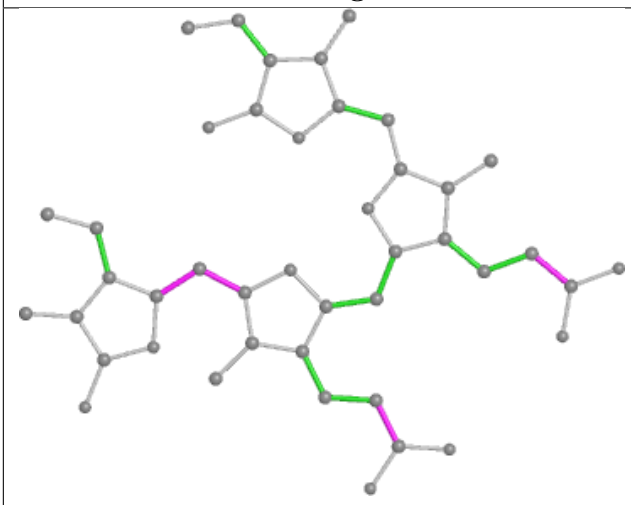

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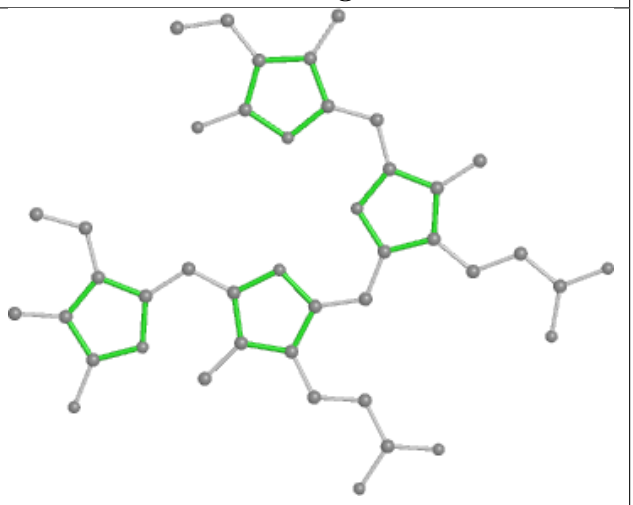
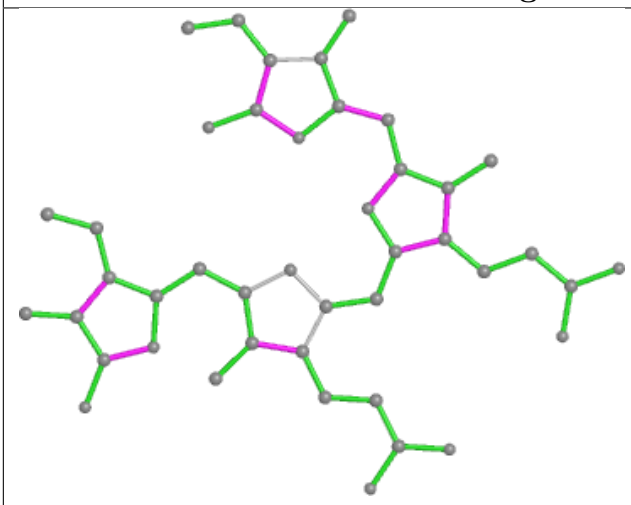


Rings

Ligand PUB gt 203



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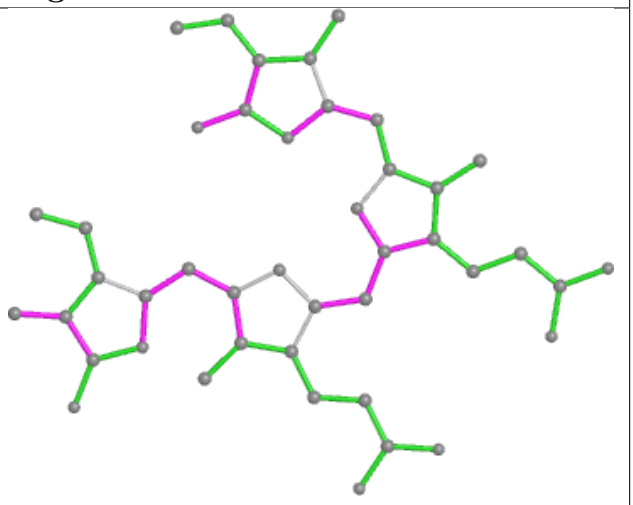

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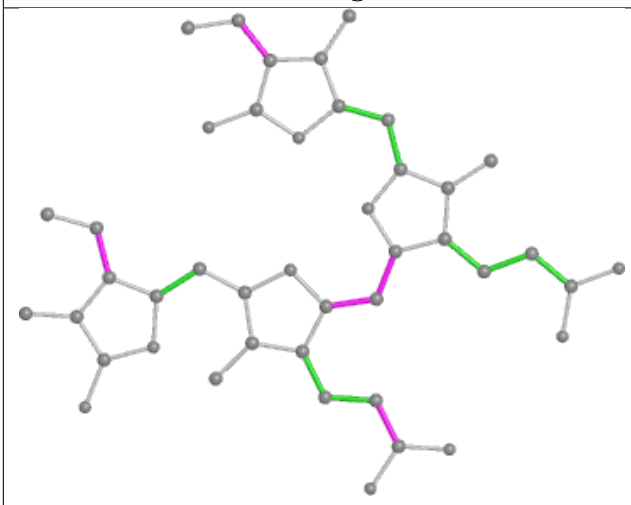

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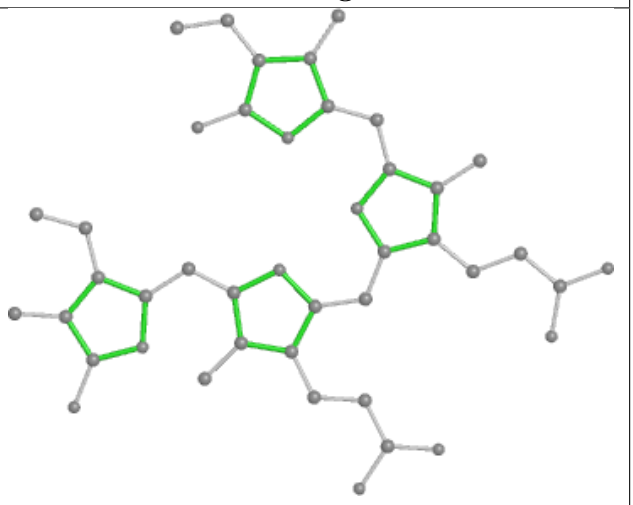

Rings

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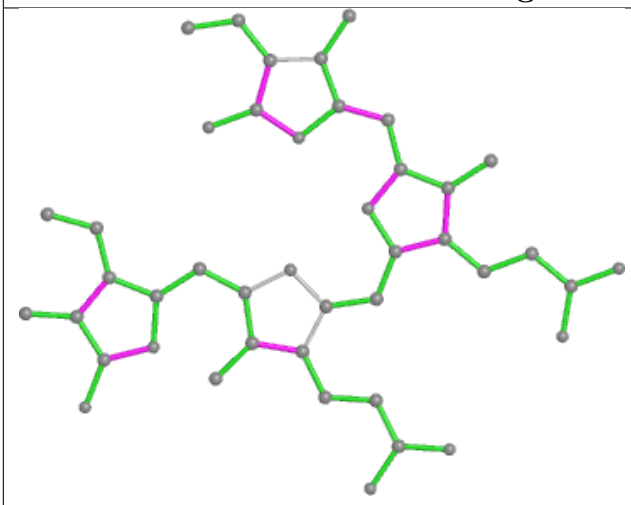

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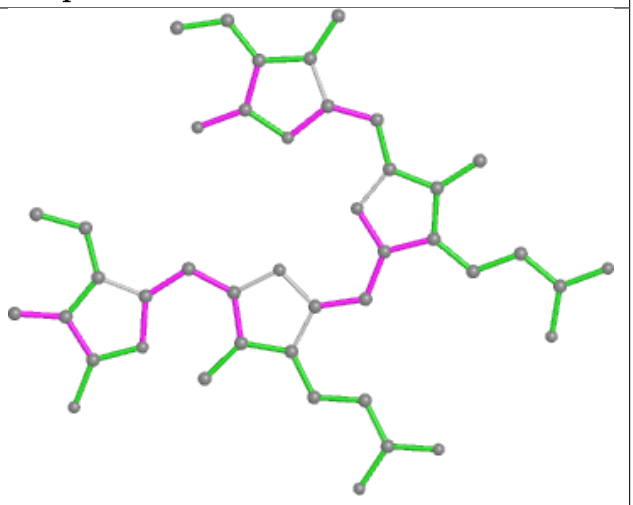

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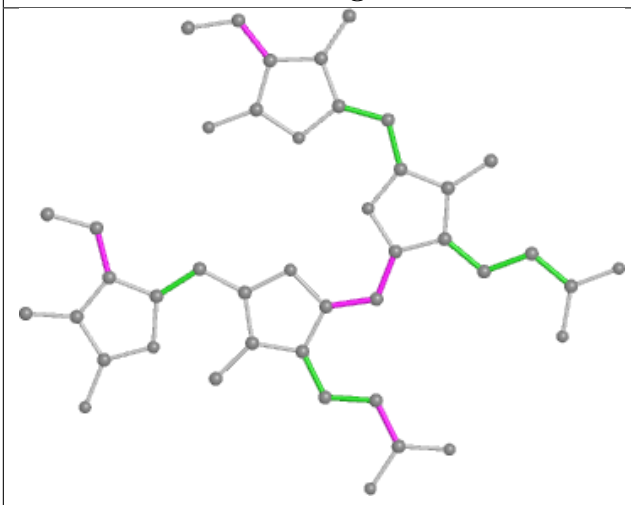

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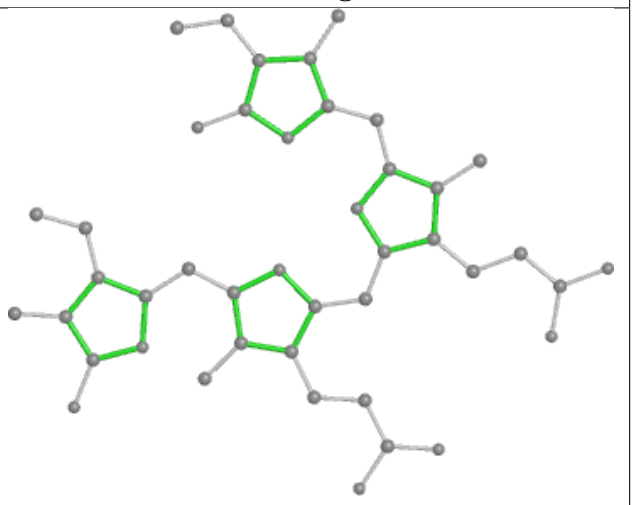
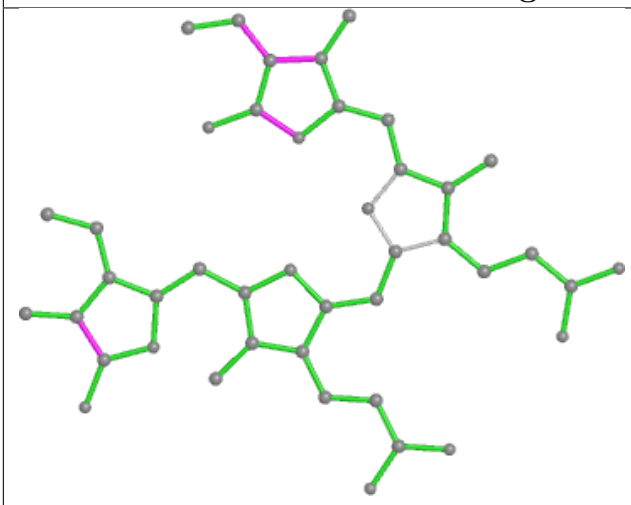


Rings

Ligand PEB x9 201



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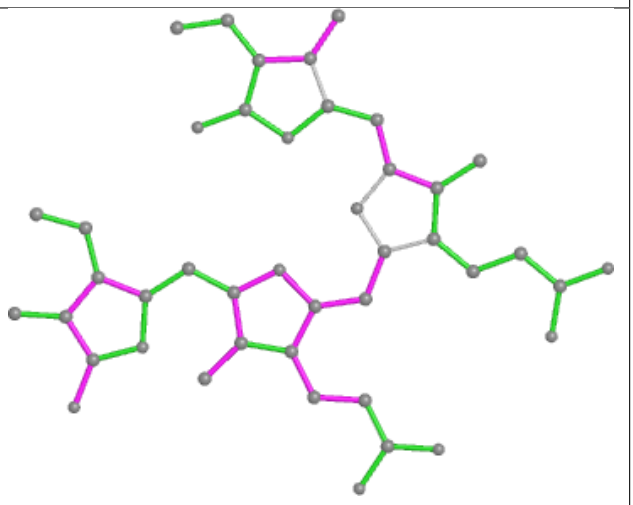

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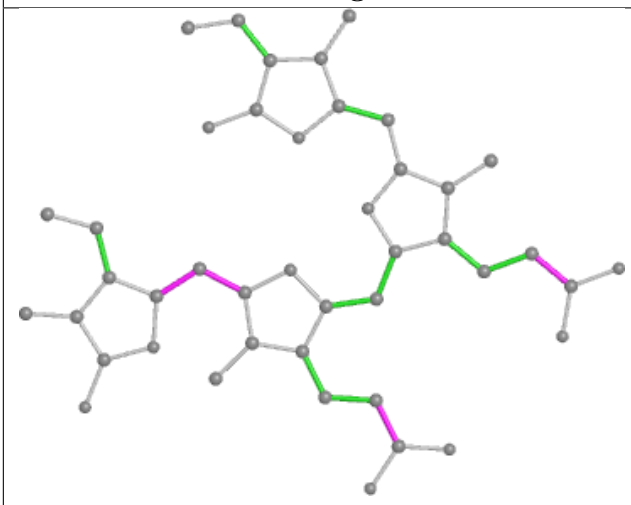
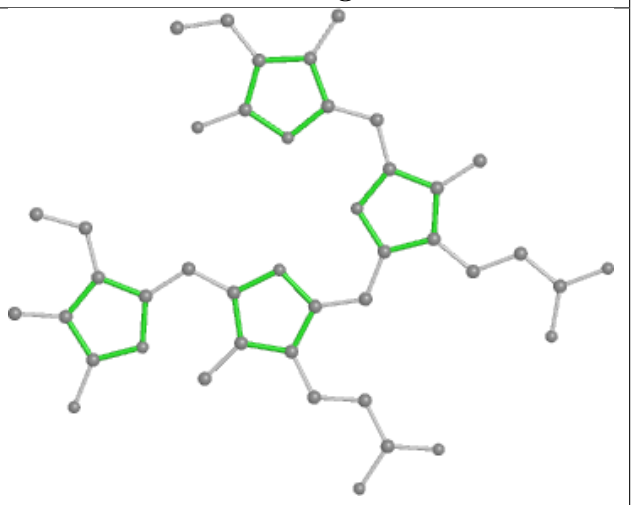
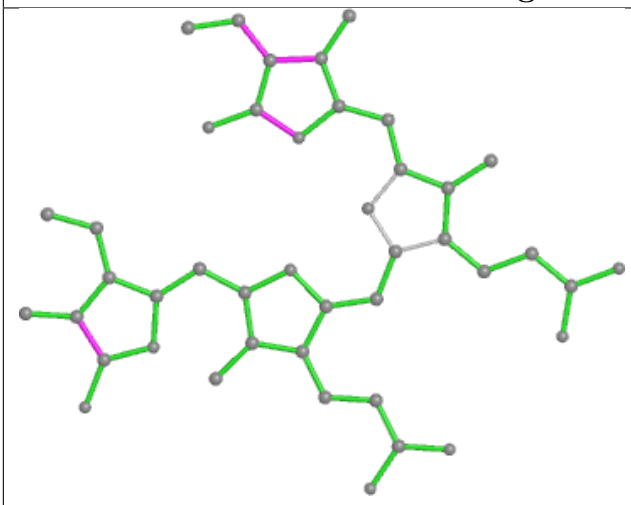


Torsions



Rings

Ligand PEB bh 201



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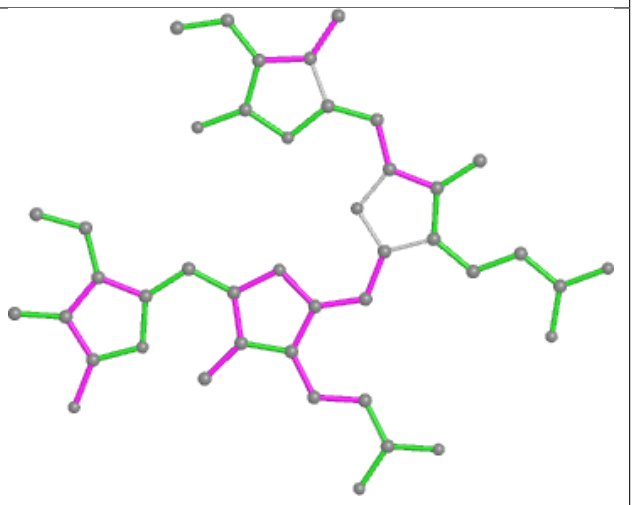

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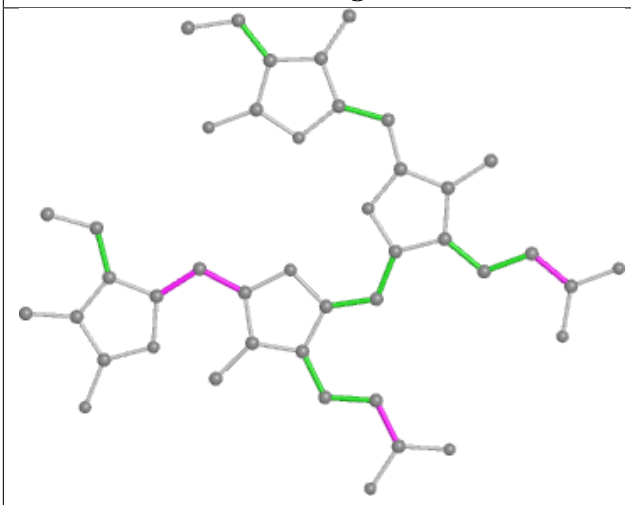

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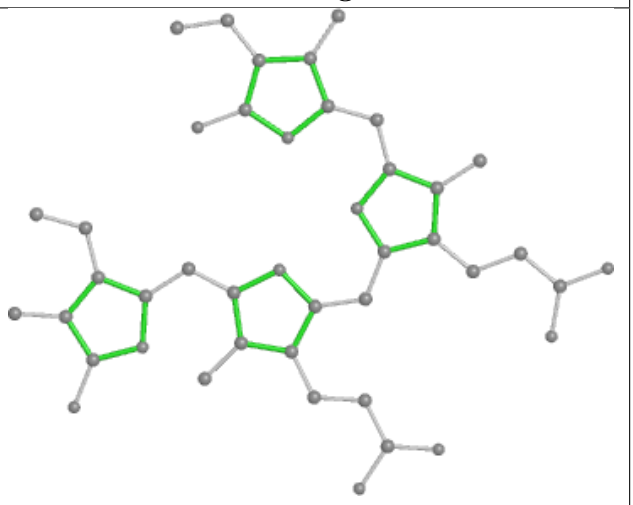
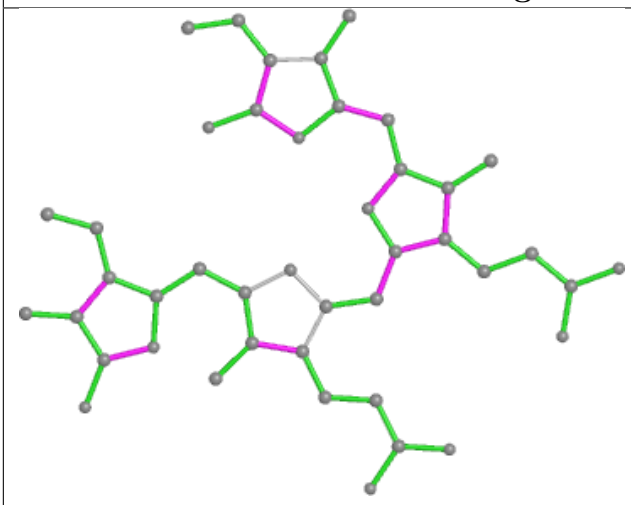


Rings

Ligand PUB eR 203



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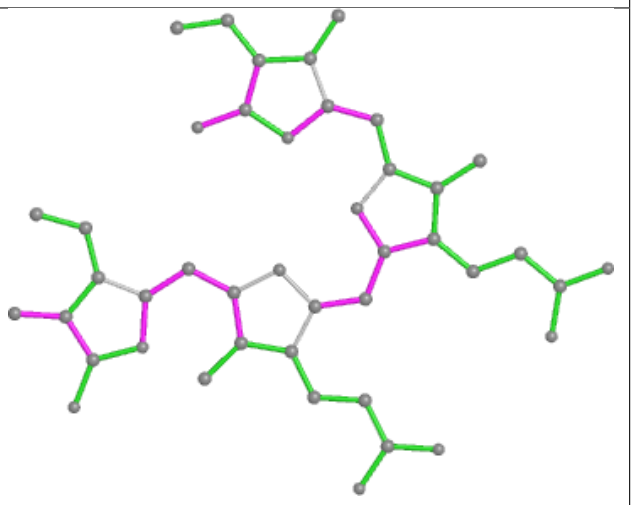

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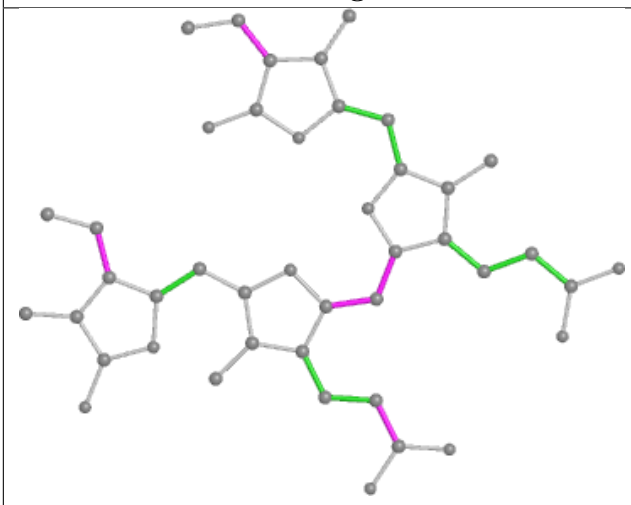

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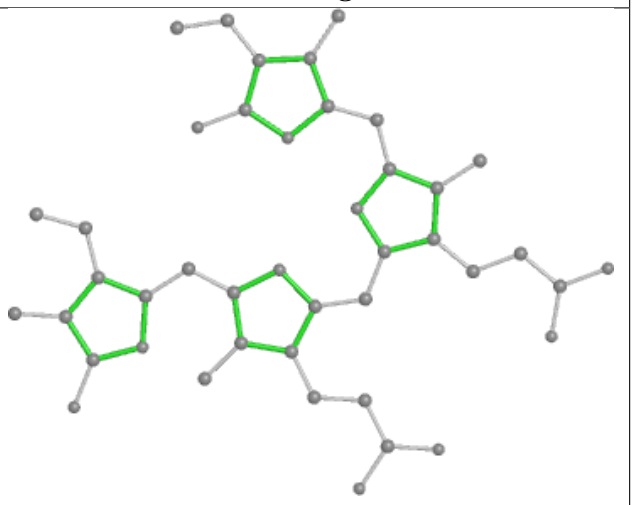
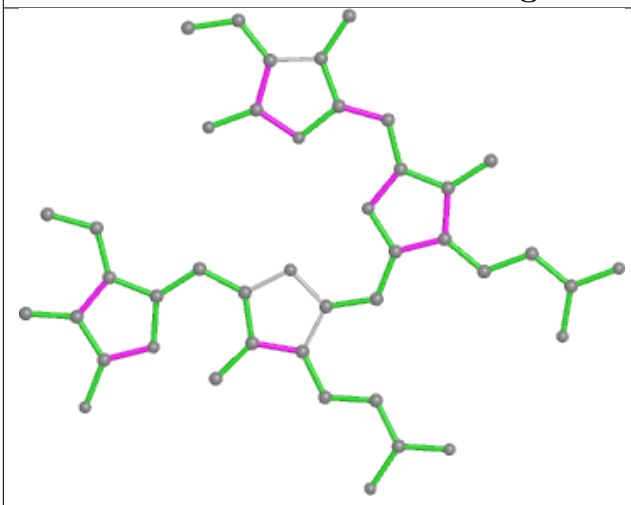


Rings

Ligand PUB at 203



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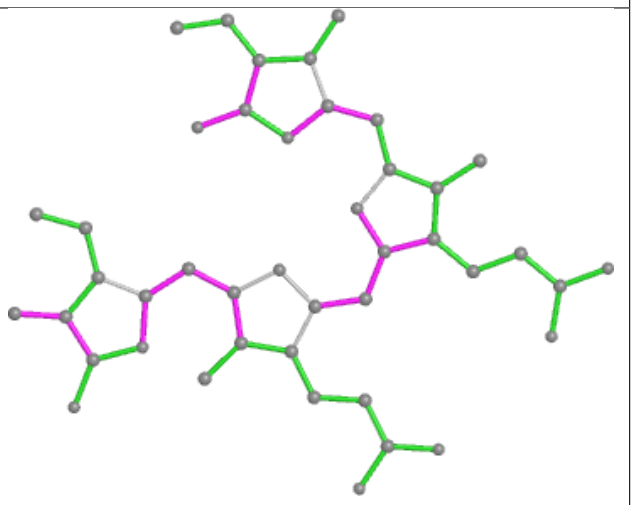

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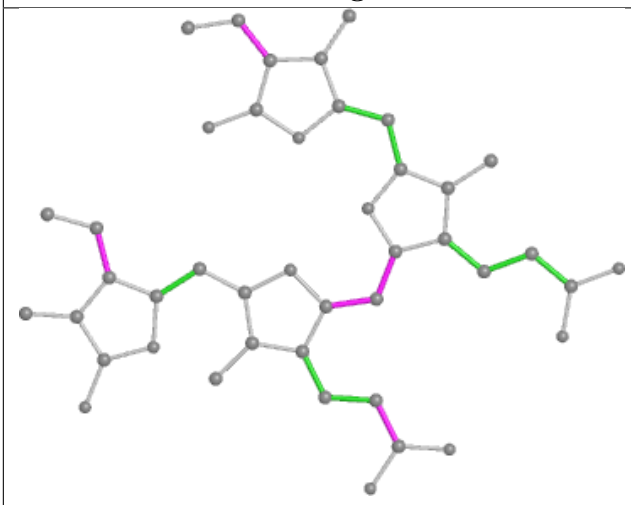

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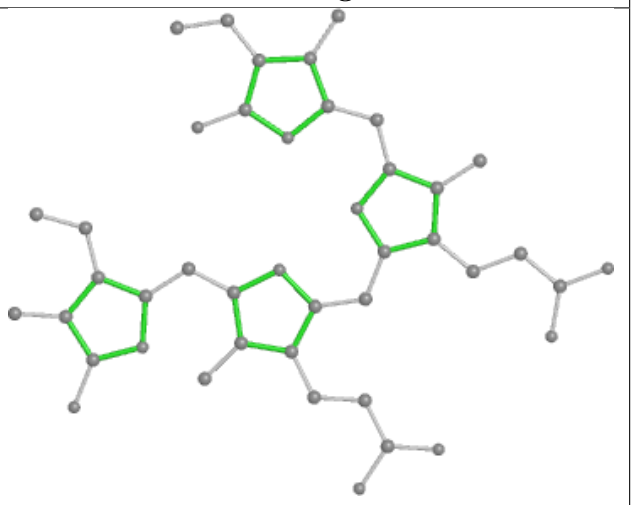
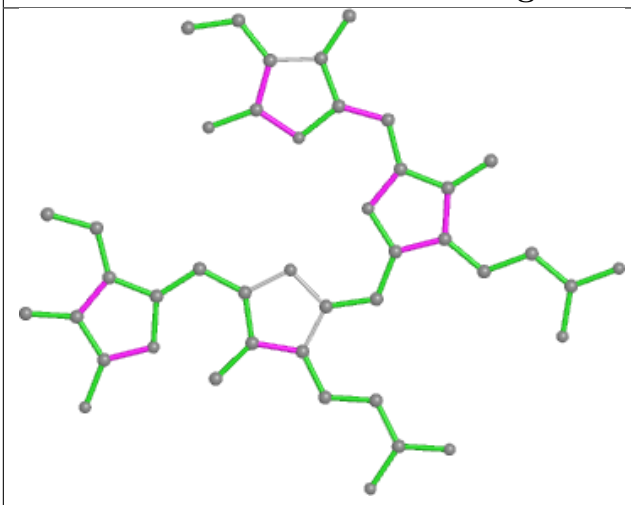


Rings

Ligand PUB v5 203



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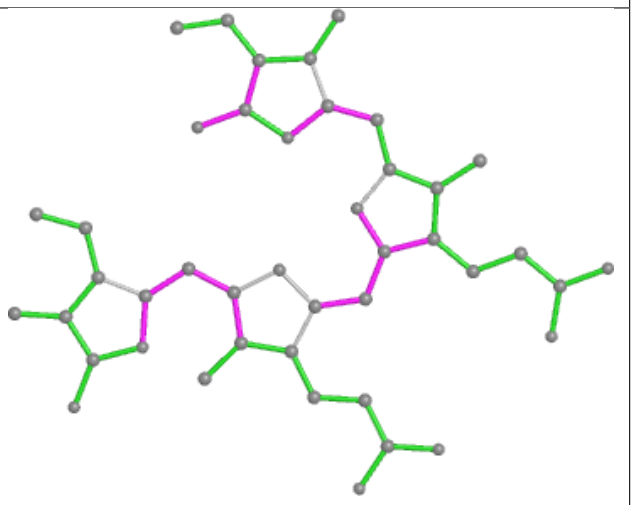

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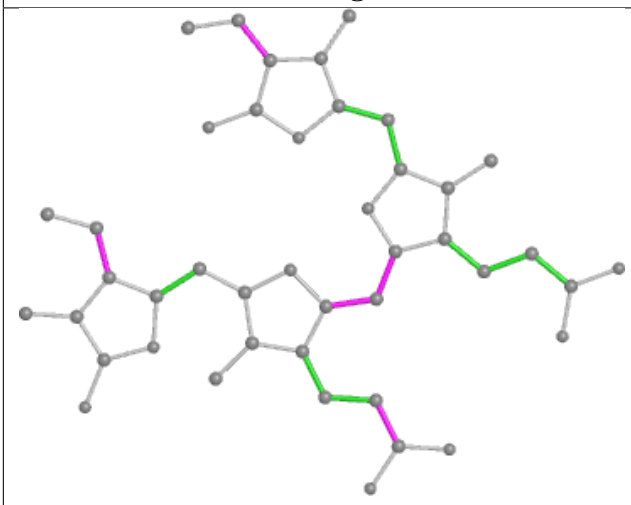

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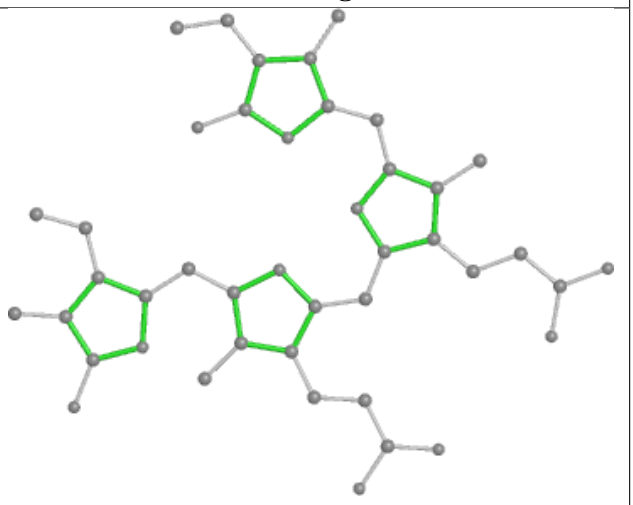
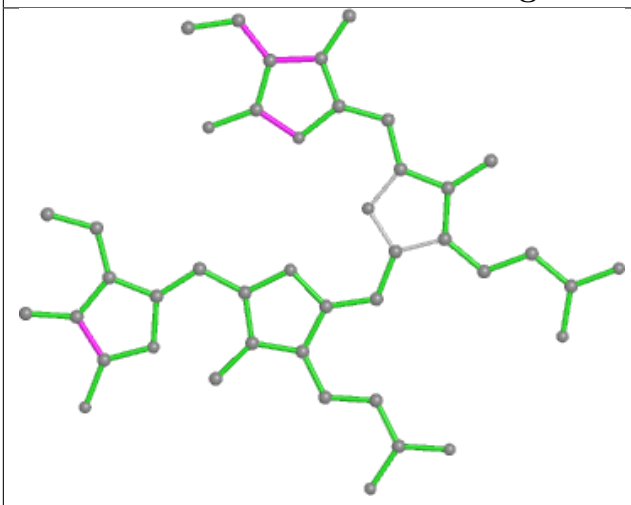


Rings

Ligand PEB y7 201



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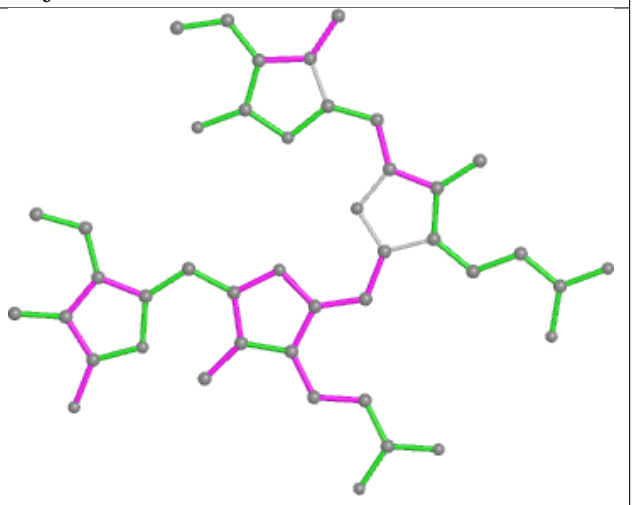

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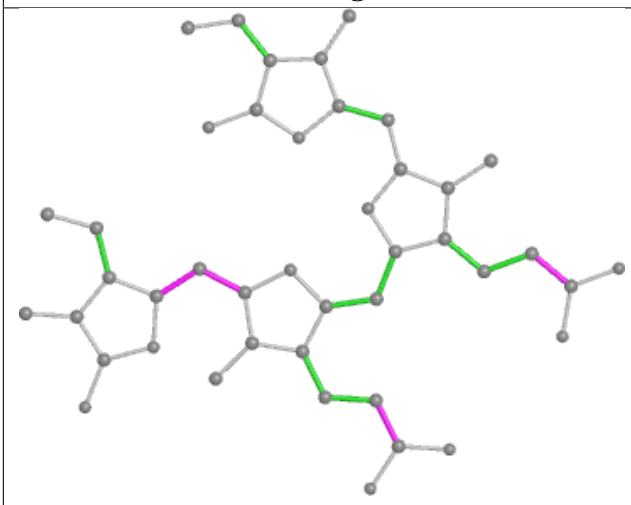

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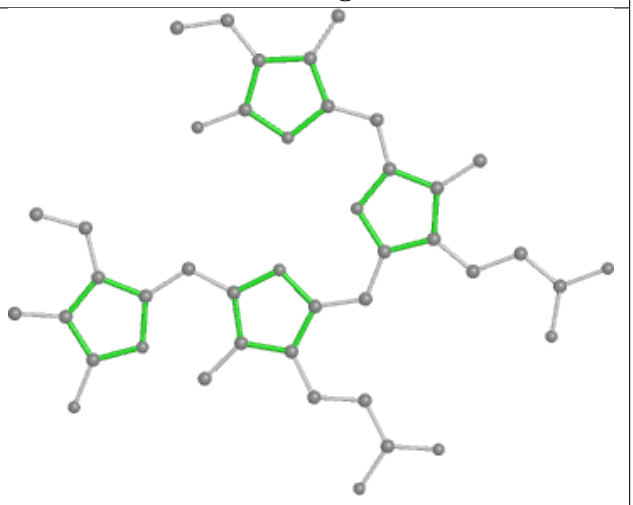

Rings

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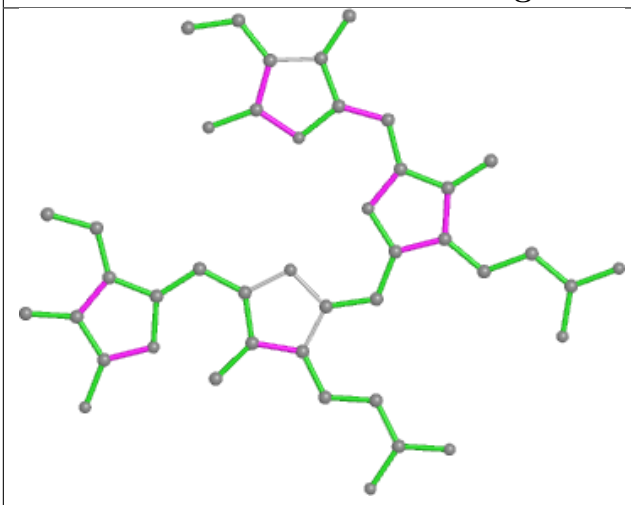

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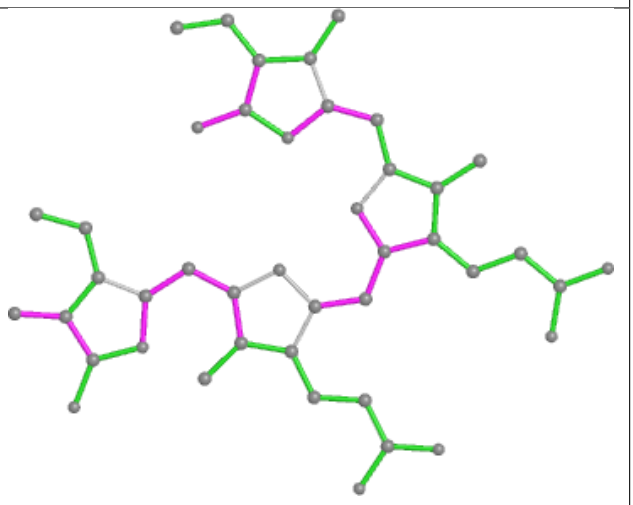

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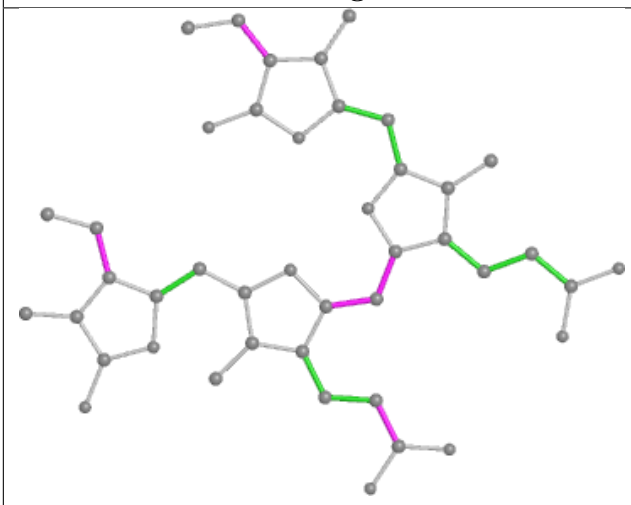

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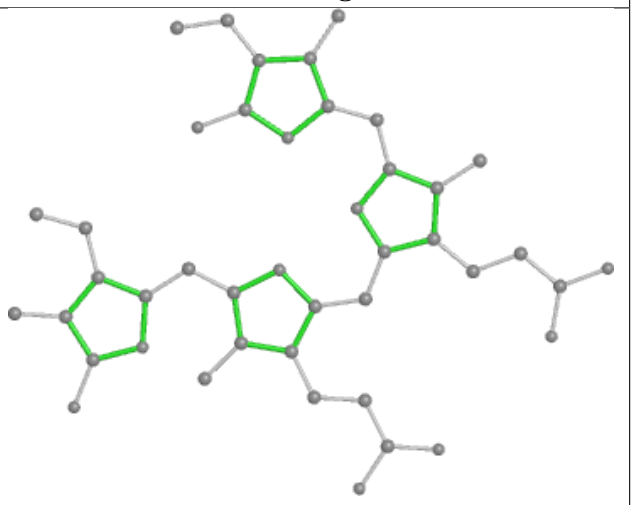

Rings

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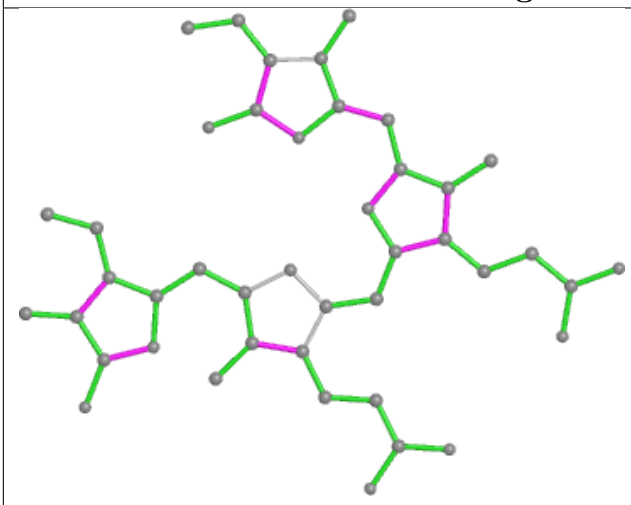

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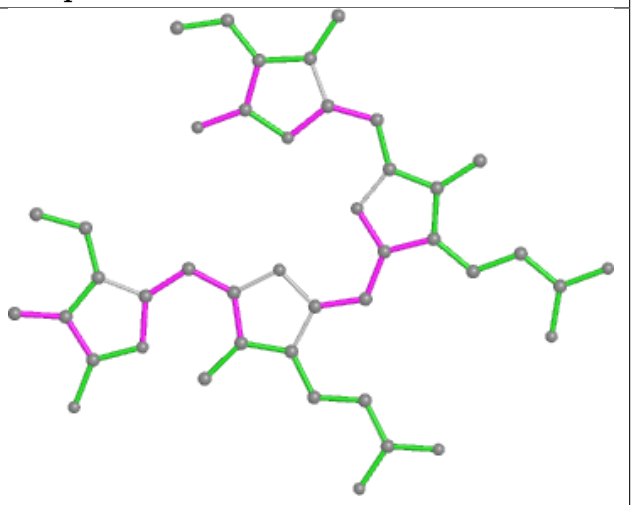

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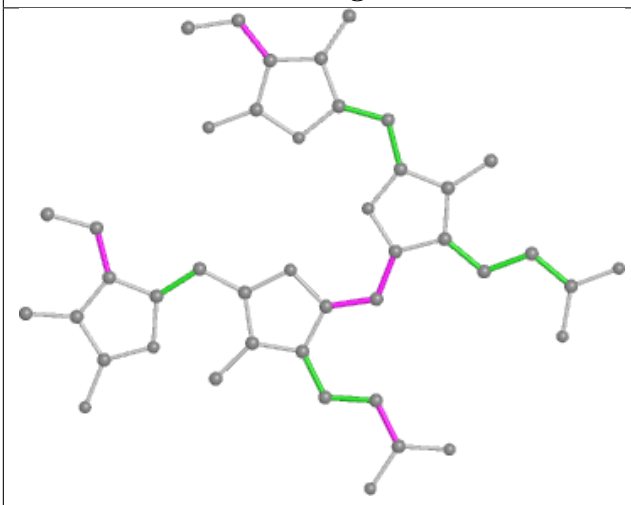

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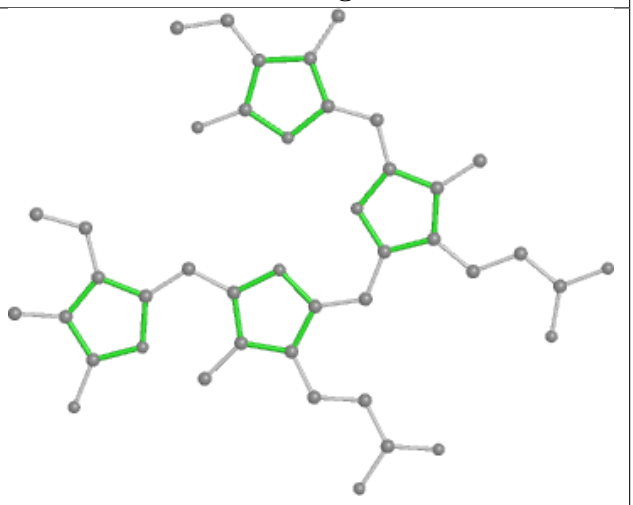
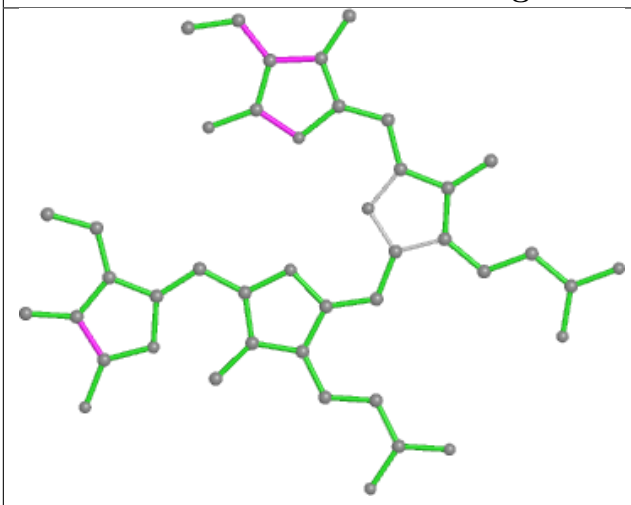


Rings

Ligand PEB aM 201



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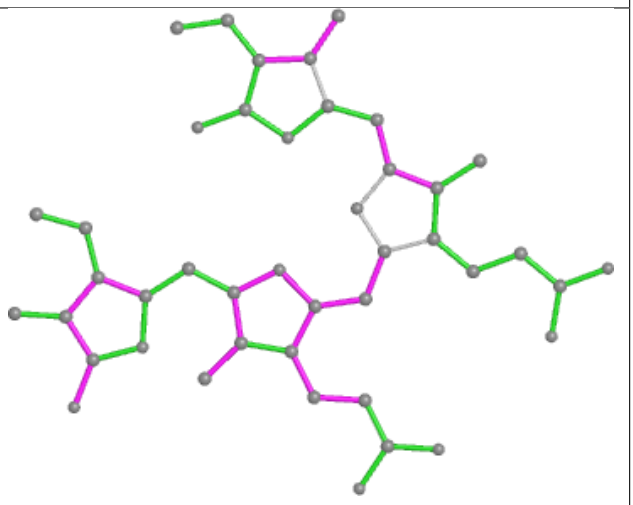

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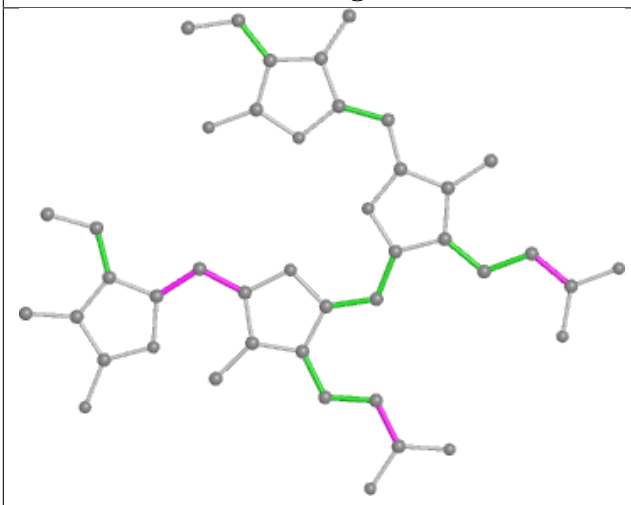

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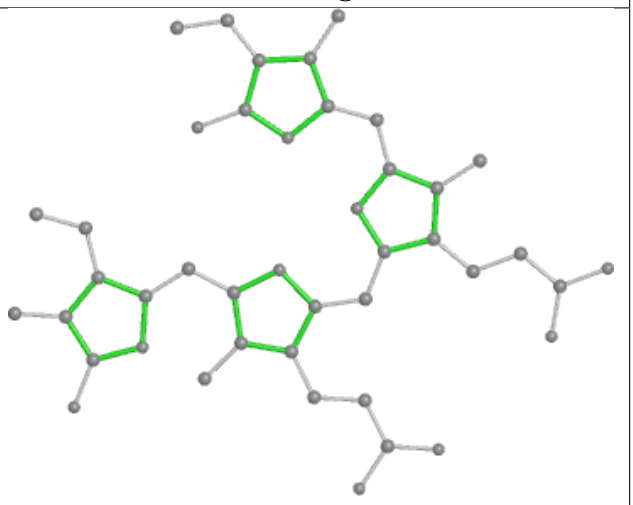

Rings

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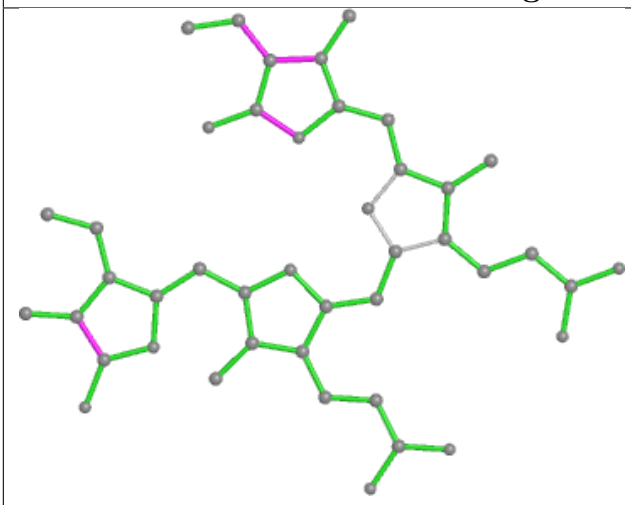

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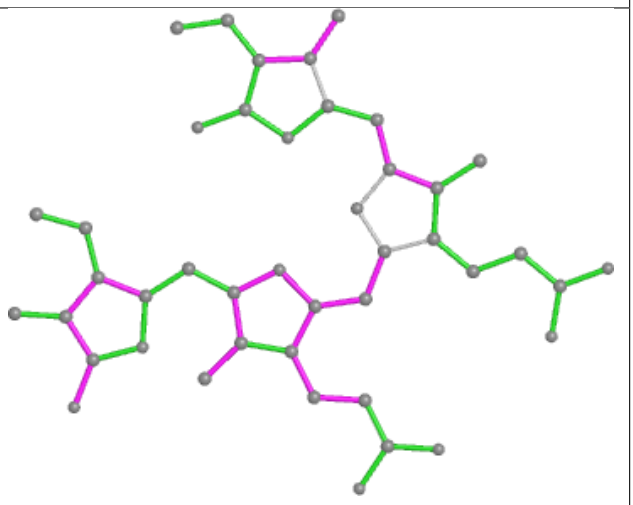

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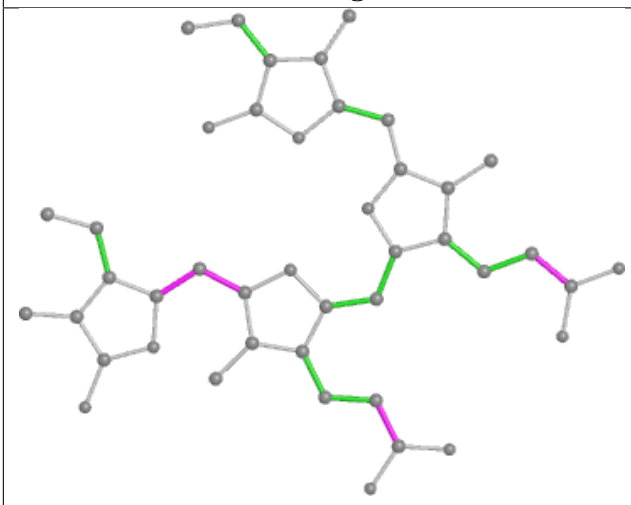

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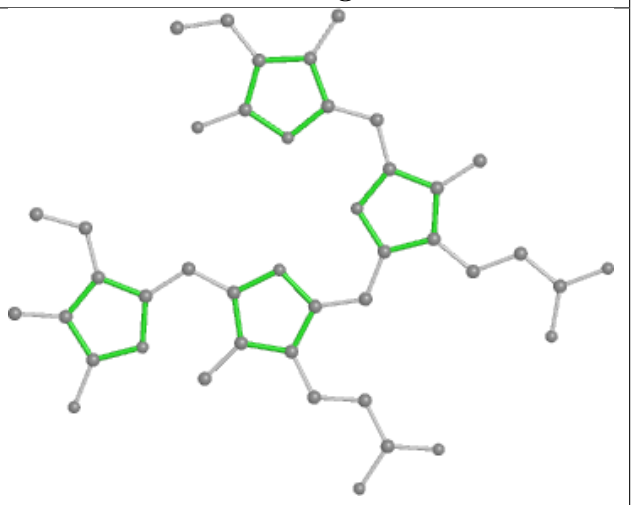

Rings

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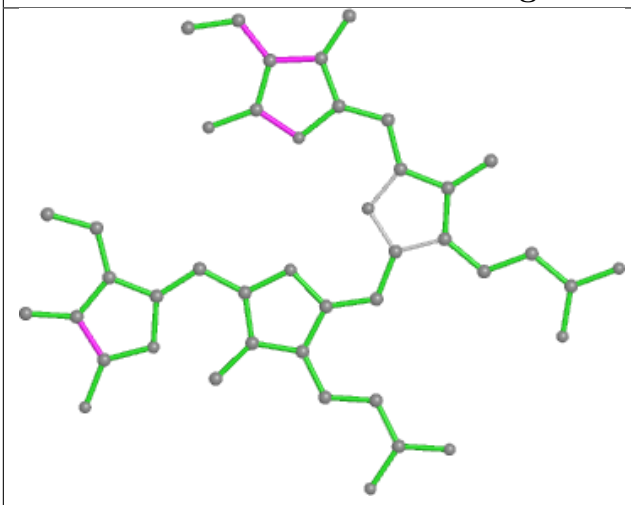

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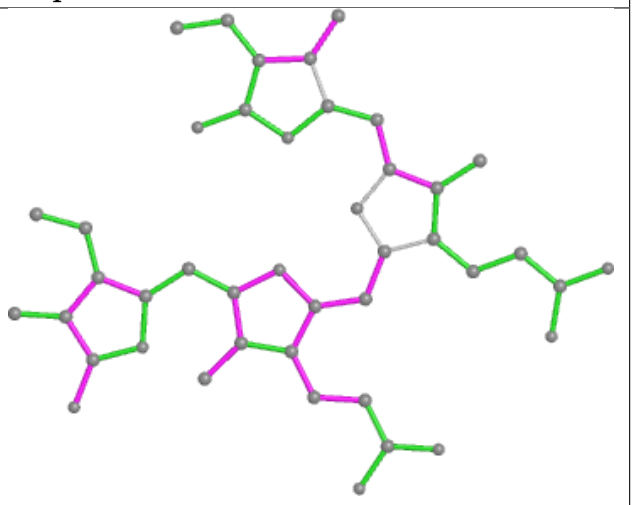

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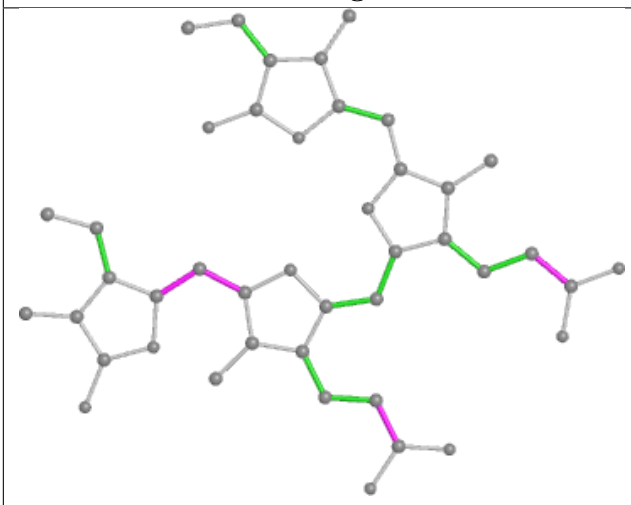

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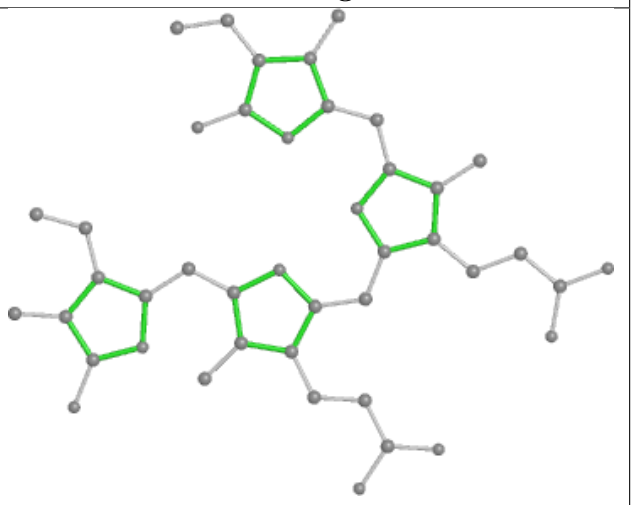
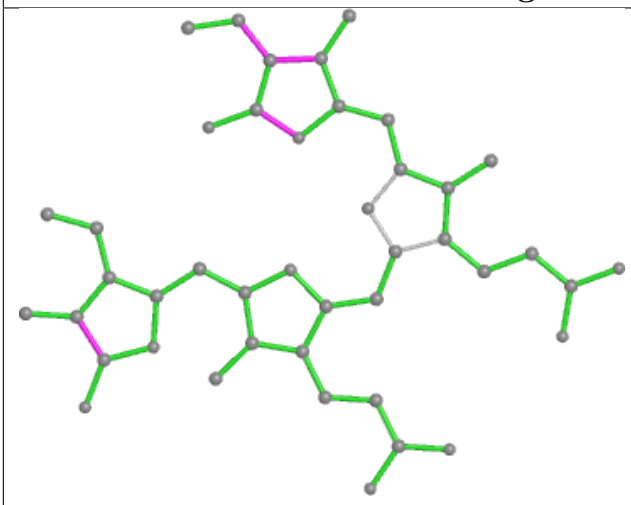


Rings

Ligand PEB Z6 201



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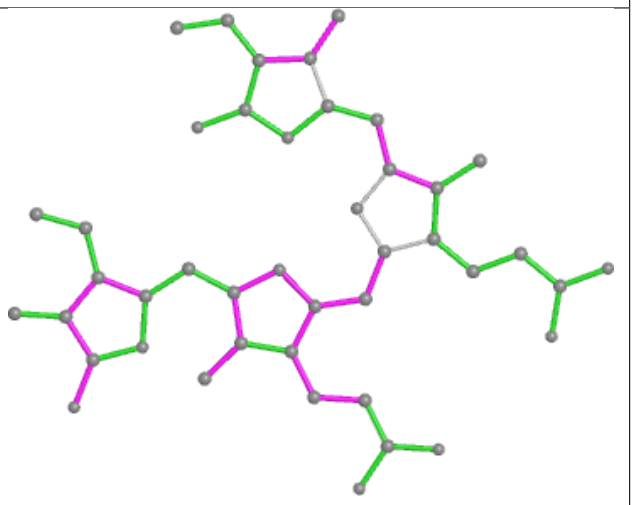

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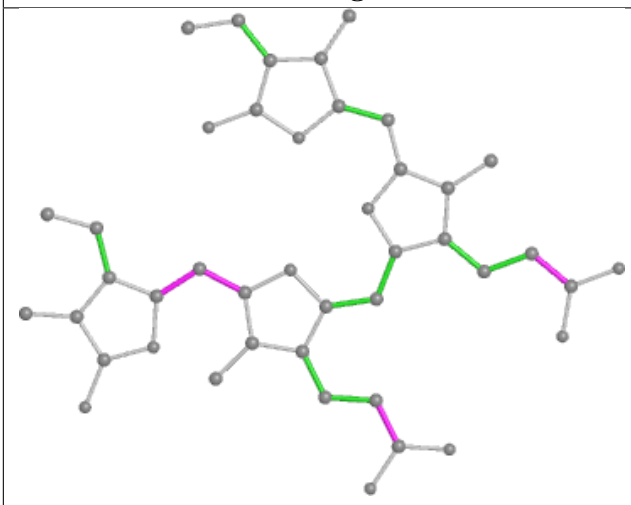

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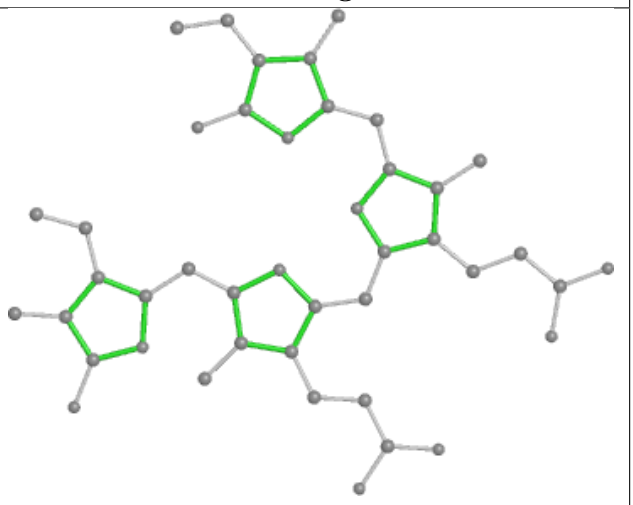

Rings

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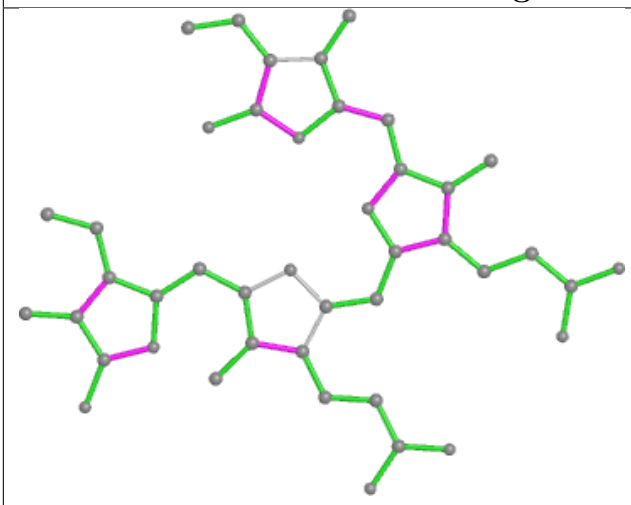

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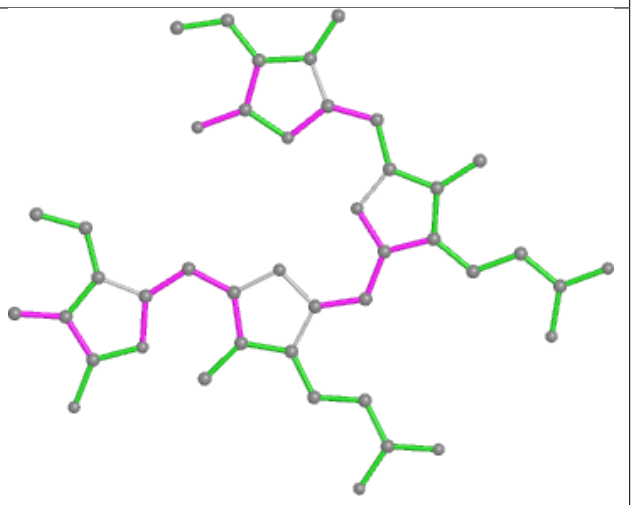

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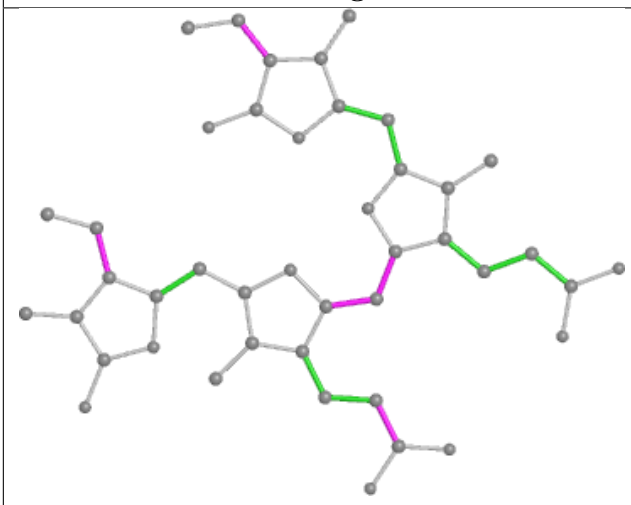

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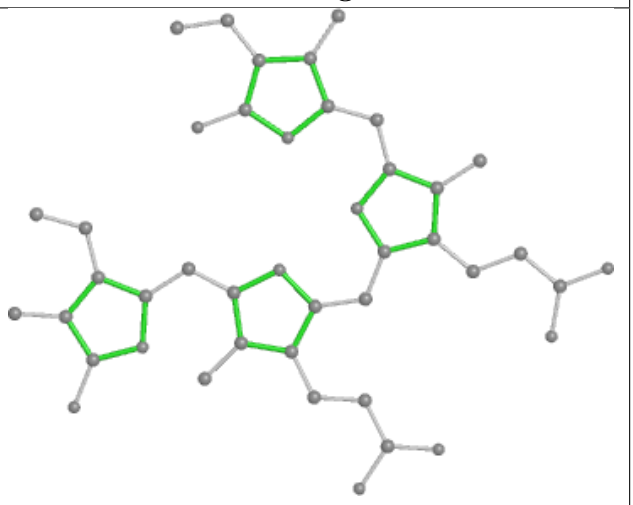
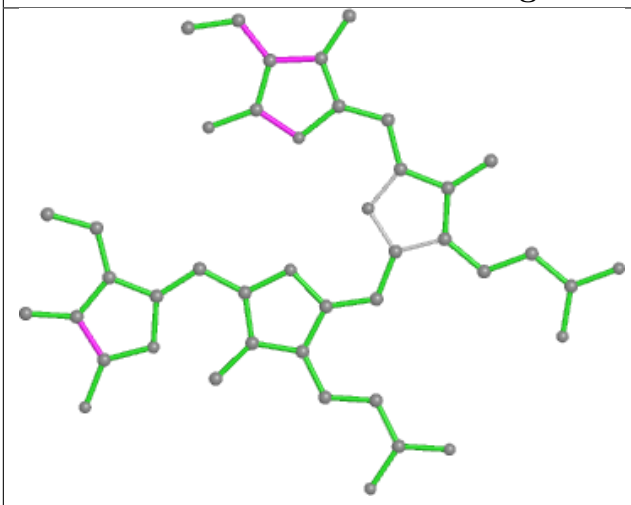


Rings

Ligand PEB y3 201



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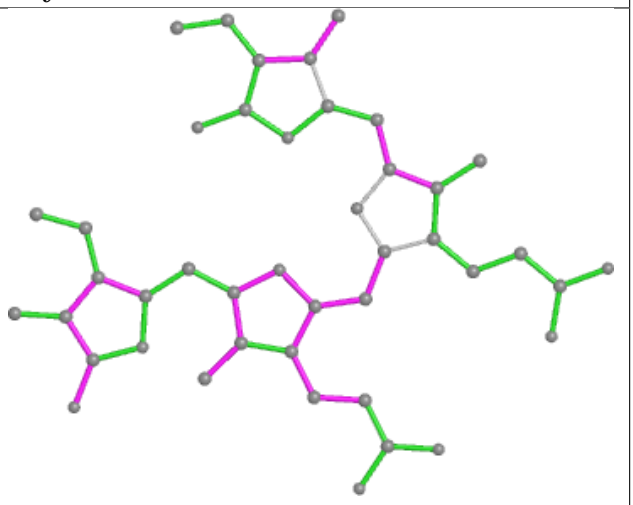
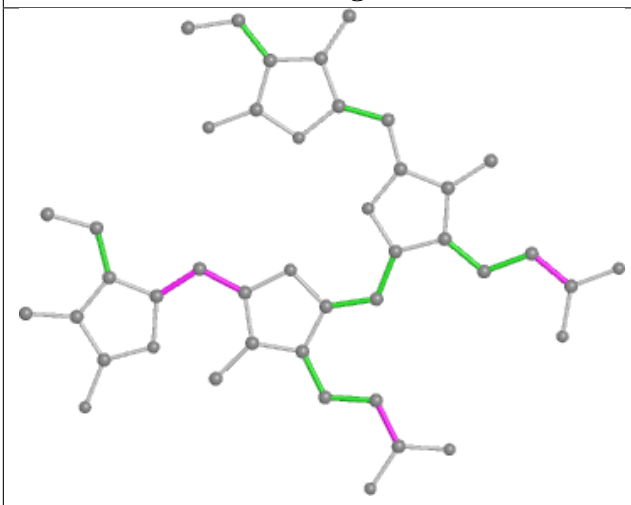
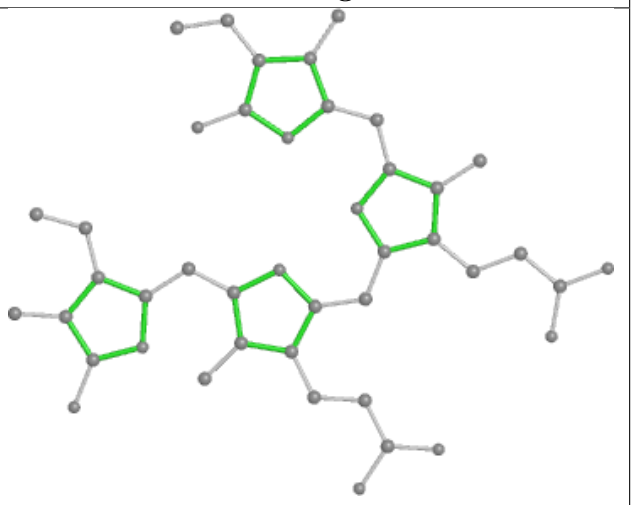


Bond angles

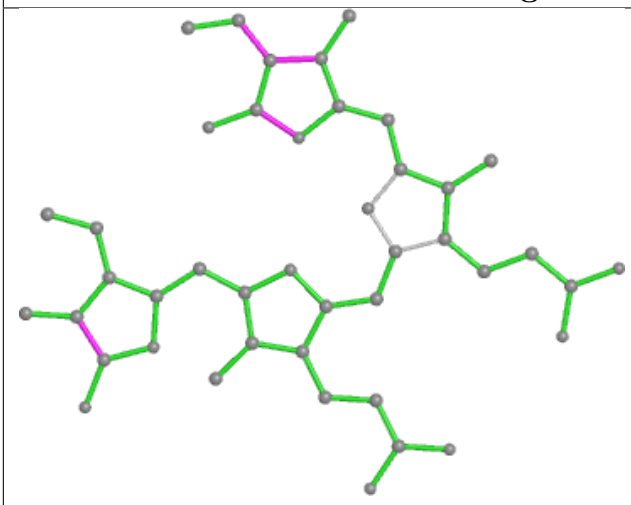


Torsions



Rings

Ligand PEB e8 302



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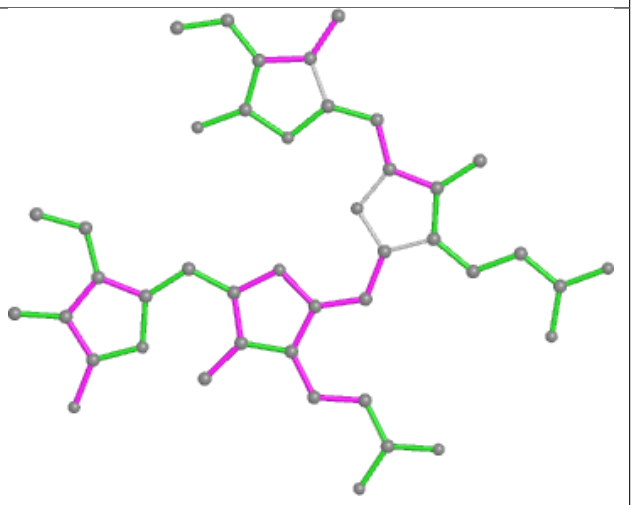
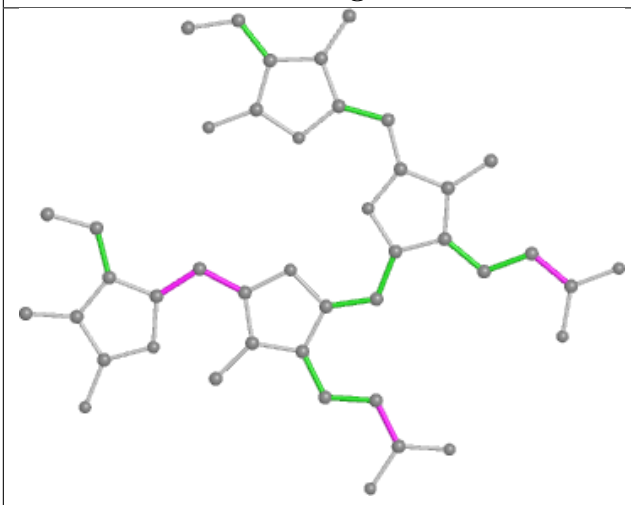
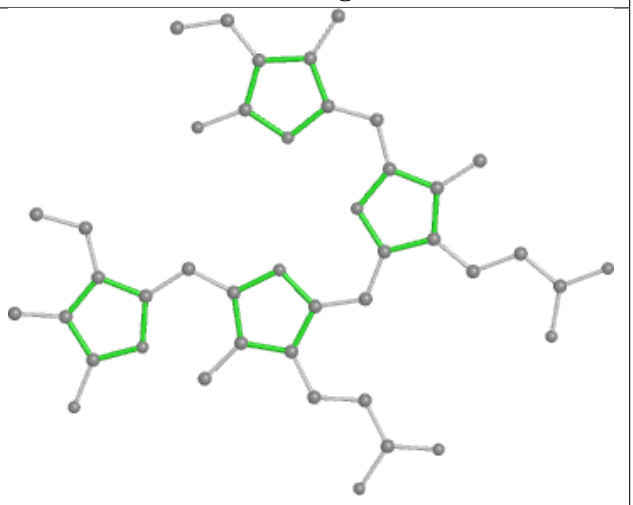


Bond angles

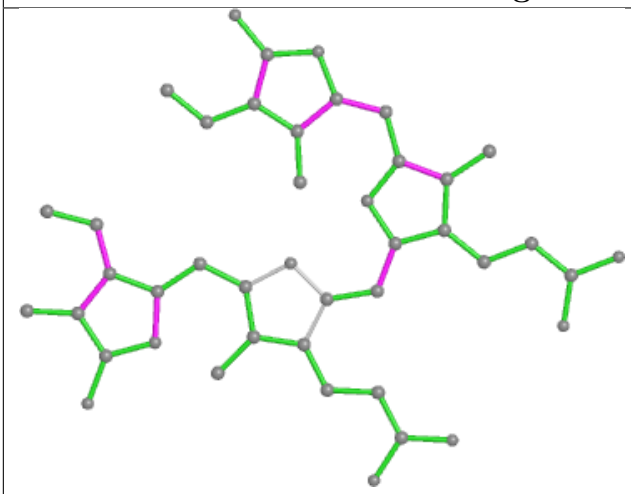


Torsions



Rings

Ligand PVN eY 403



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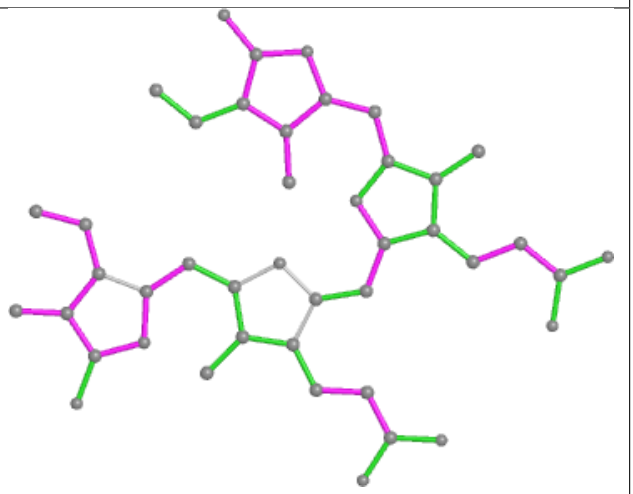

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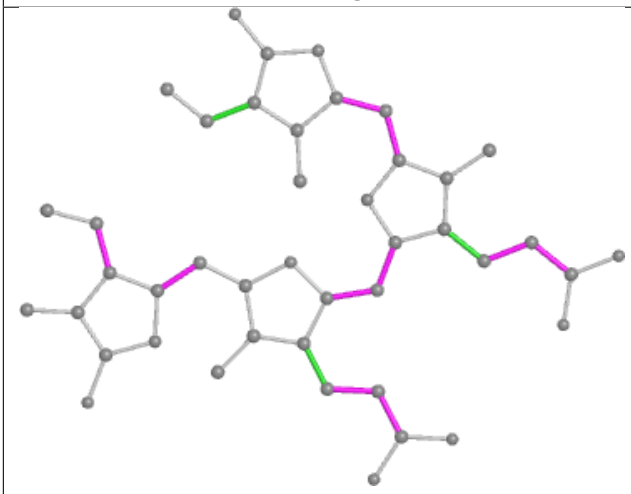

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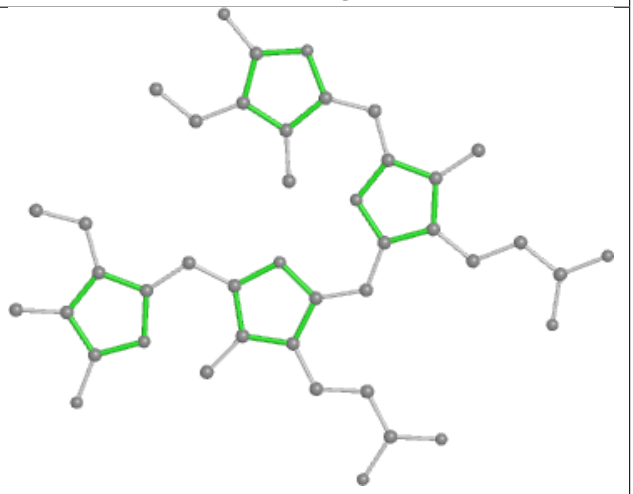
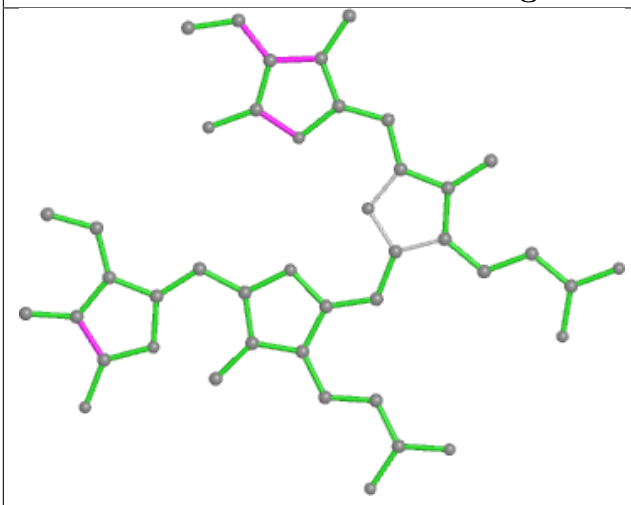


Rings

Ligand PEB a4 201



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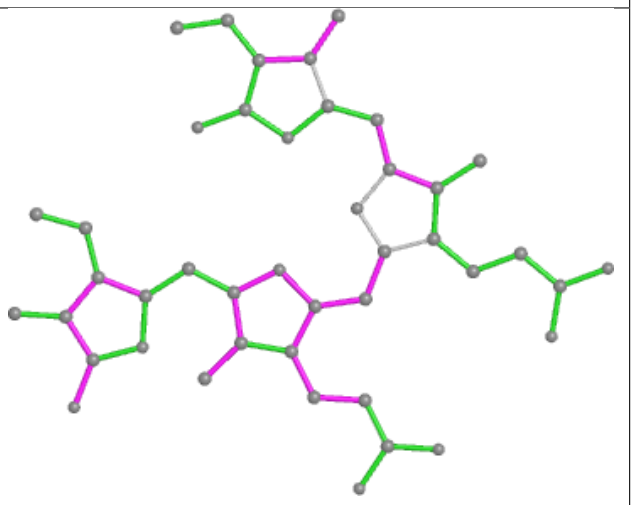
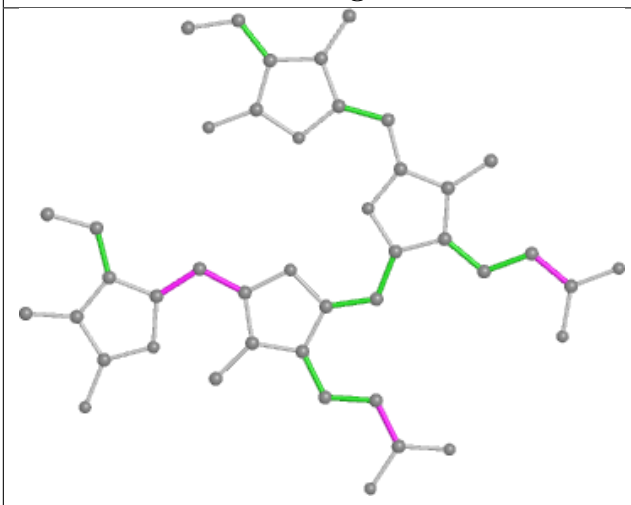


Bond angles



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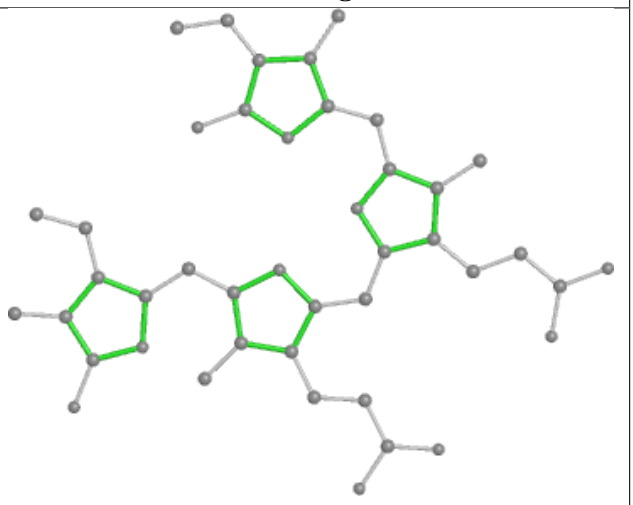
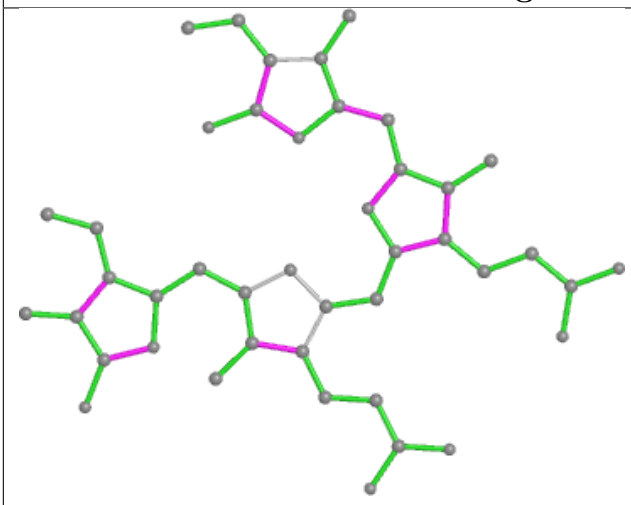


Rings

Ligand PUB Z3 203



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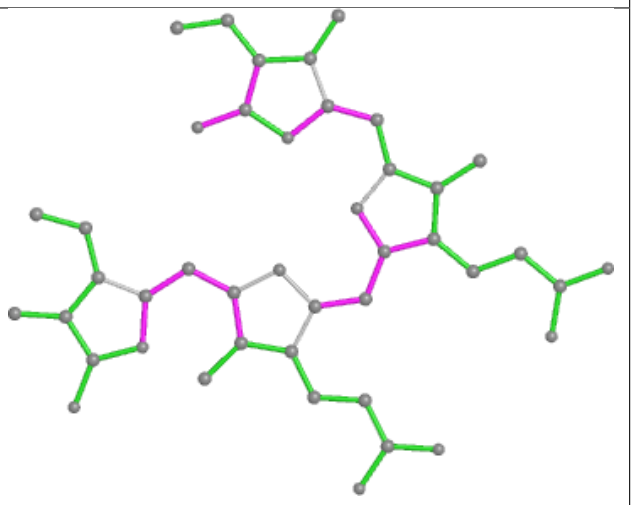

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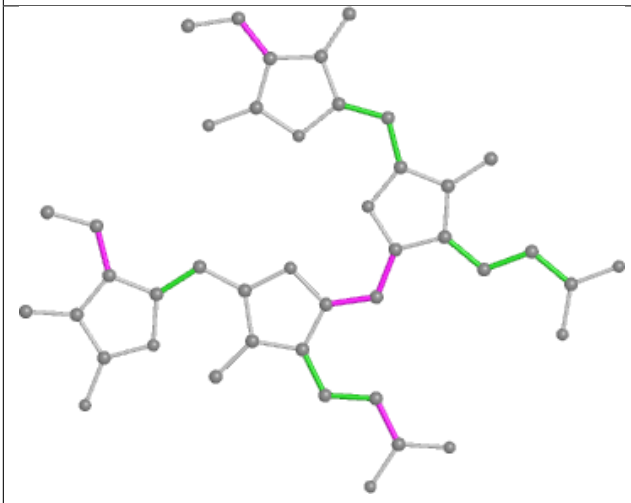

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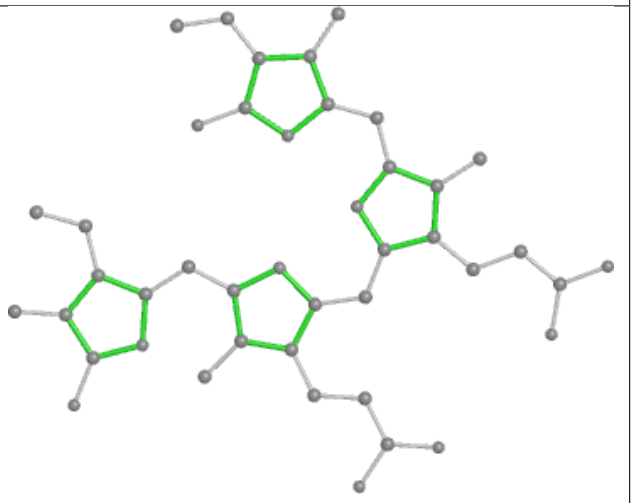
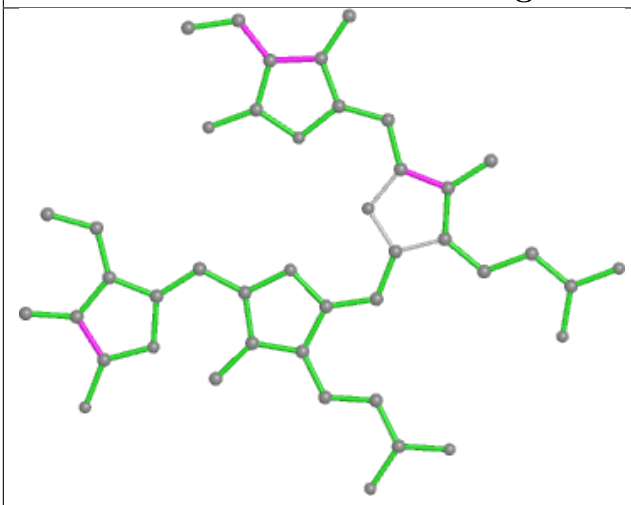


Rings

Ligand PEB V6 202



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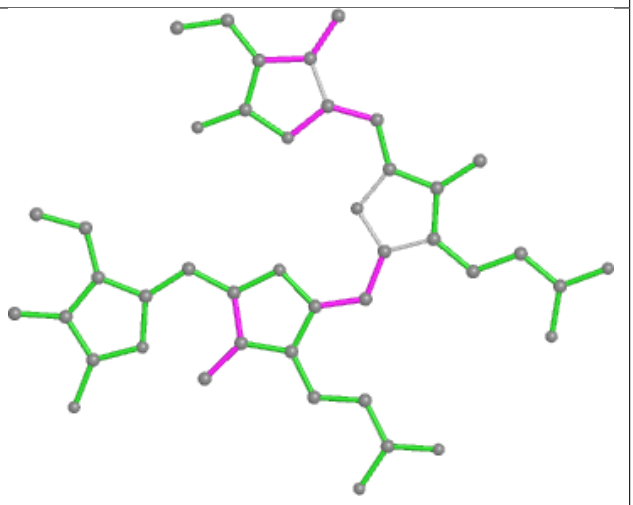

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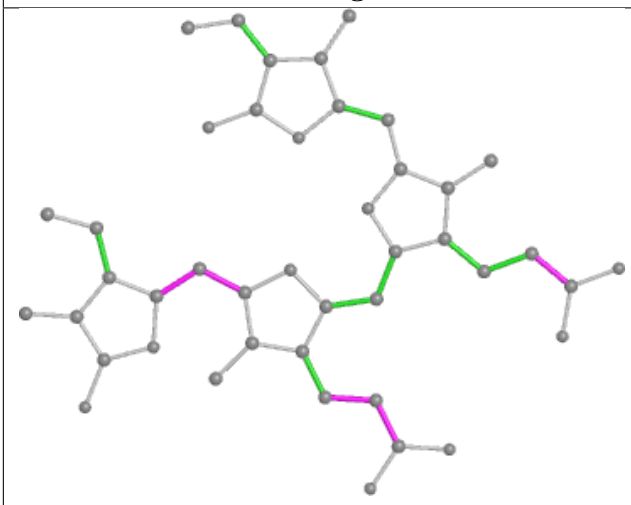

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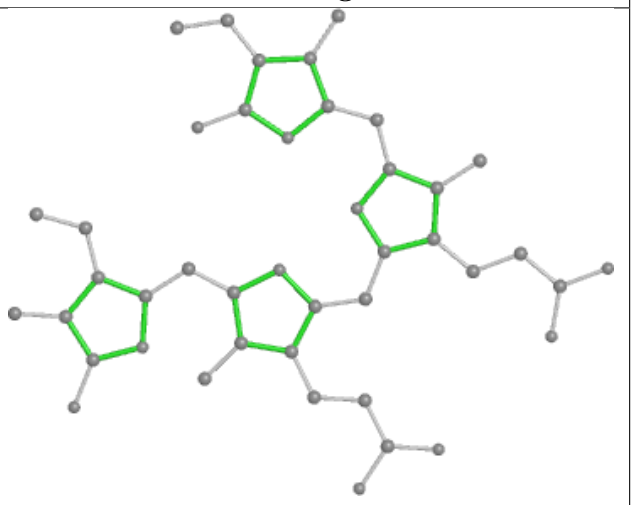
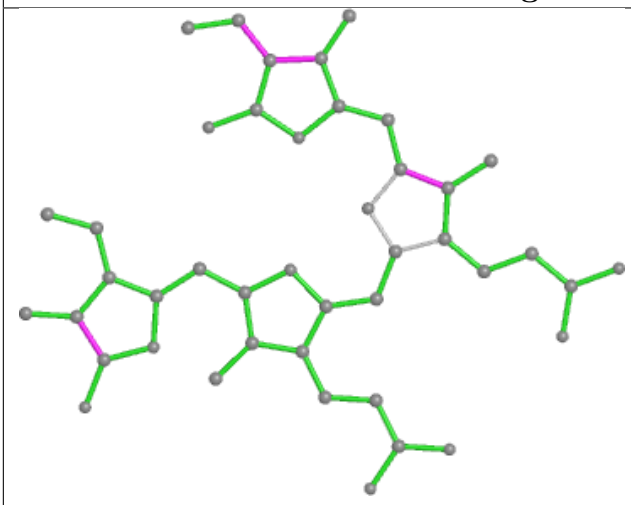


Rings

Ligand PEB hI 202



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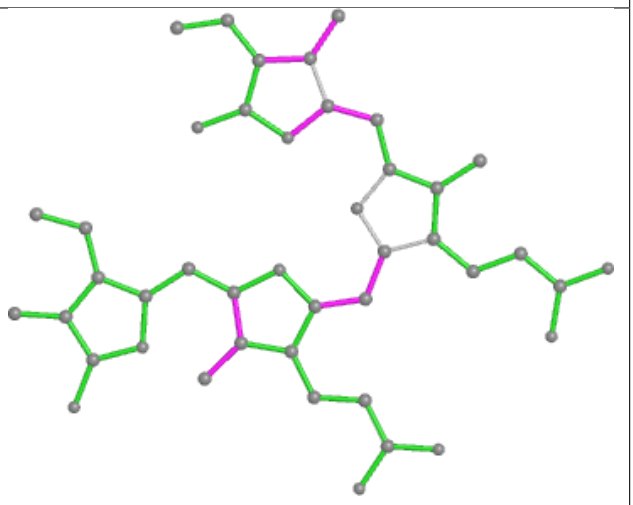

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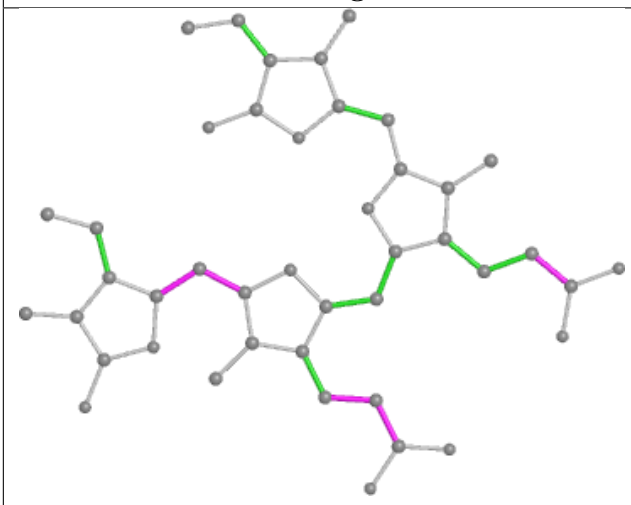

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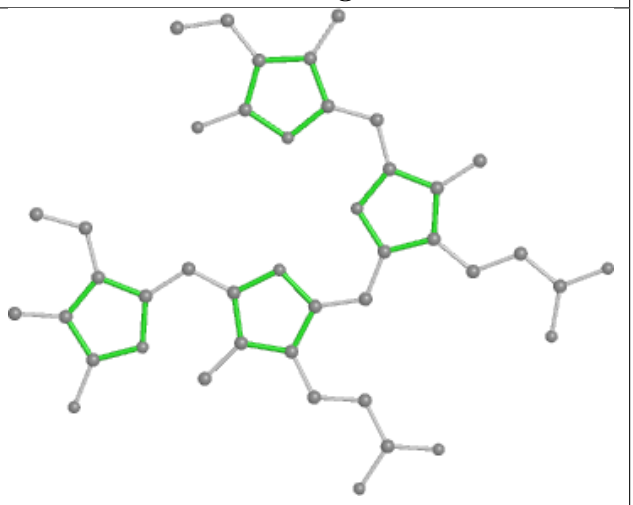

Rings

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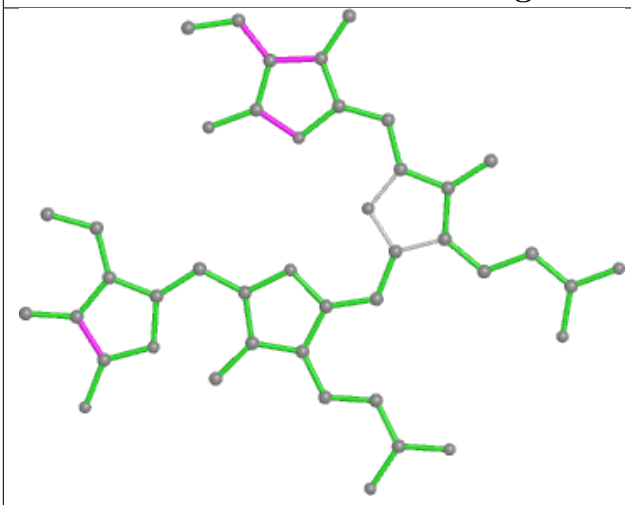

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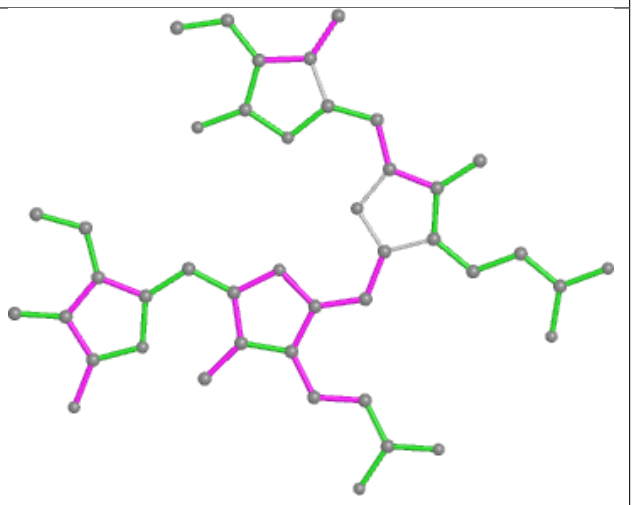

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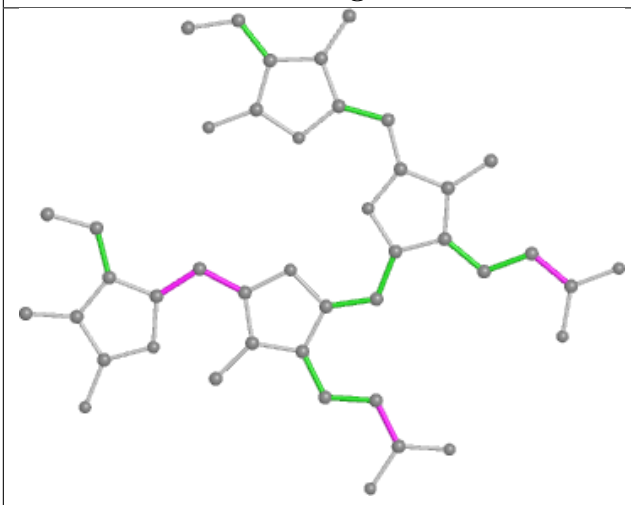

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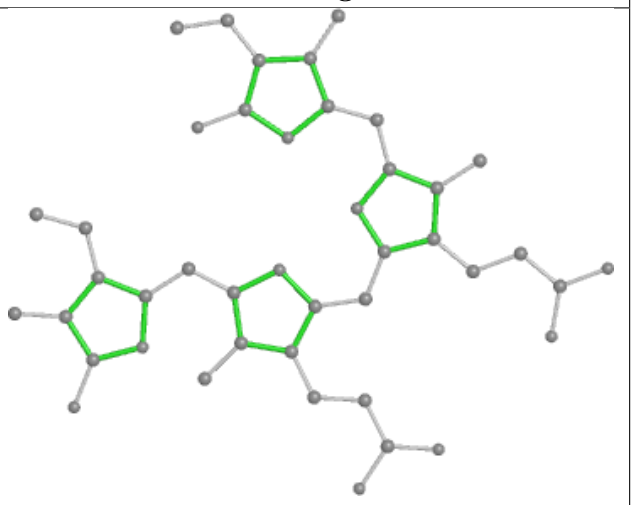
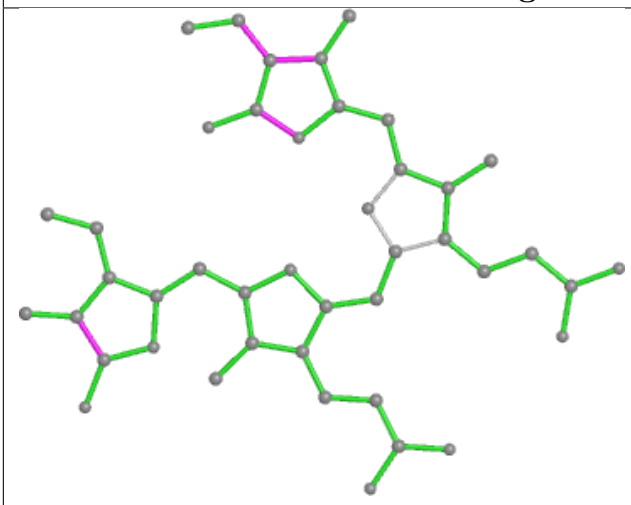


Rings

Ligand PEB u7 201



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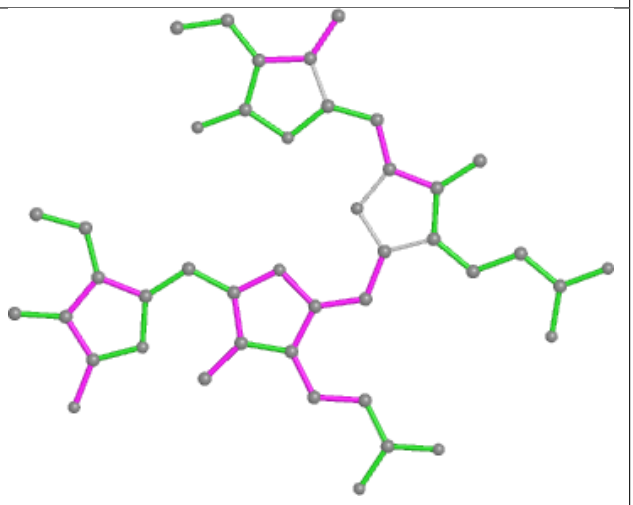

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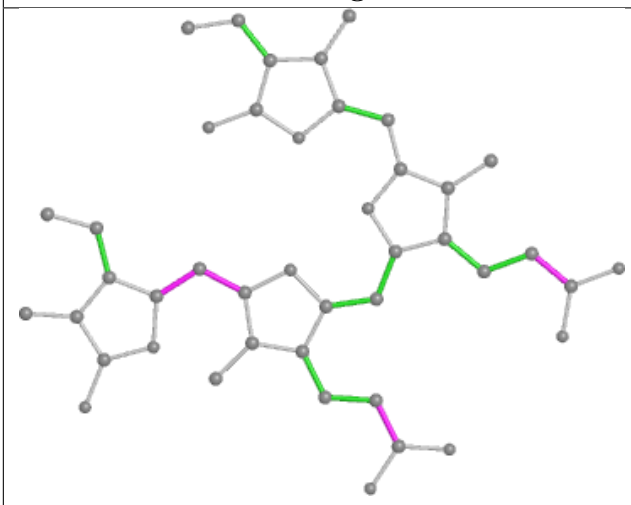

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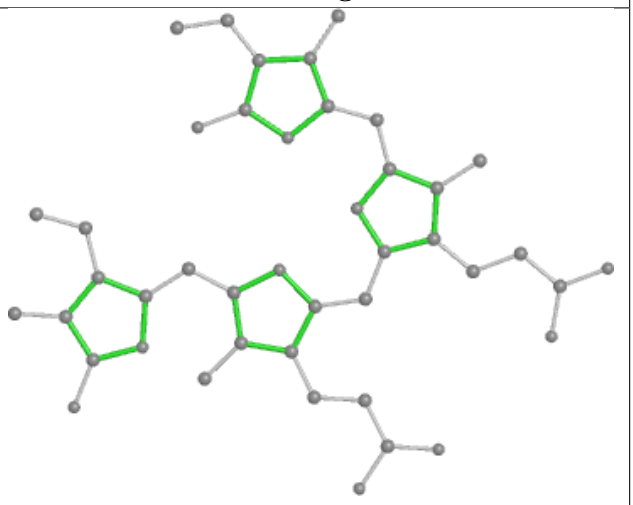

Rings

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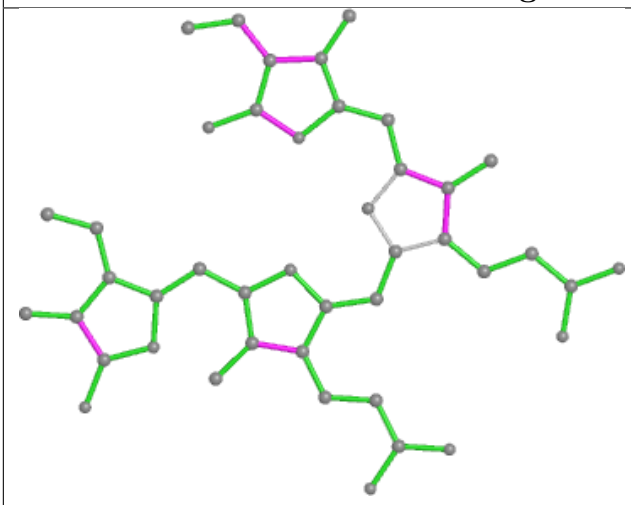

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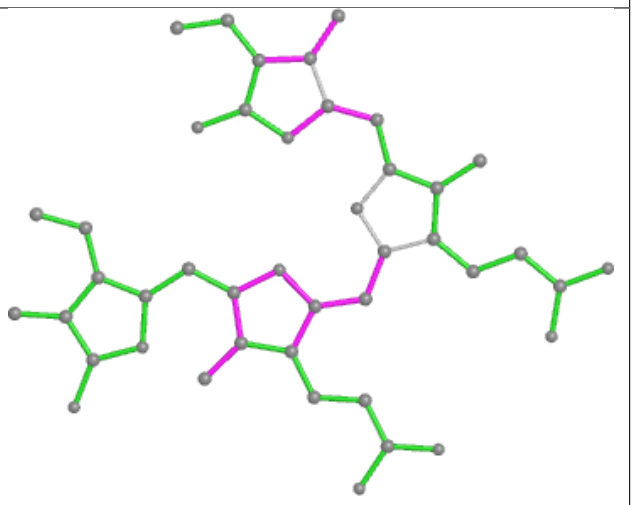

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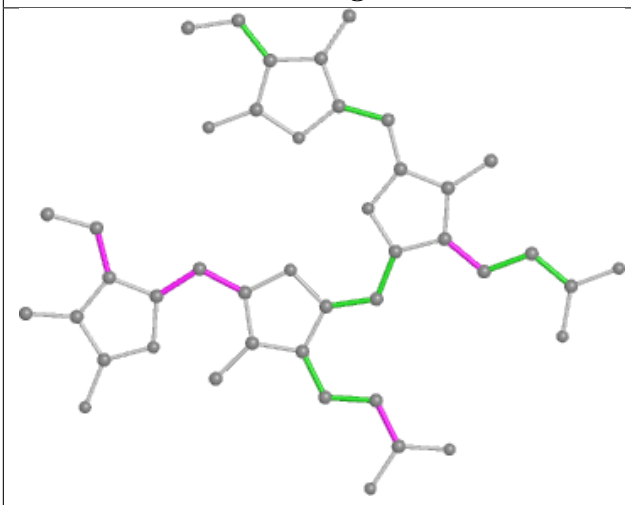

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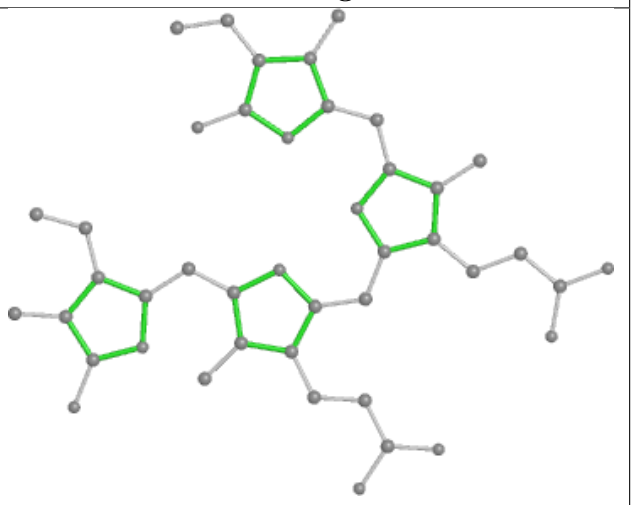
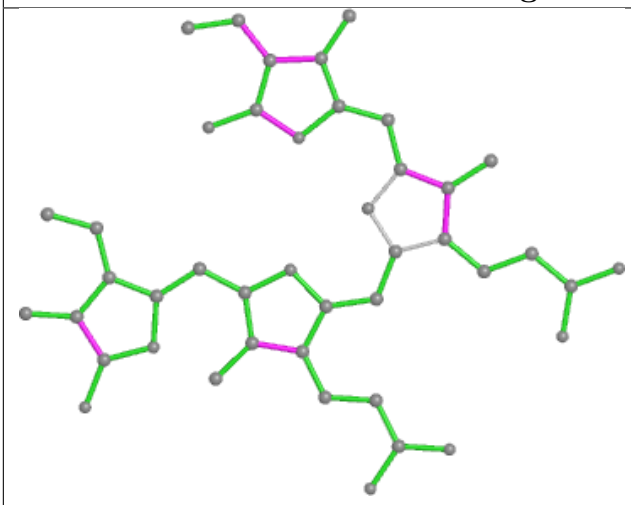


Rings

Ligand PEB ga 202



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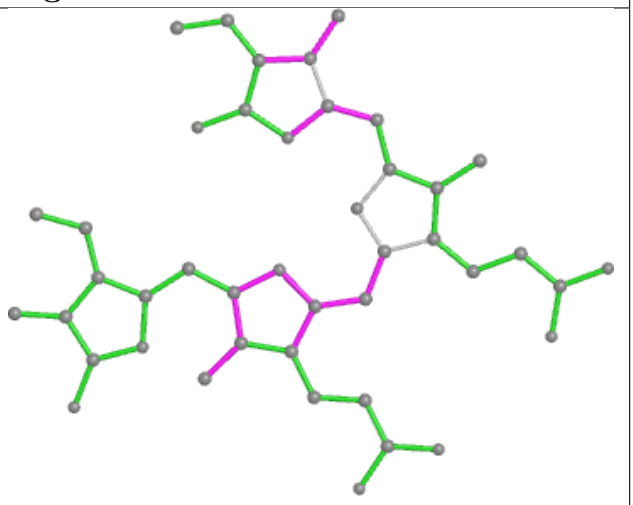

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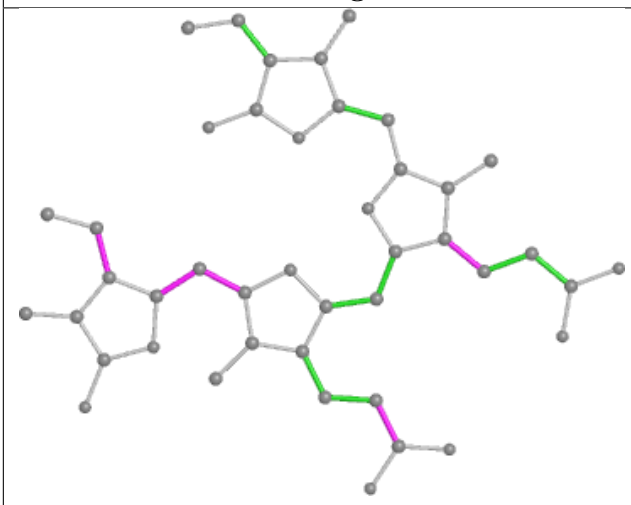

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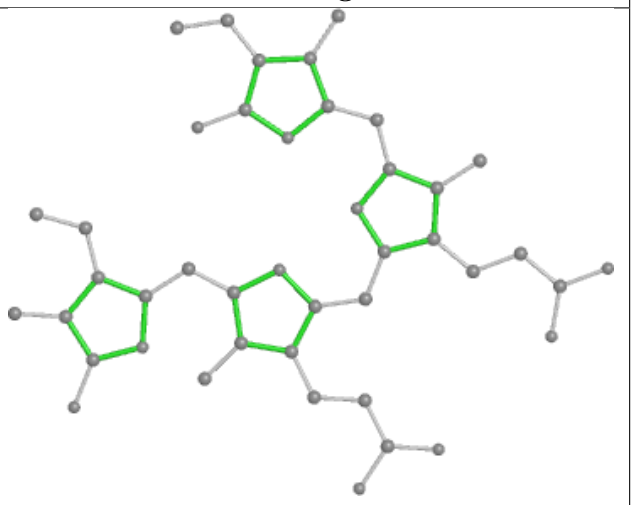

Rings

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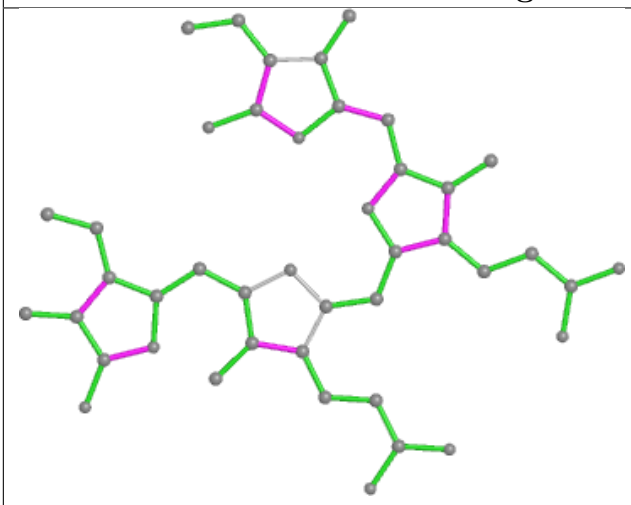

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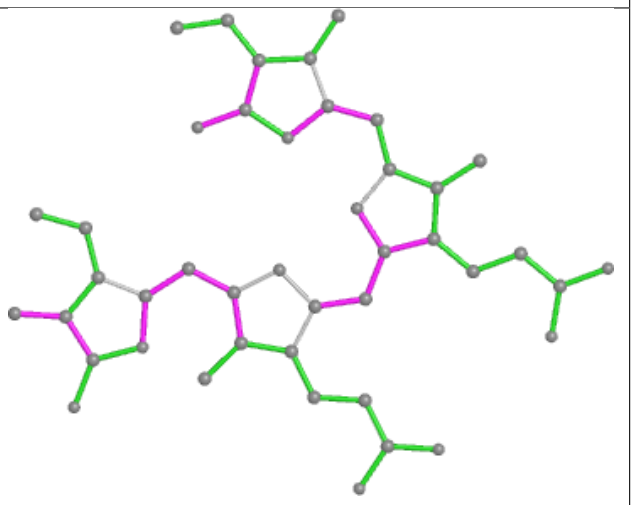

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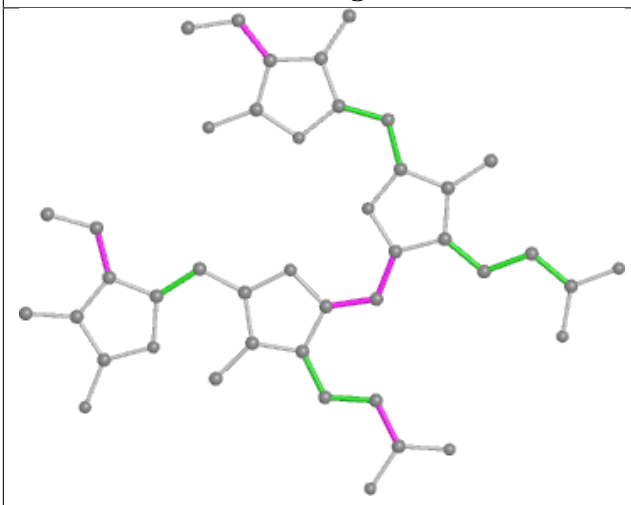

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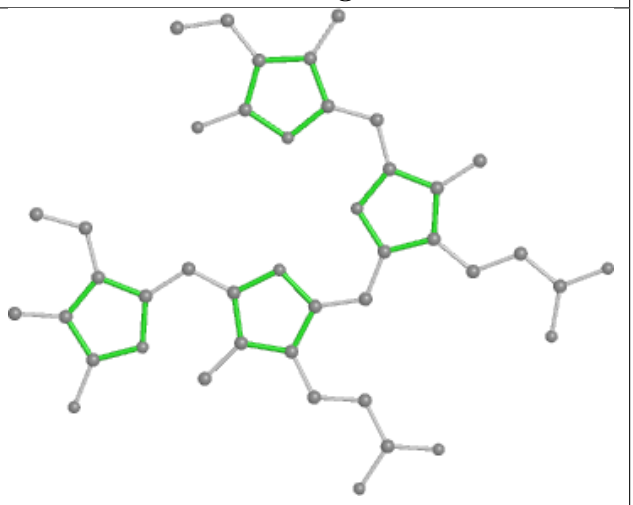

Rings

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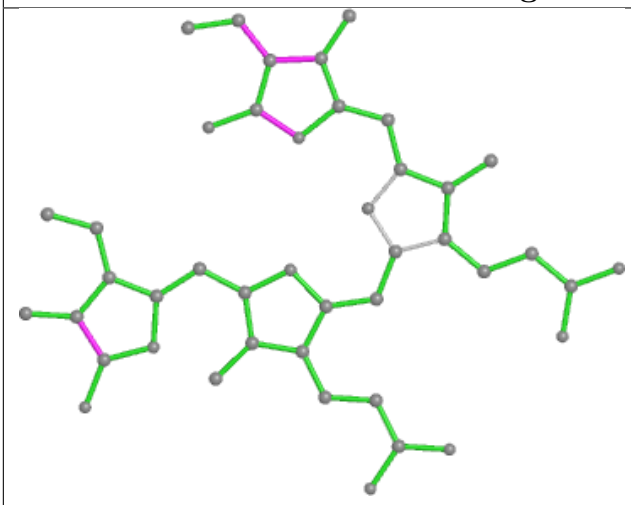

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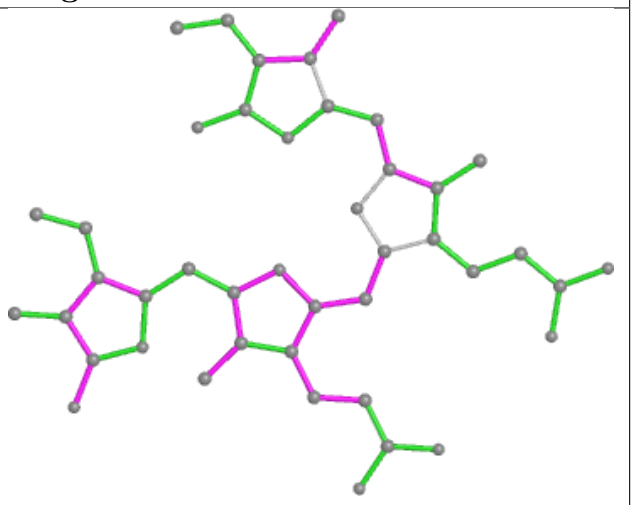

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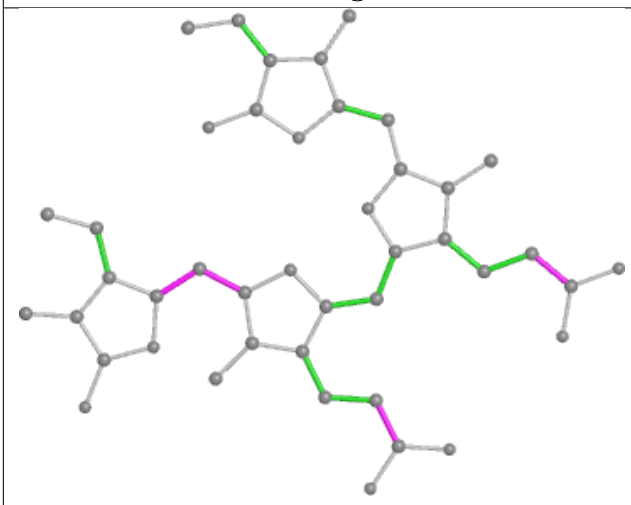

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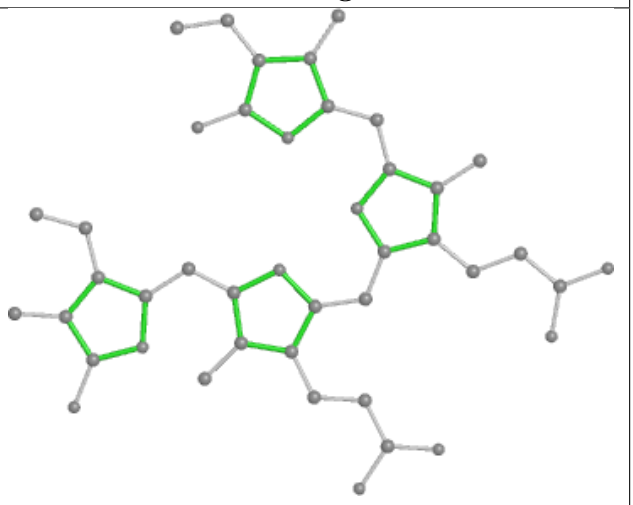

Rings

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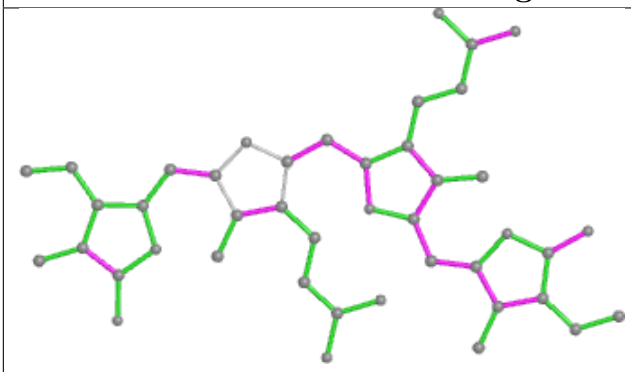

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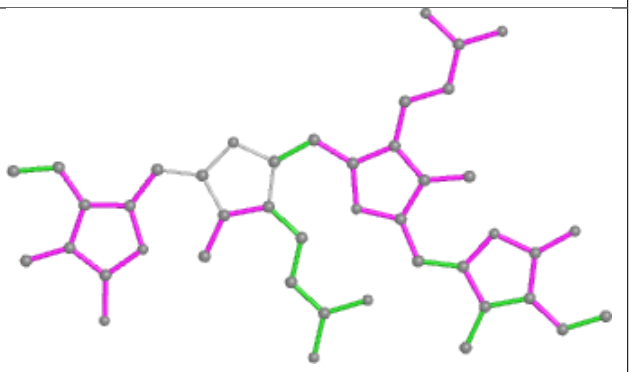

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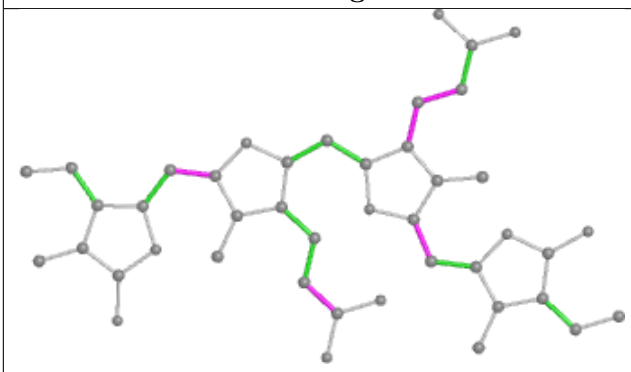

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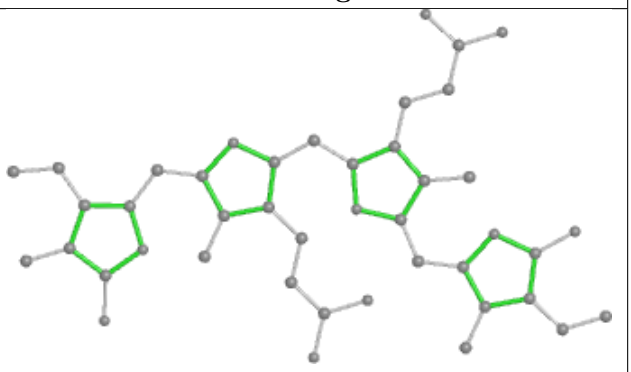
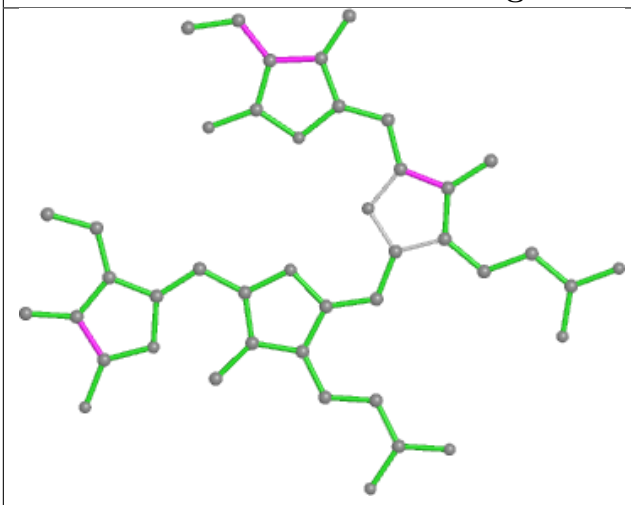
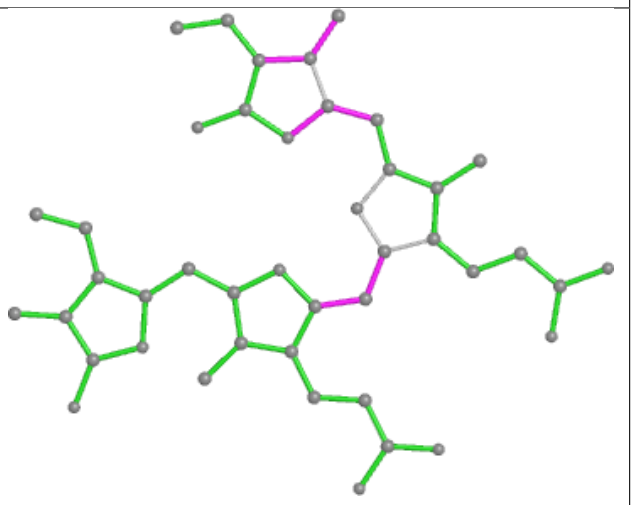


Rings

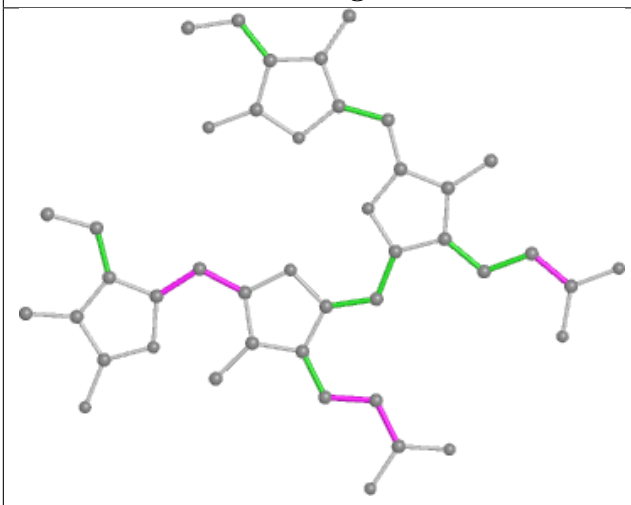
Ligand PEB w7 1002



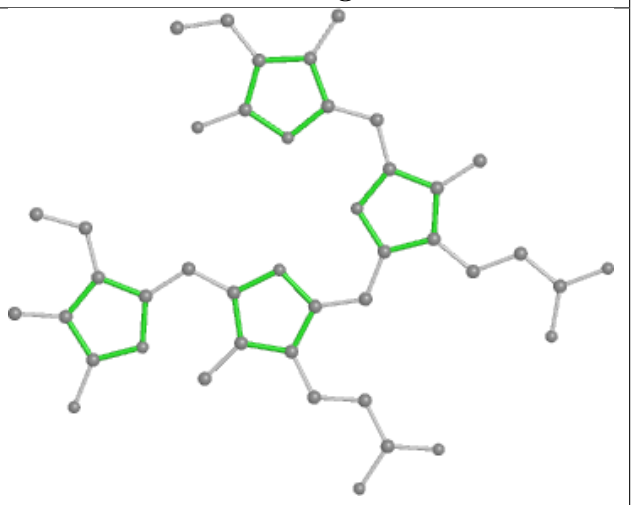
Bond lengths



Bond angles

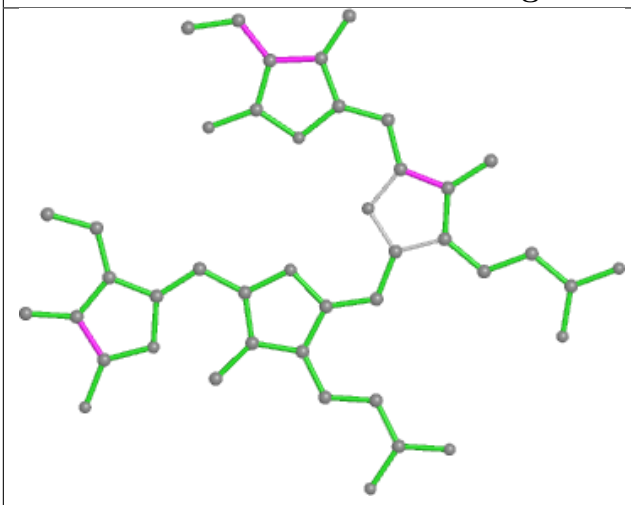


Torsions



Rings

Ligand PEB s7 202



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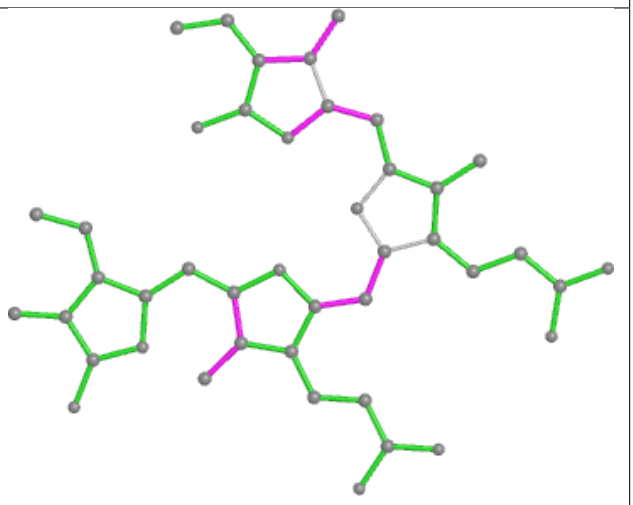

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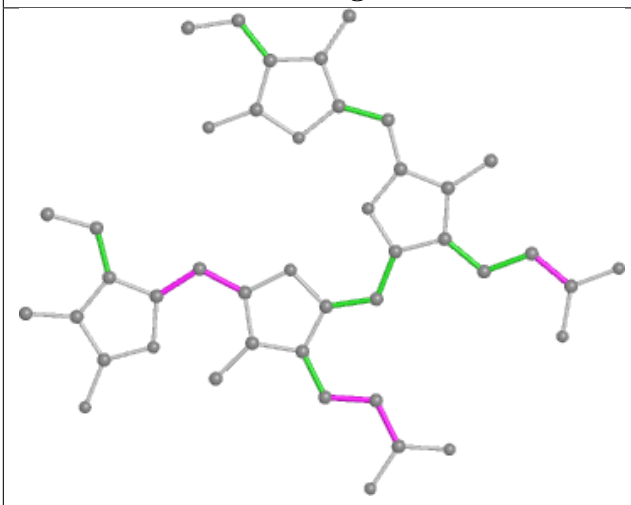

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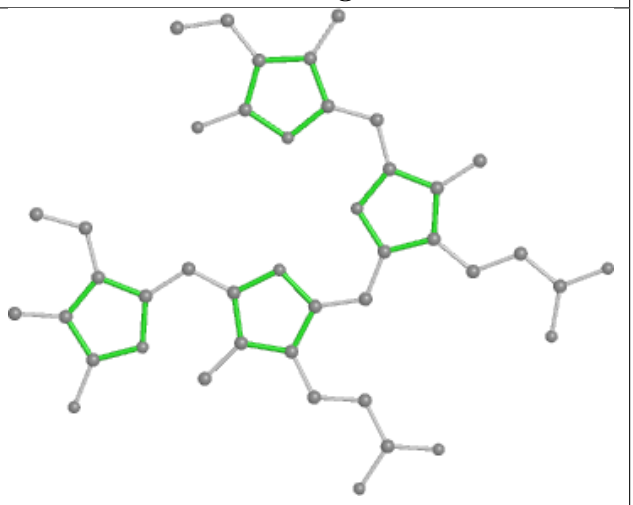
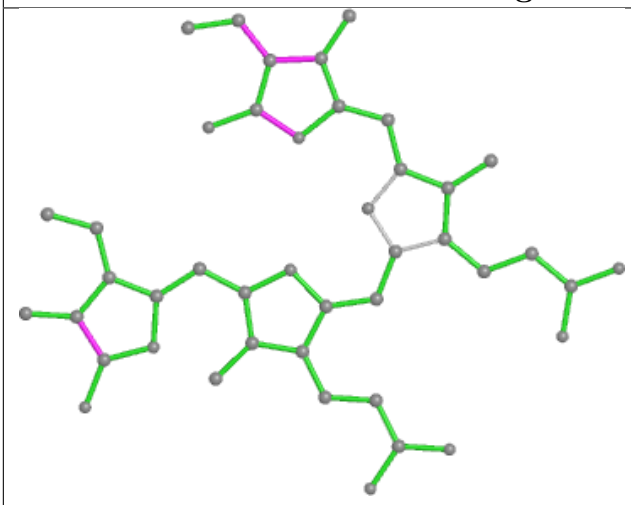


Rings

Ligand PEB X5 401



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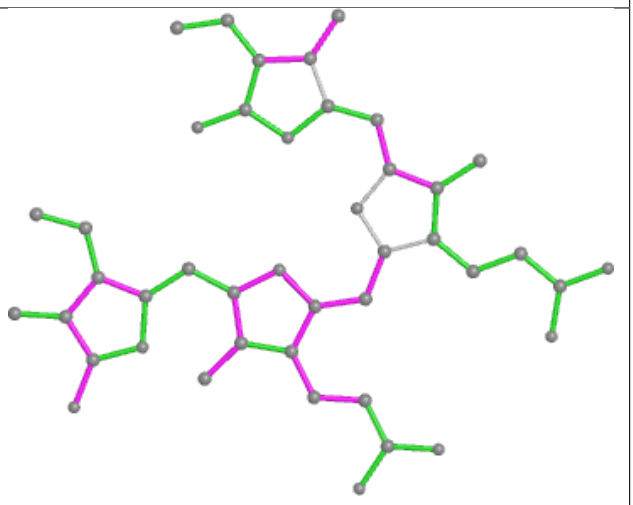

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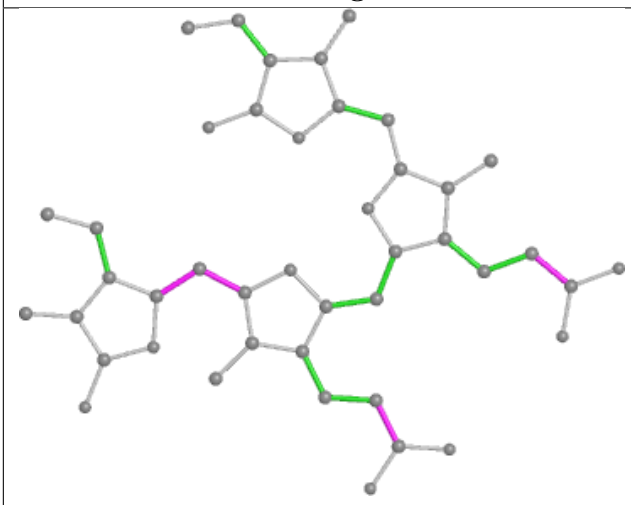

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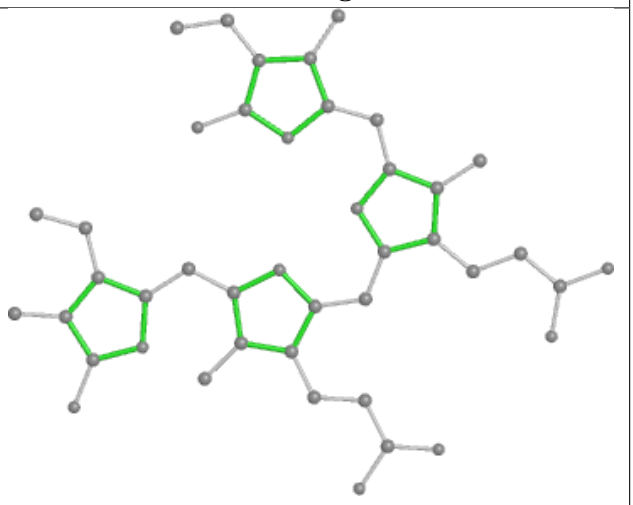
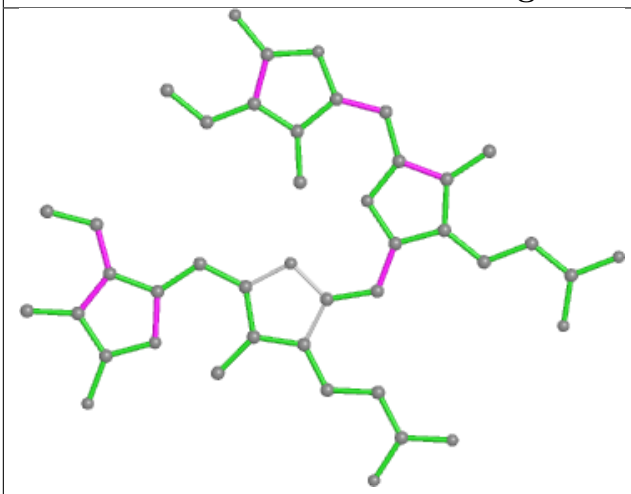


Rings

Ligand PVN c9 303



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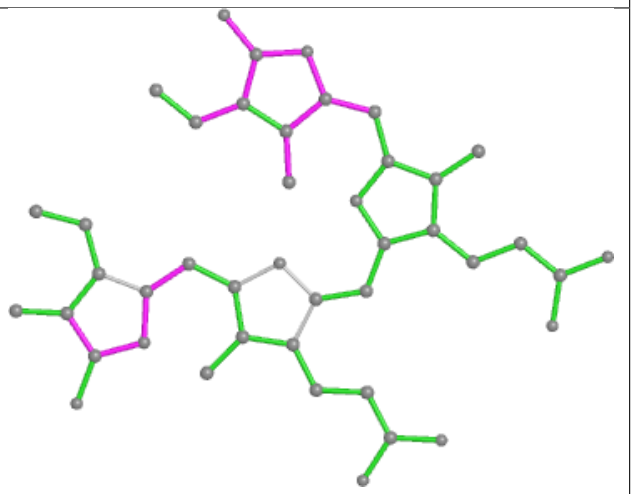

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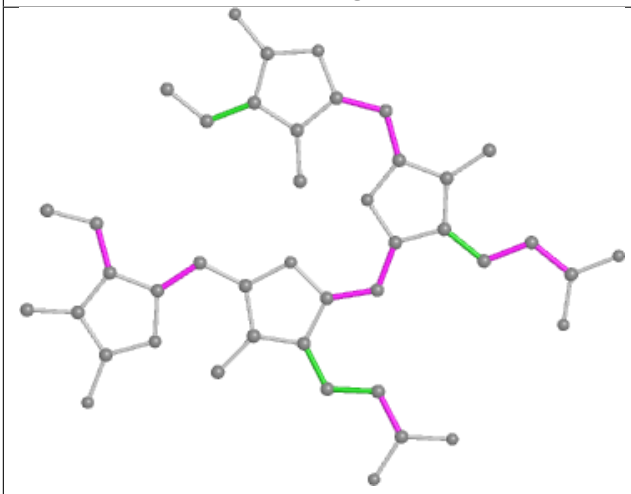

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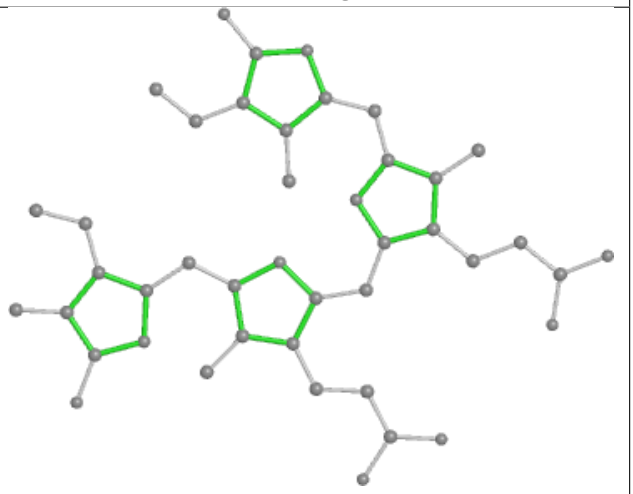

Rings

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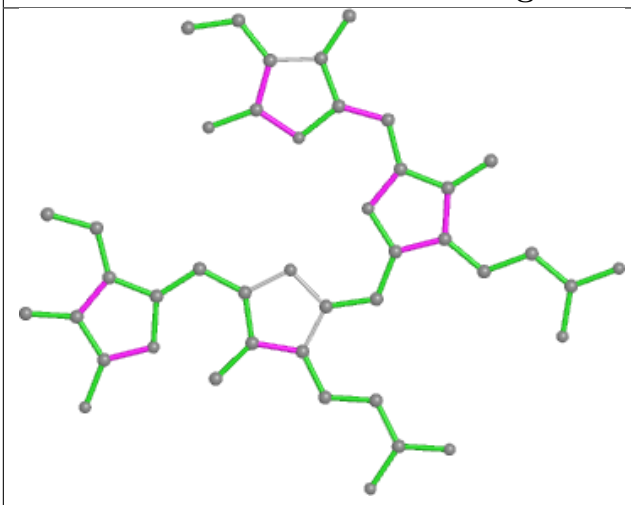

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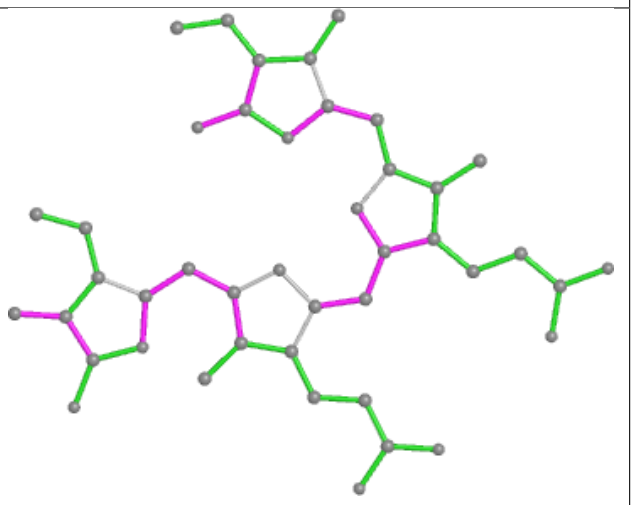

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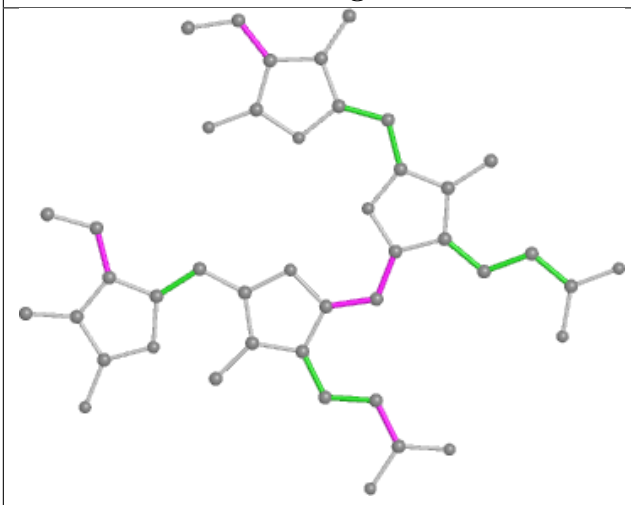

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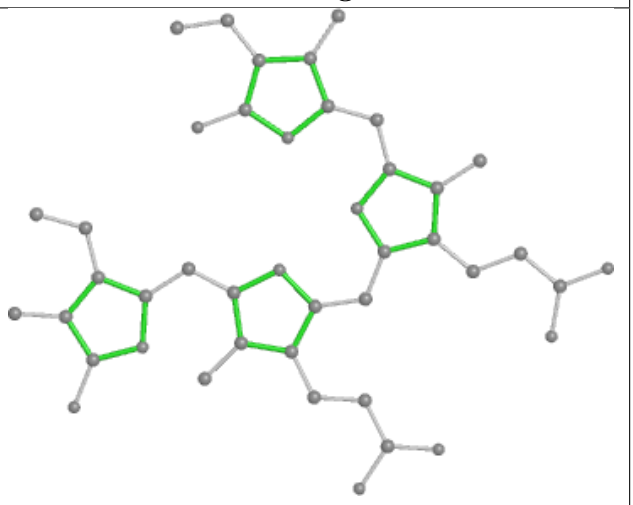

Rings

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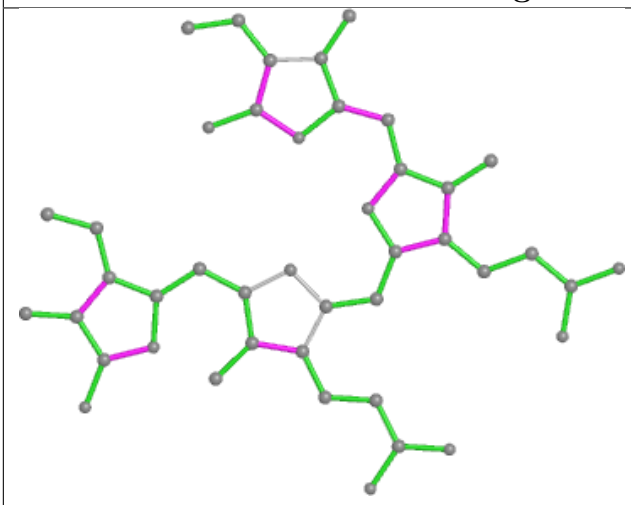

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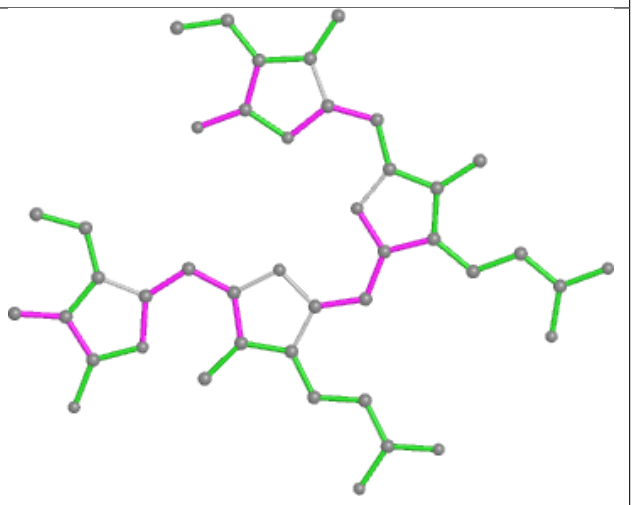

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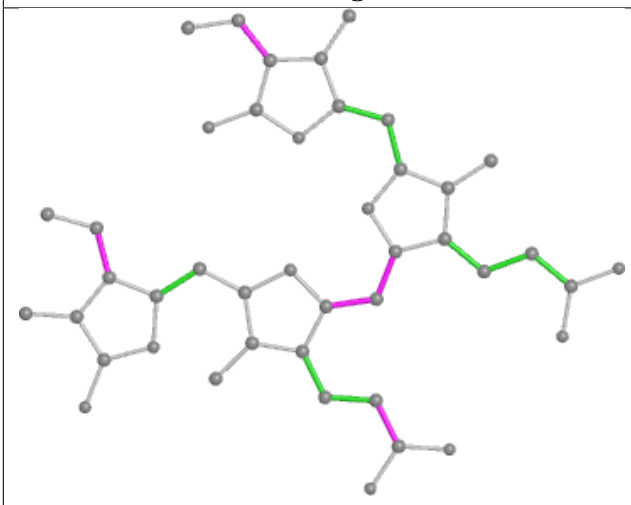

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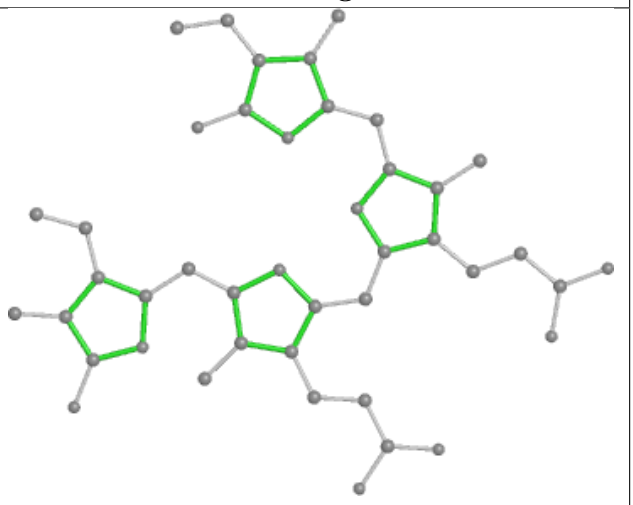
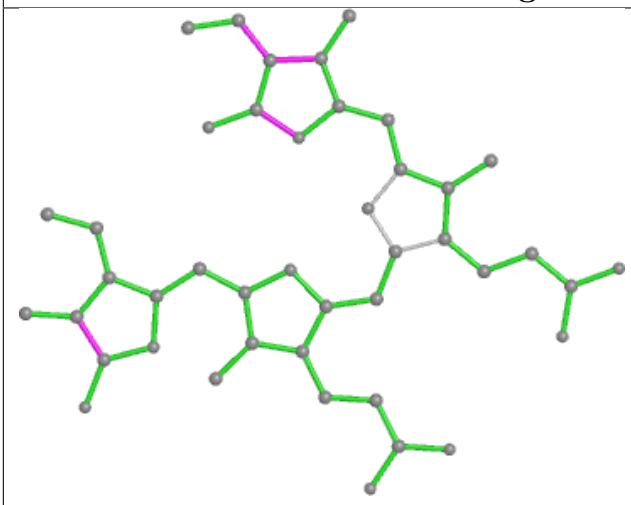


Rings

Ligand PEB S3 201



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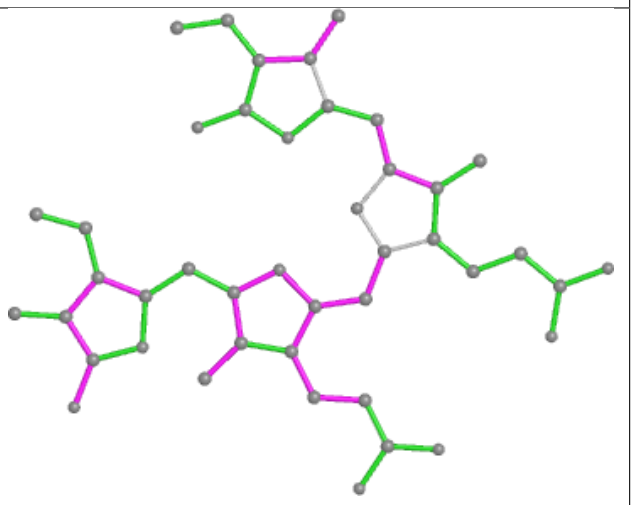

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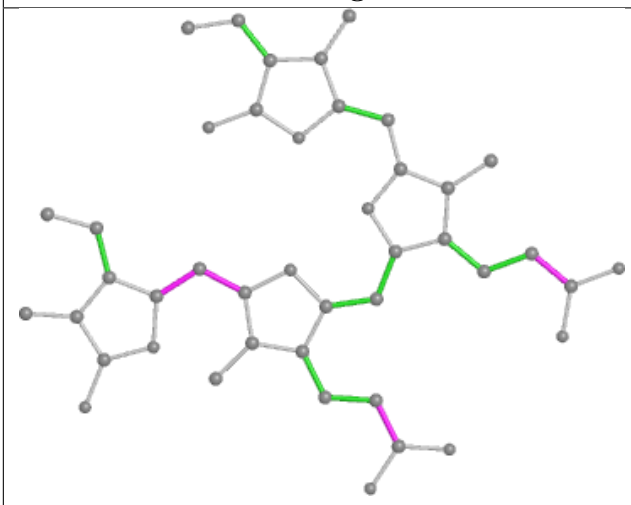

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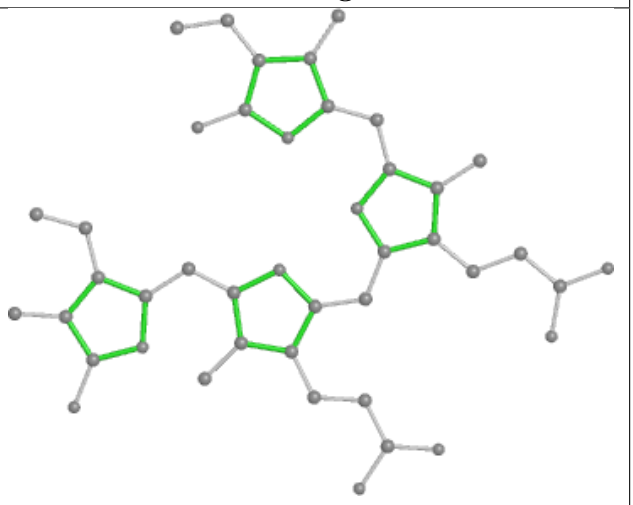
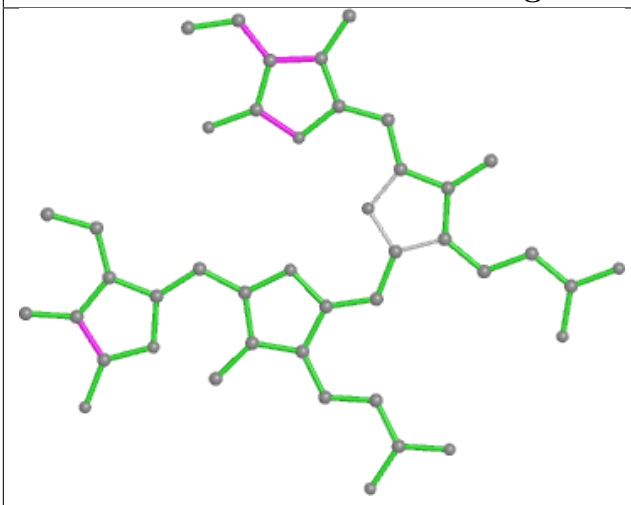


Rings

Ligand PEB ej 202



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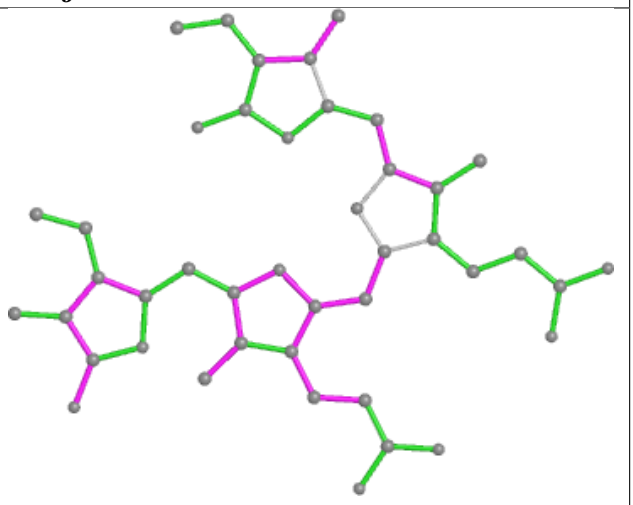

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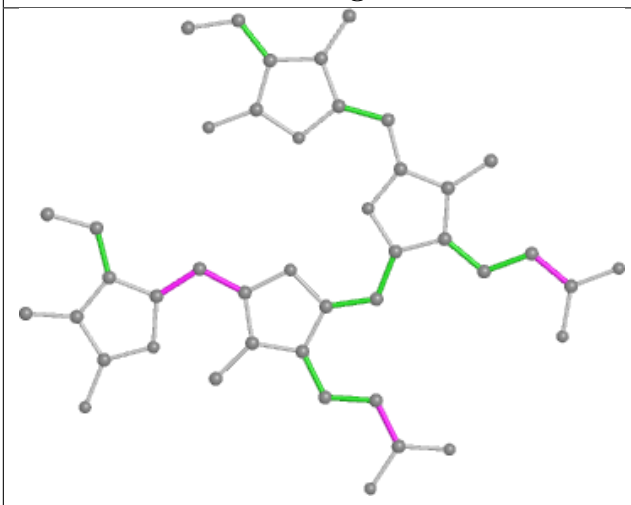

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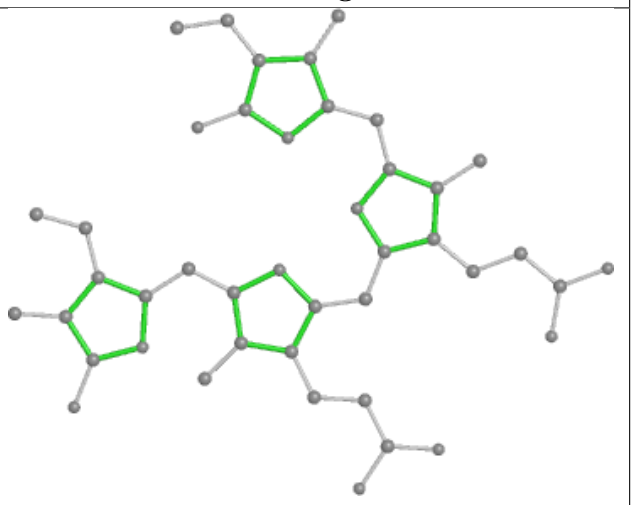
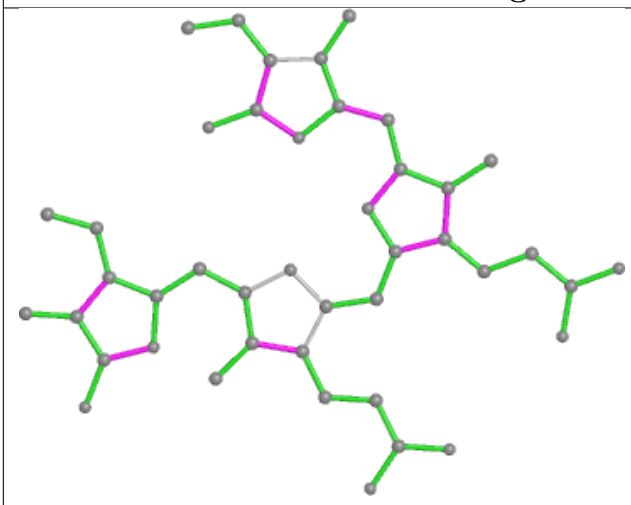


Rings

Ligand PUB c6 1004



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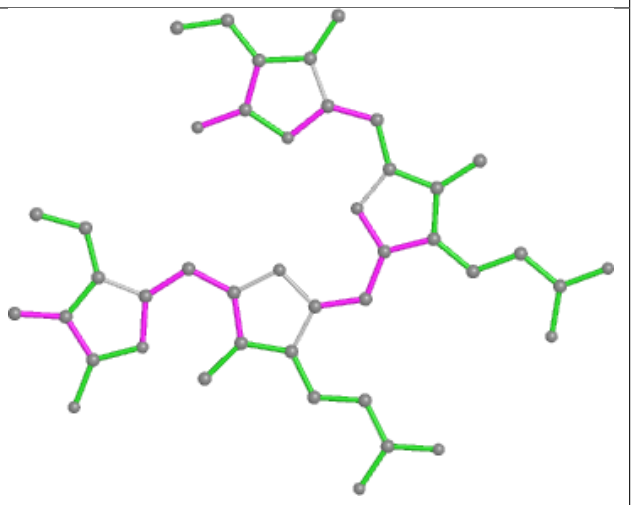

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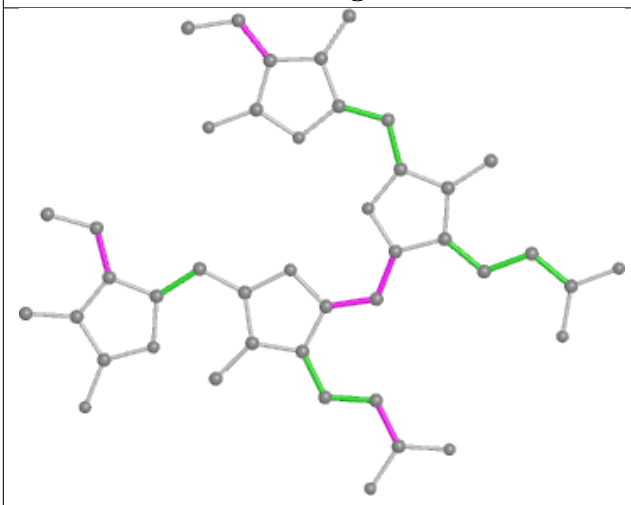

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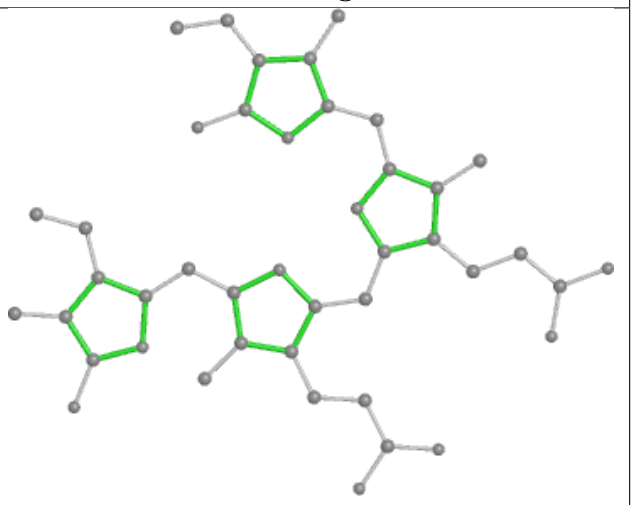

Rings

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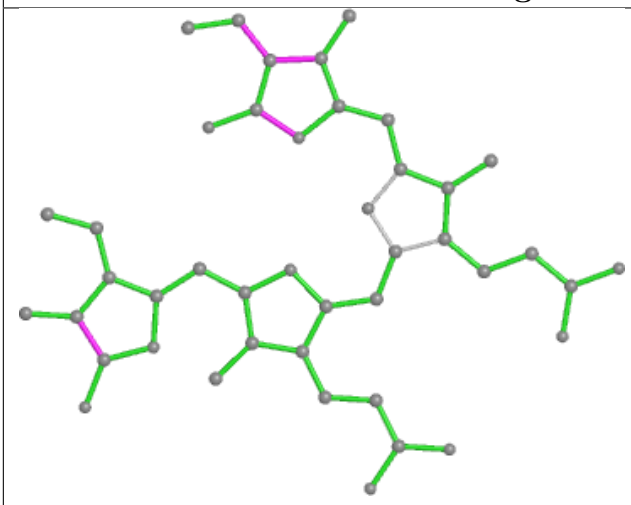

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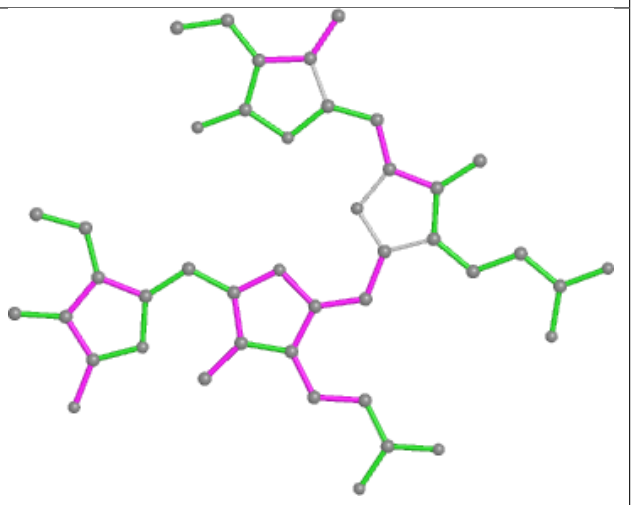

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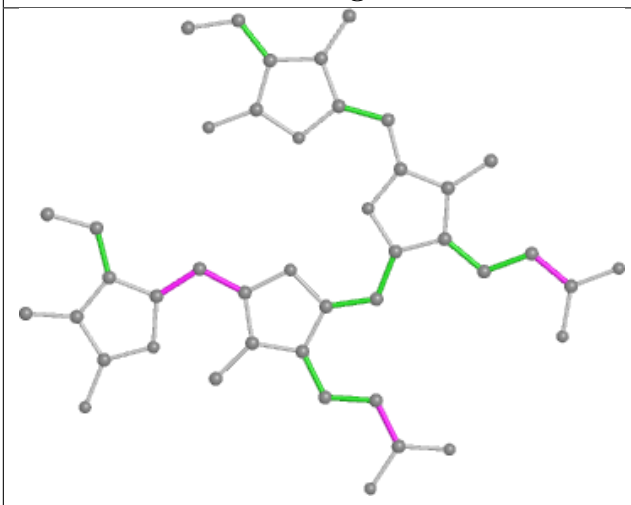

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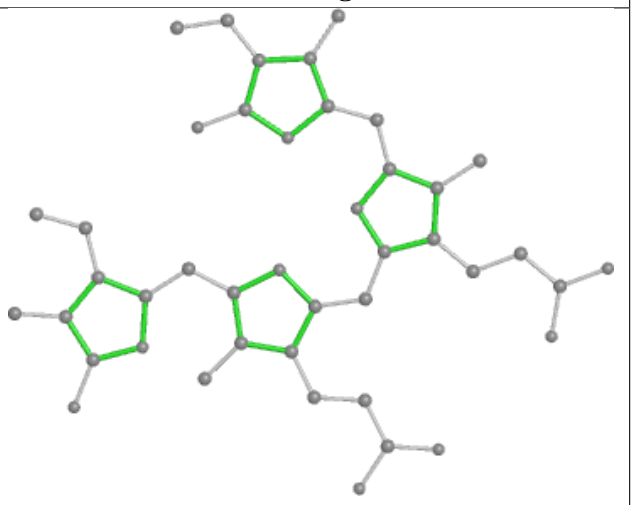

Rings

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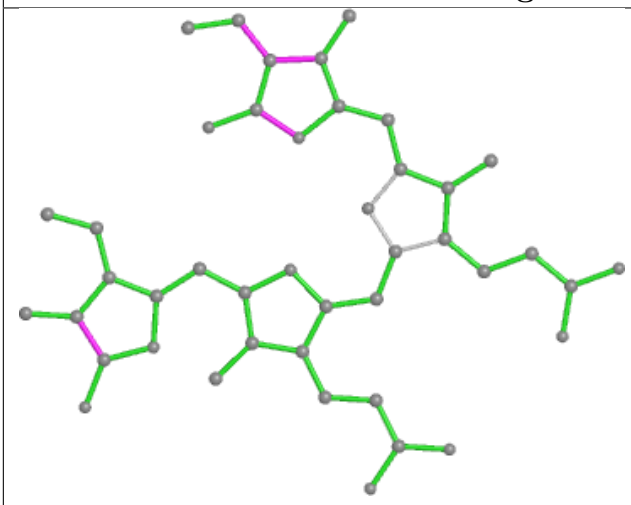

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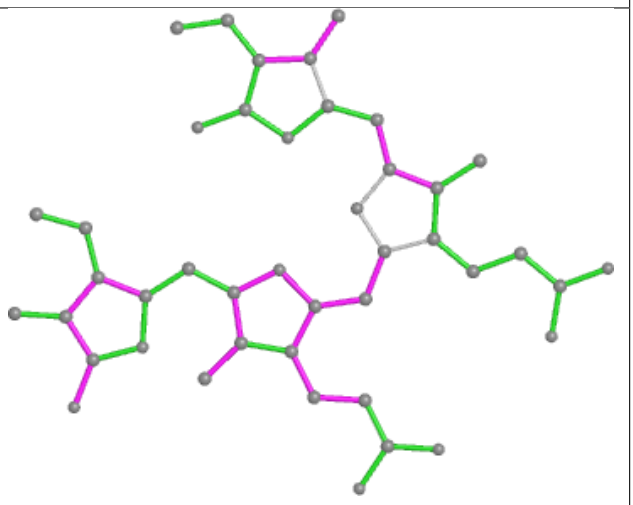

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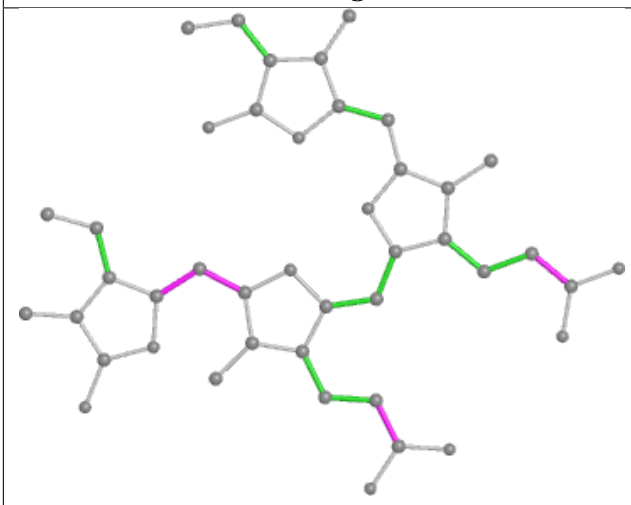

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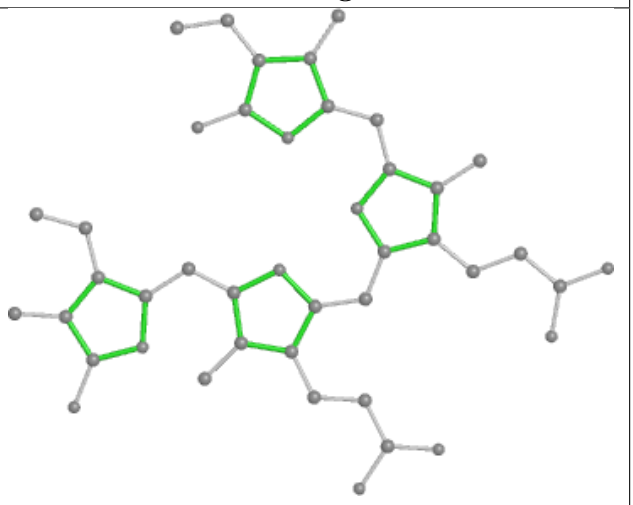
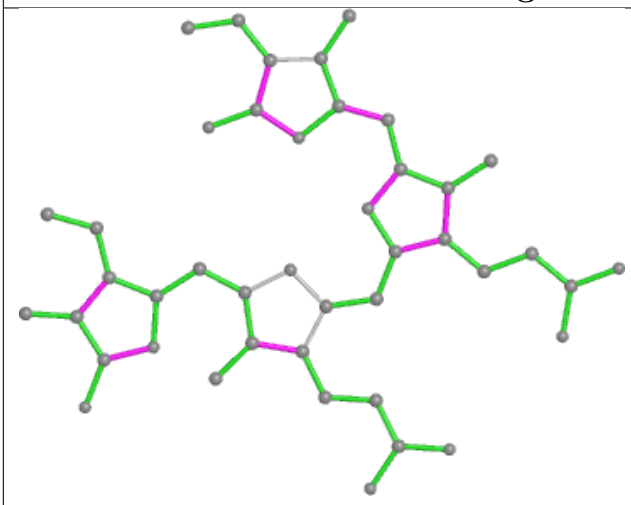


Rings

Ligand PUB J3 203



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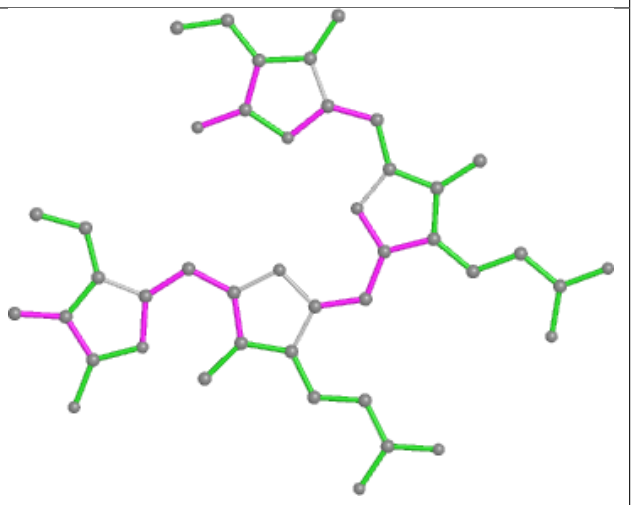

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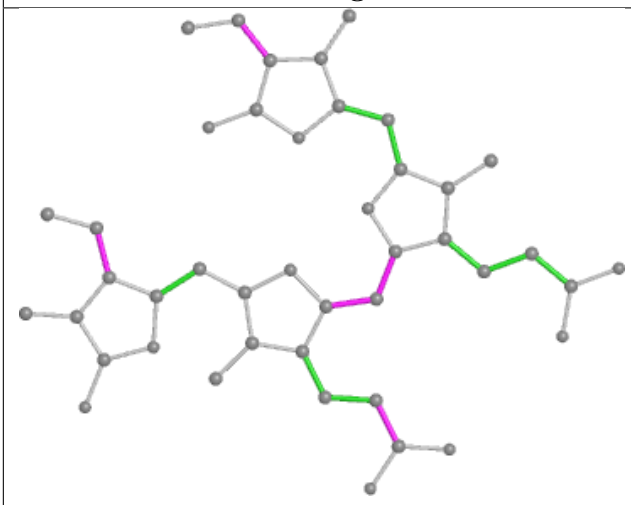

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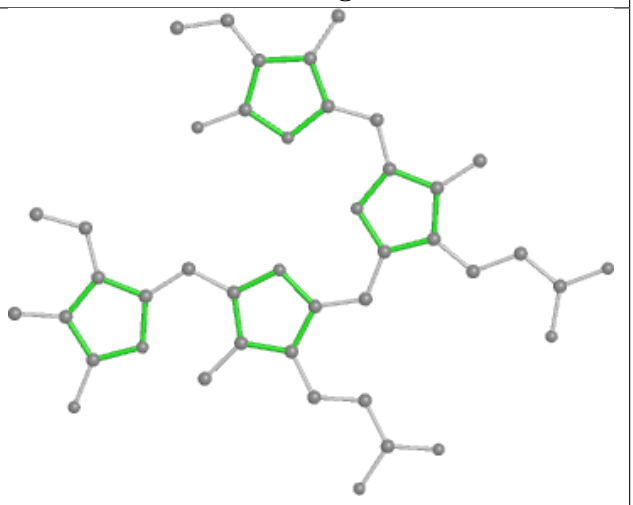

Rings

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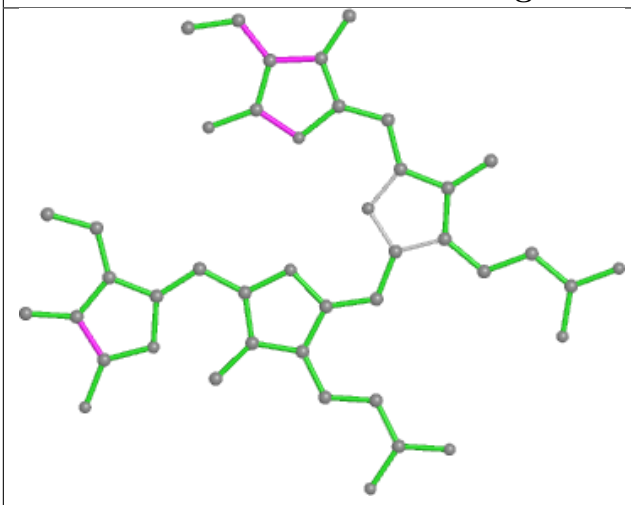

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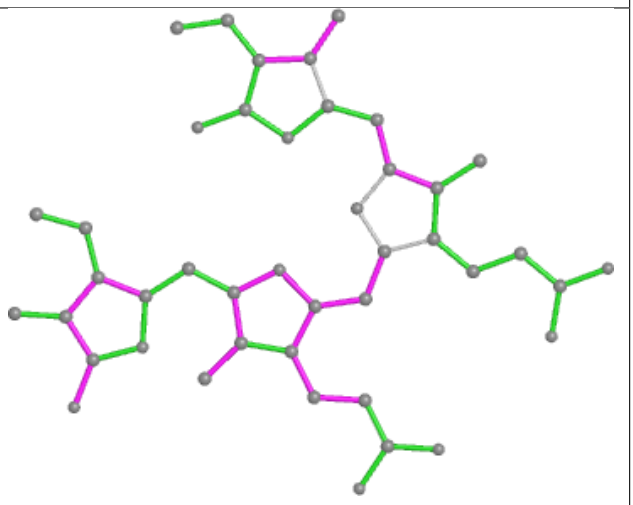

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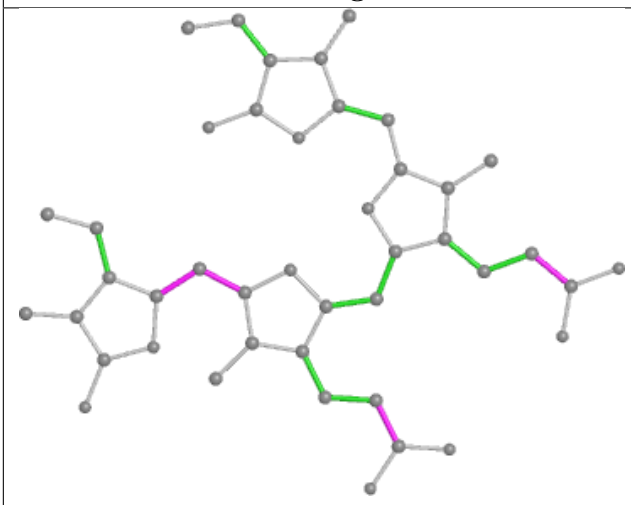

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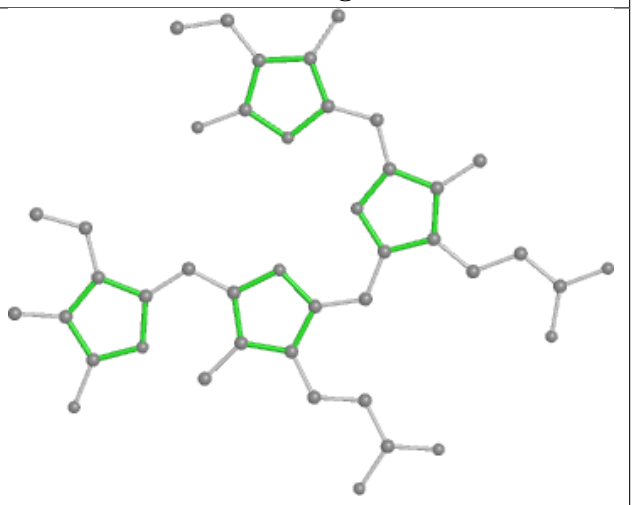

Rings

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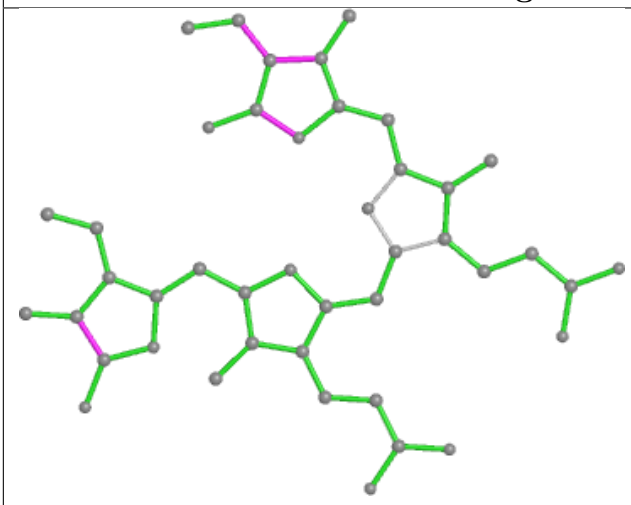

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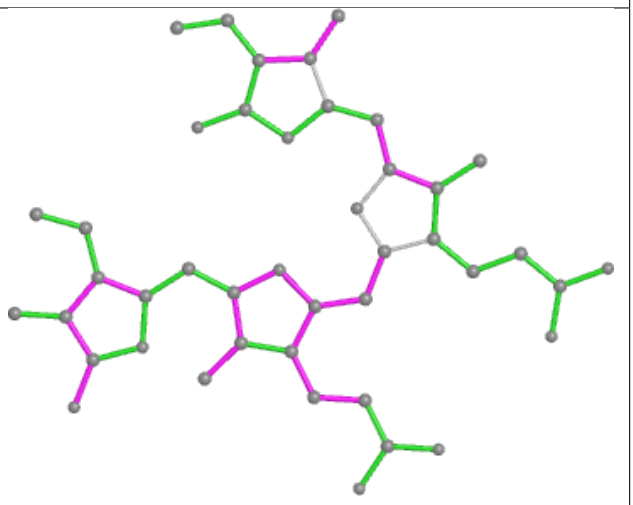
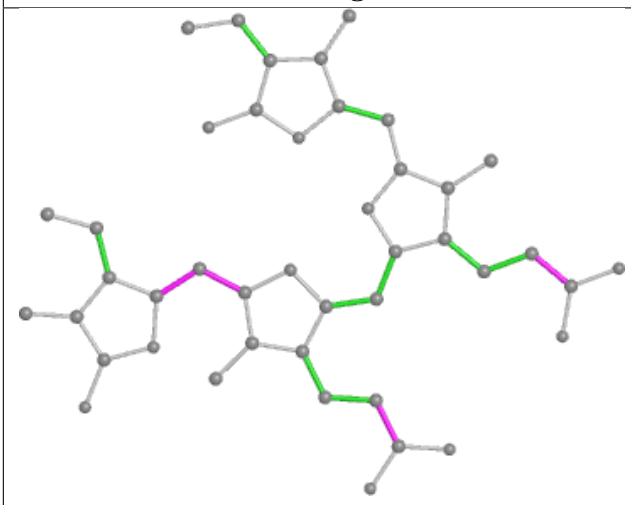
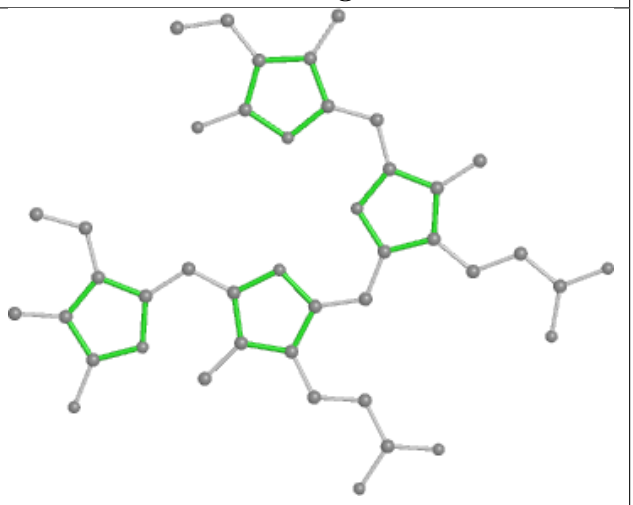


Bond angles

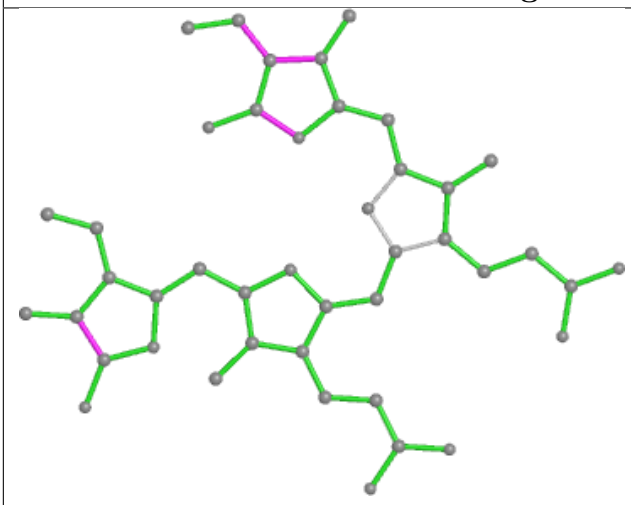


Torsions



Rings

Ligand PEB cg 201



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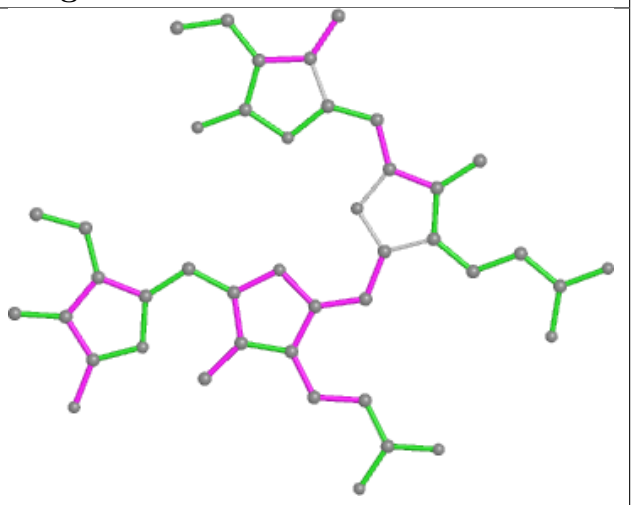

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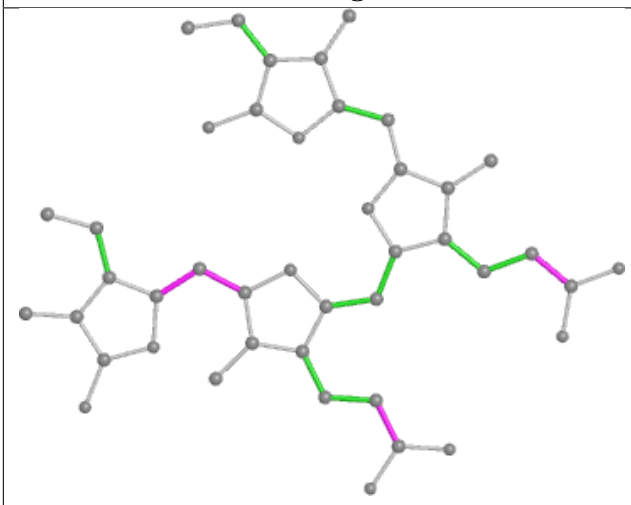
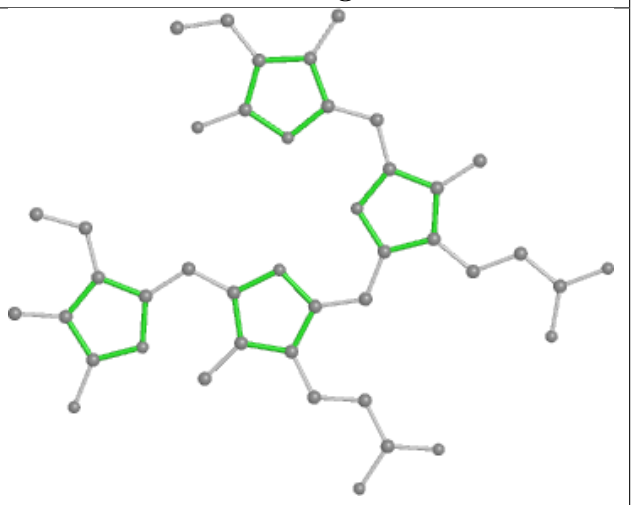
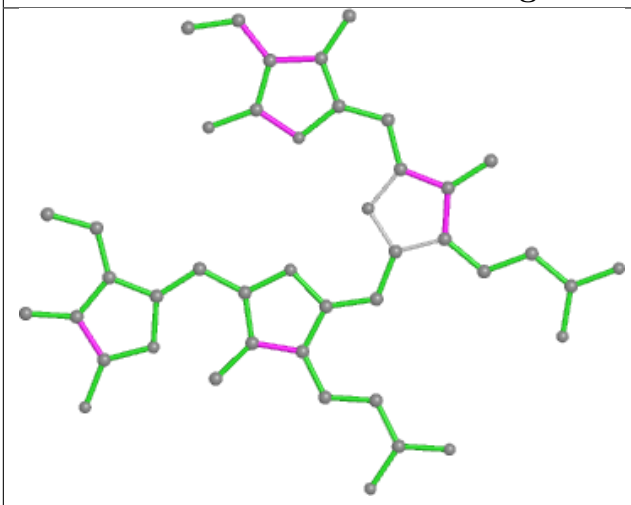


Torsions



Rings

Ligand PEB x3 202



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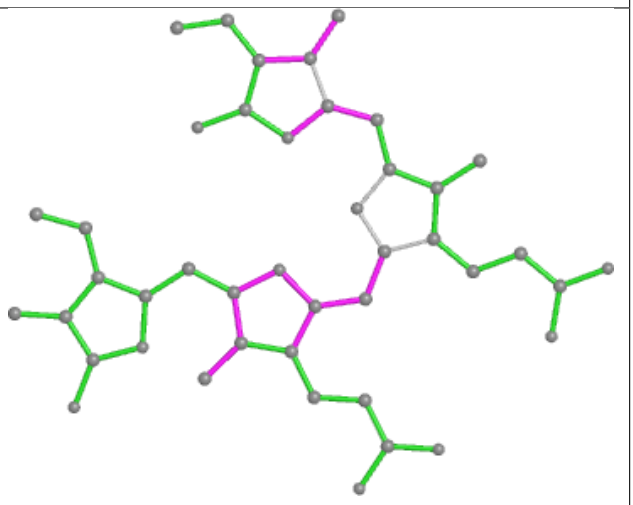
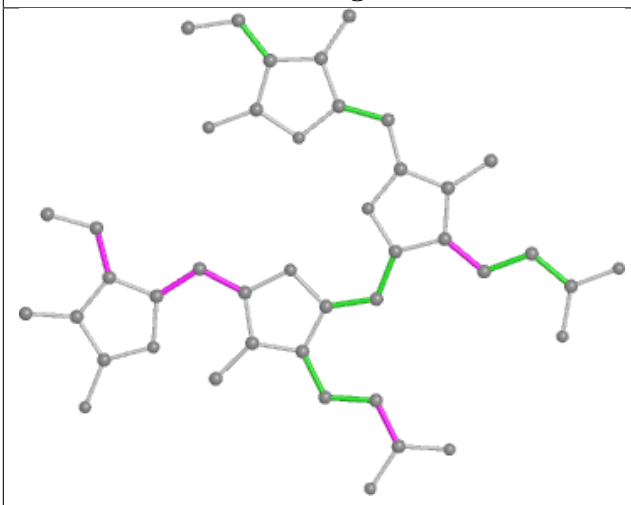


Bond angles



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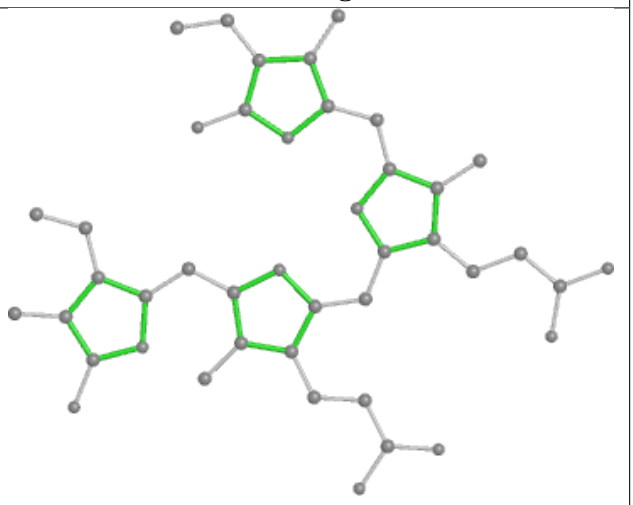
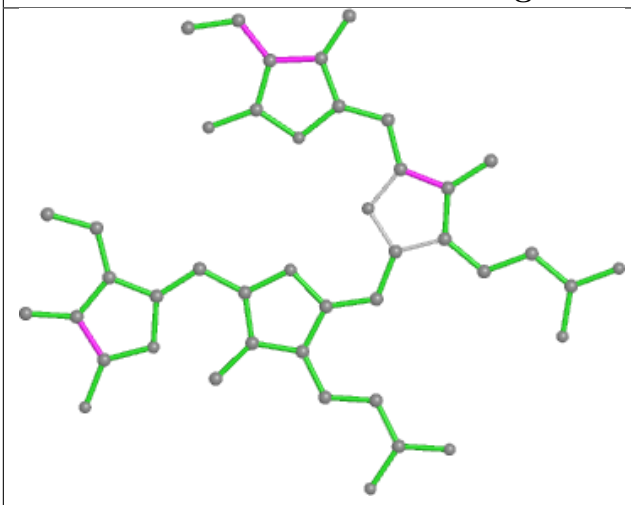


Rings

Ligand PEB N6 202



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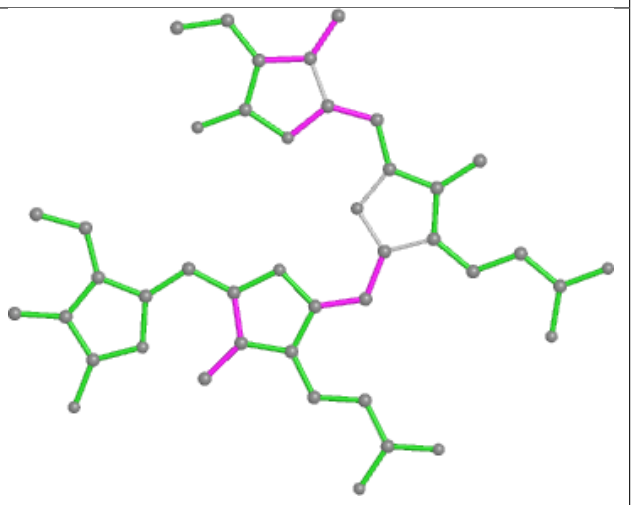

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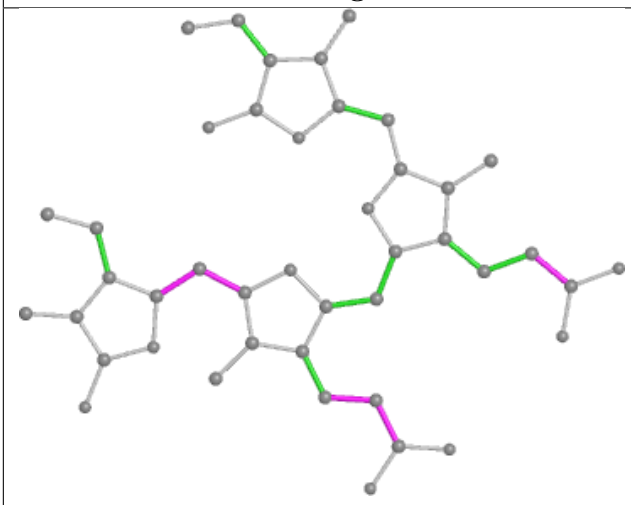

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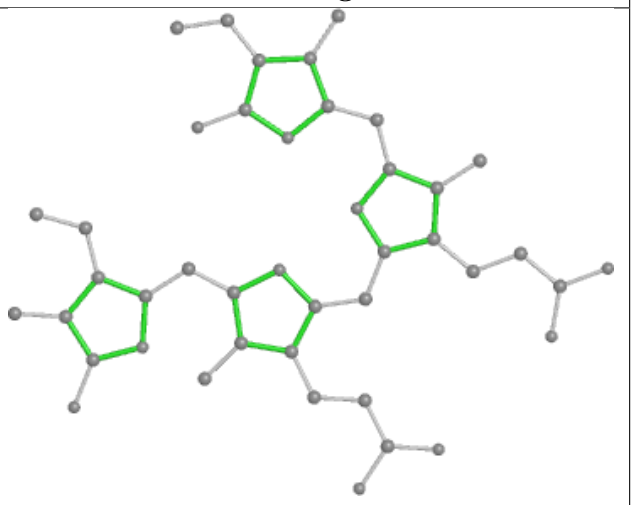
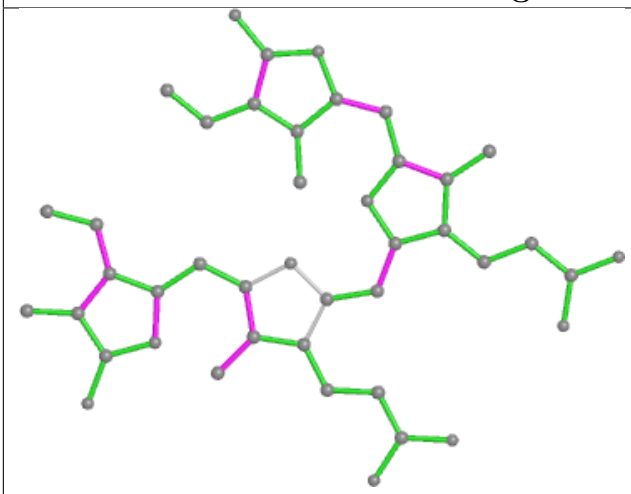


Rings

Ligand PVN aY 403



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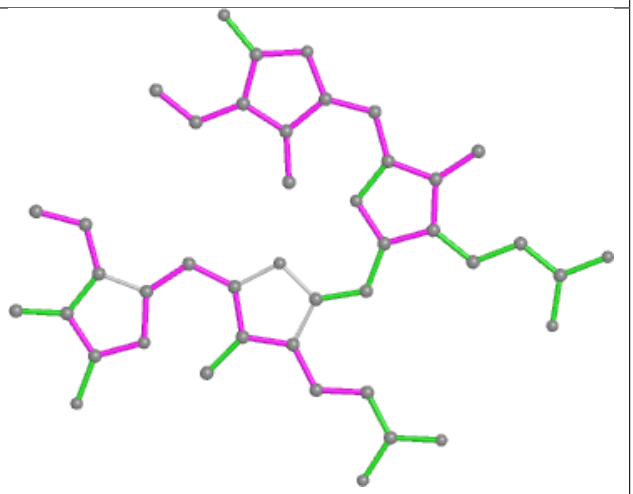
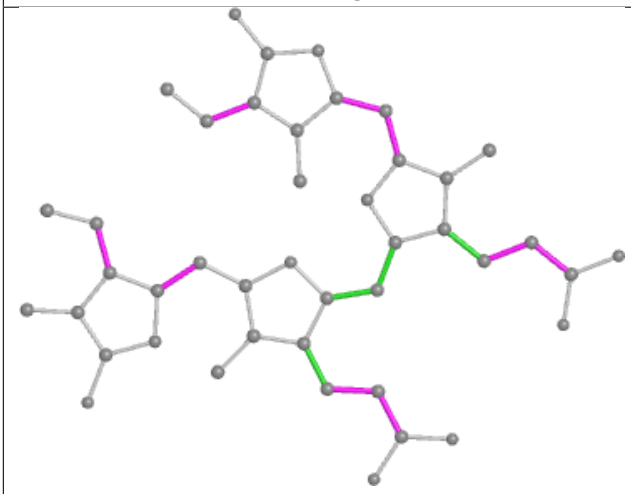


Bond angles



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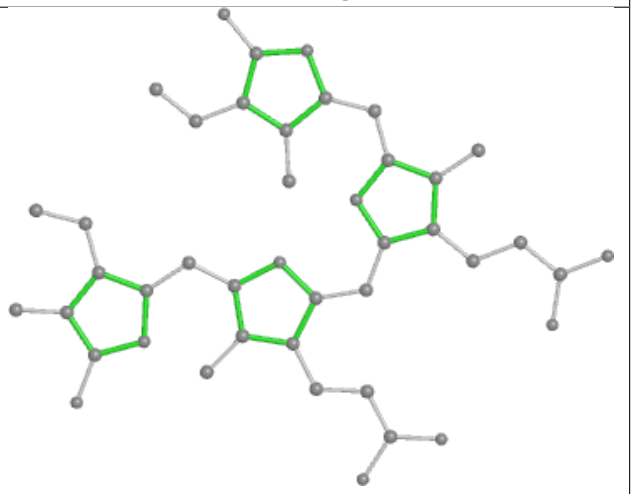
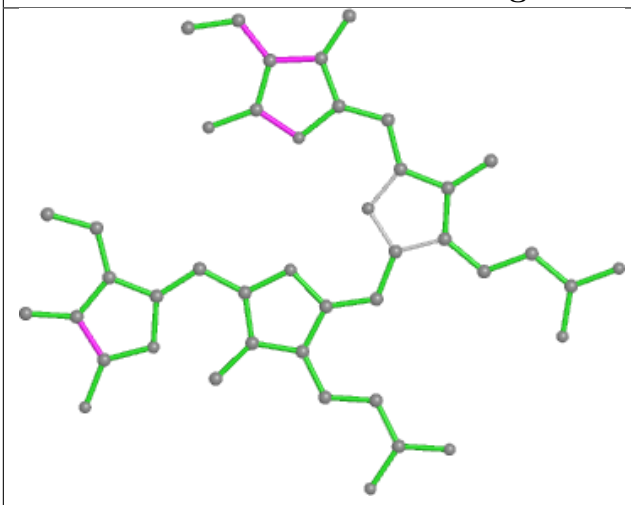


Rings

Ligand PEB dW 201



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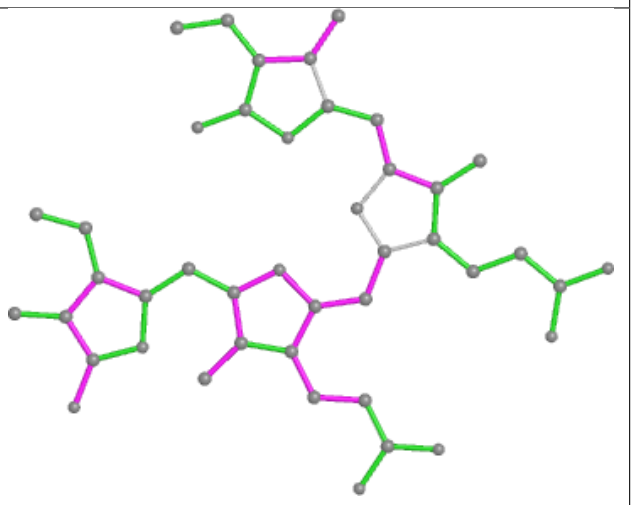

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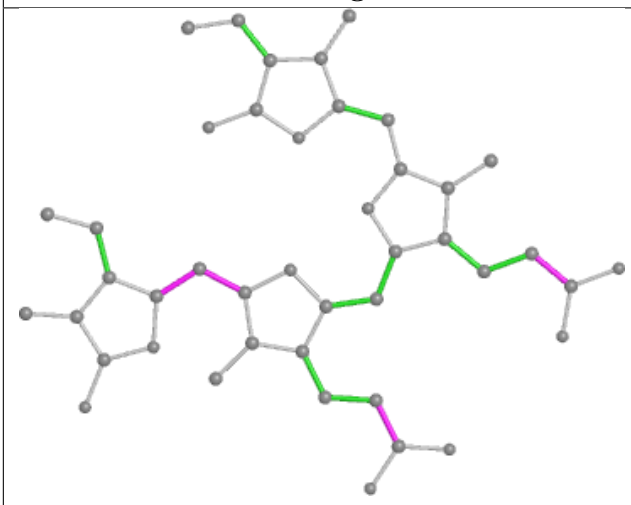

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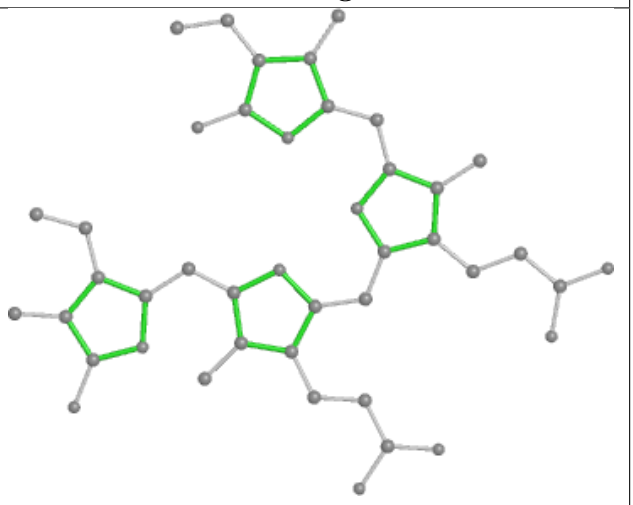

Rings

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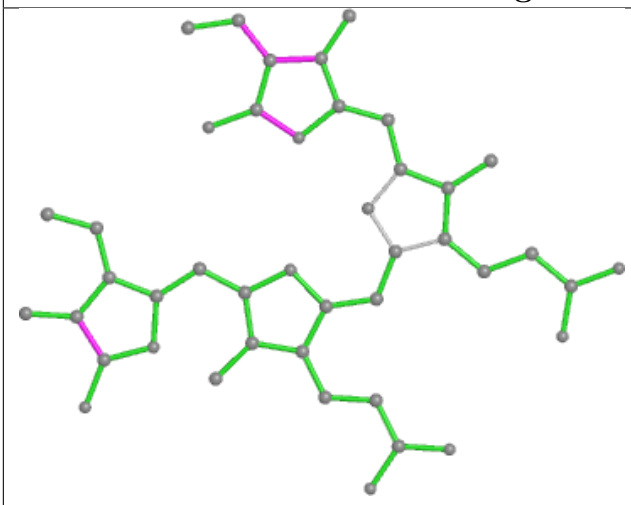

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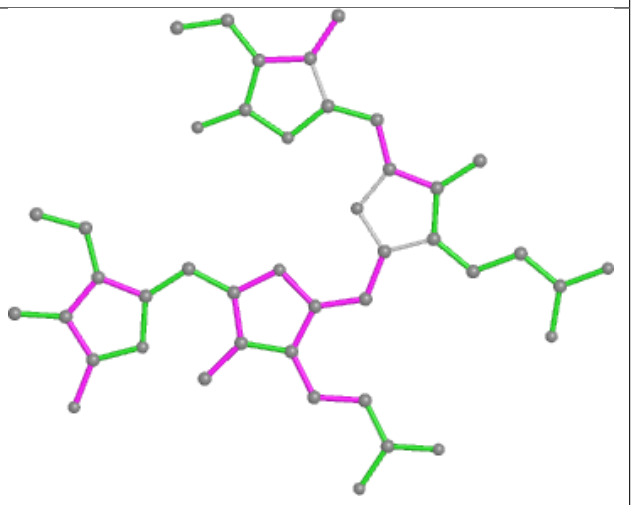

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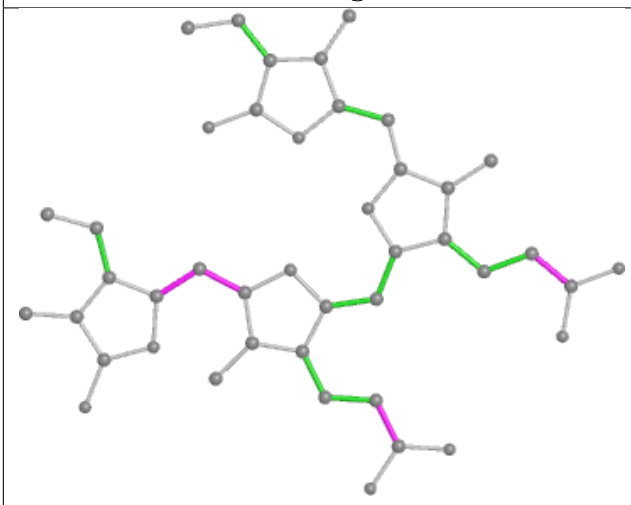

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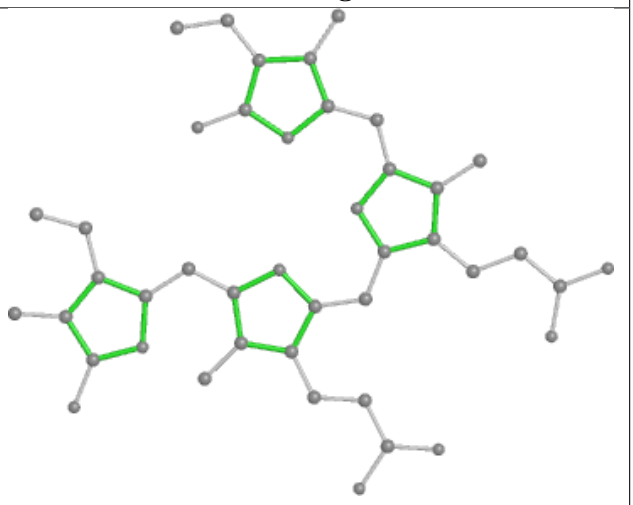

Rings

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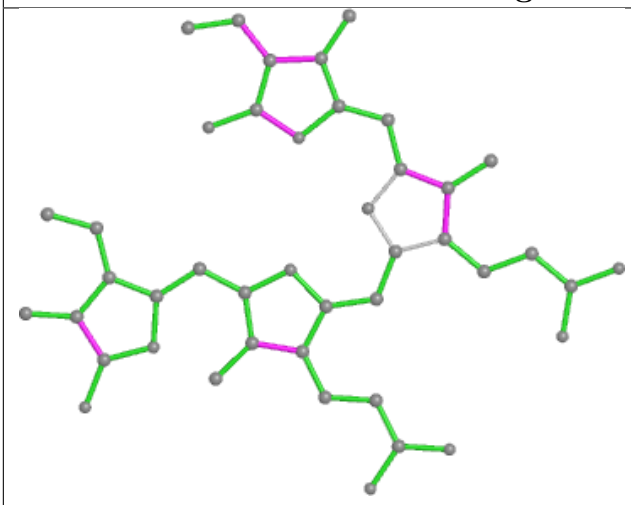

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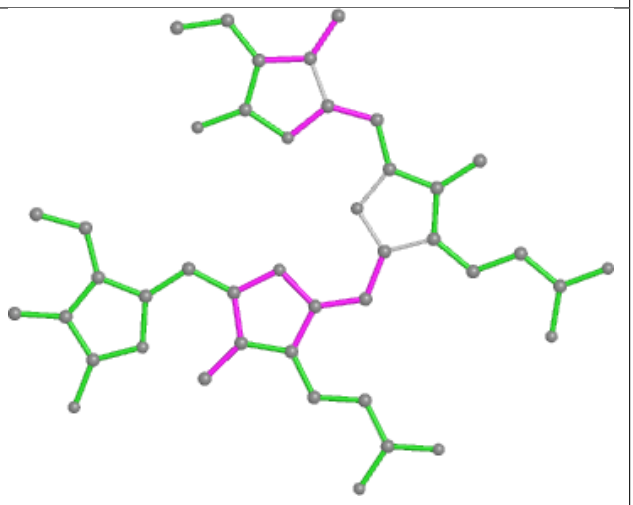

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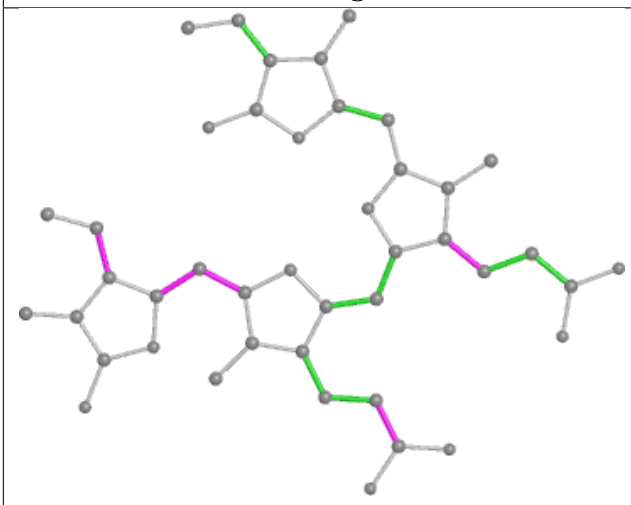

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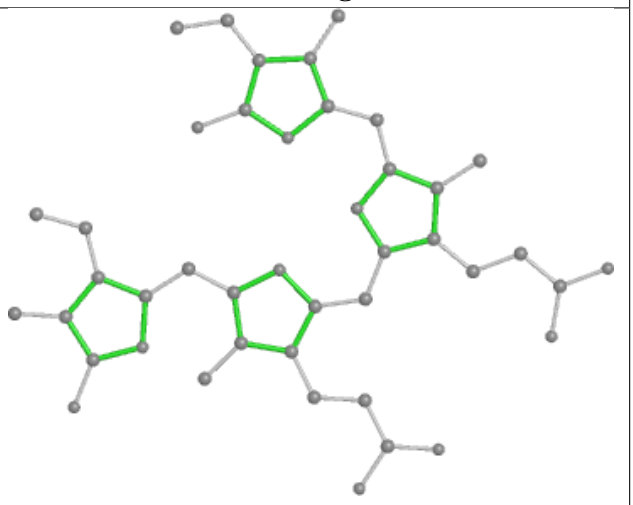
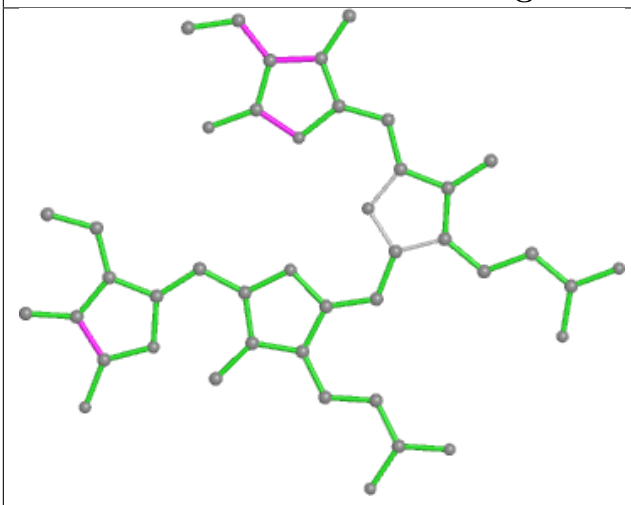


Rings

Ligand PEB C2 302



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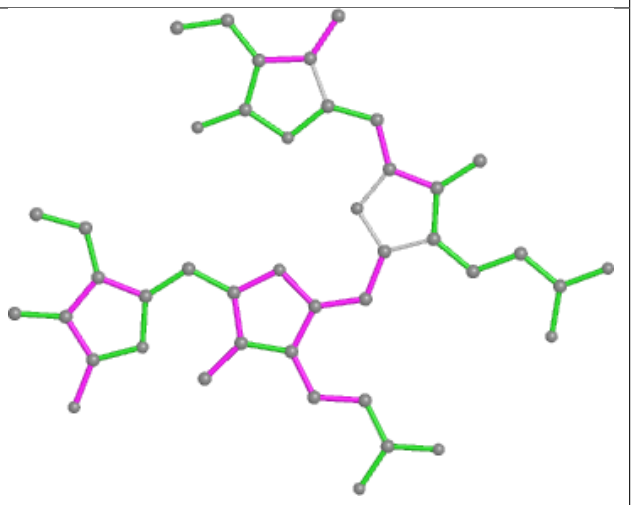
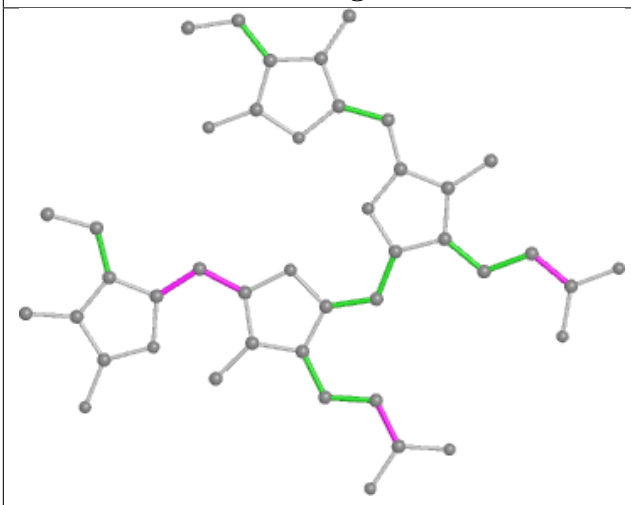


Bond angles



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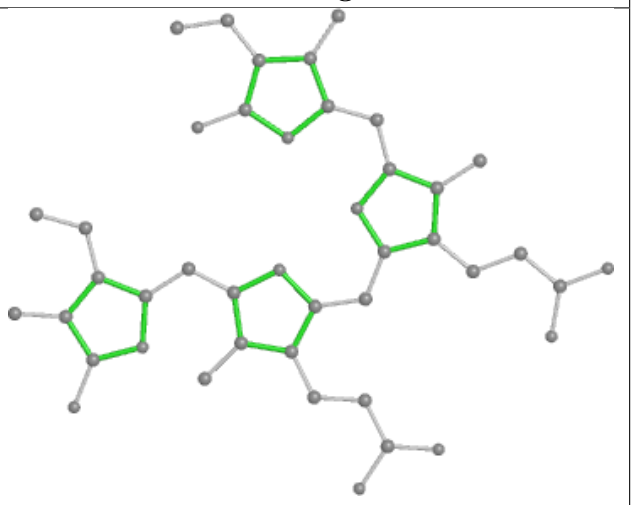

Rings

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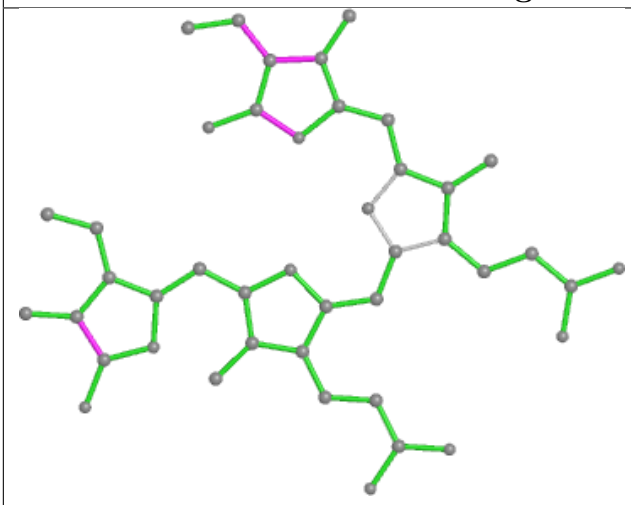

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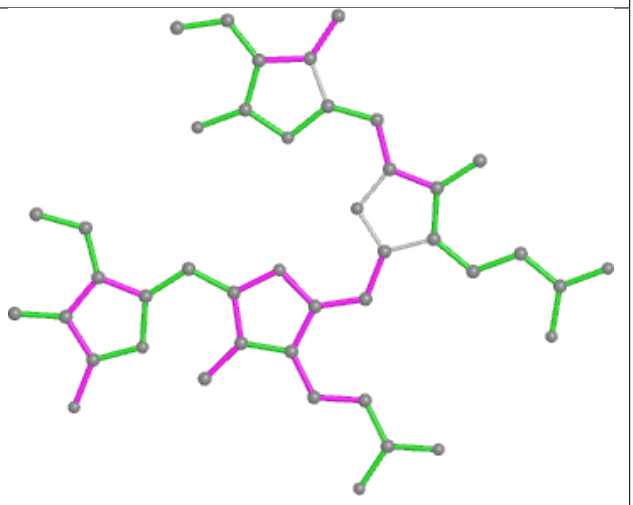

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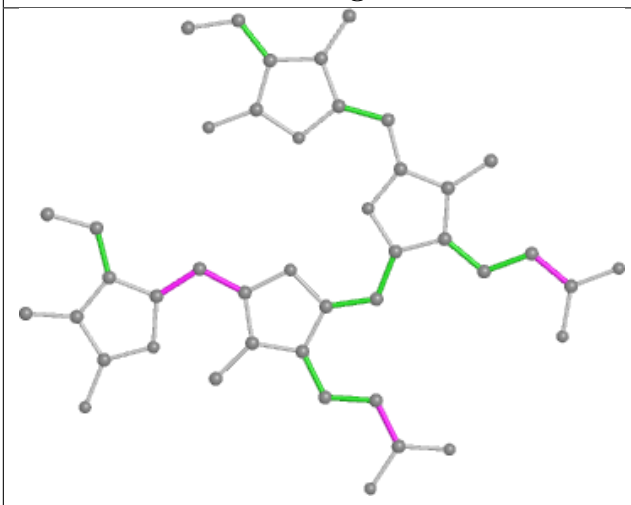

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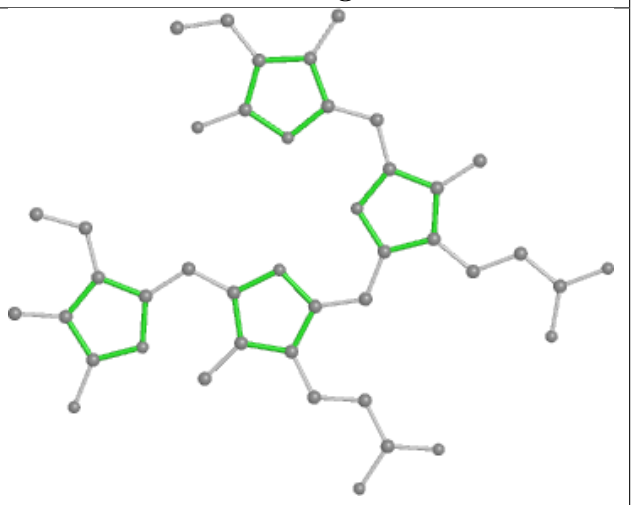
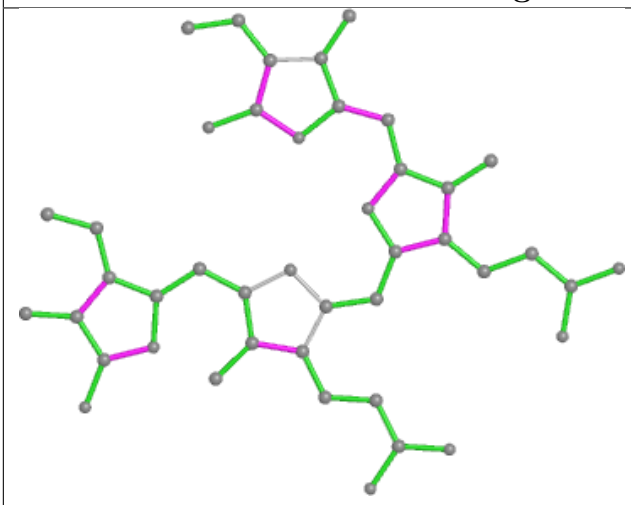


Rings

Ligand PUB V5 203



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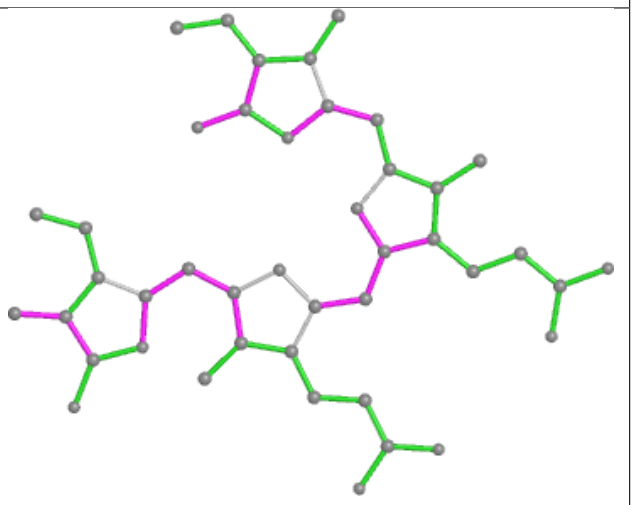

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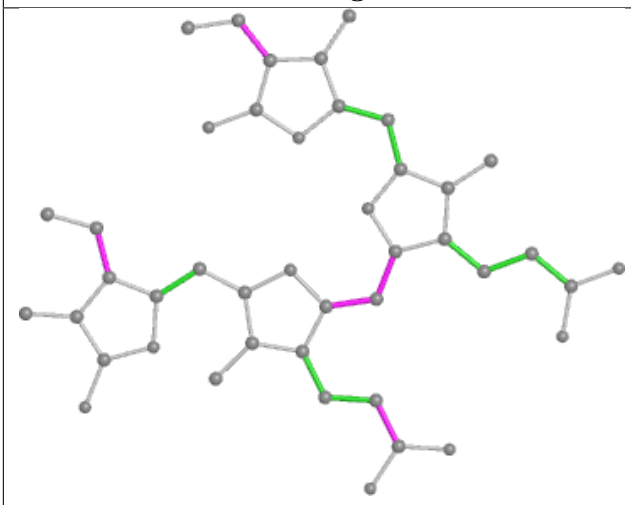

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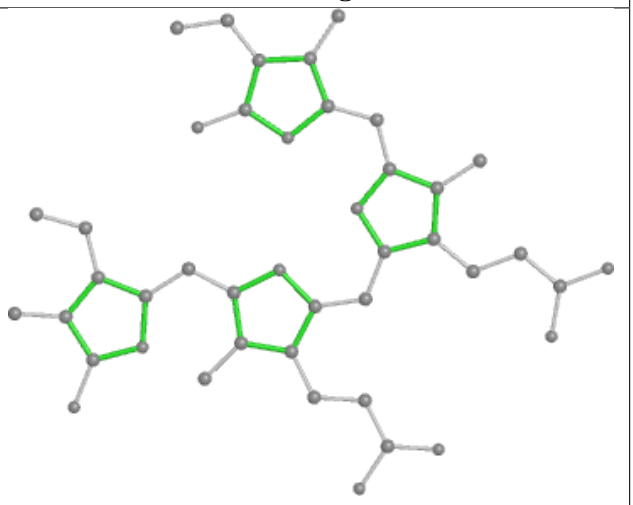
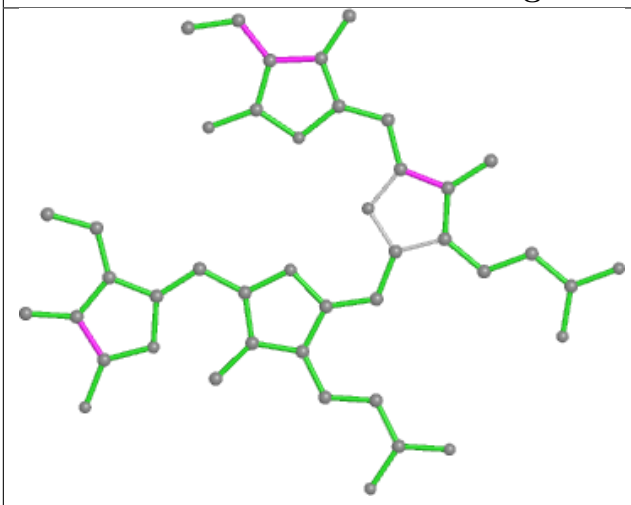


Rings

Ligand PEB lo 202



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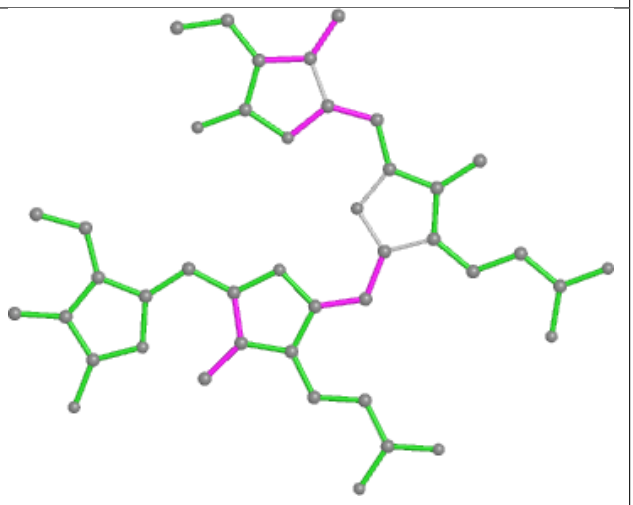

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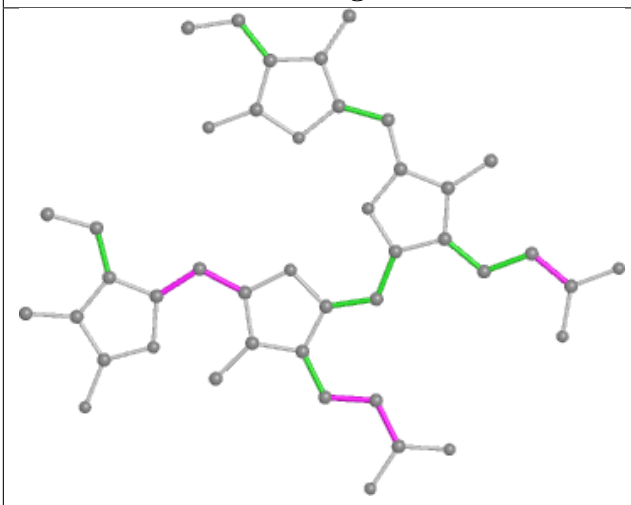

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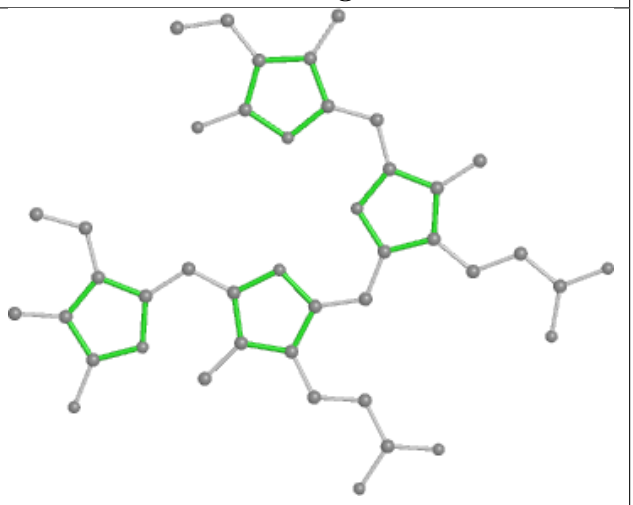

Rings

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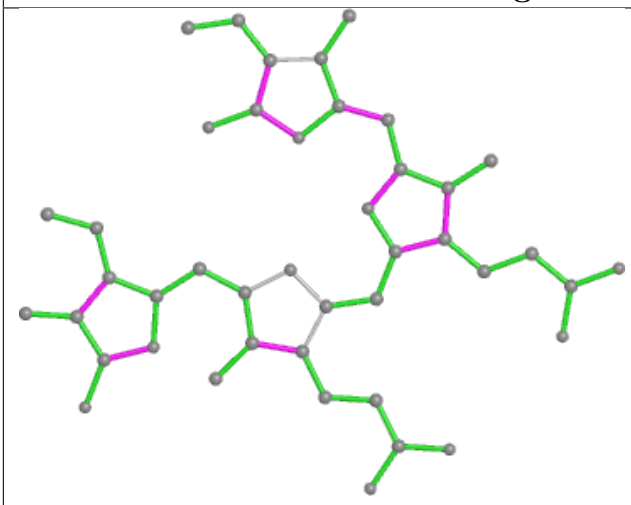

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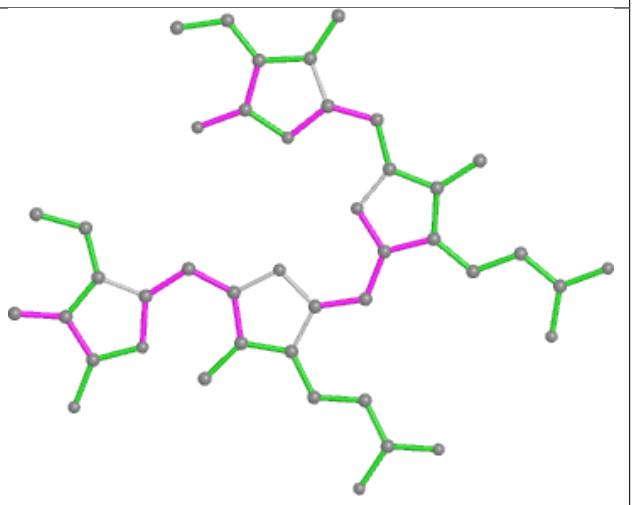

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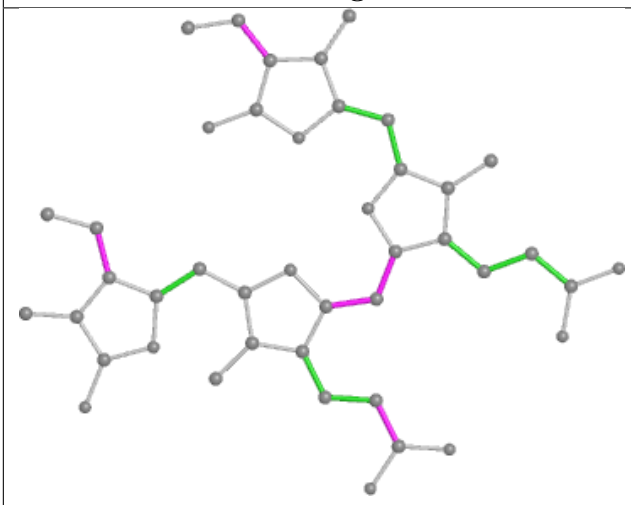

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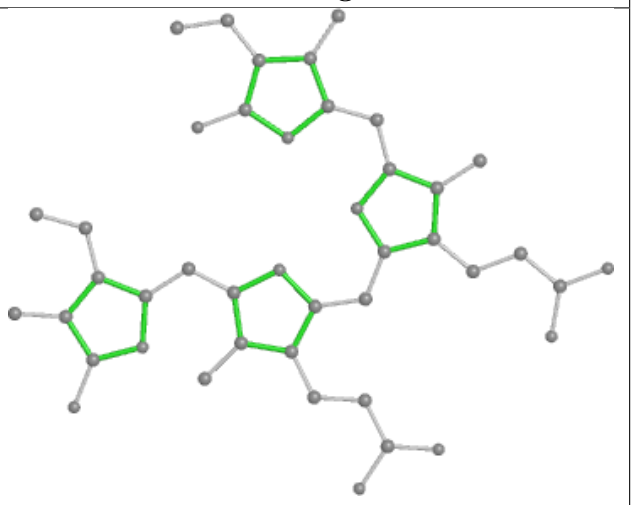
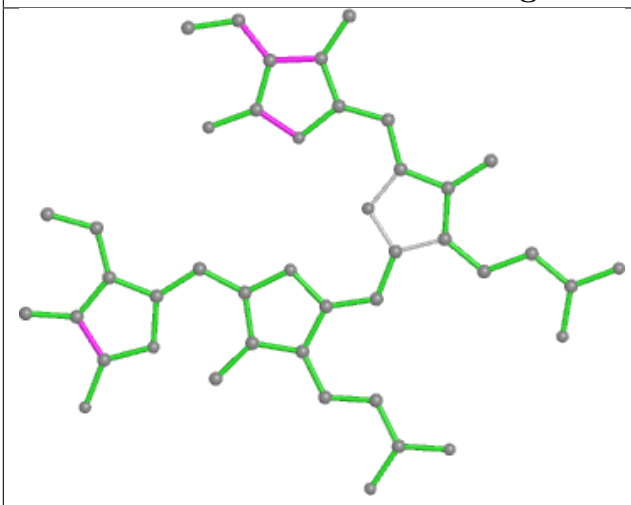


Rings

Ligand PEB dc 203



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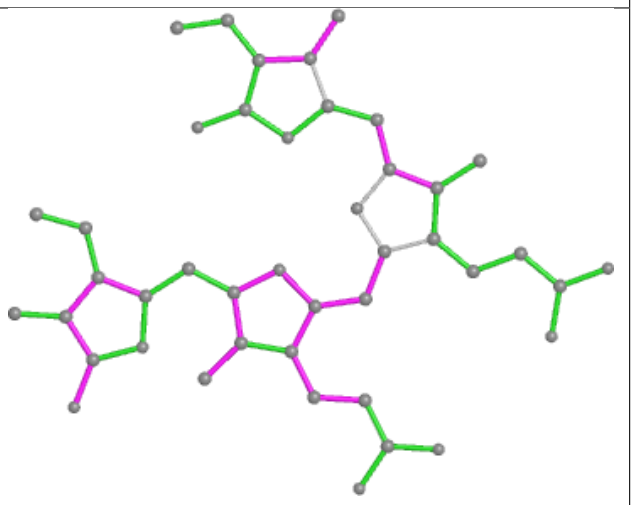

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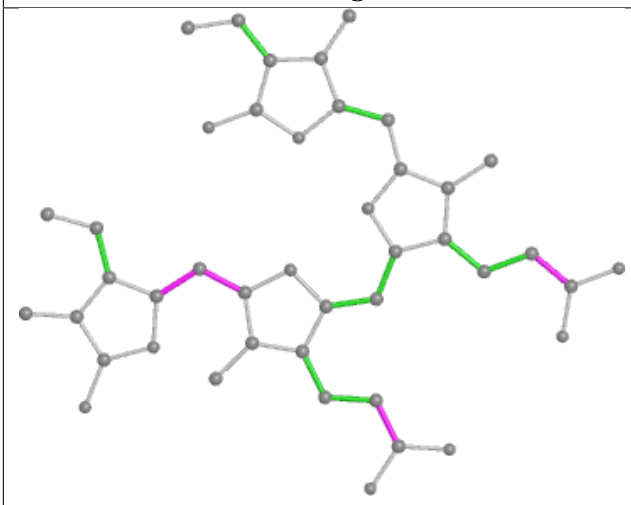
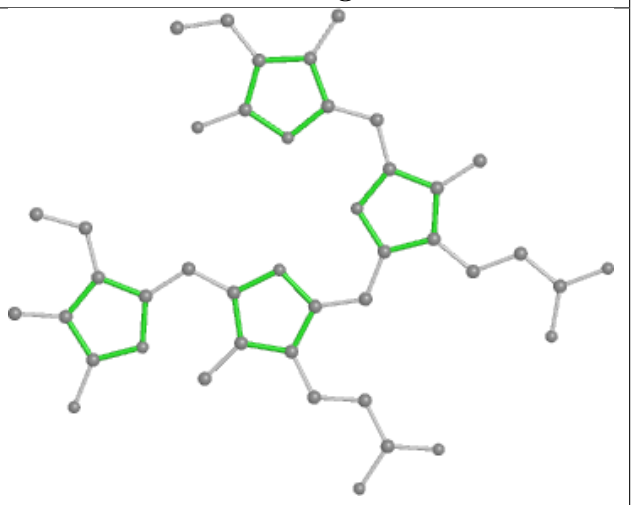
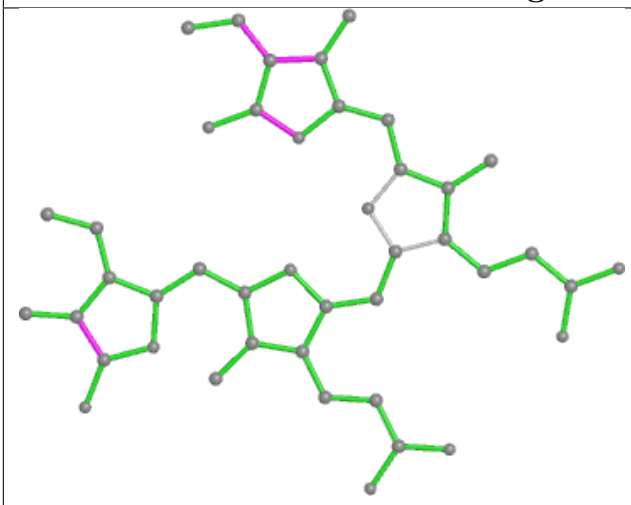


Torsions



Rings

Ligand PEB ff 201



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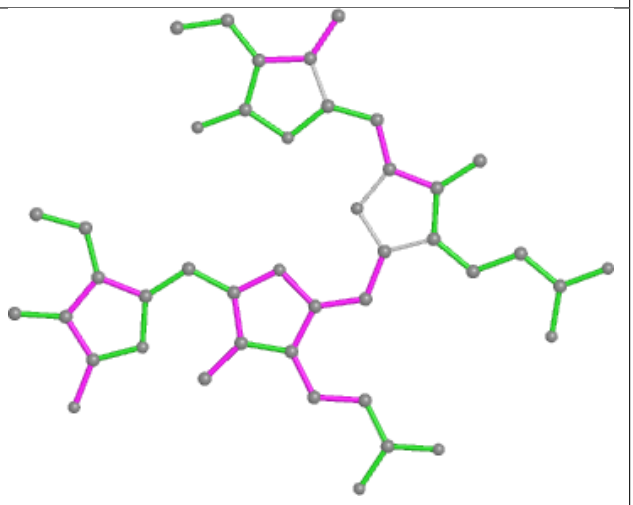

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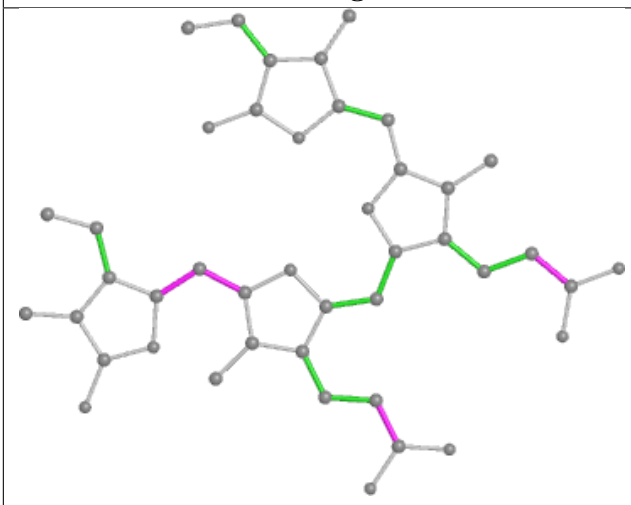

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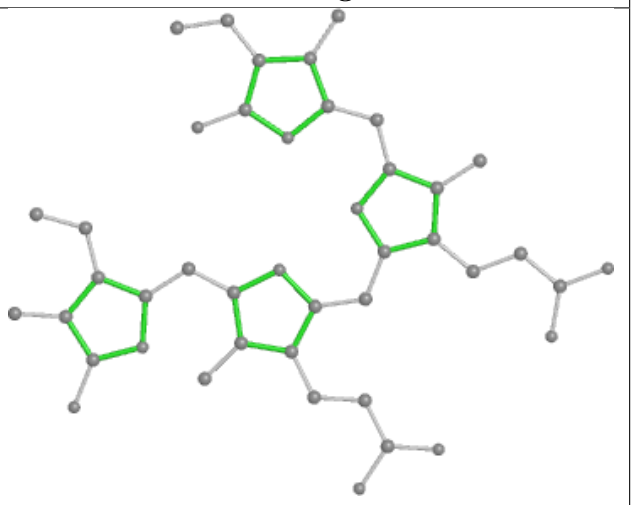
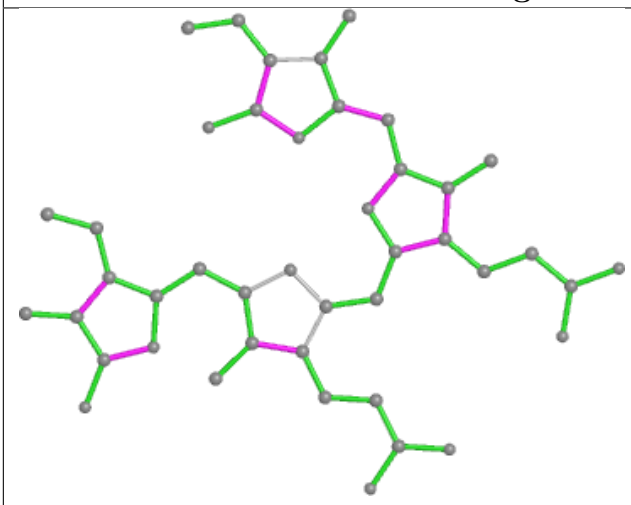


Rings

Ligand PUB R5 203



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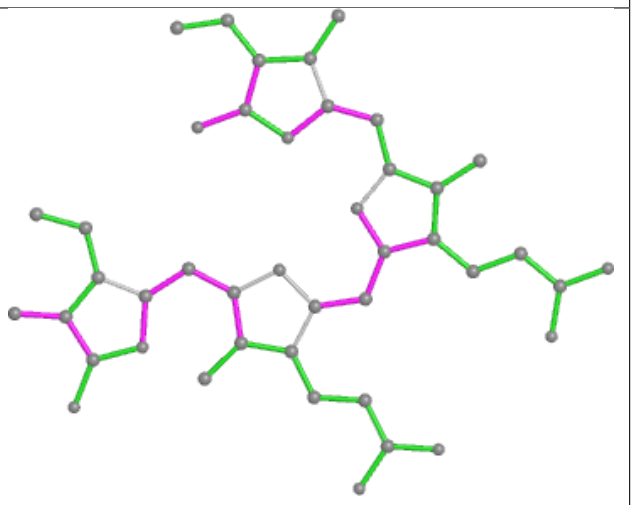

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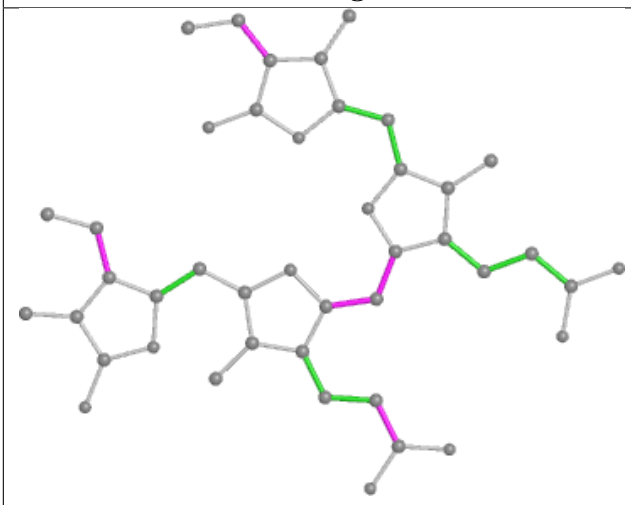

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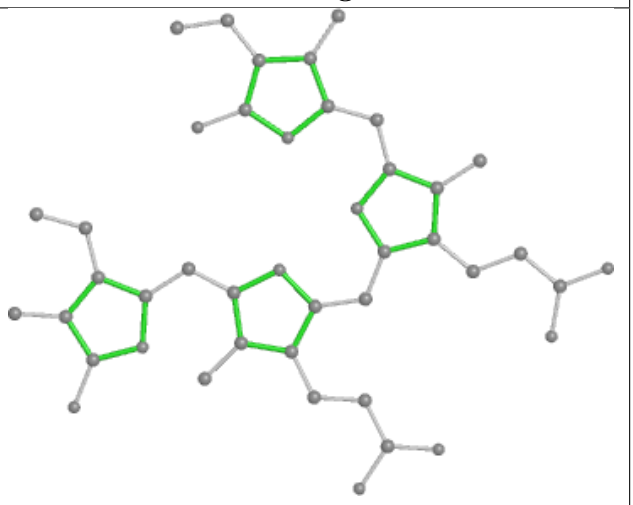

Rings

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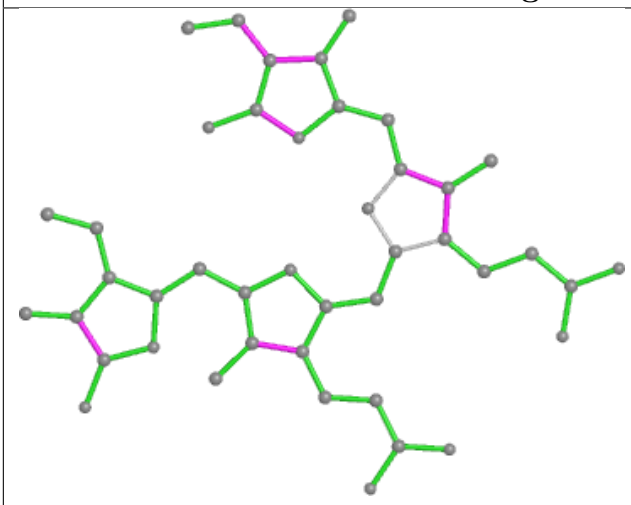

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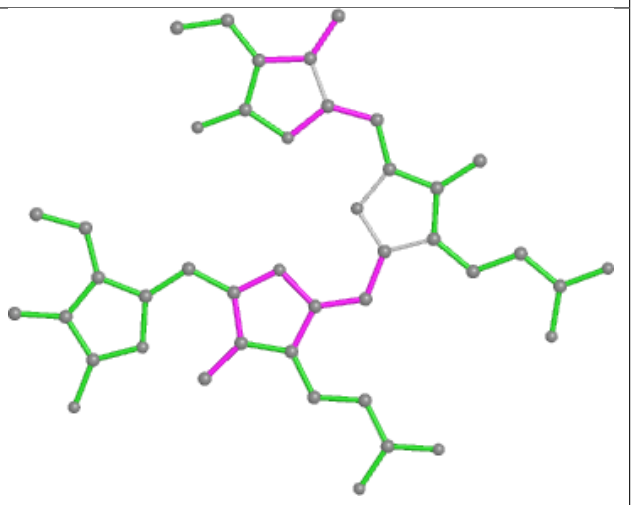

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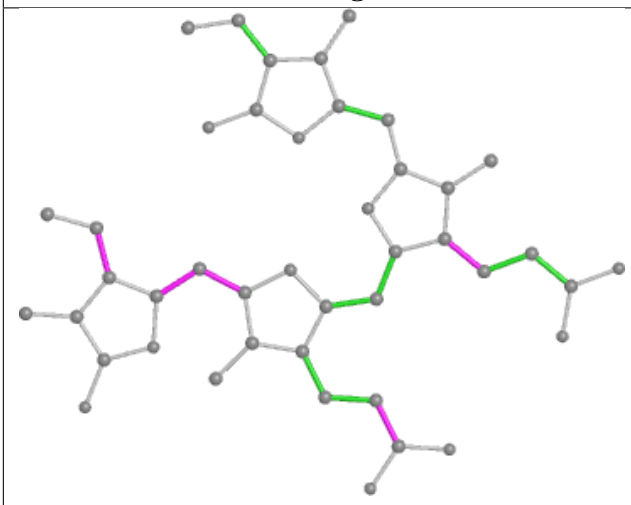

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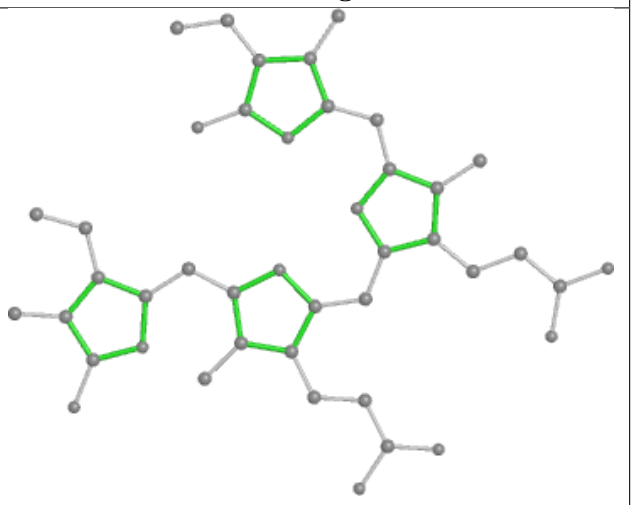
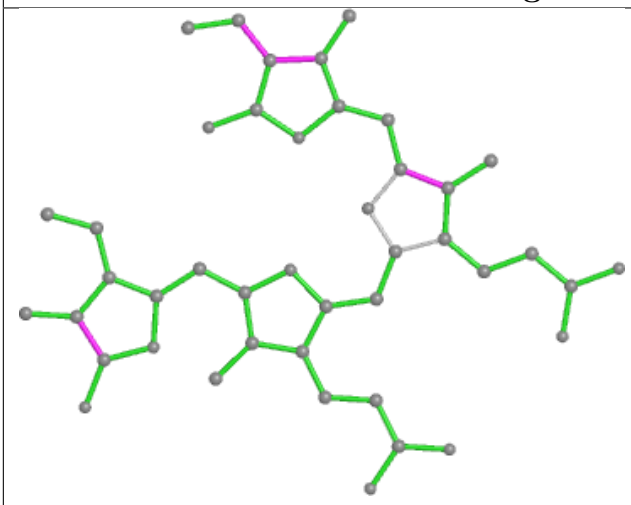


Rings

Ligand PEB f6 202



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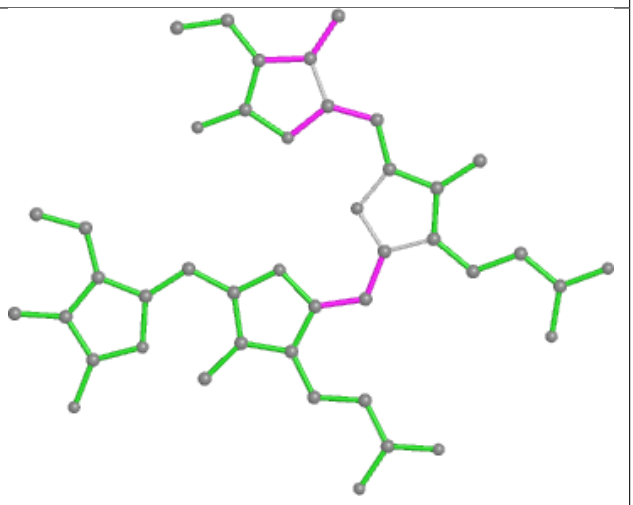

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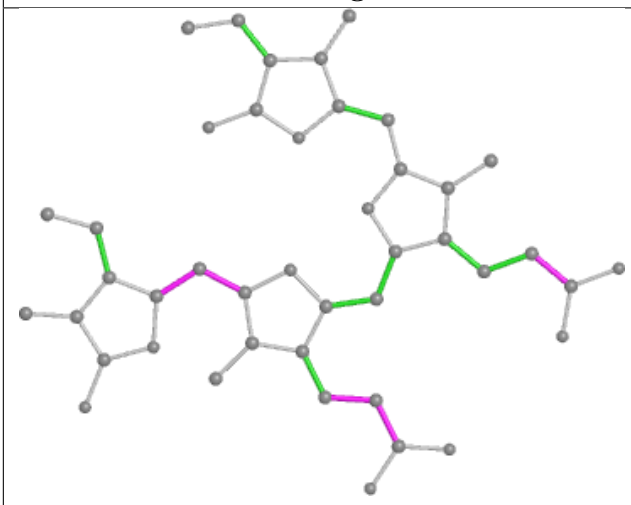

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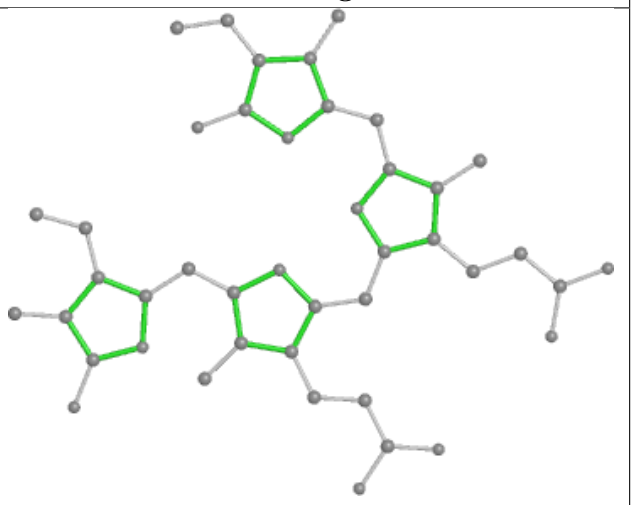
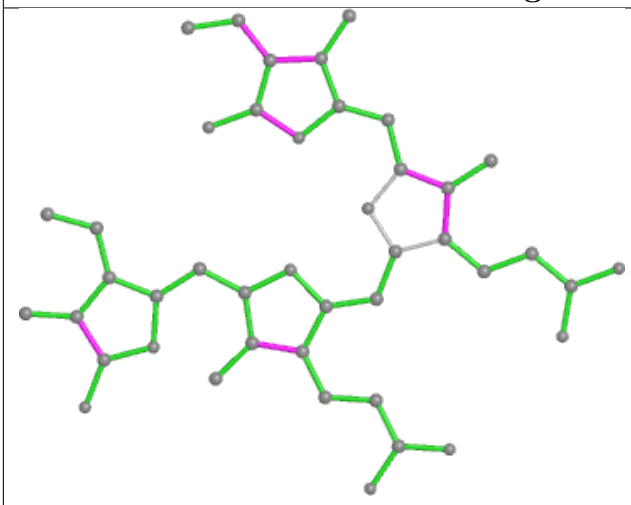


Rings

Ligand PEB al 202



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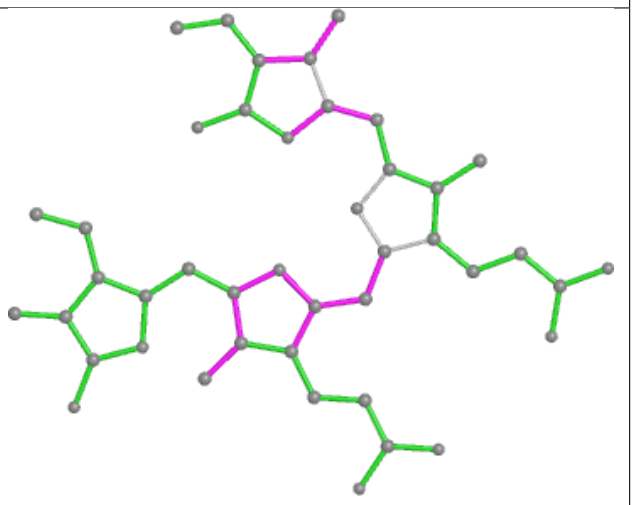

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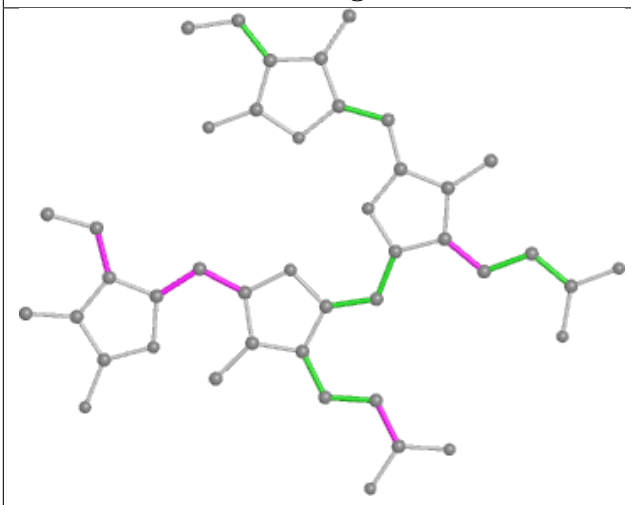

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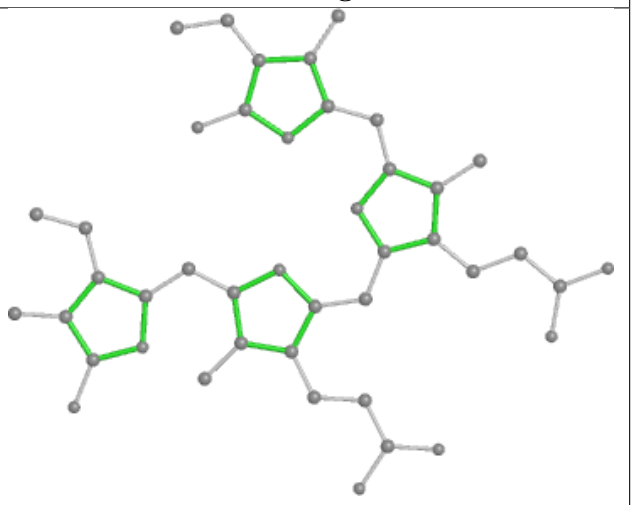

Rings

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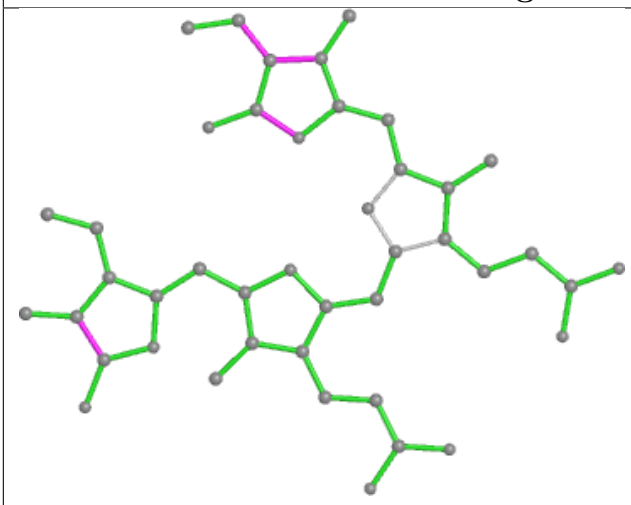

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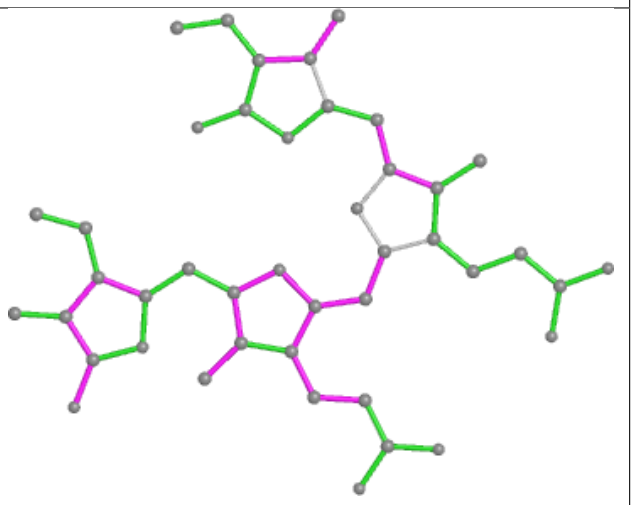

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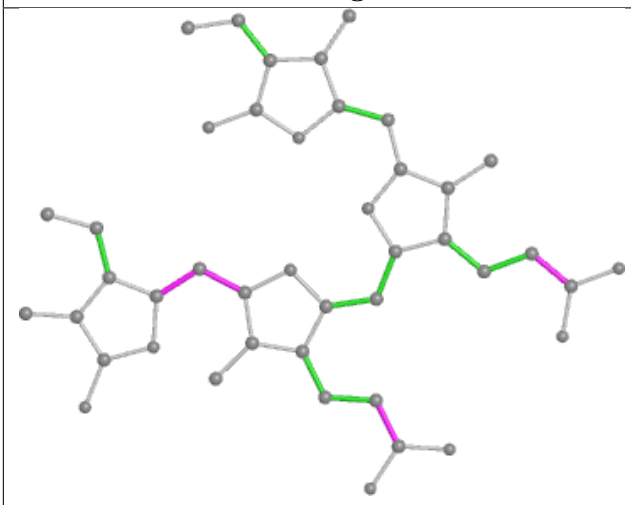

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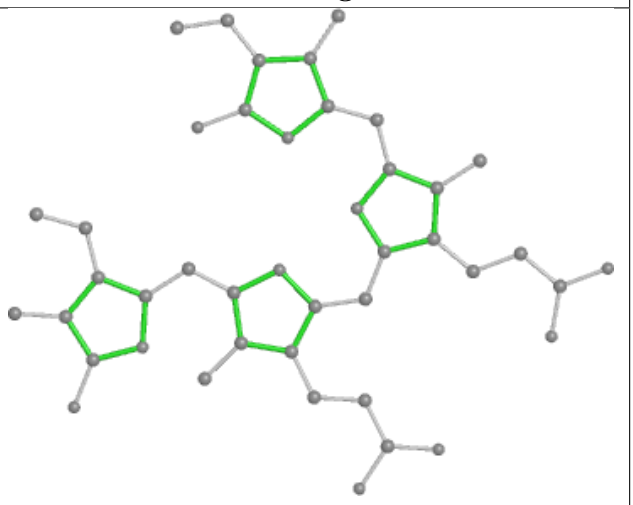

Rings

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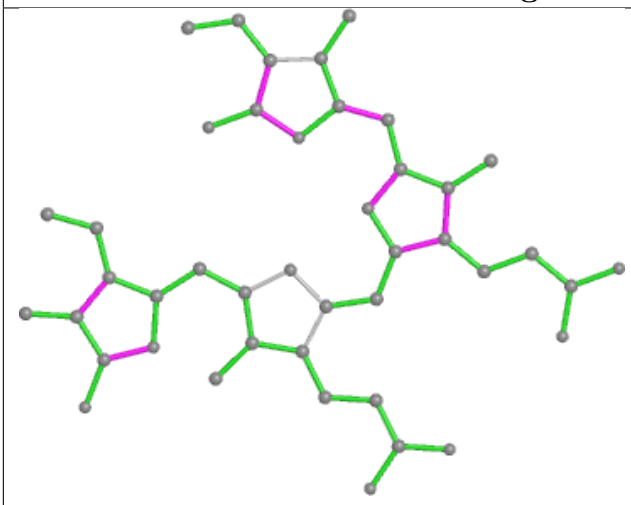

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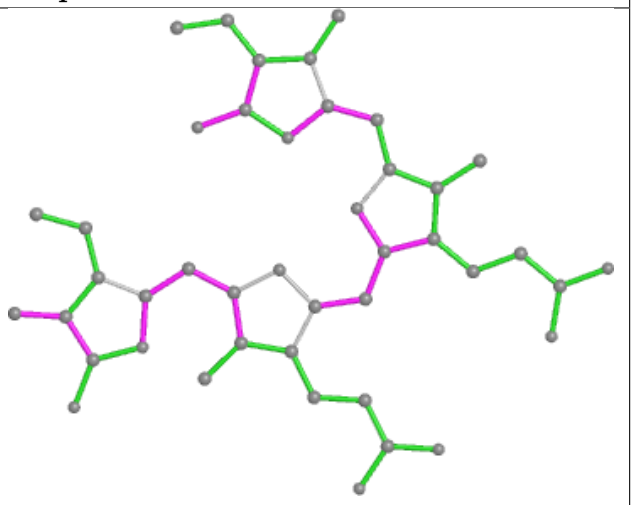

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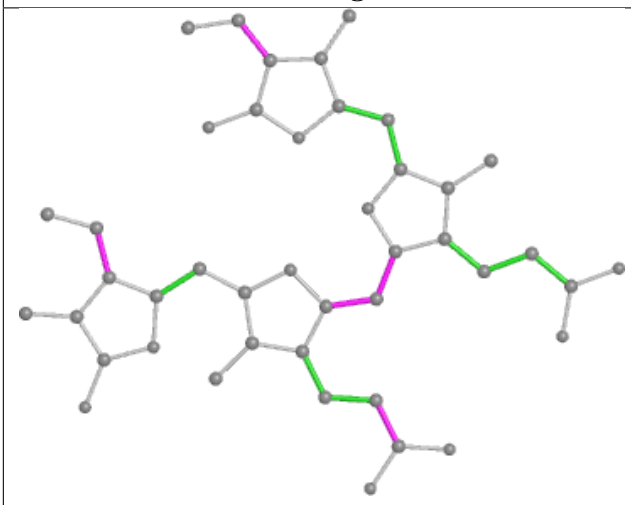

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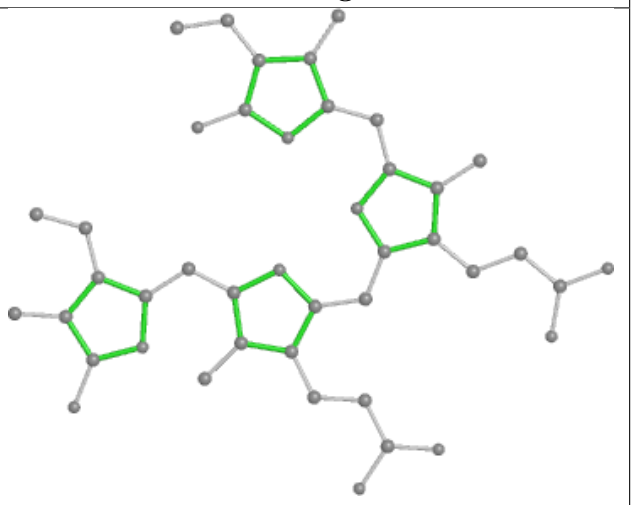

Rings

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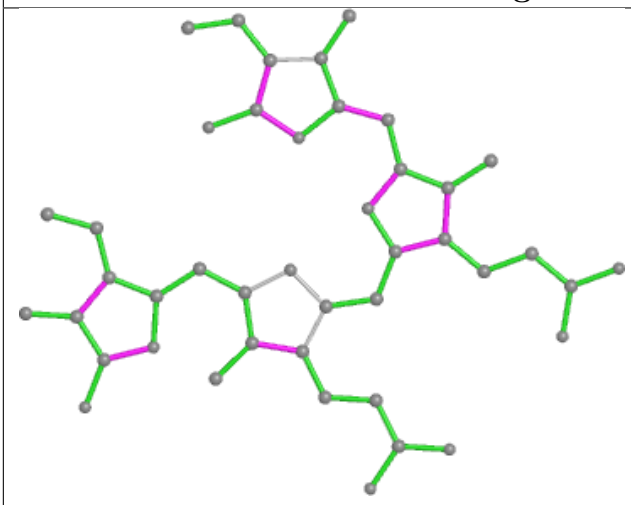

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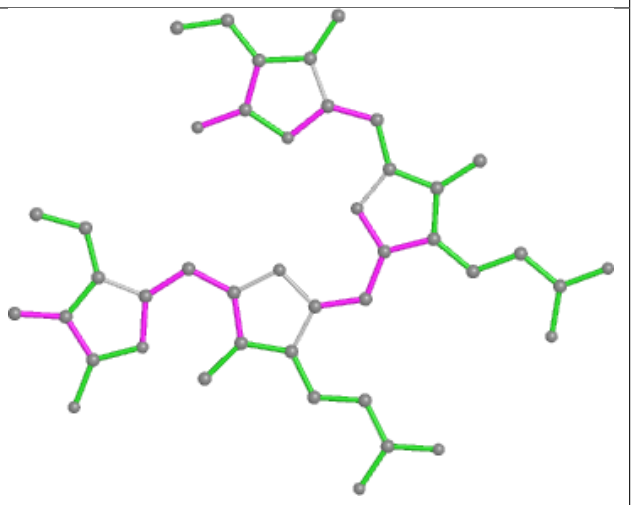

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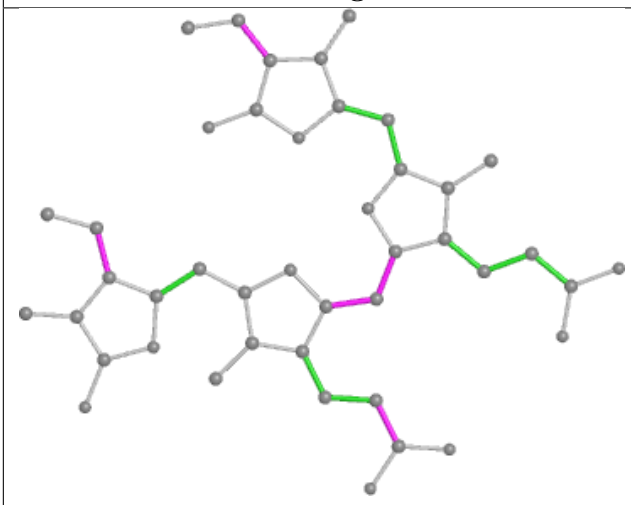

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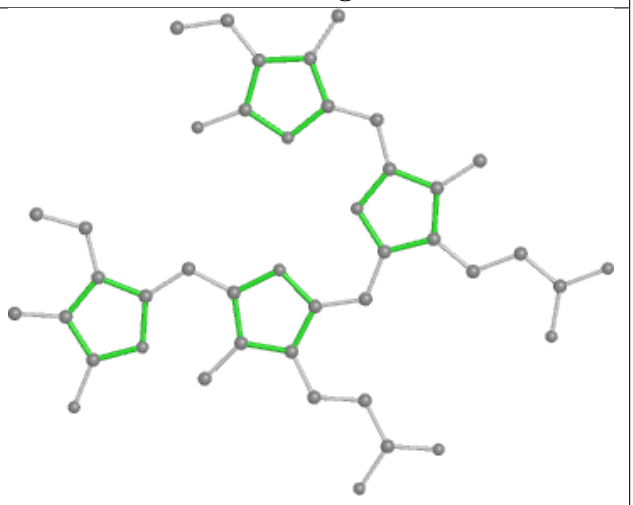

Rings

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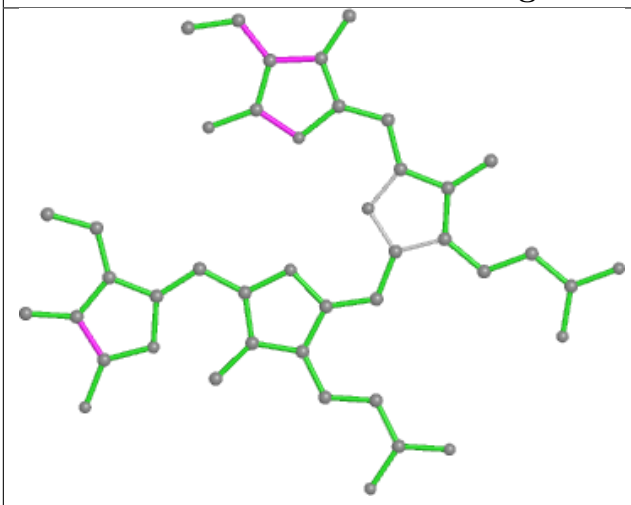

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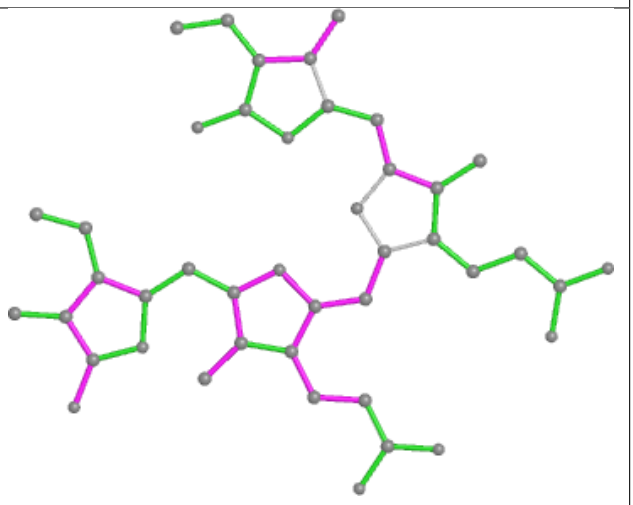

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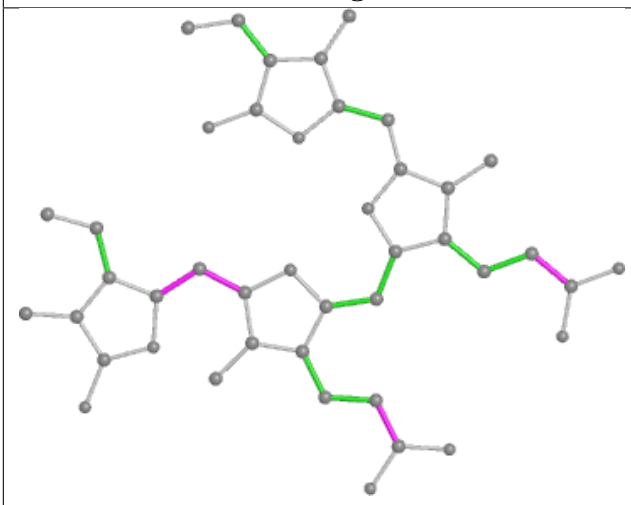

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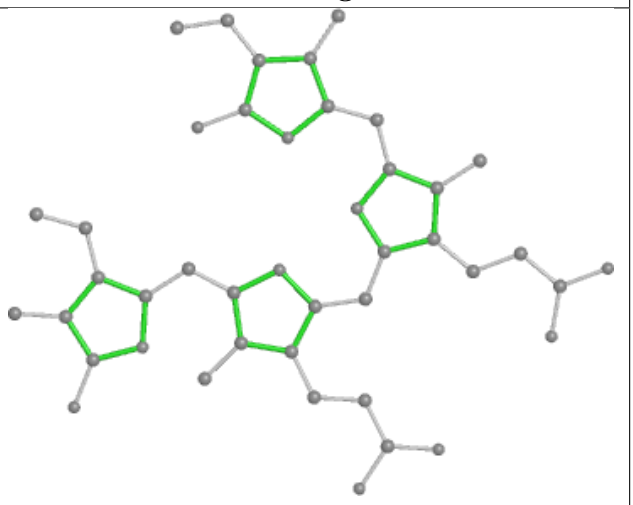
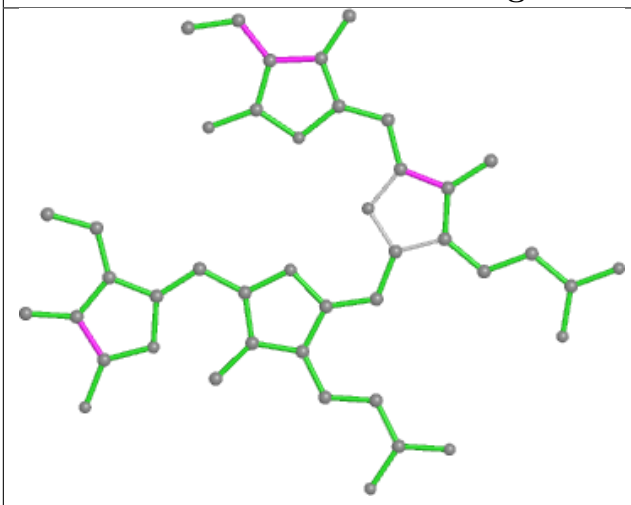


Rings

Ligand PEB dZ 1002



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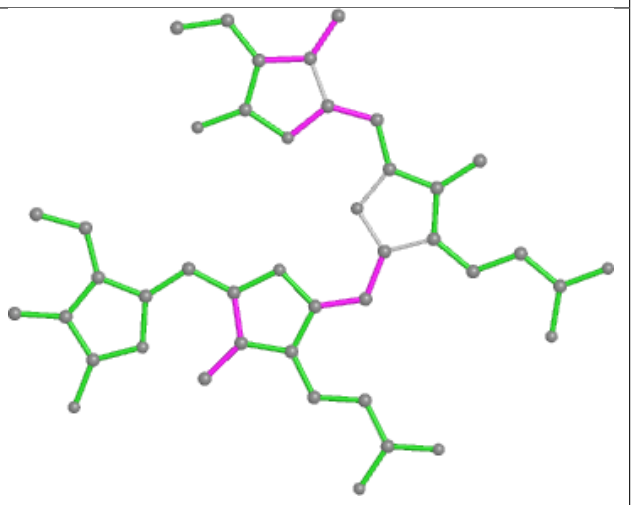

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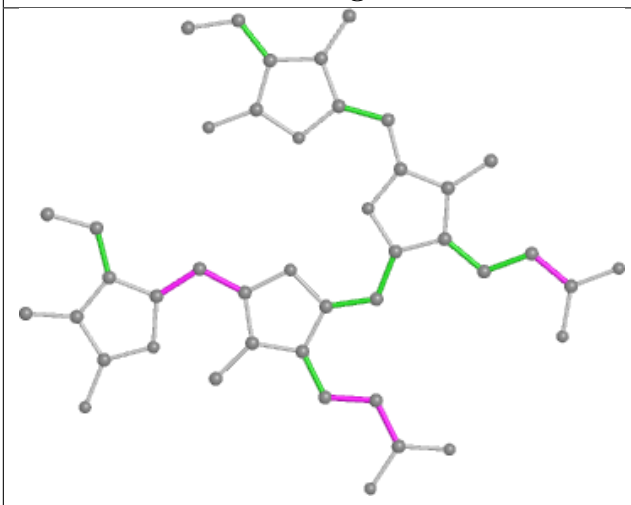

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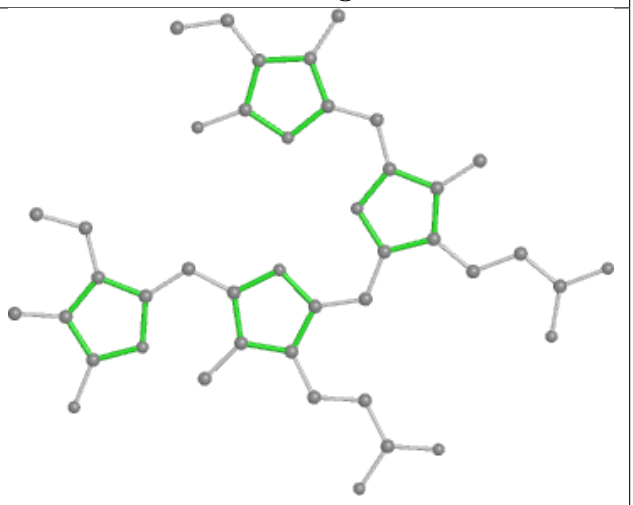

Rings

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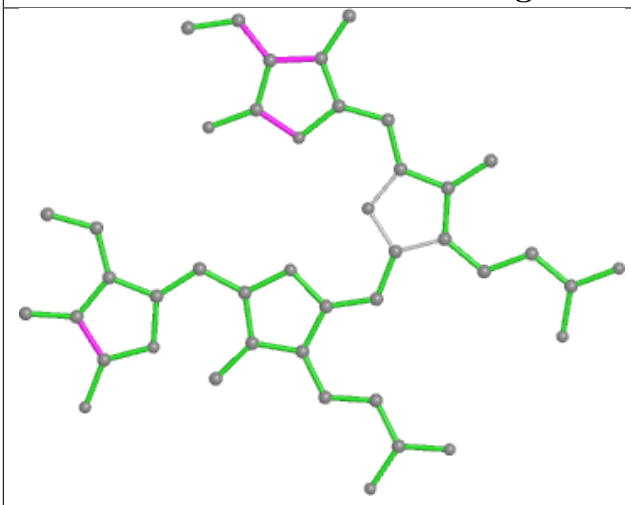

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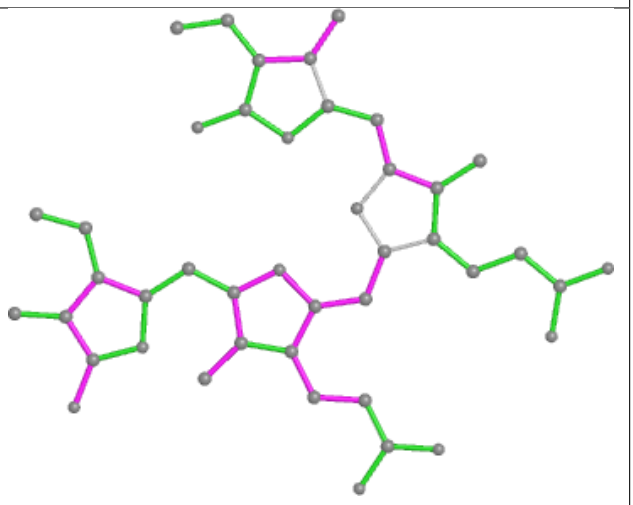

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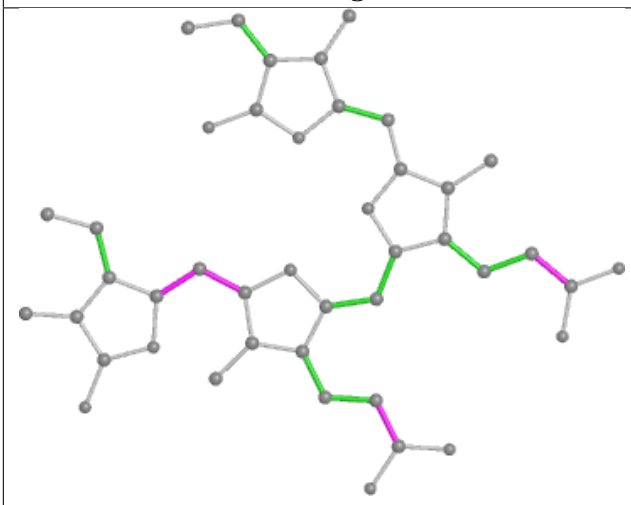

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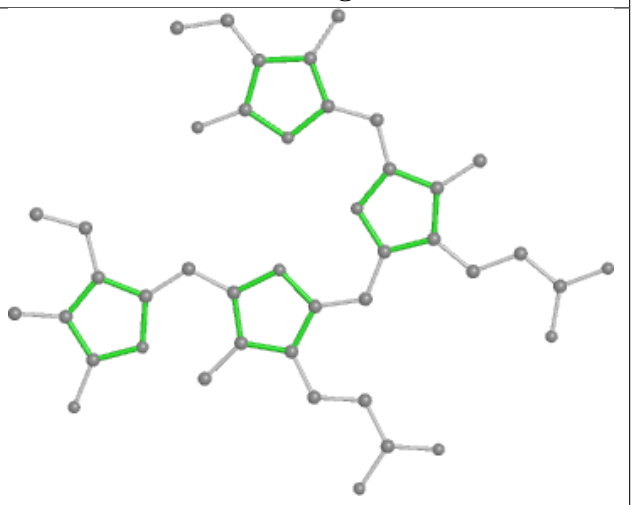
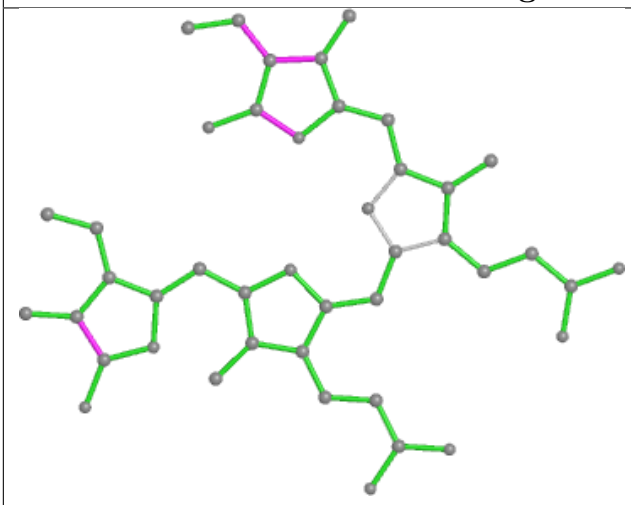


Rings

Ligand PEB d9 302



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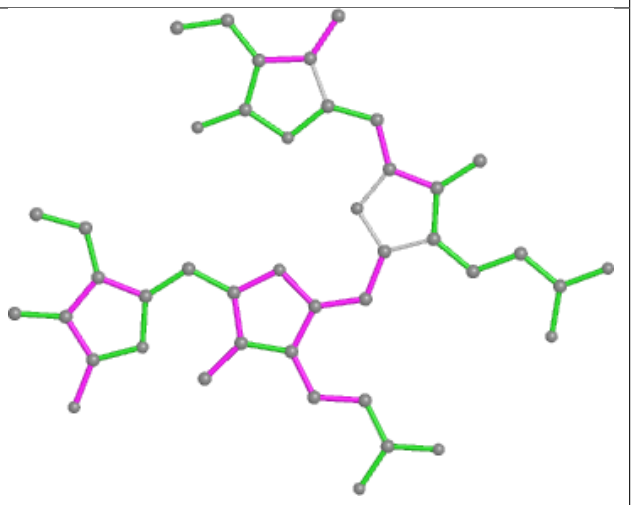

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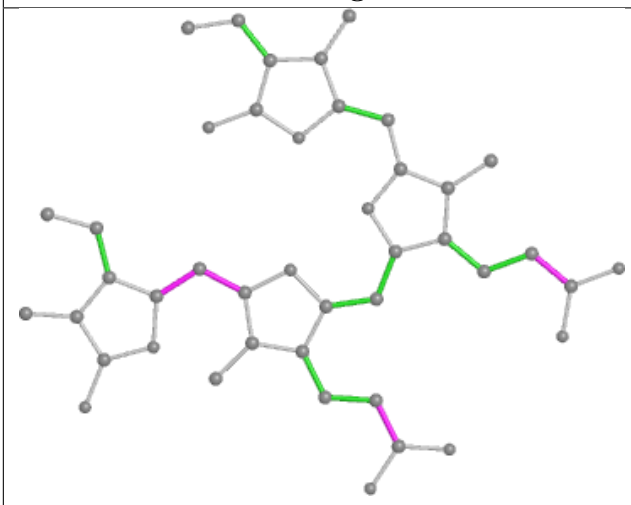

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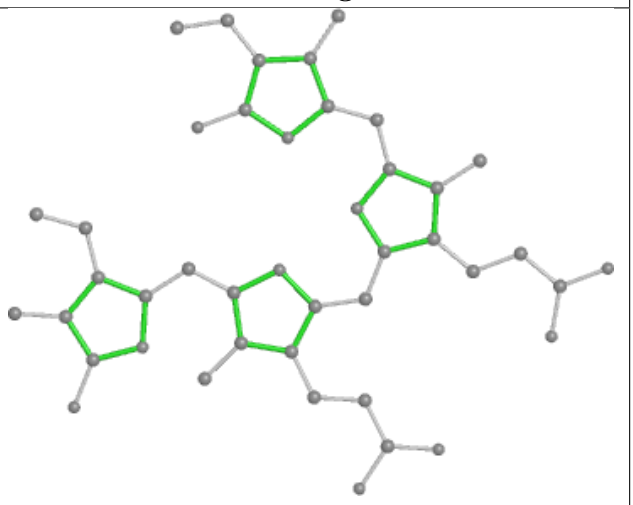
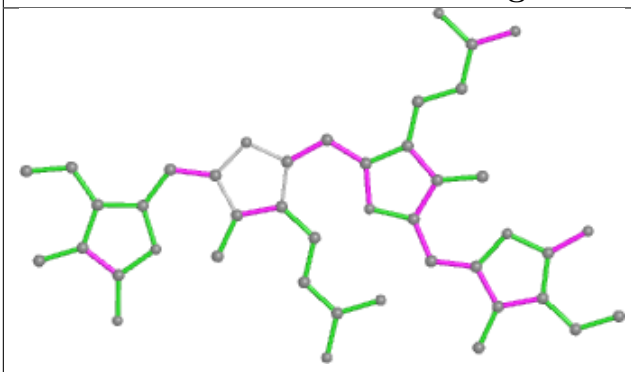


Rings

Ligand CYC o1 1001



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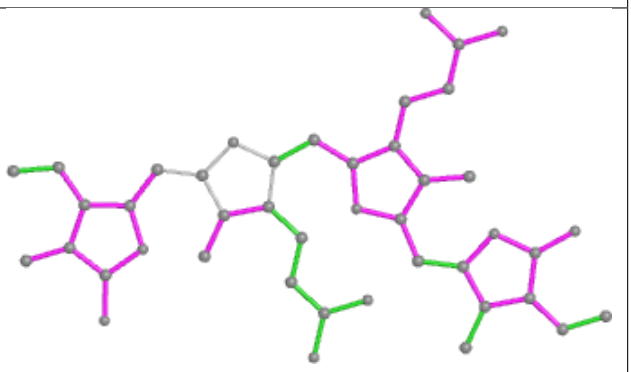

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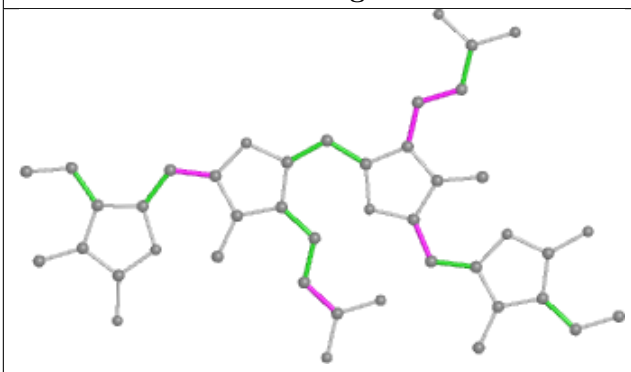

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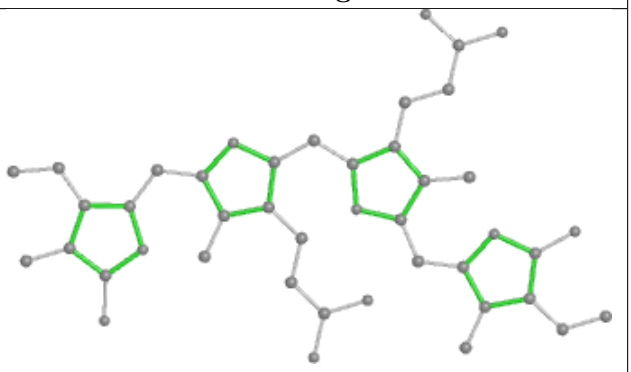
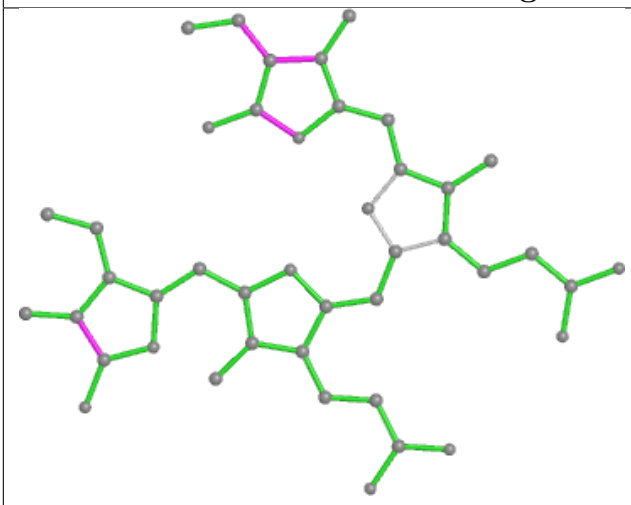
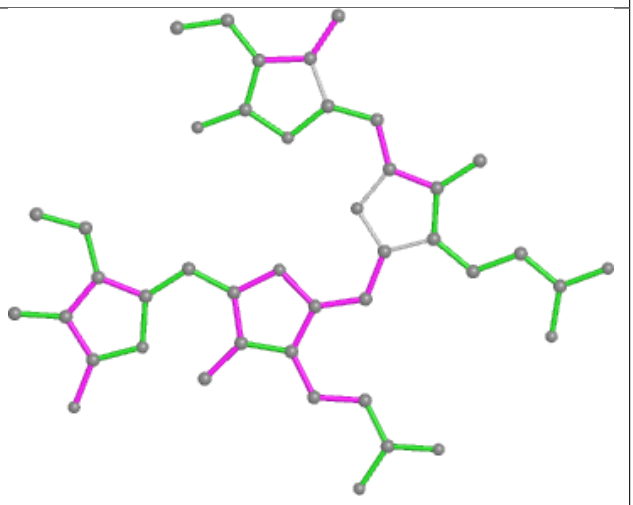


Rings

Ligand PEB 44 302



Bond lengths



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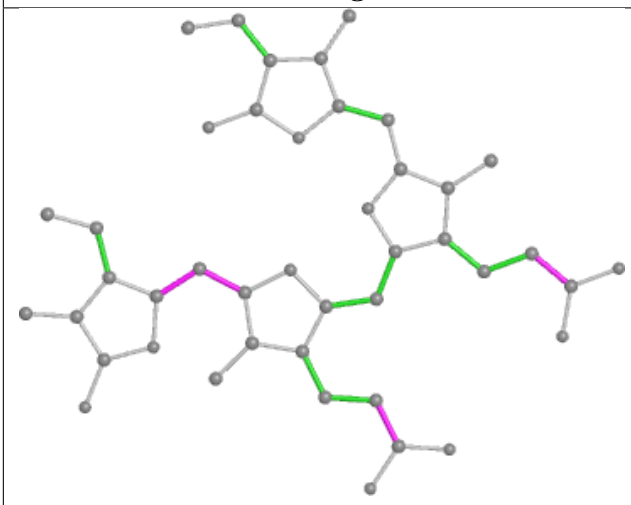
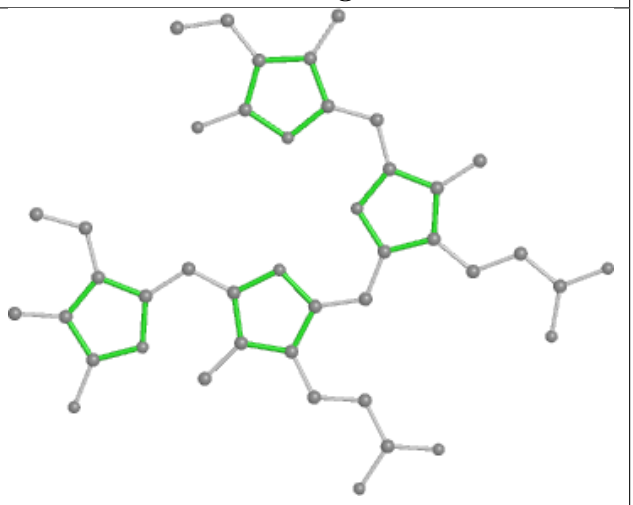
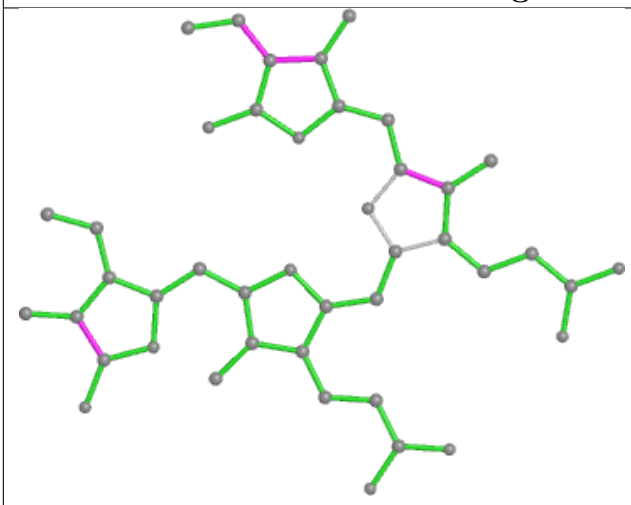


Torsions



Rings

Ligand PEB M5 202



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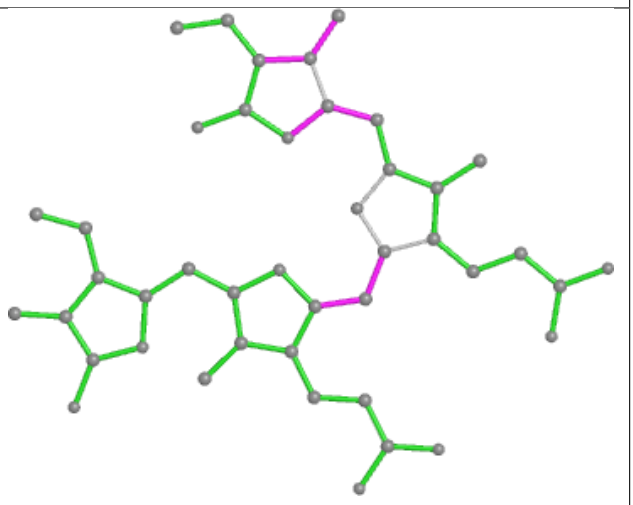

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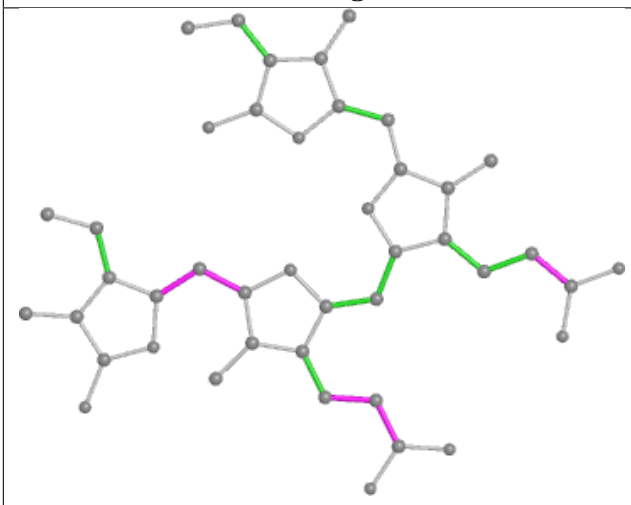

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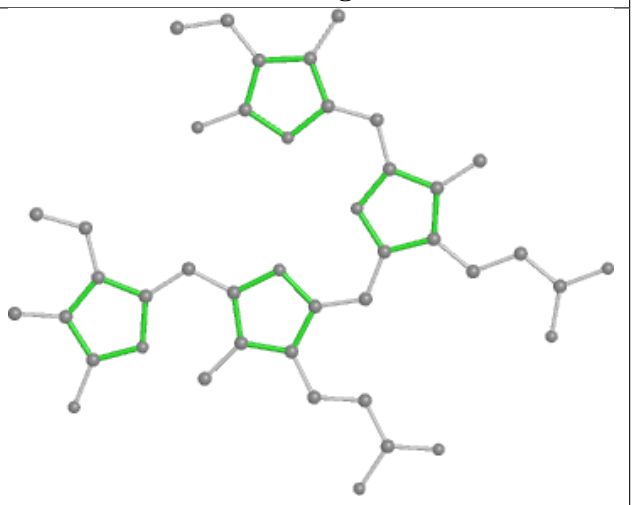
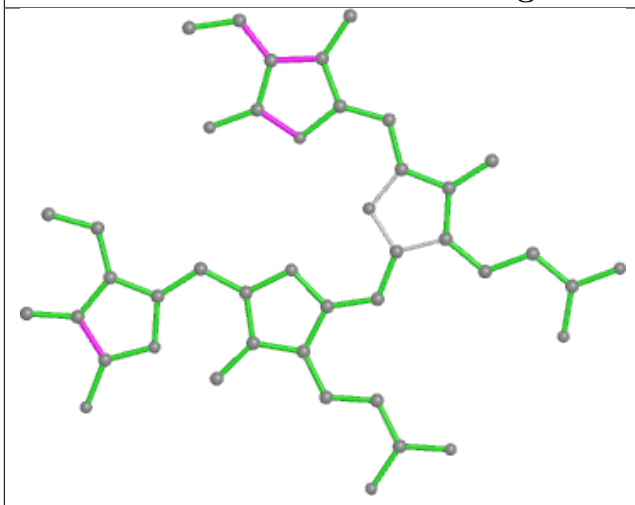


Rings

Ligand PEB cV 203



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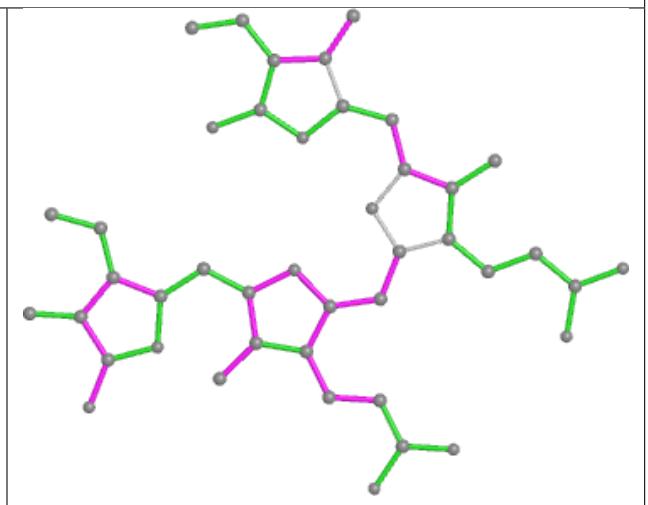

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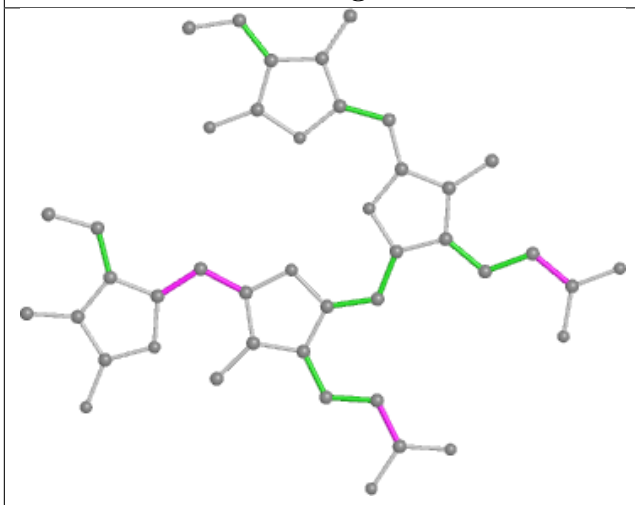

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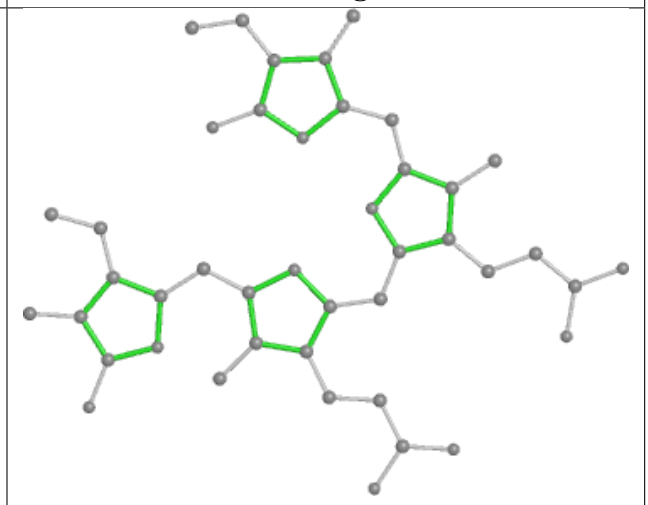
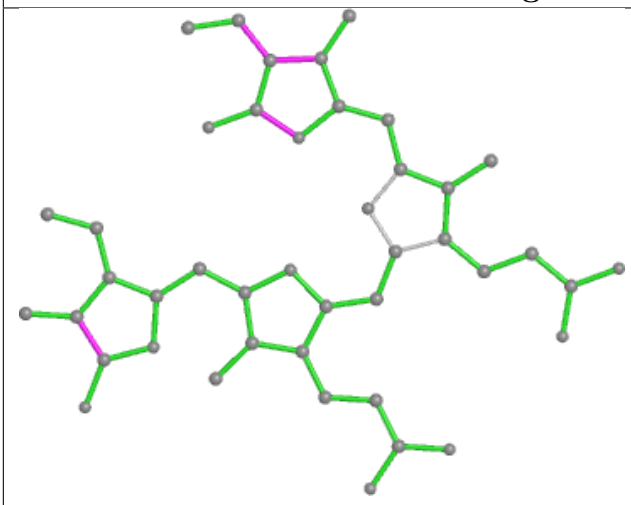


Rings

Ligand PEB df 201



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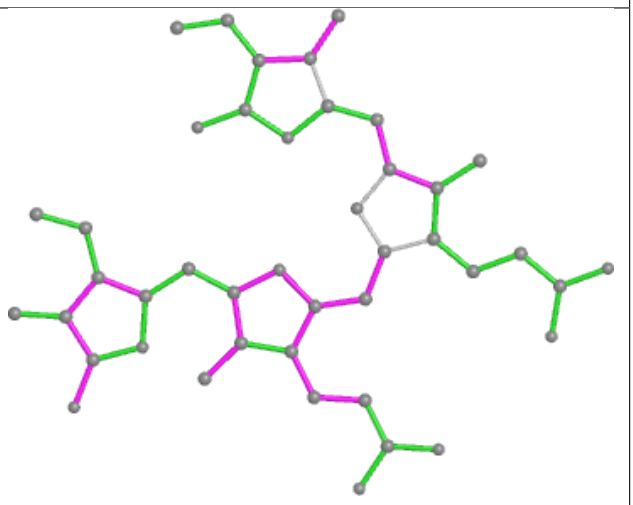

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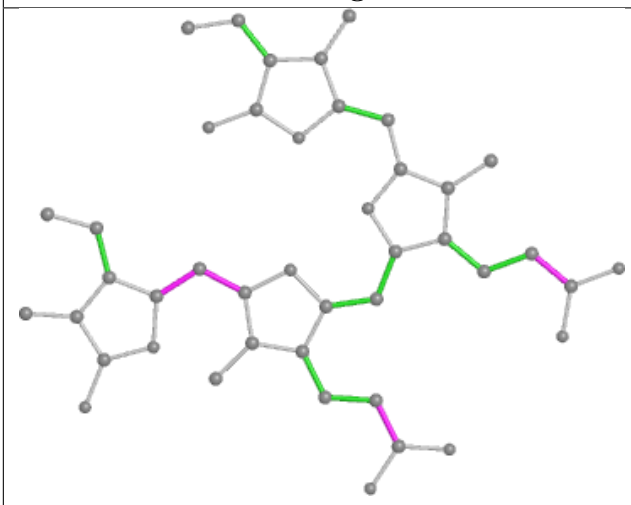

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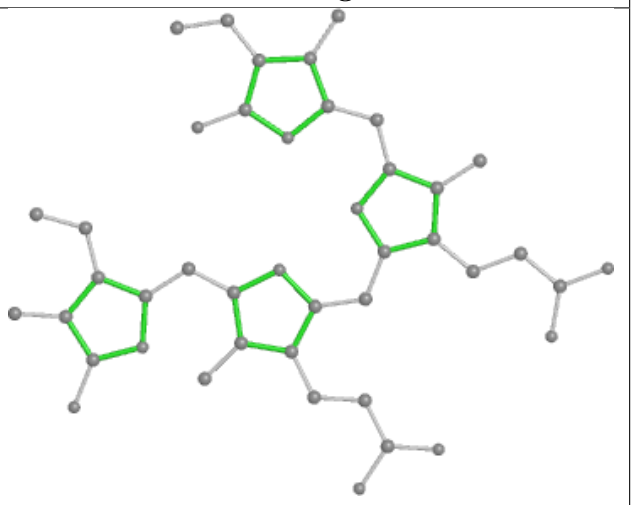
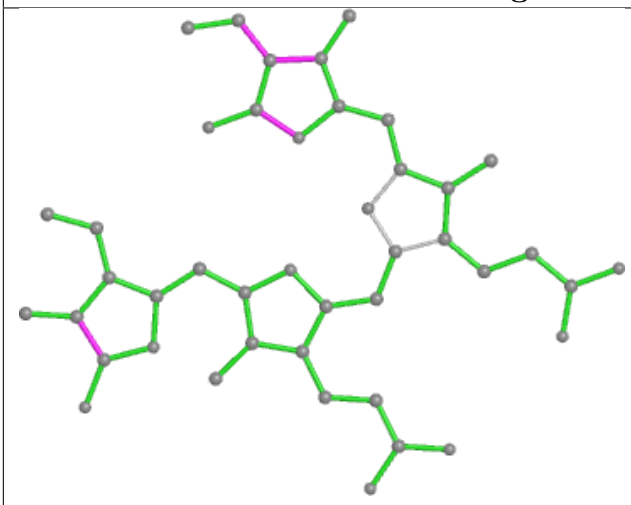


Rings

Ligand PEB iC 1001



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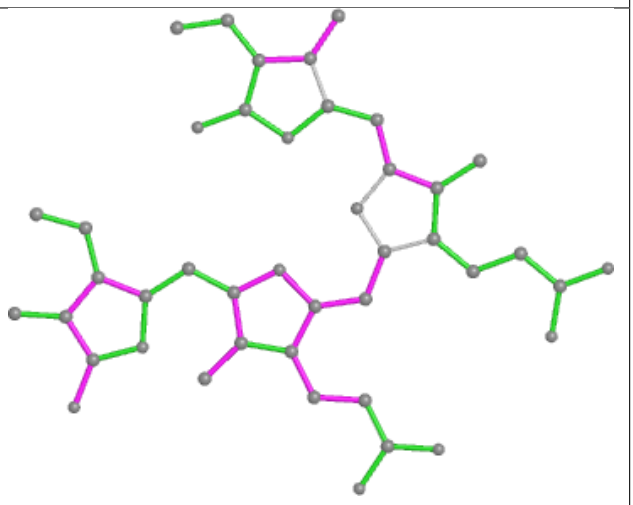

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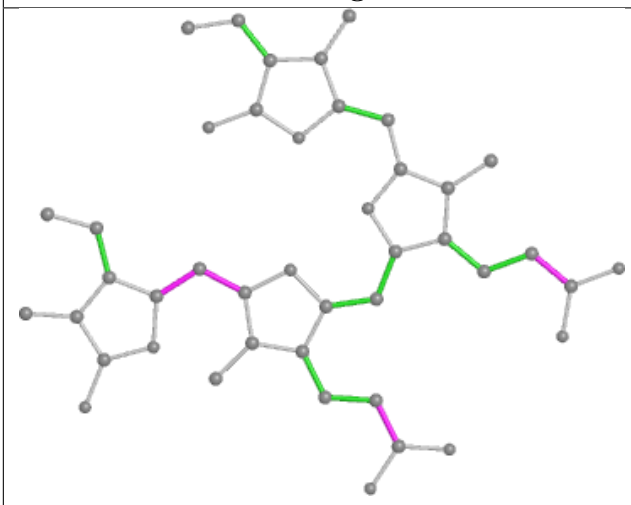

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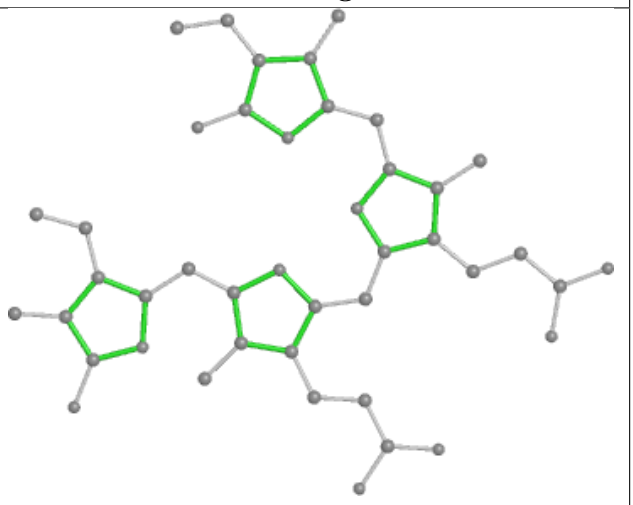

Rings

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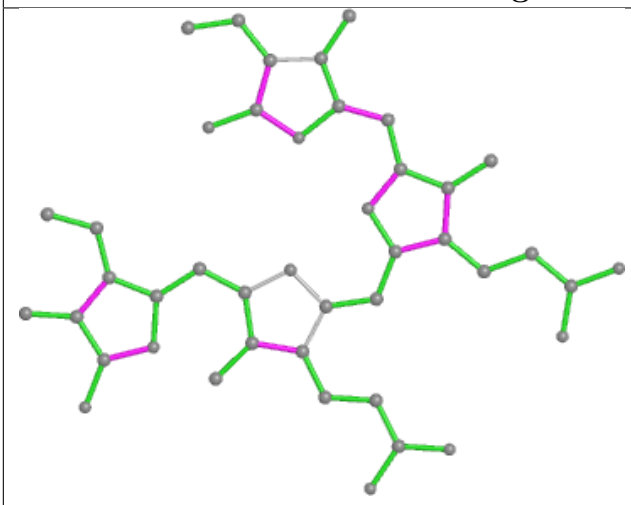

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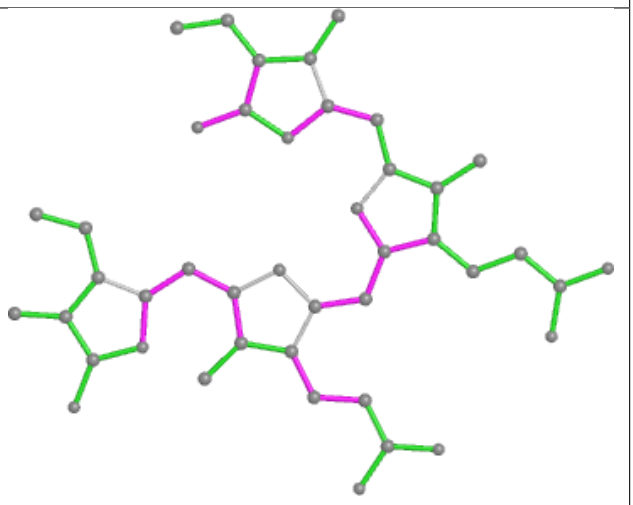

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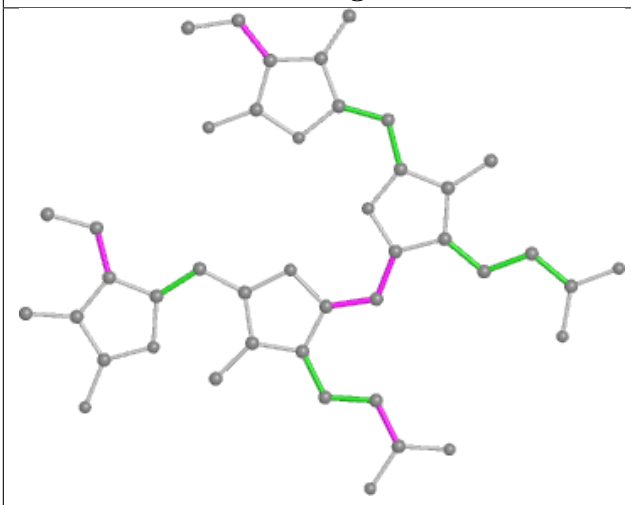

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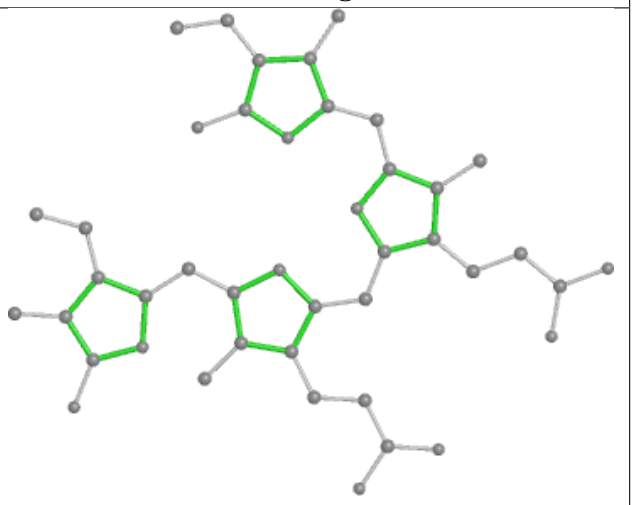

Rings

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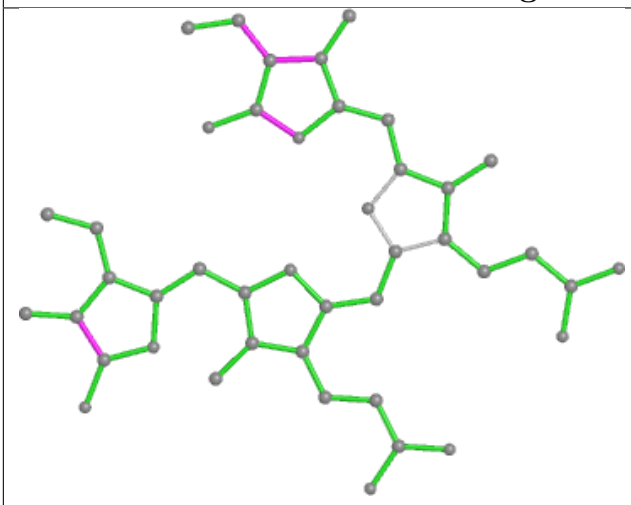

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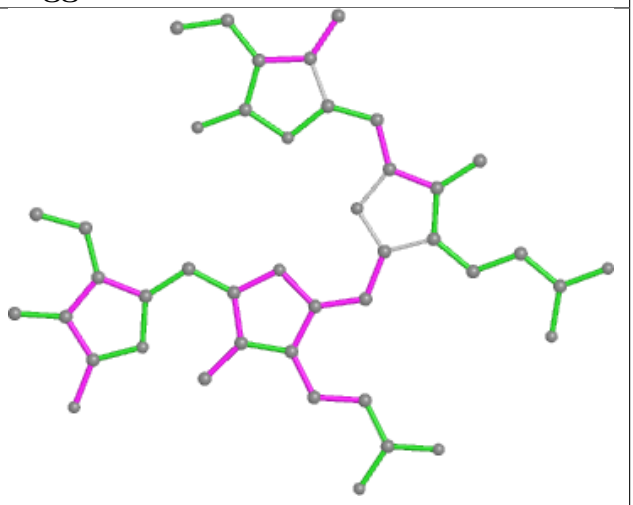

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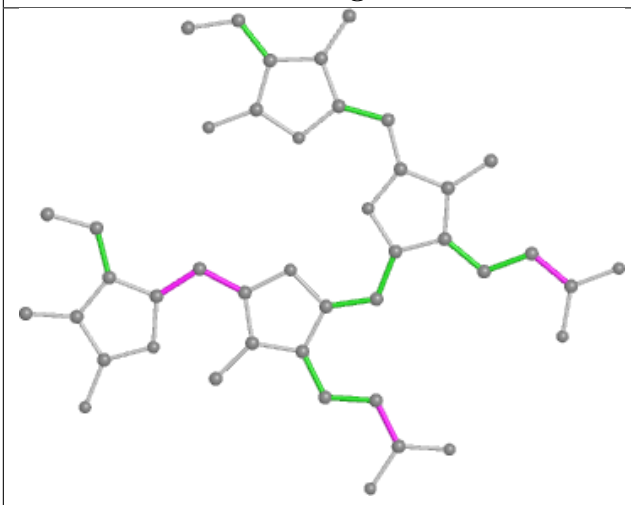

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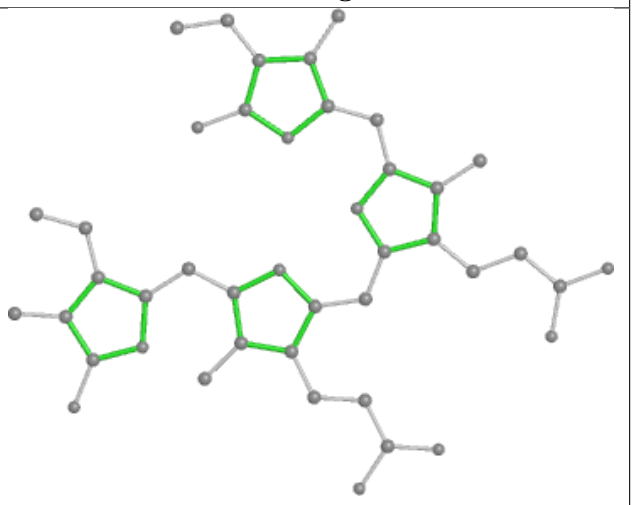
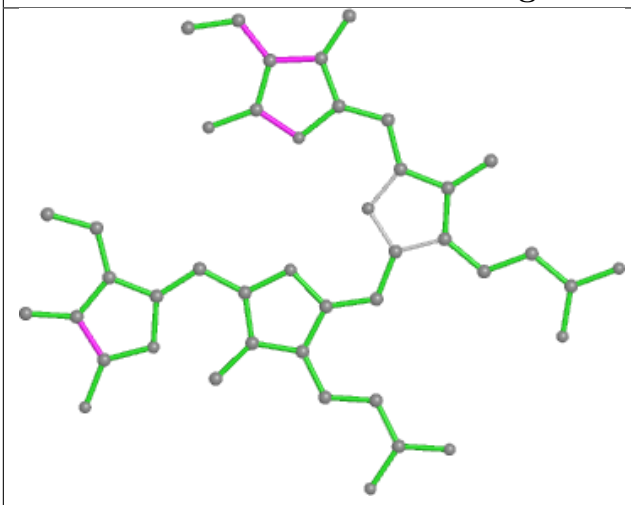


Rings

Ligand PEB n4 201



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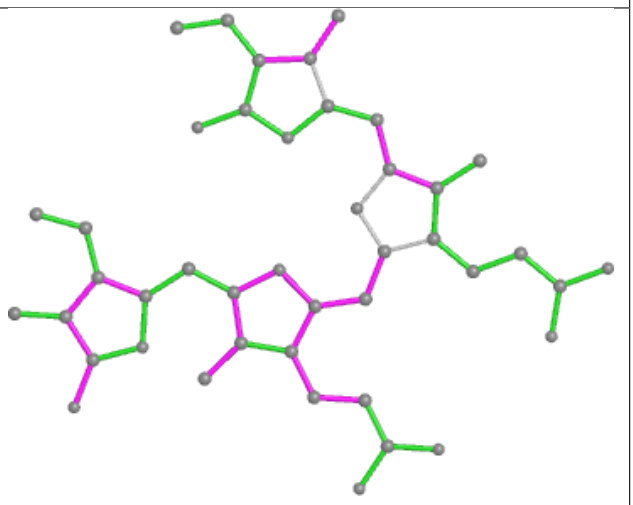

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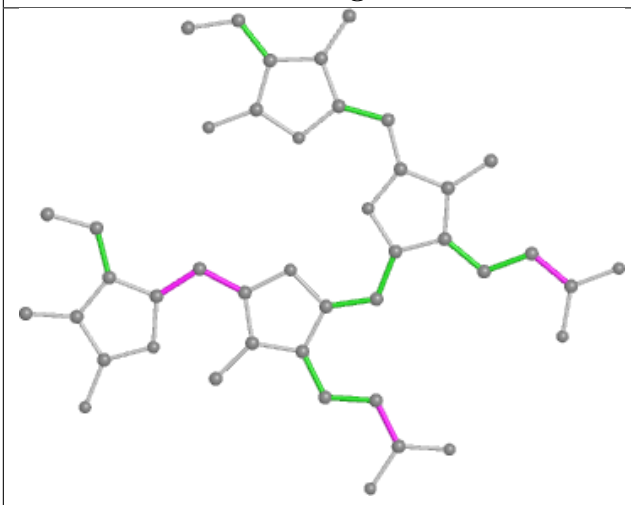

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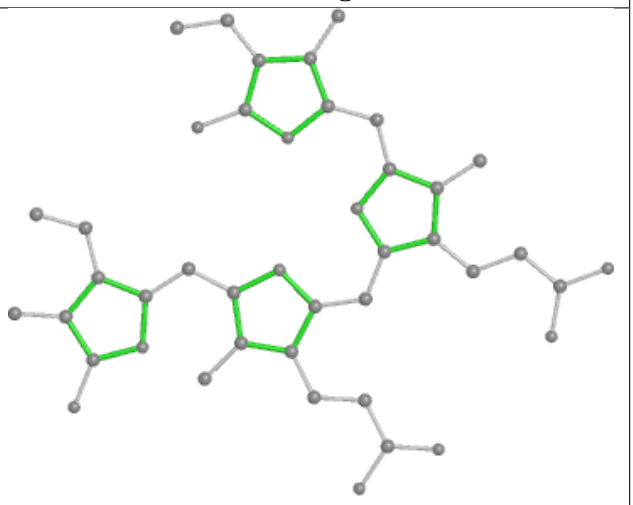
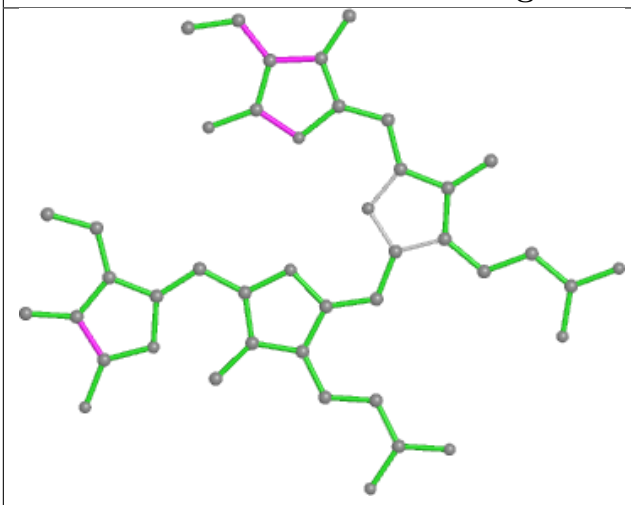


Rings

Ligand PEB jI 1001



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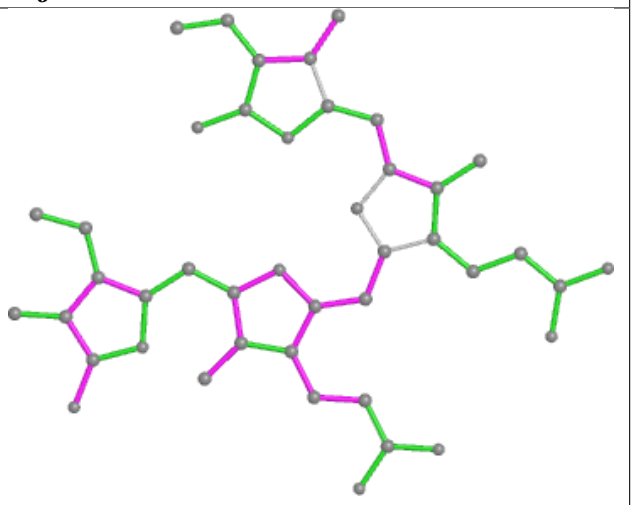

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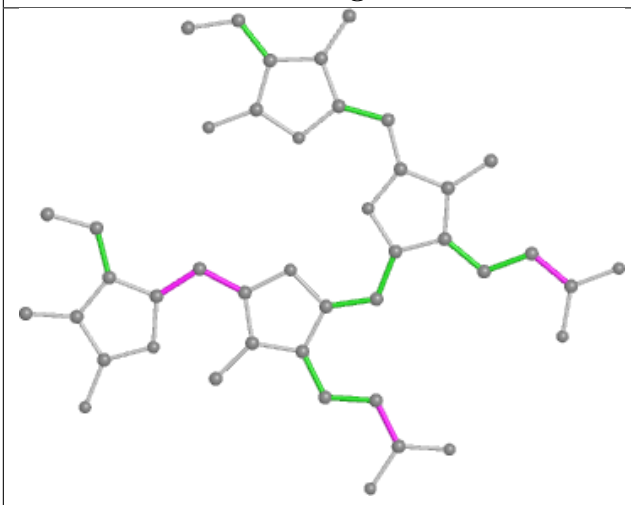

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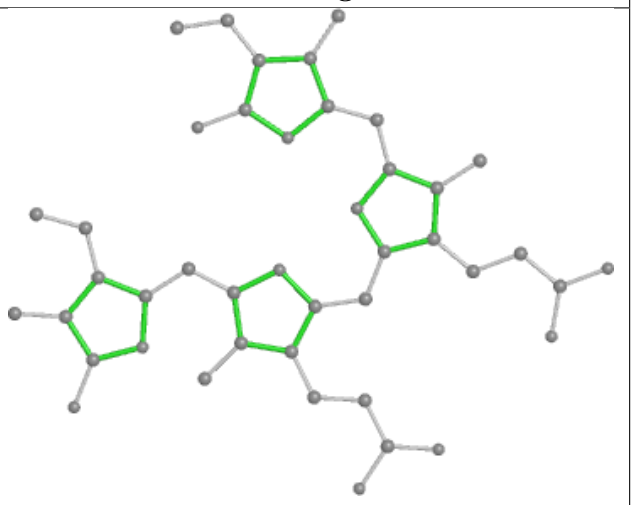
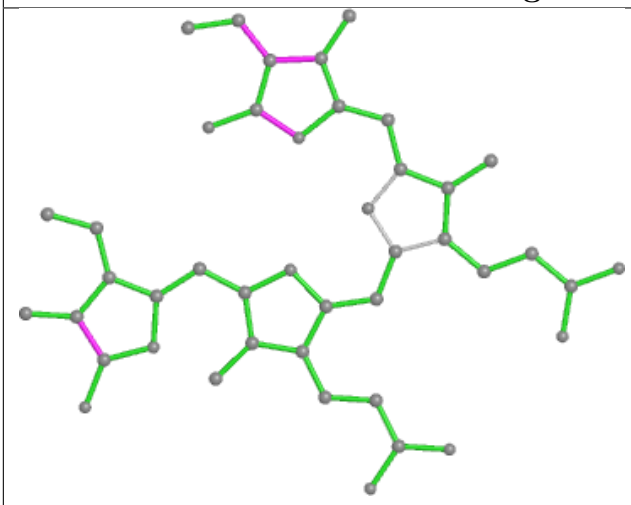


Rings

Ligand PEB lv 201



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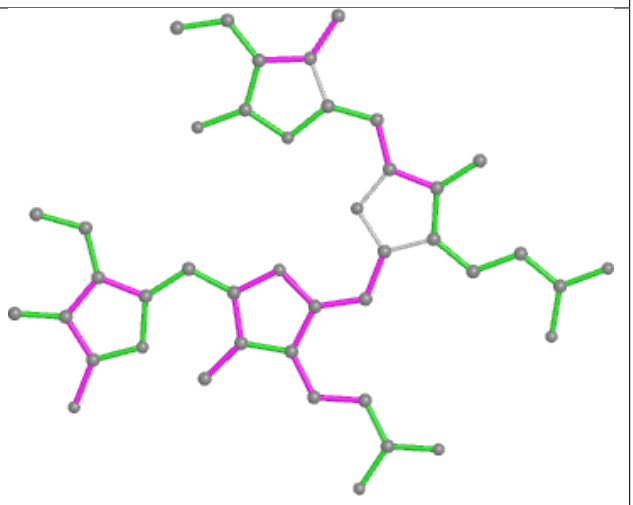

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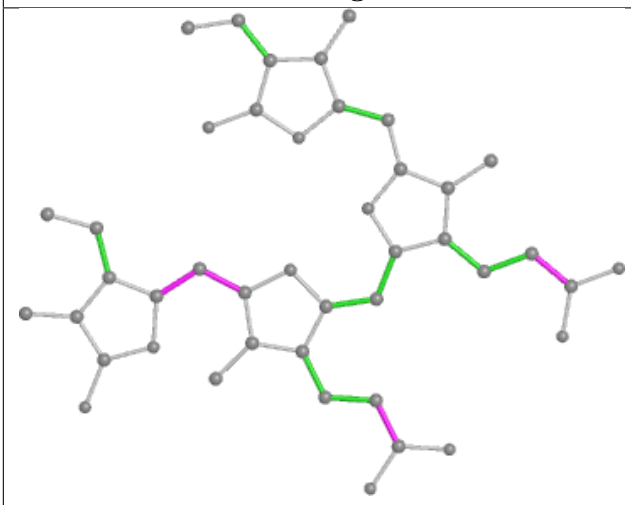

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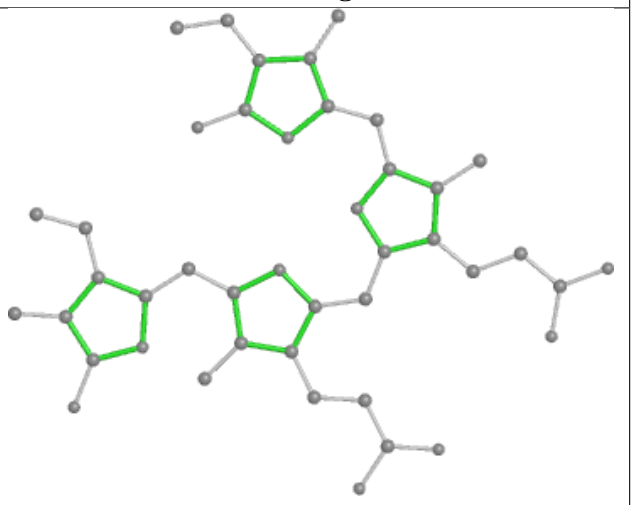
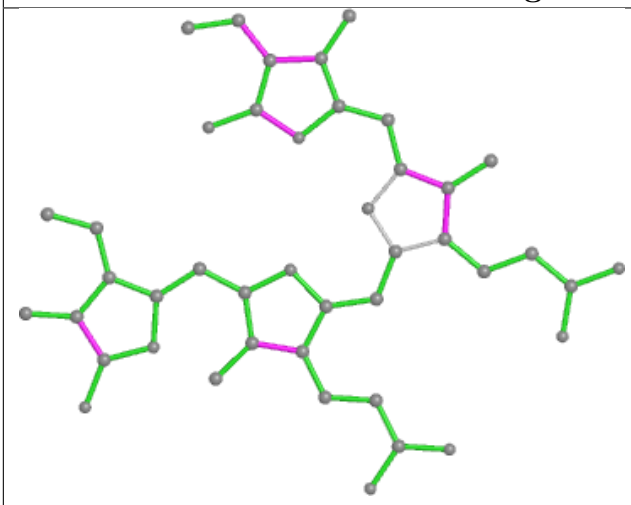


Rings

Ligand PEB fc 202



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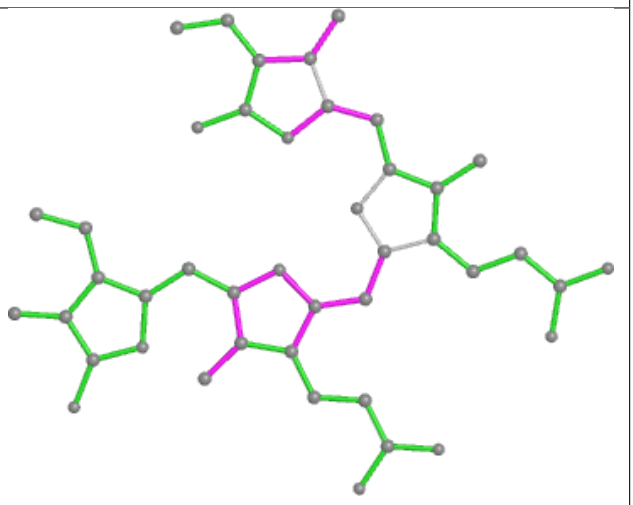

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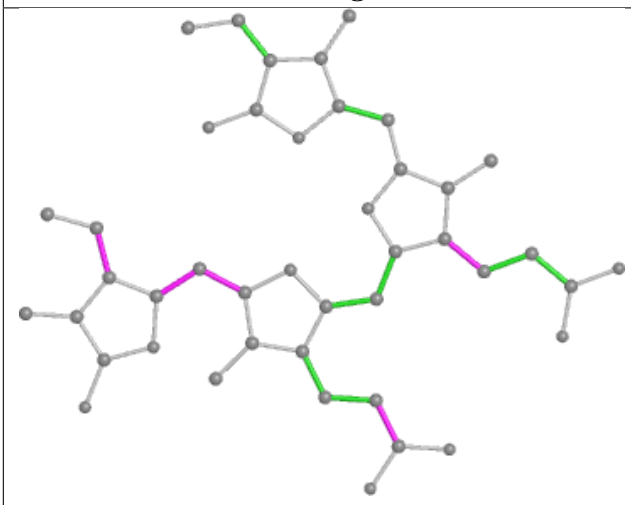

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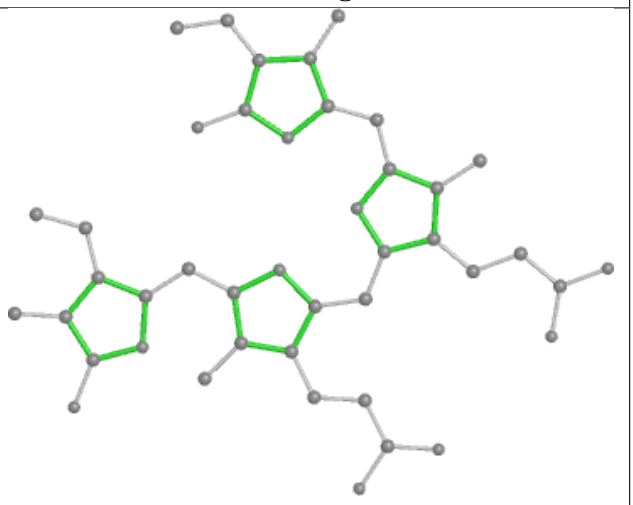
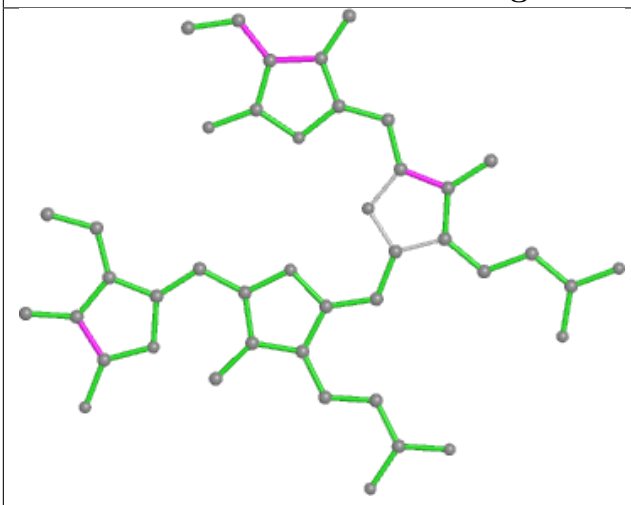


Rings

Ligand PEB iA 1002



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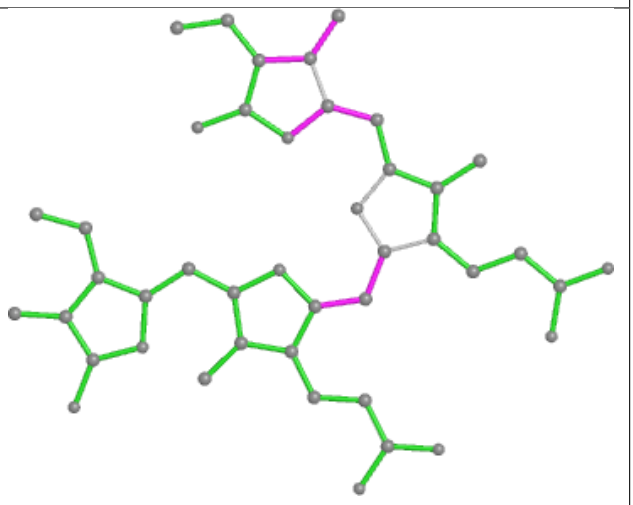

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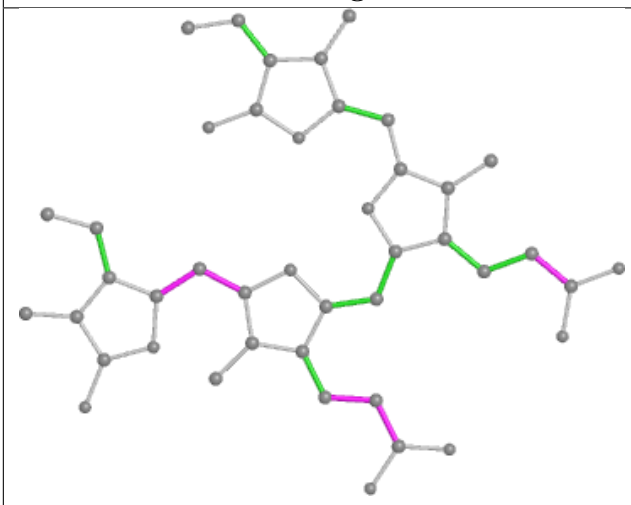

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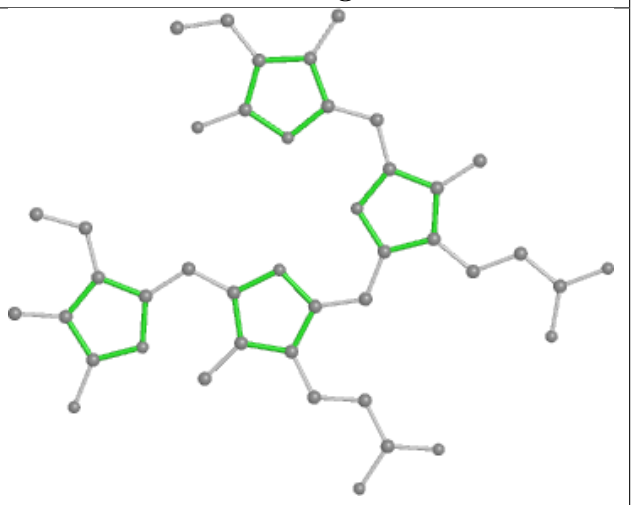
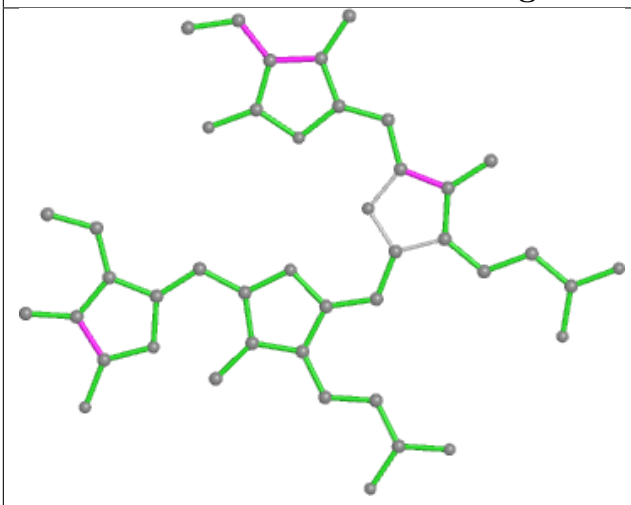


Rings

Ligand PEB S5 202



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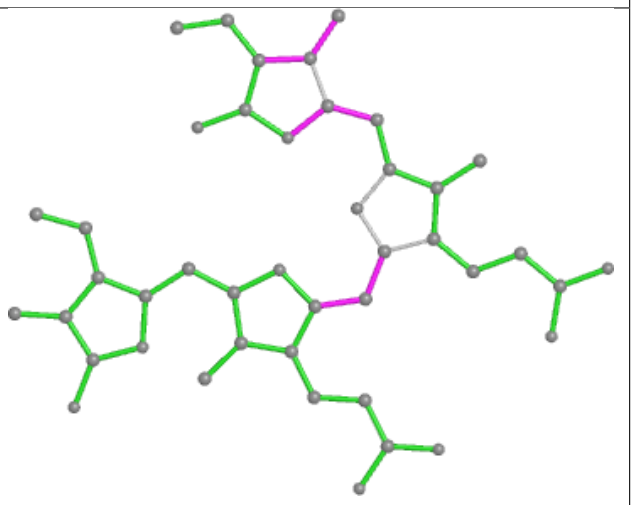

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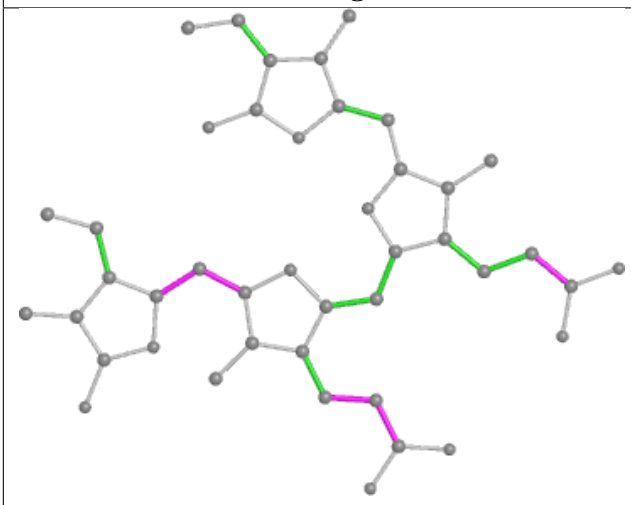

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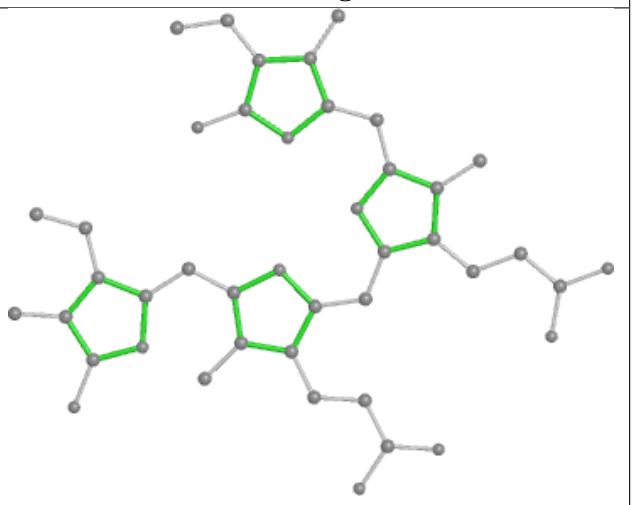
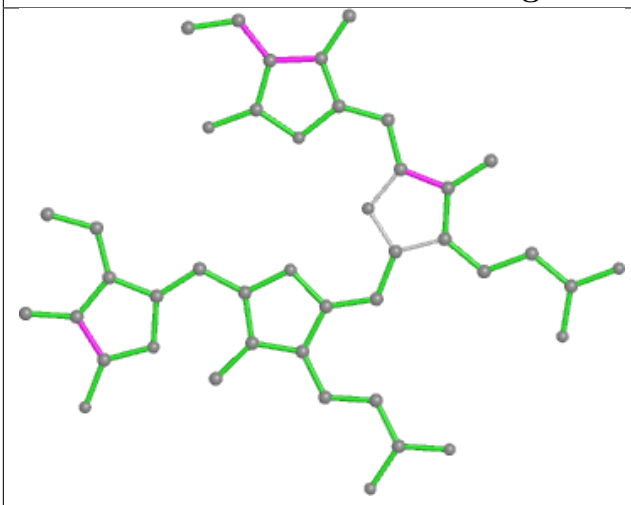
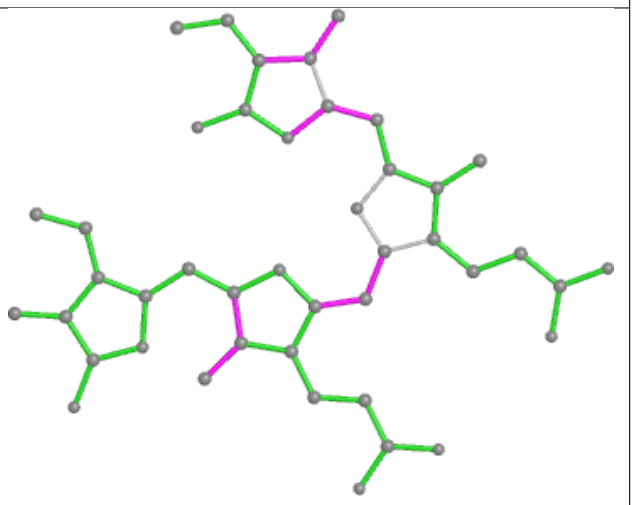


Rings

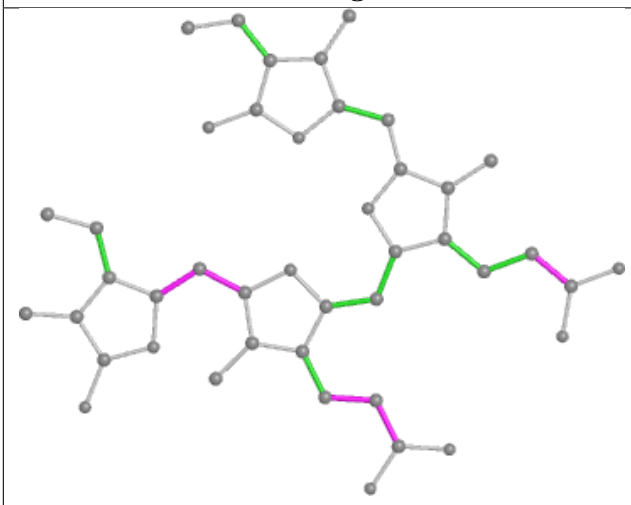
Ligand PEB I5 202



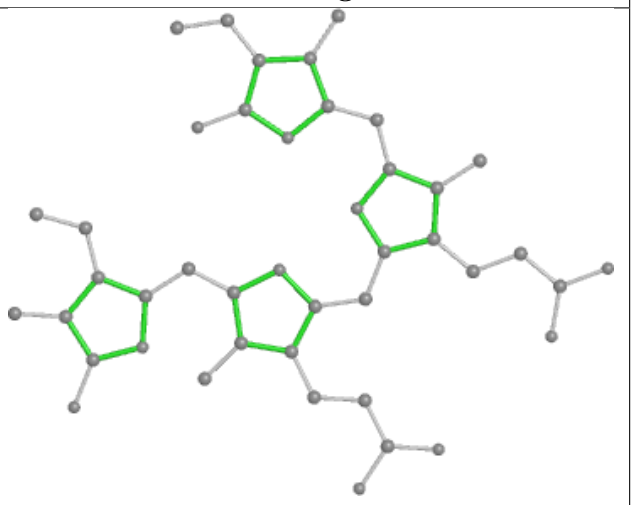
Bond lengths



Bond angles

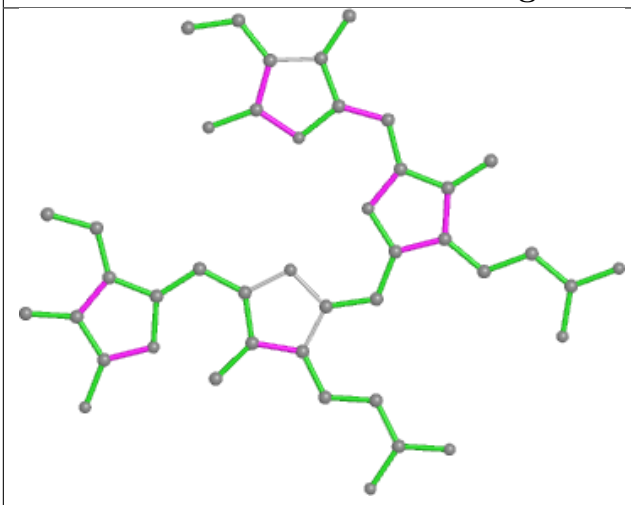


Torsions



Rings

Ligand PUB e8 304



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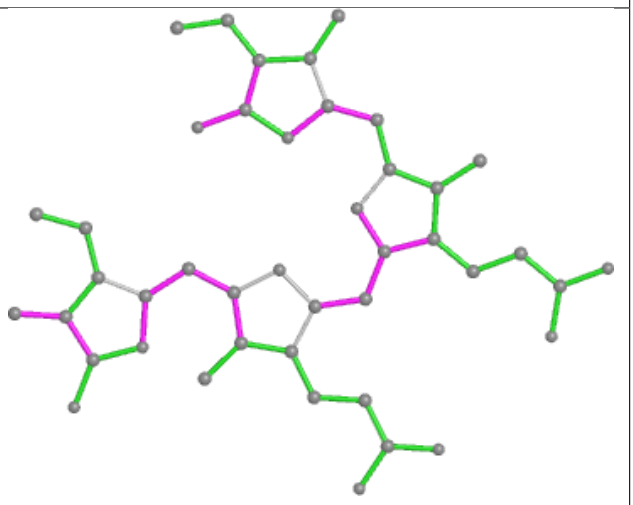

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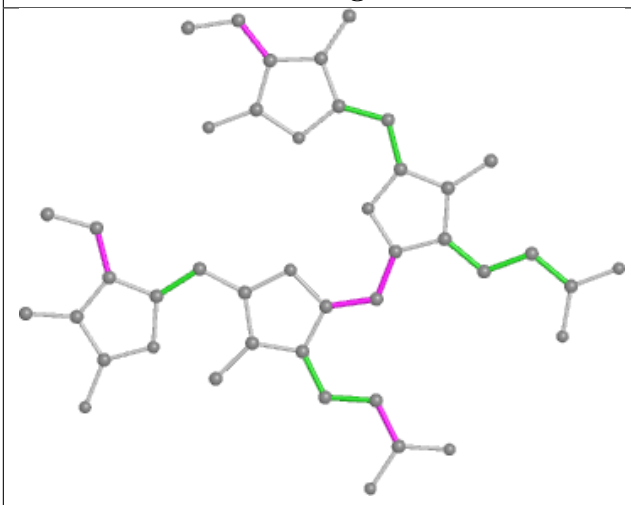

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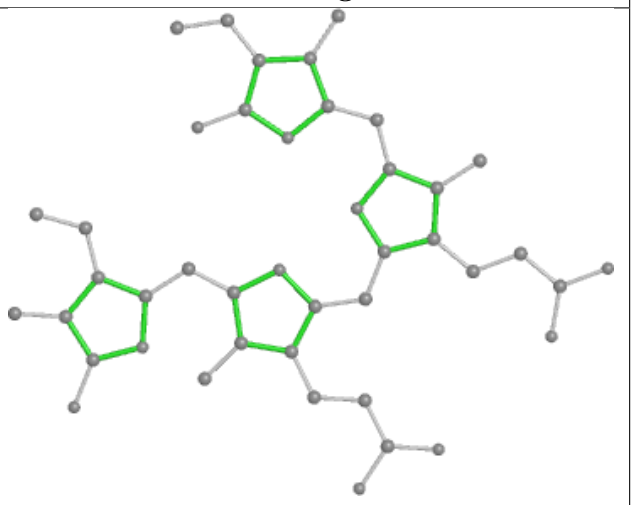
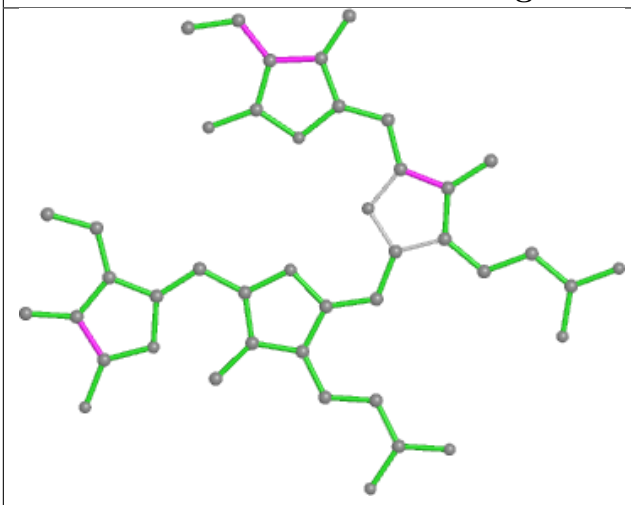


Rings

Ligand PEB Q5 202



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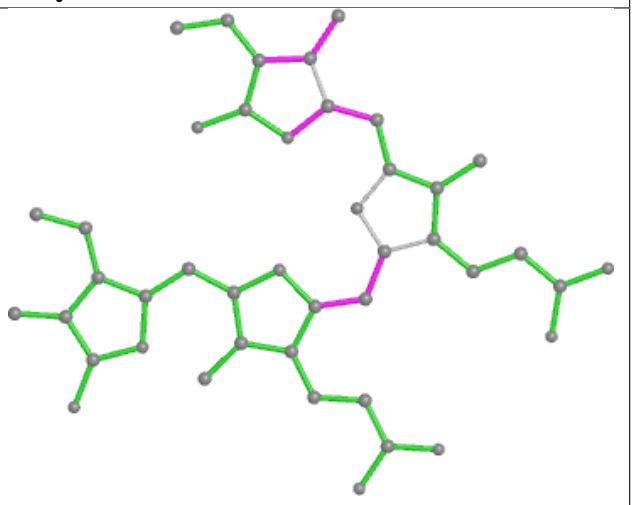

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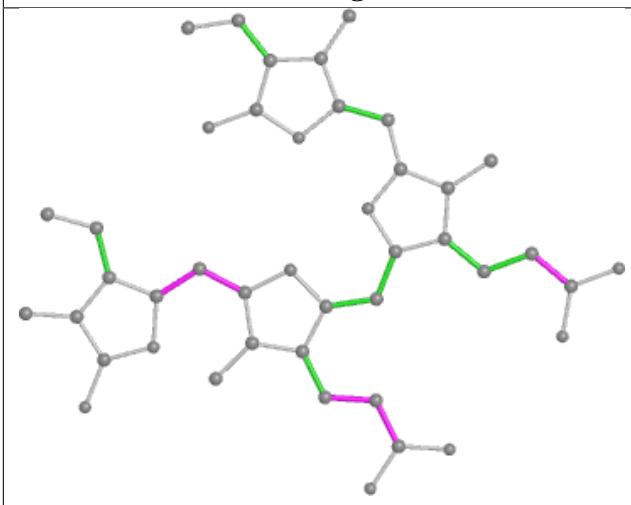

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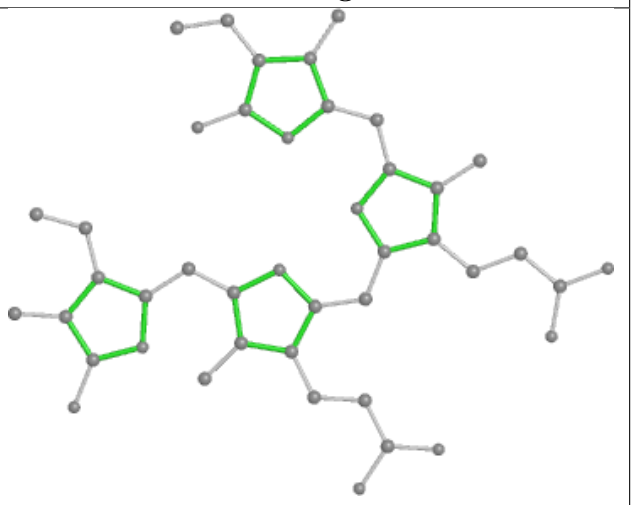
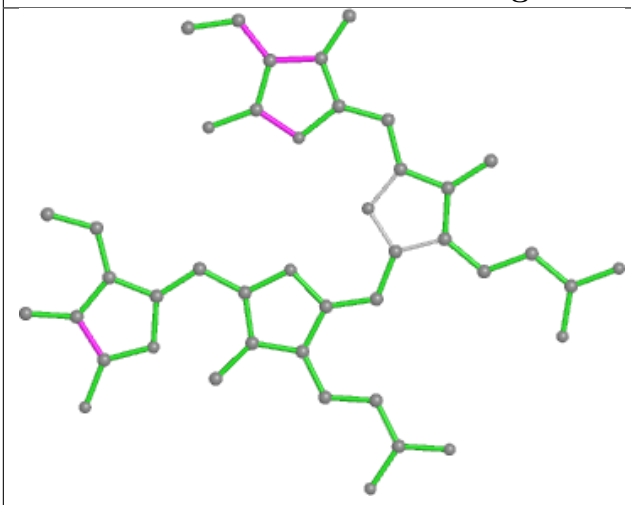


Rings

Ligand PEB aa 1001



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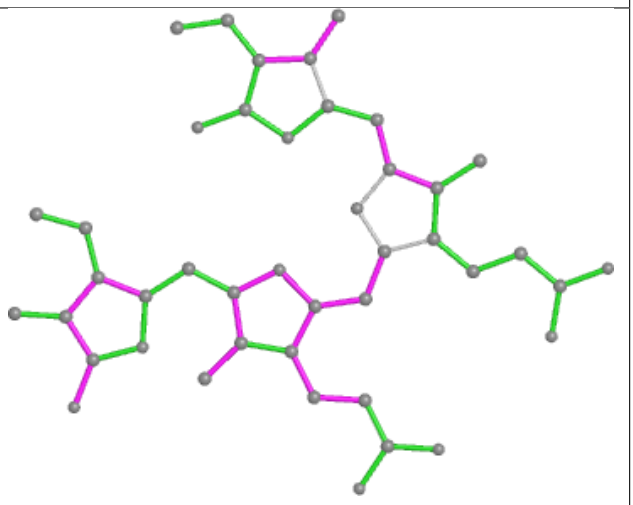

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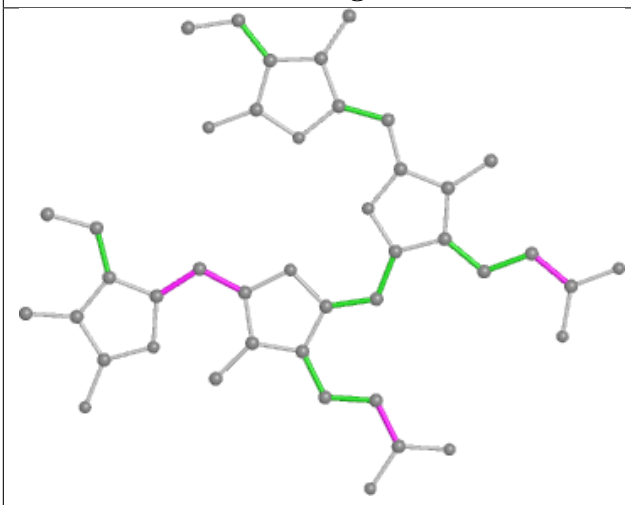

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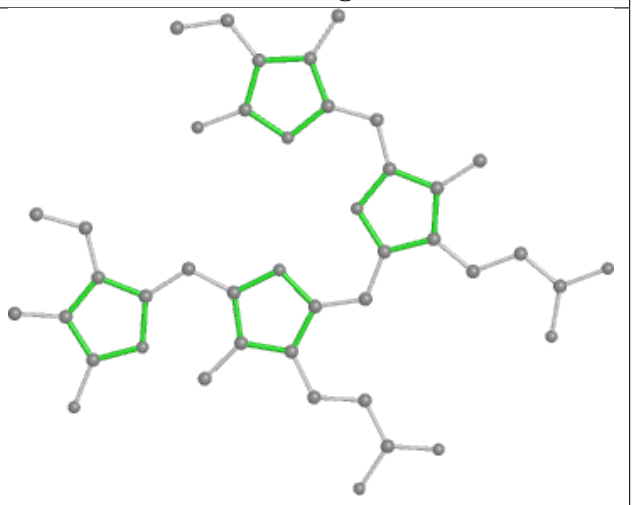
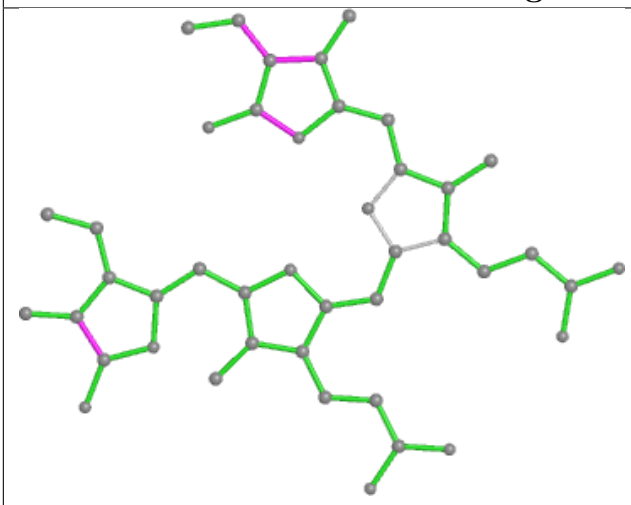


Rings

Ligand PEB lr 201



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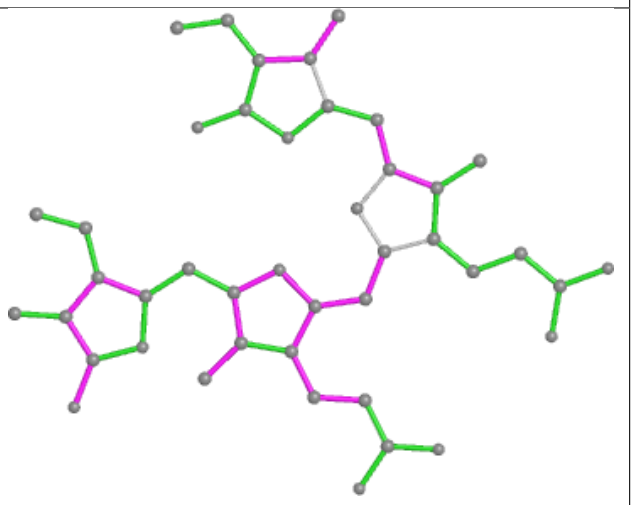

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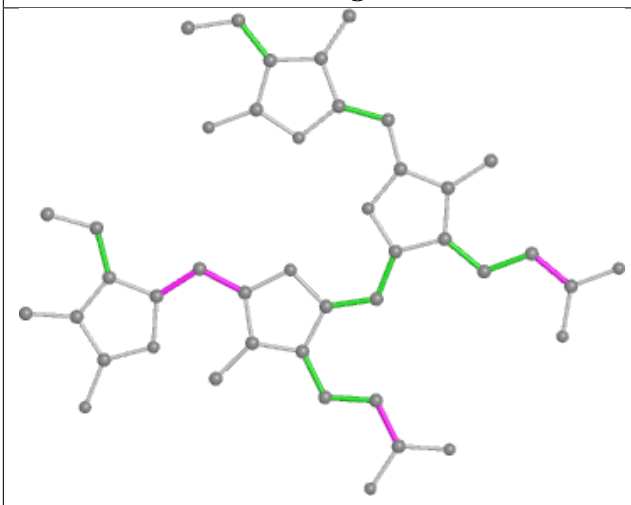

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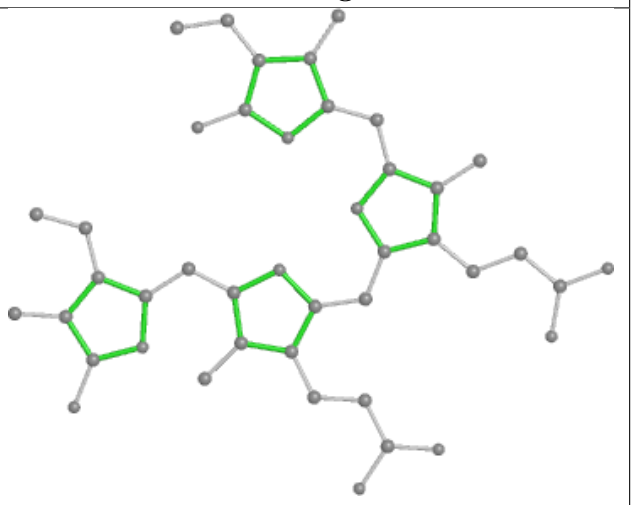

Rings

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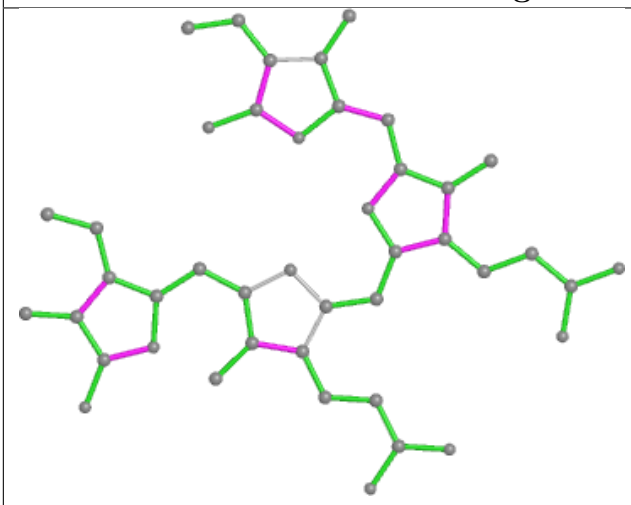

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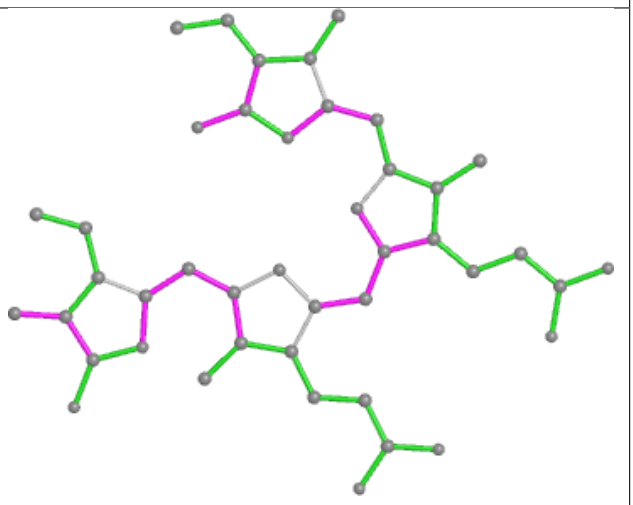

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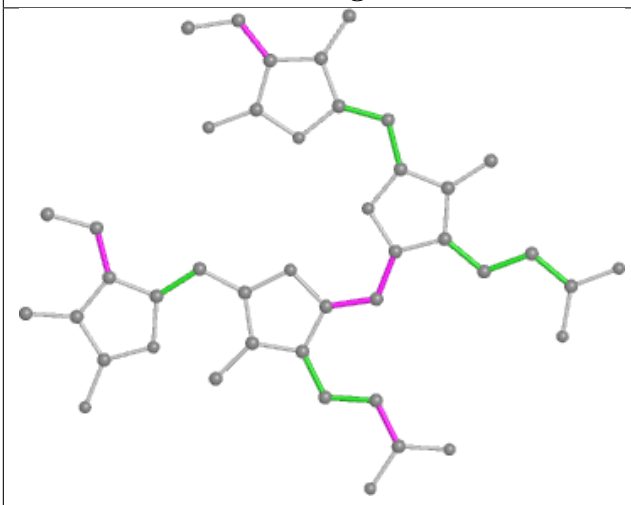

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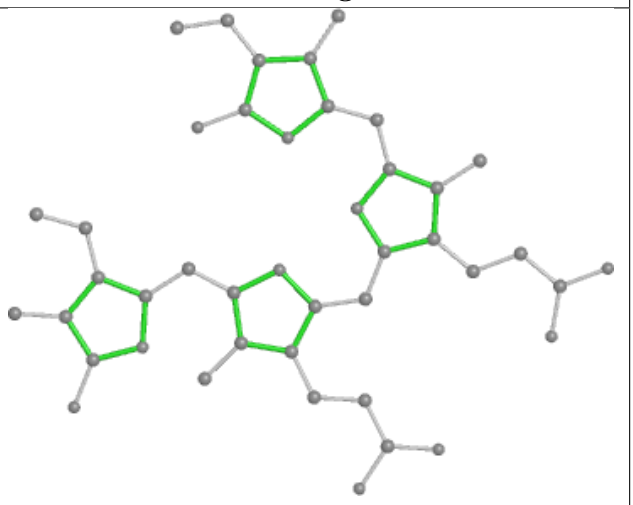
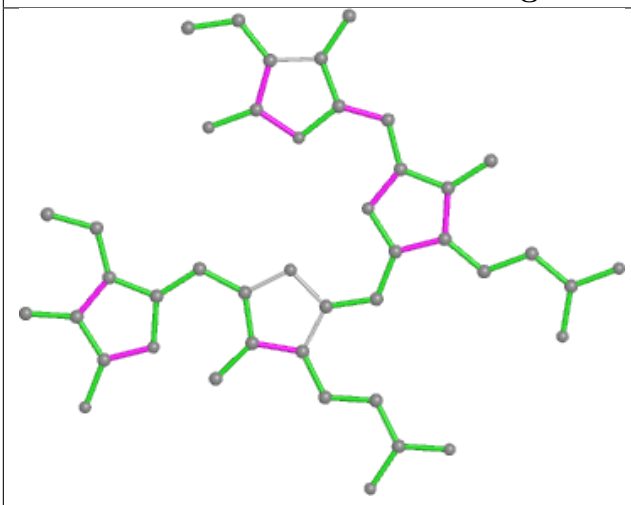


Rings

Ligand PUB lb 203



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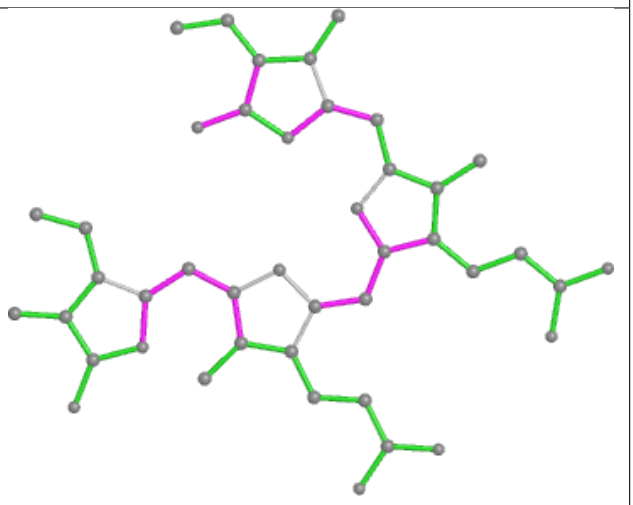

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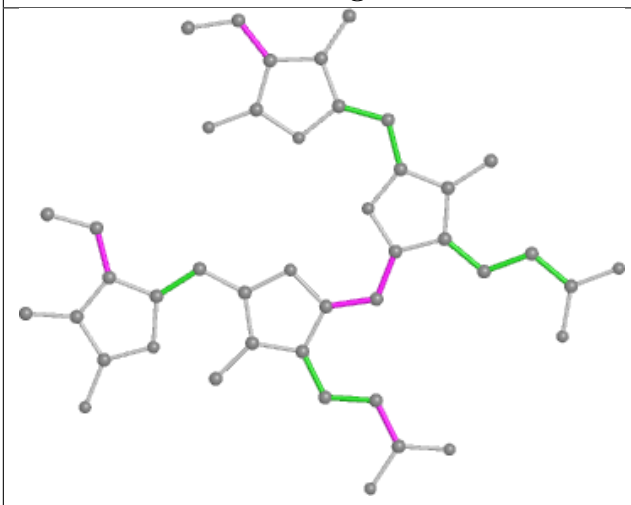

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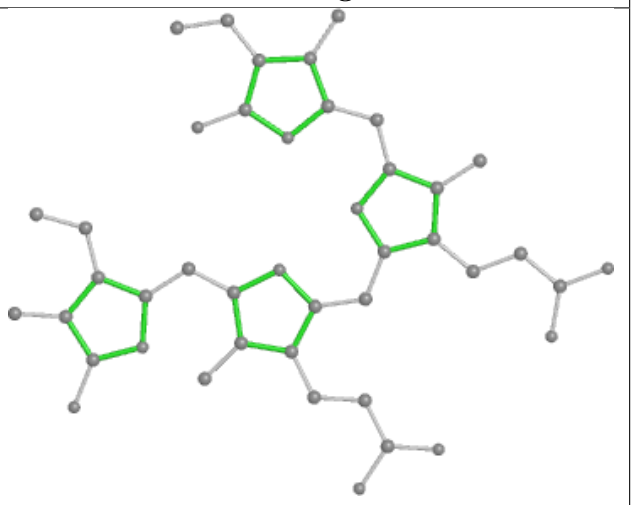
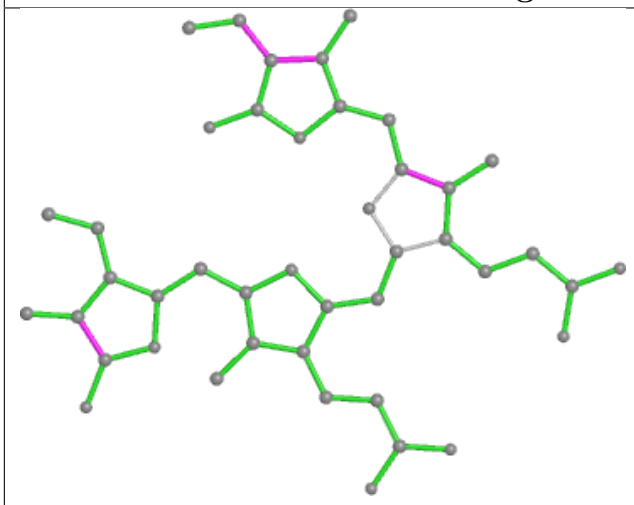


Rings

Ligand PEB Q3 202



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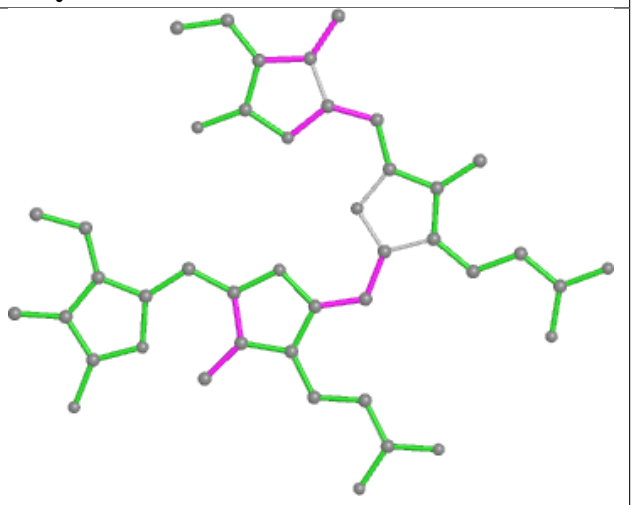

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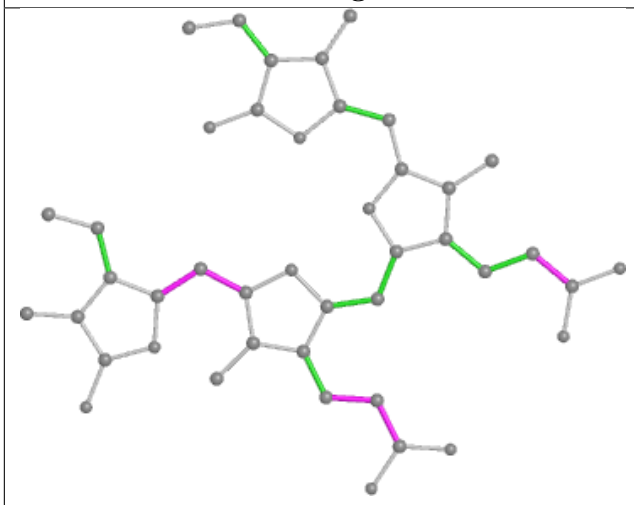

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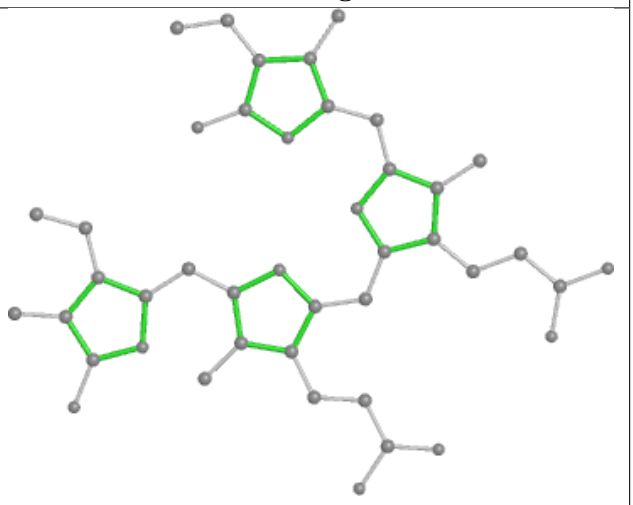
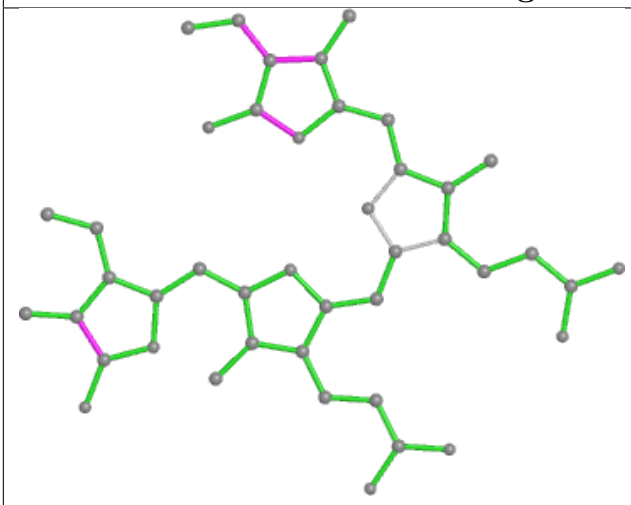


Rings

Ligand PEB cP 201



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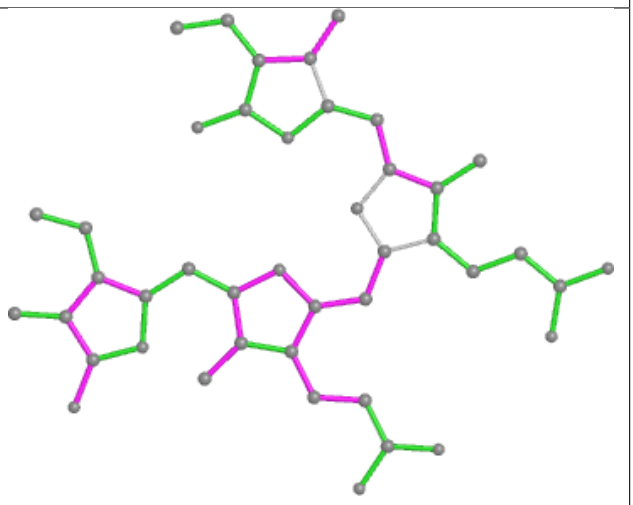

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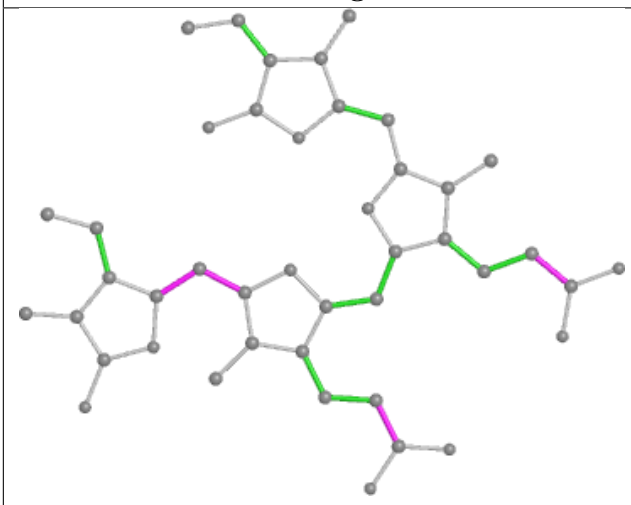

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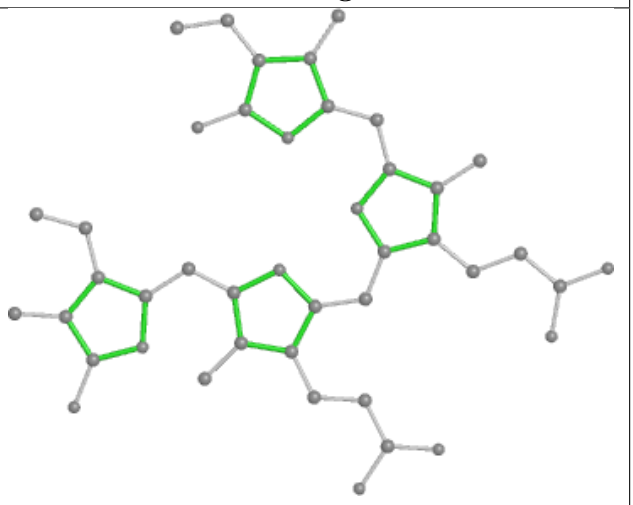
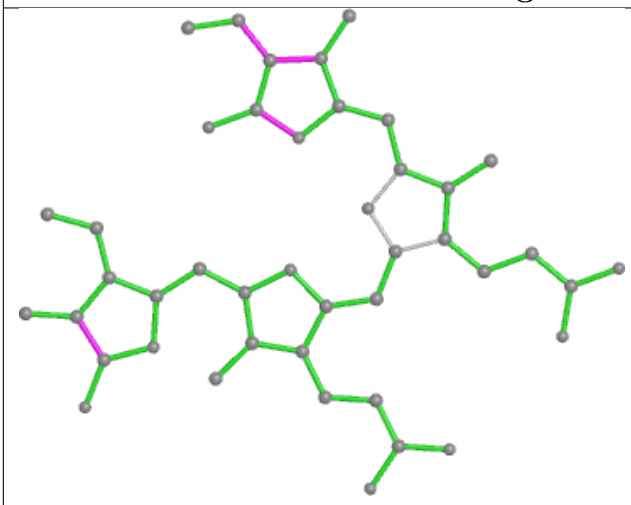


Rings

Ligand PEB P2 201



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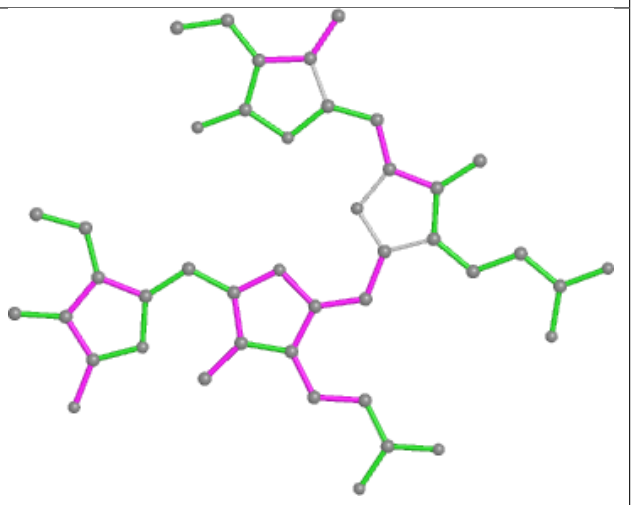

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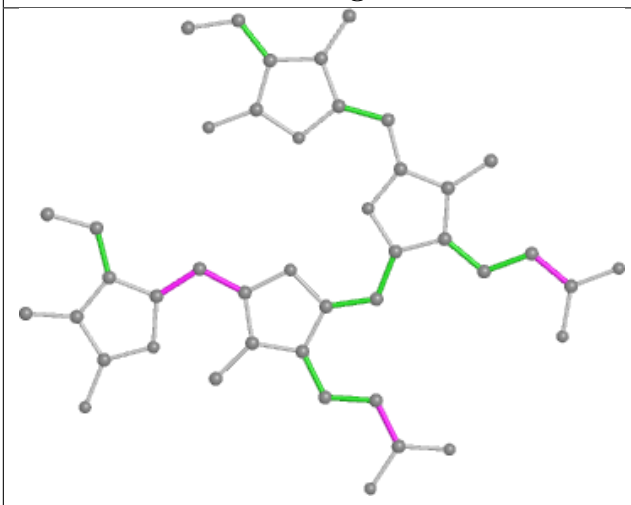

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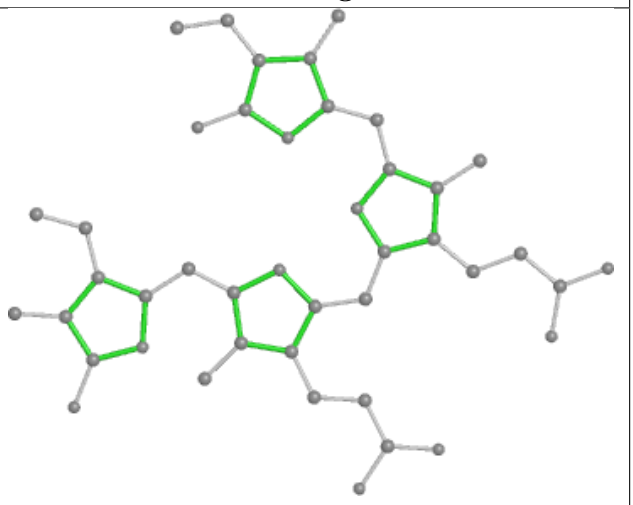
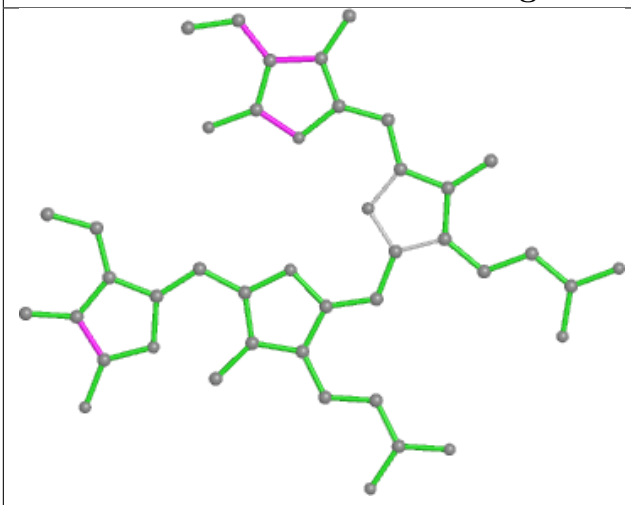


Rings

Ligand PEB k9 201



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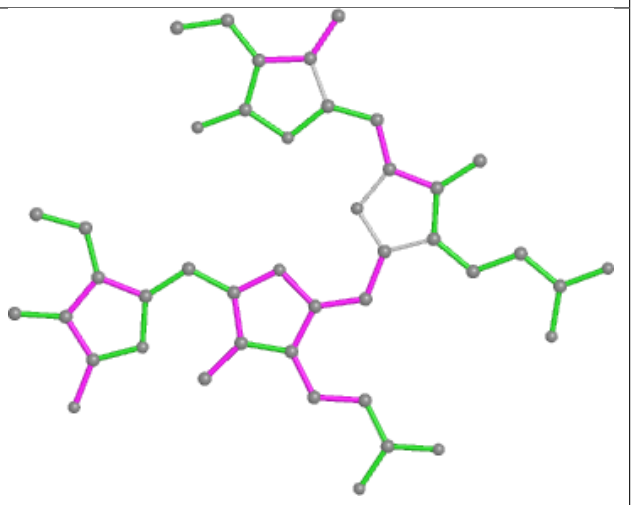

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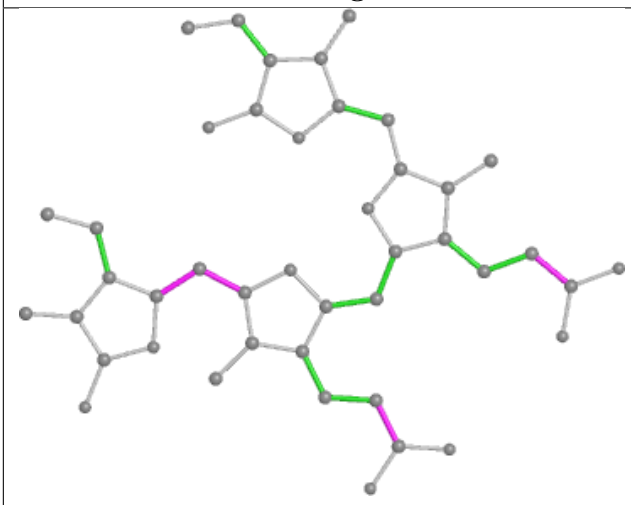

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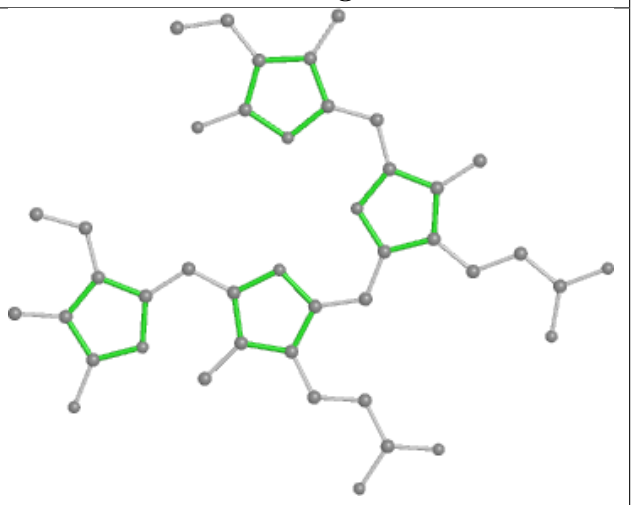
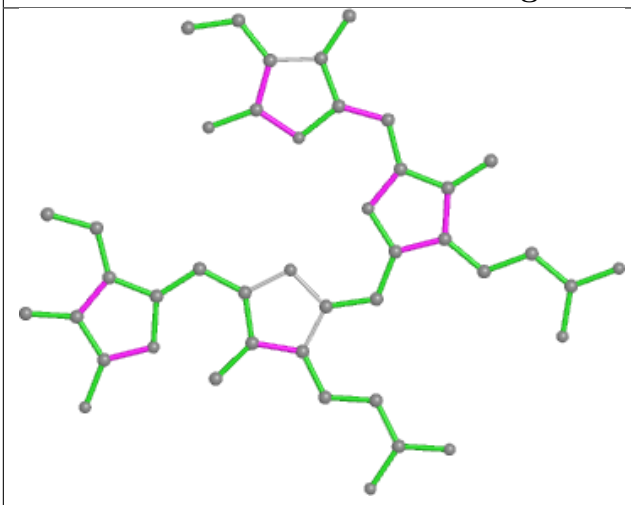


Rings

Ligand PUB ld 203



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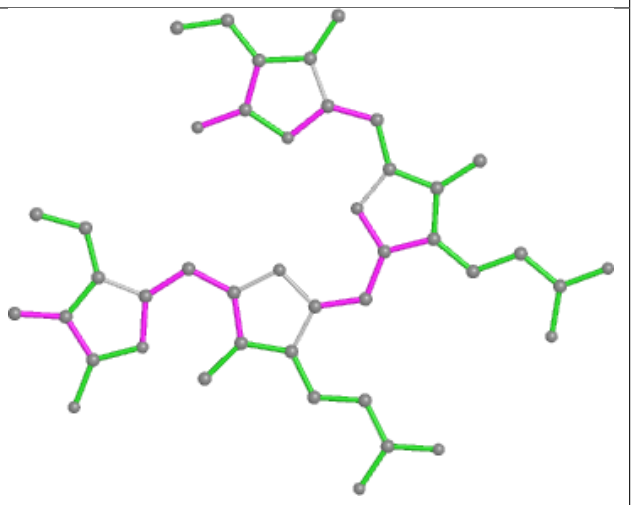

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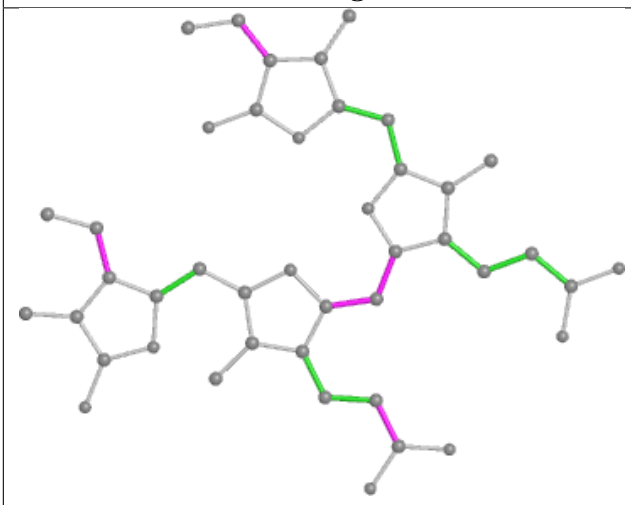

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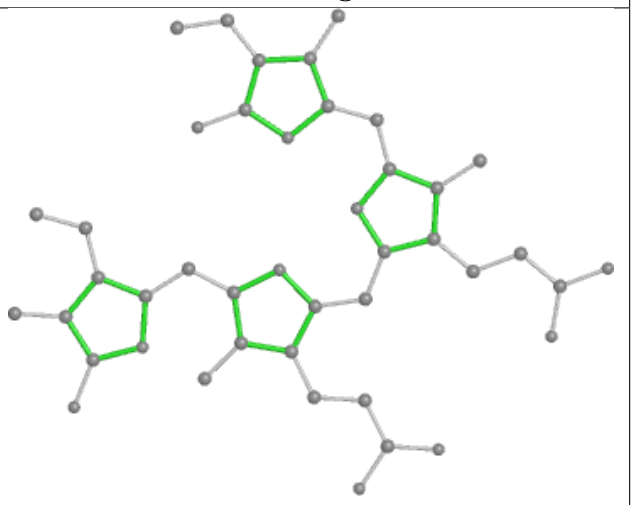
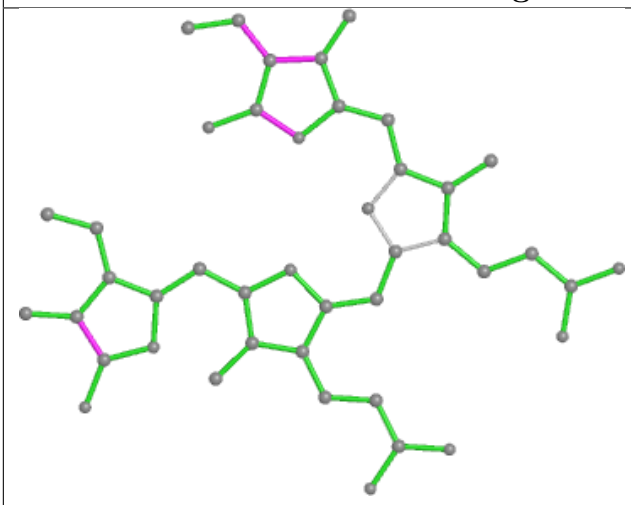


Rings

Ligand PEB iF 1001



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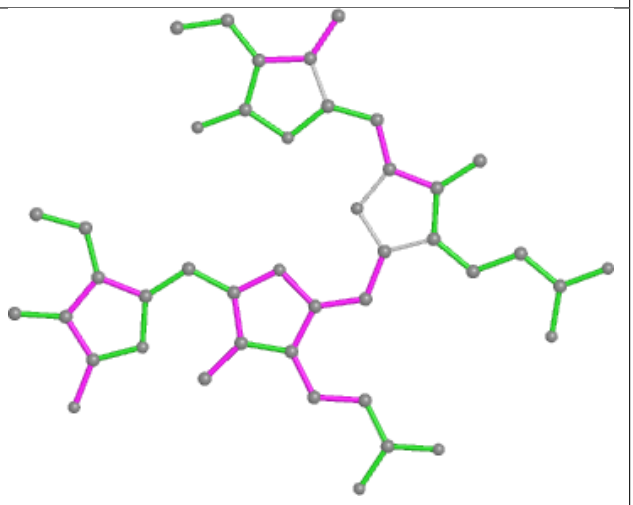
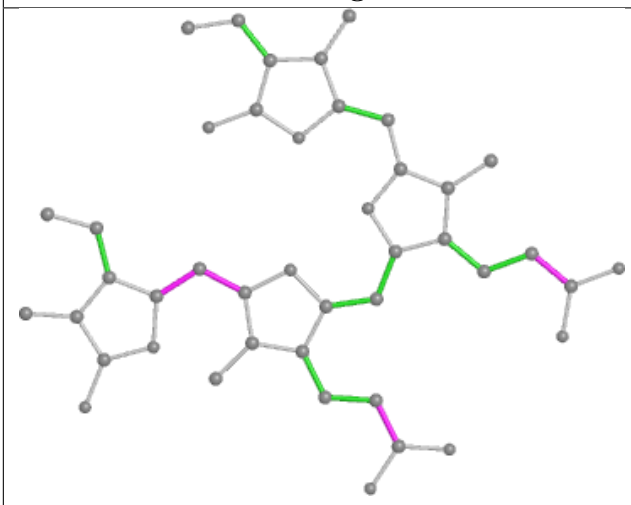


Bond angles



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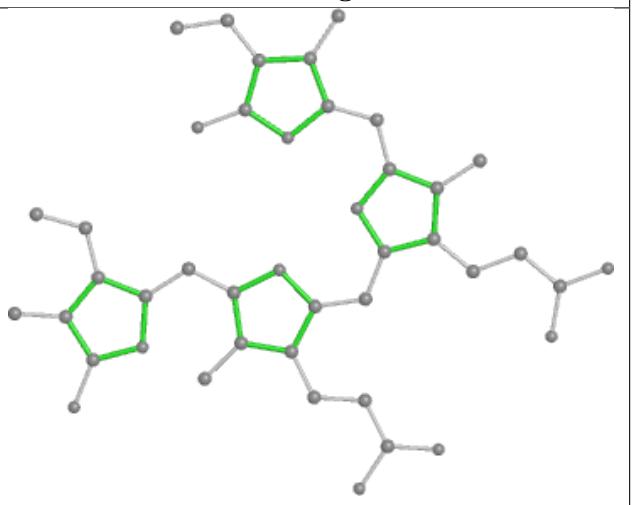
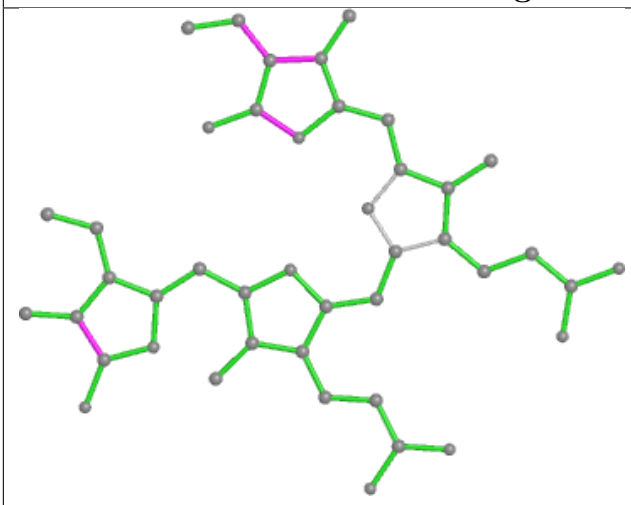


Rings

Ligand PEB bD 201



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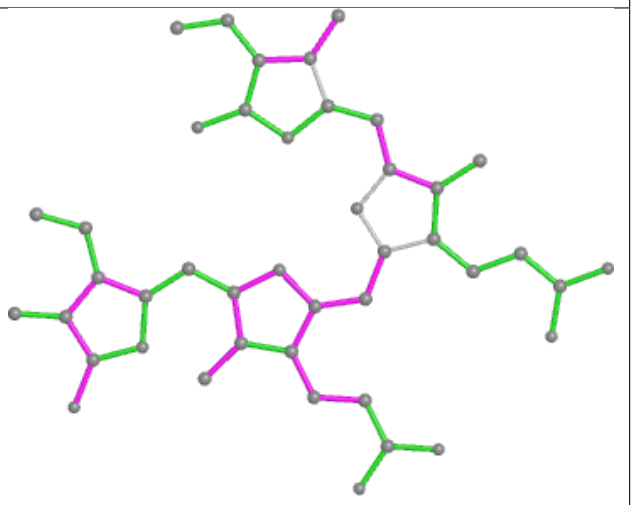
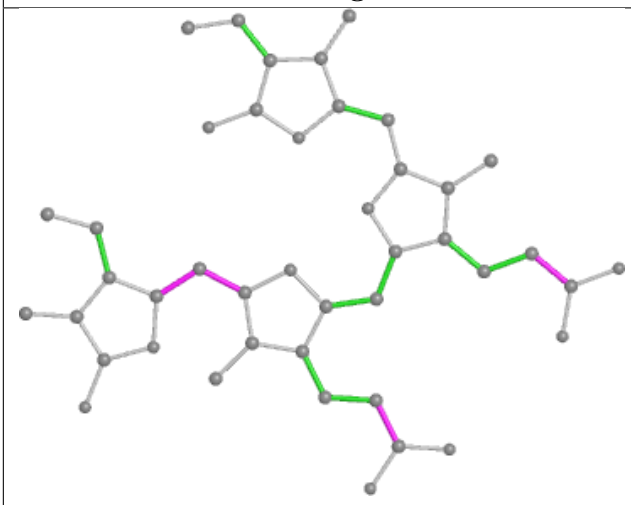
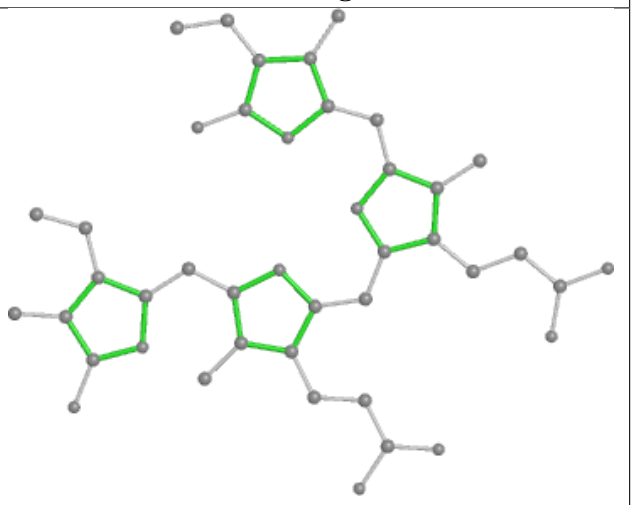


Bond angles

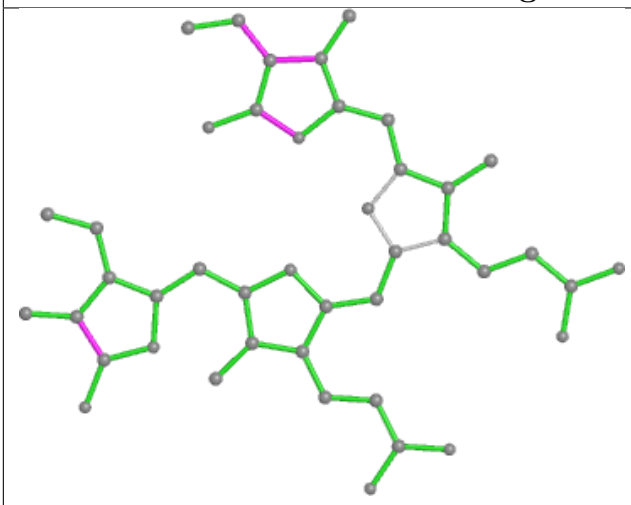


Torsions



Rings

Ligand PEB v8 202



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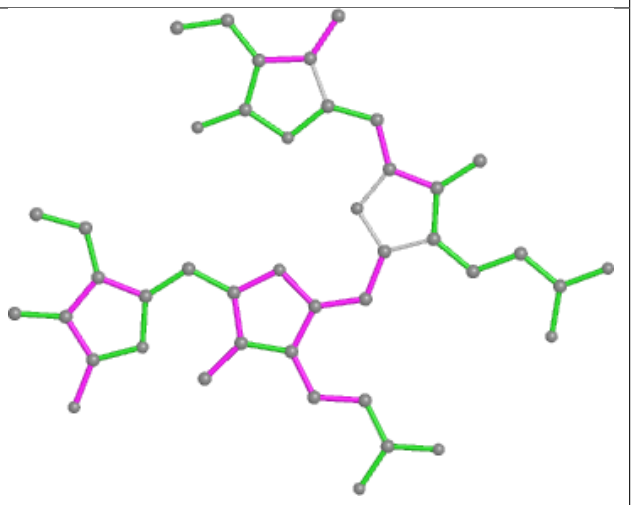
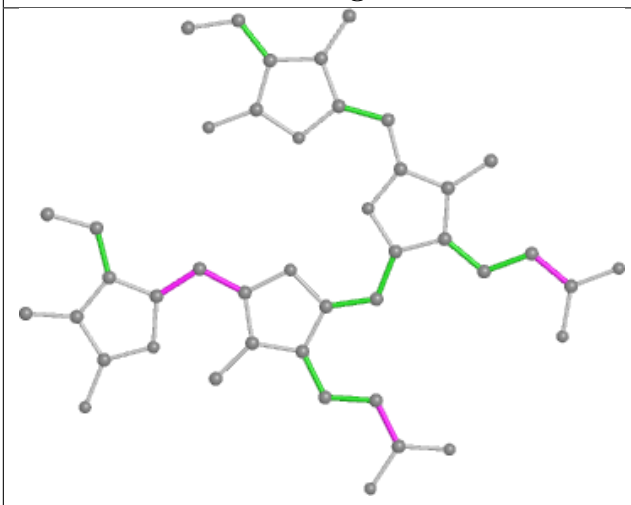


Bond angles



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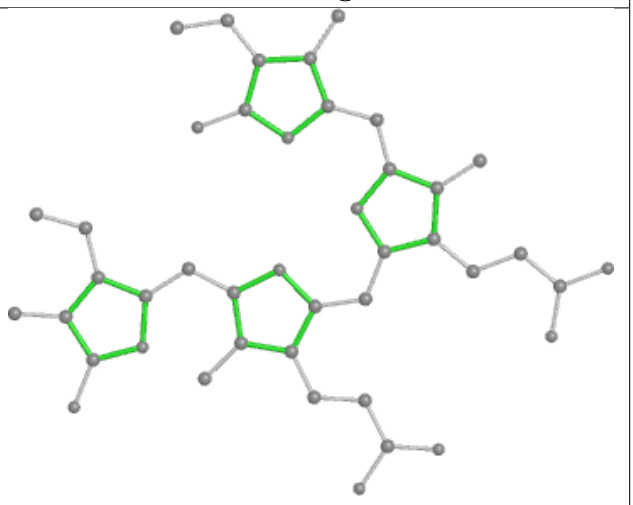
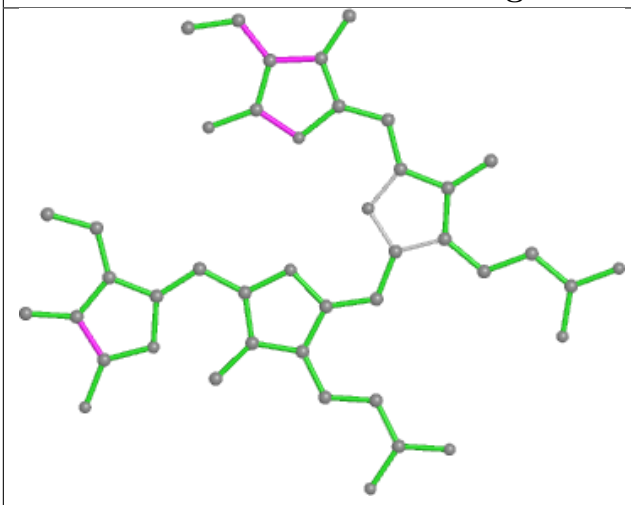


Rings

Ligand PEB U8 1001



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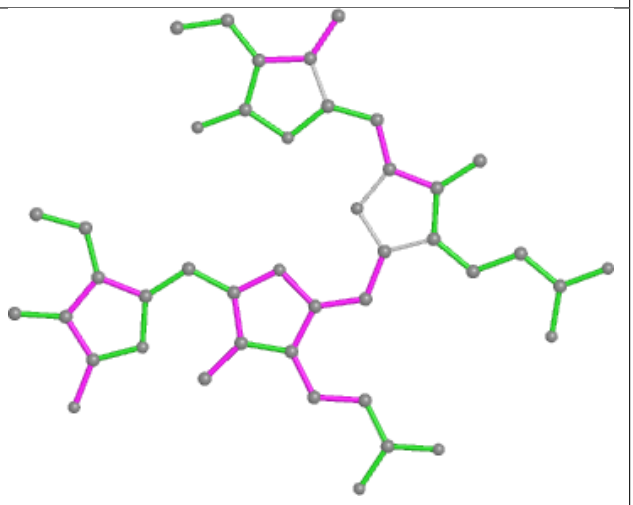

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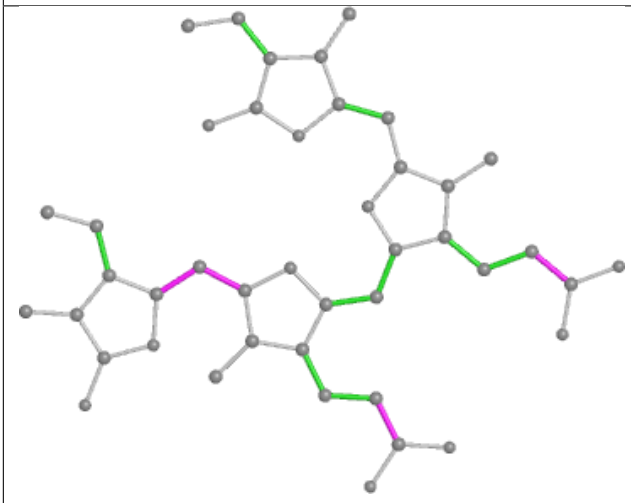

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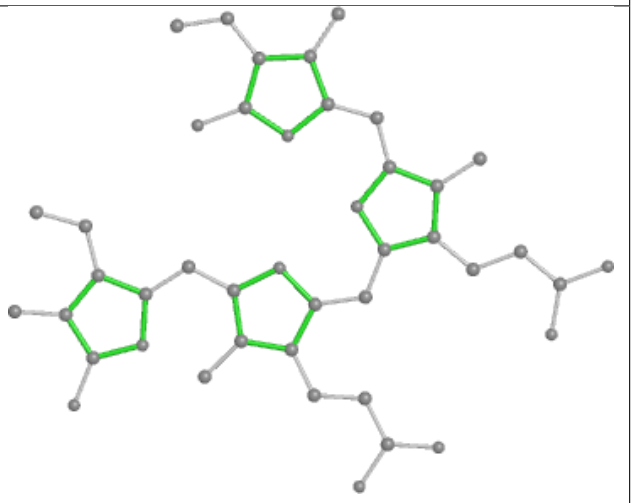
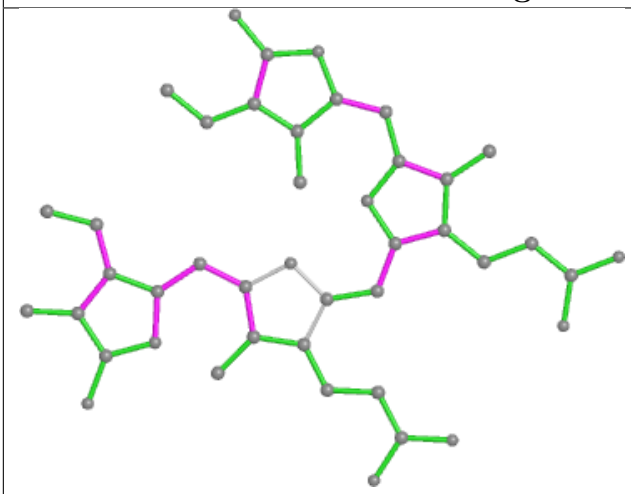


Rings

Ligand PVN hZ 403



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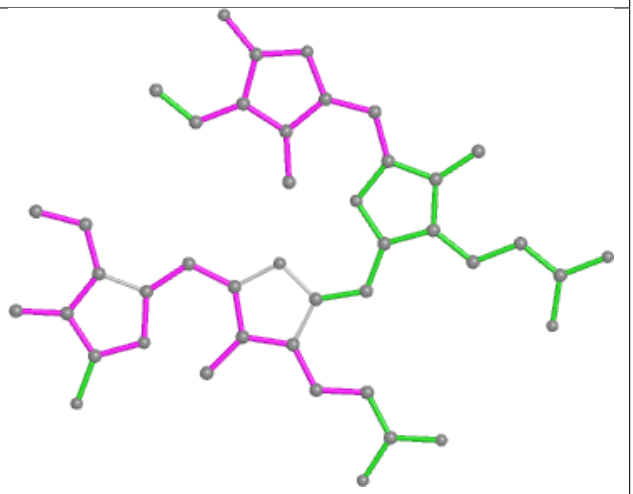

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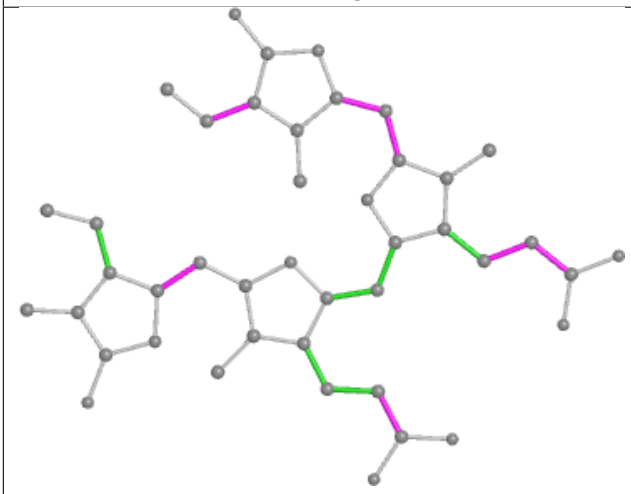

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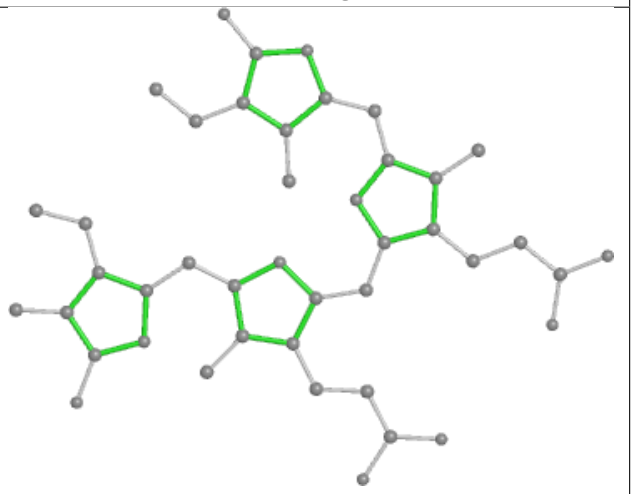
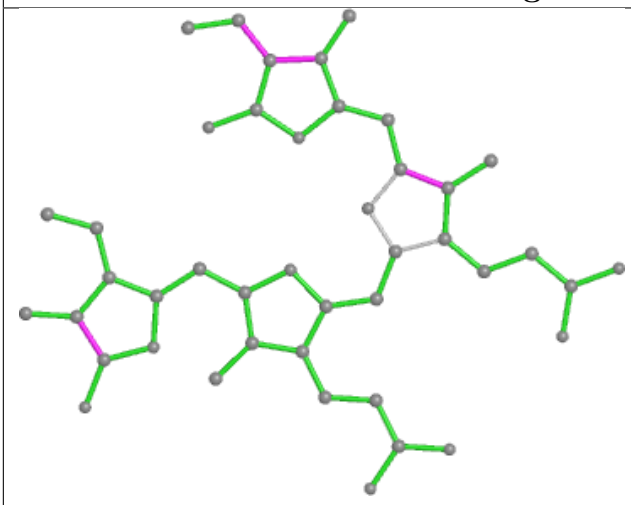


Rings

Ligand PEB lk 202



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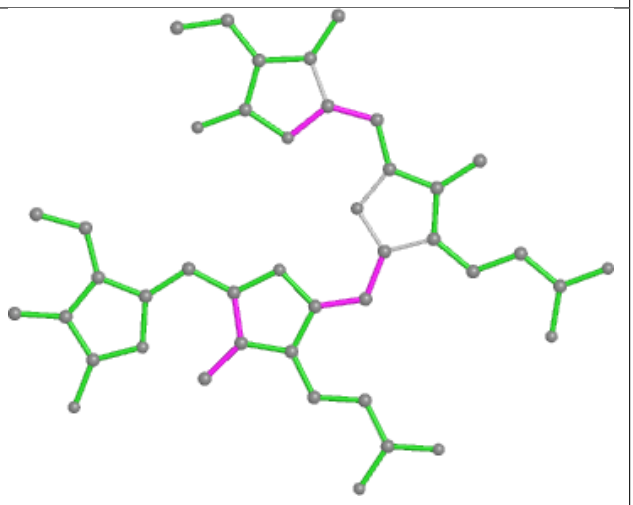

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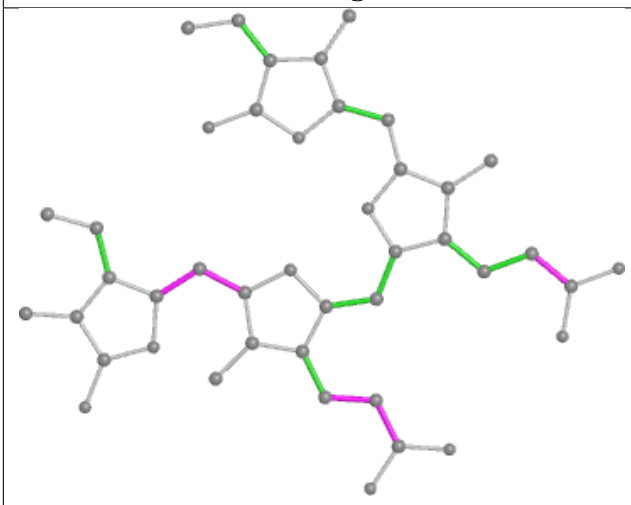

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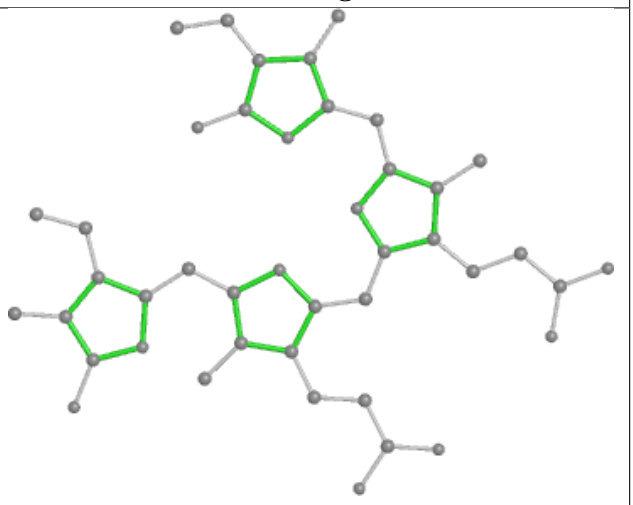

Rings

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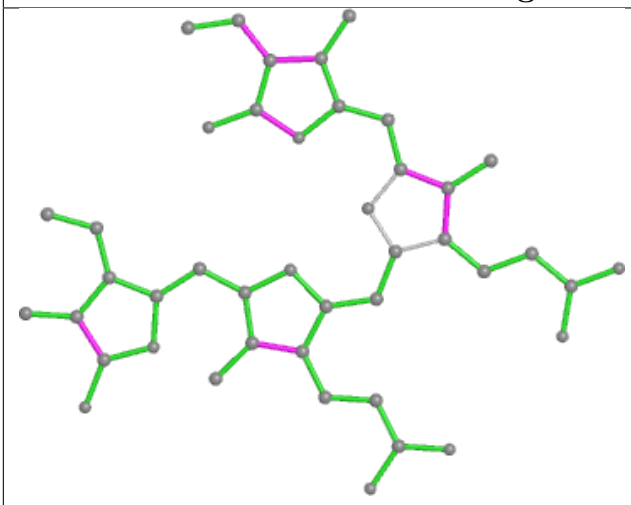

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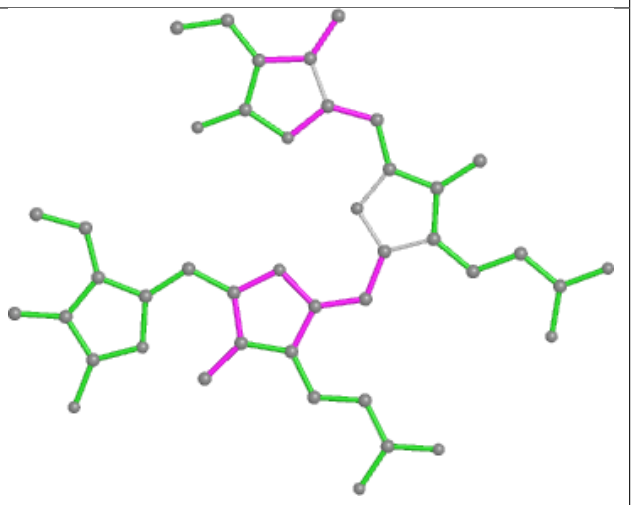

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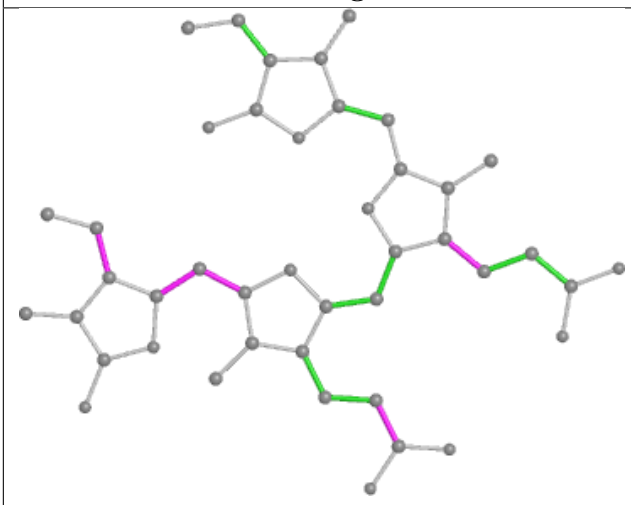

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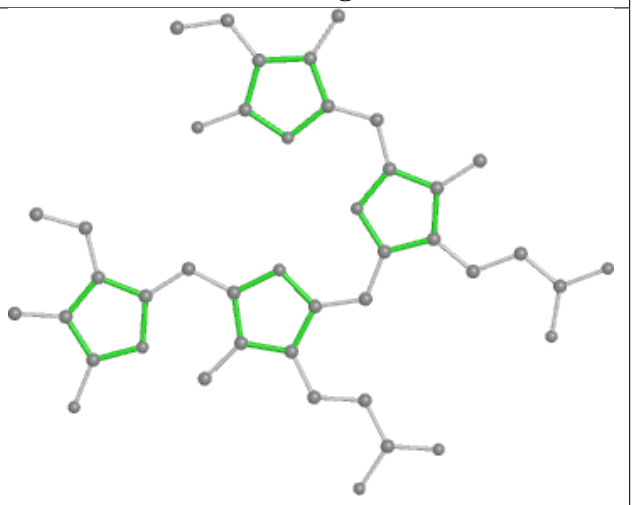

Rings

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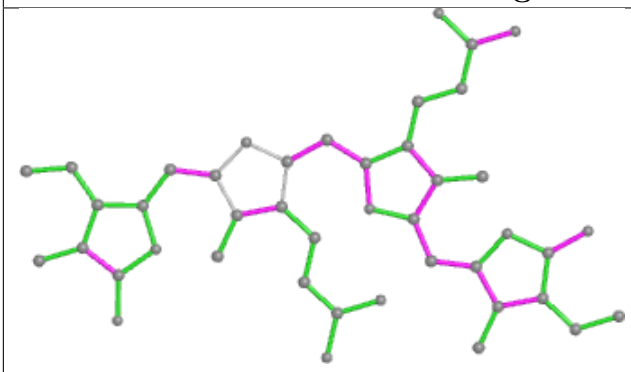

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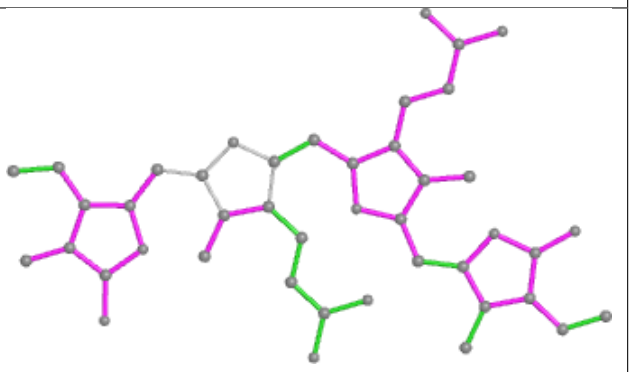

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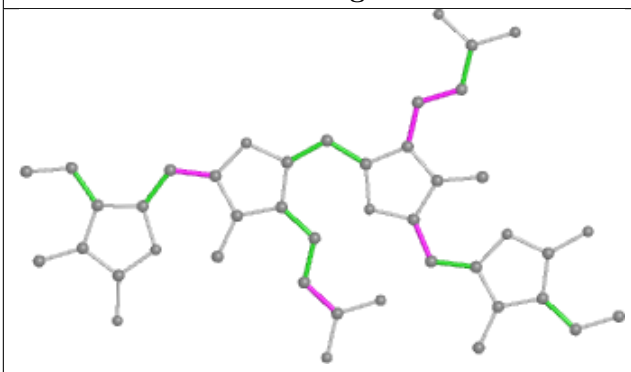

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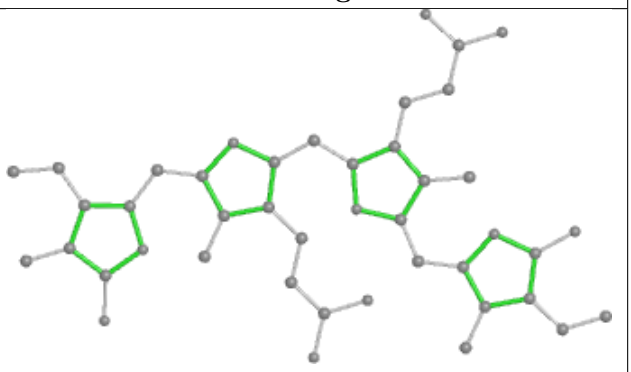
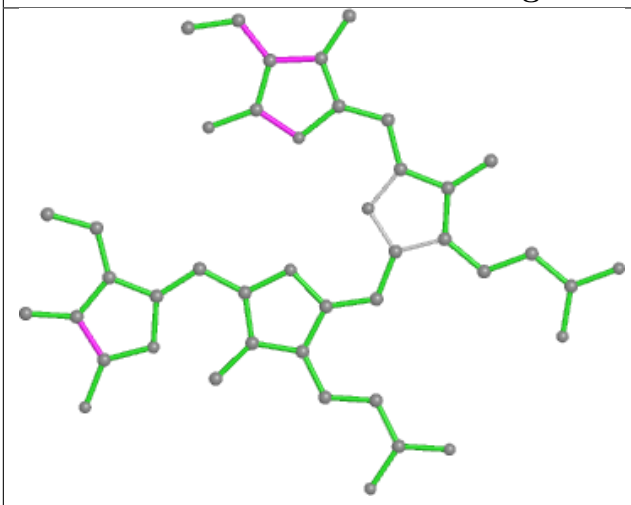


Rings

Ligand PEB aI 202



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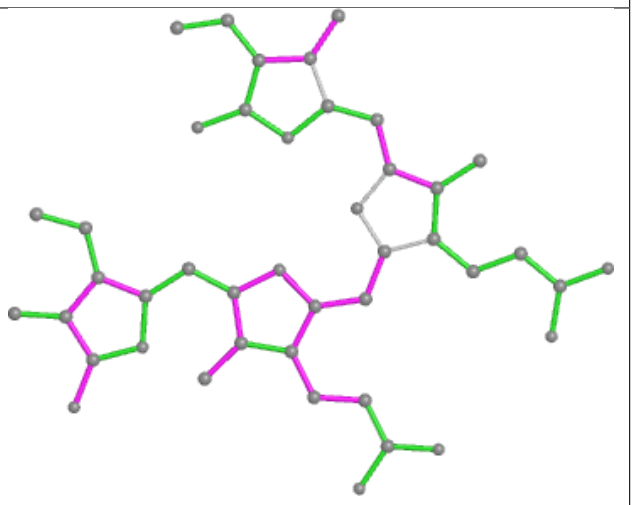

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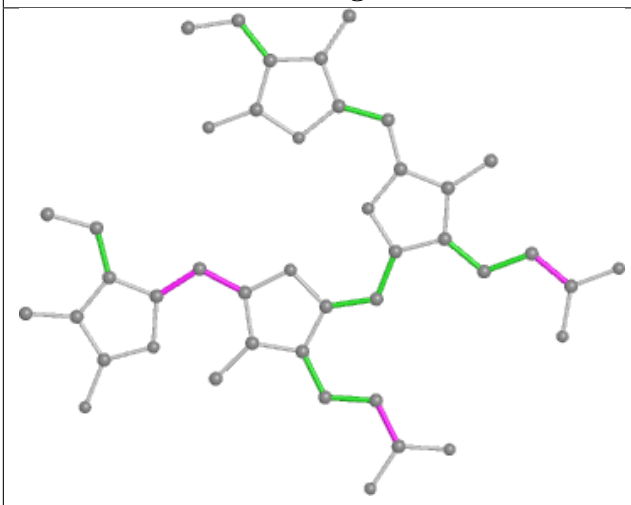

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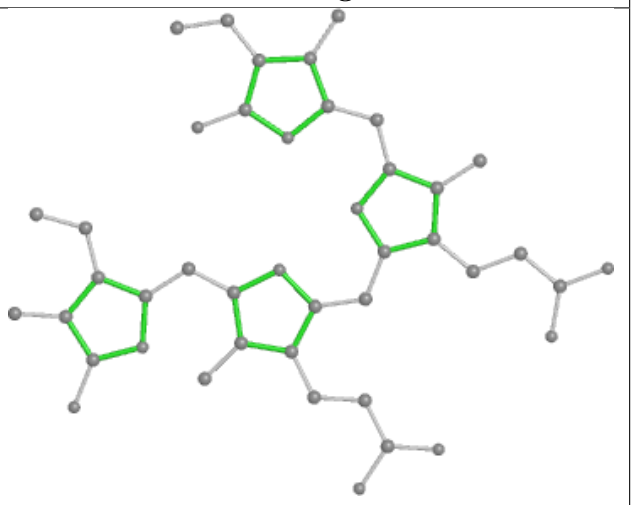
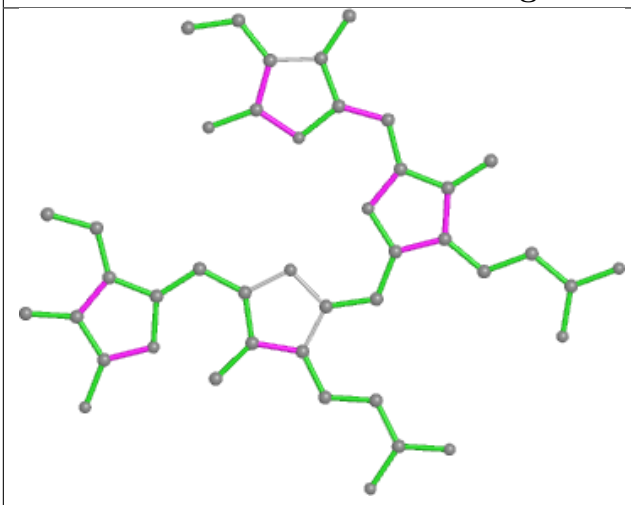


Rings

Ligand PUB t4 203



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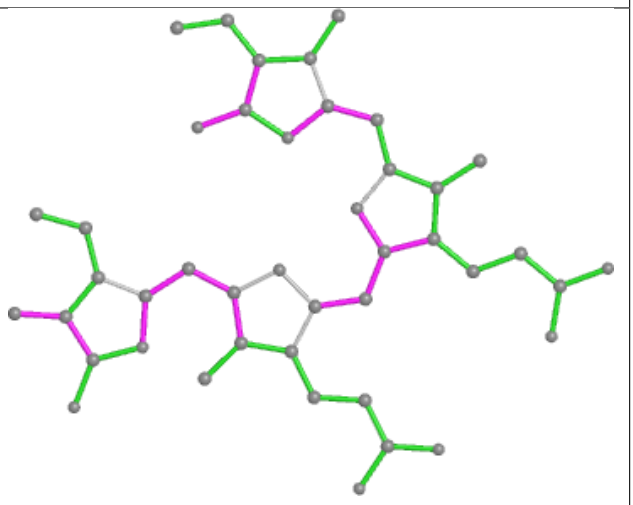

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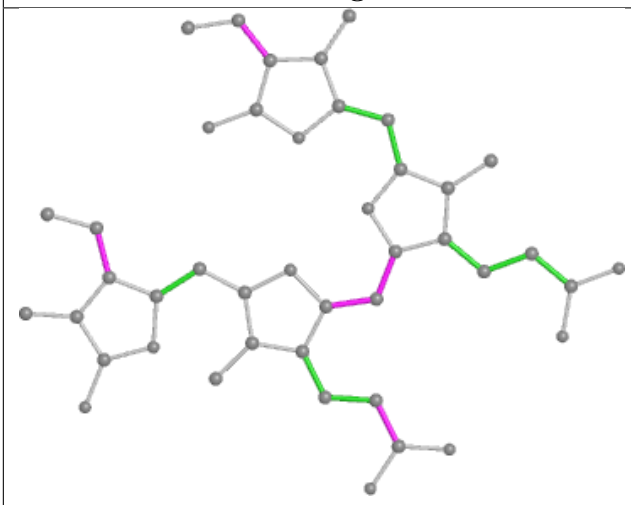

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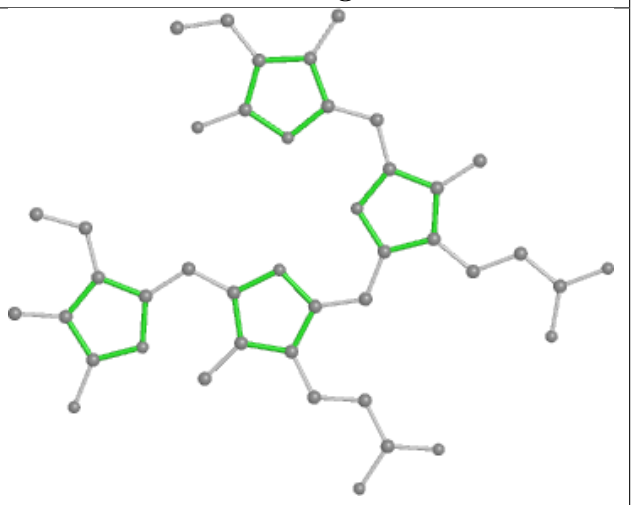

Rings

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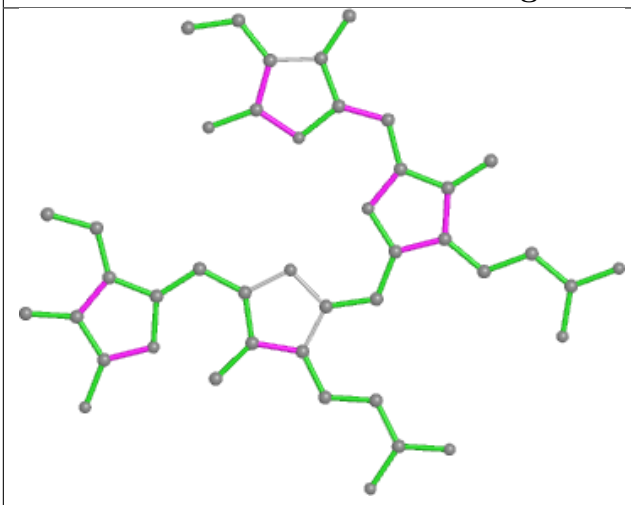

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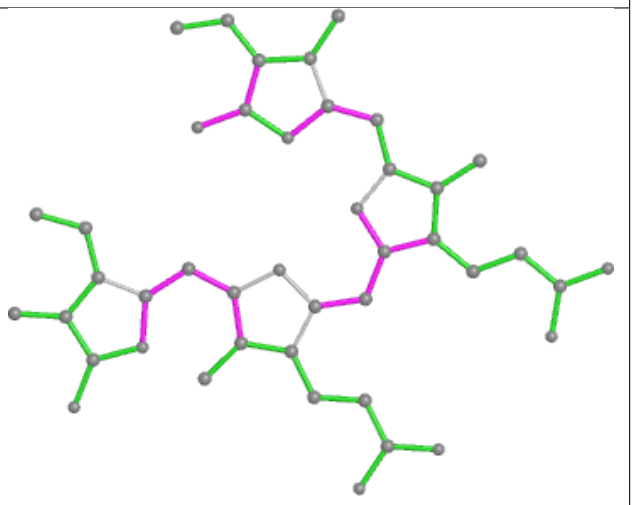

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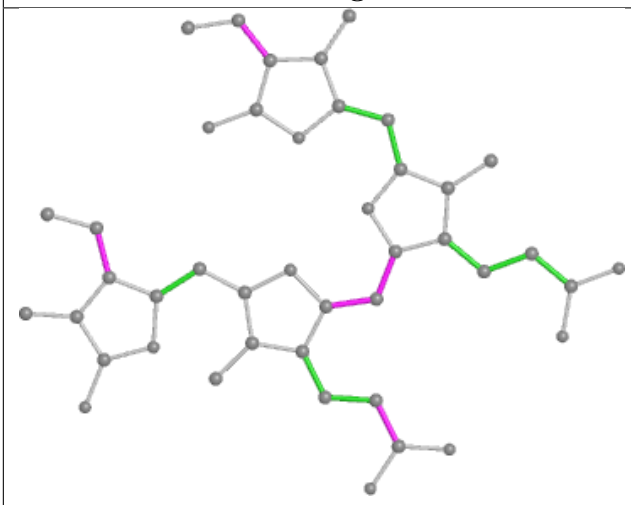

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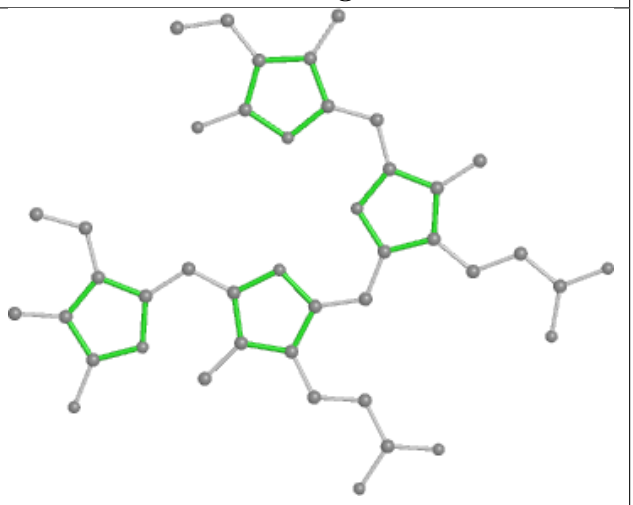
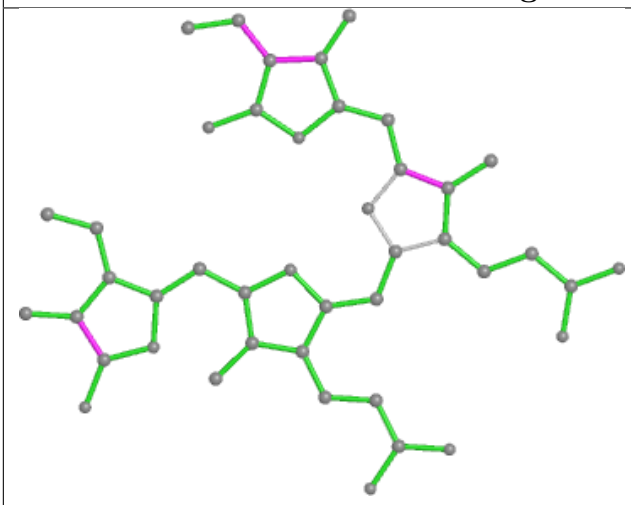


Rings

Ligand PEB ao 202



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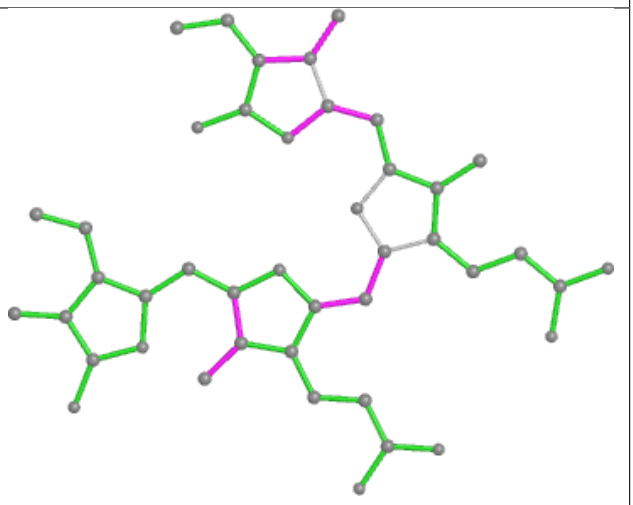

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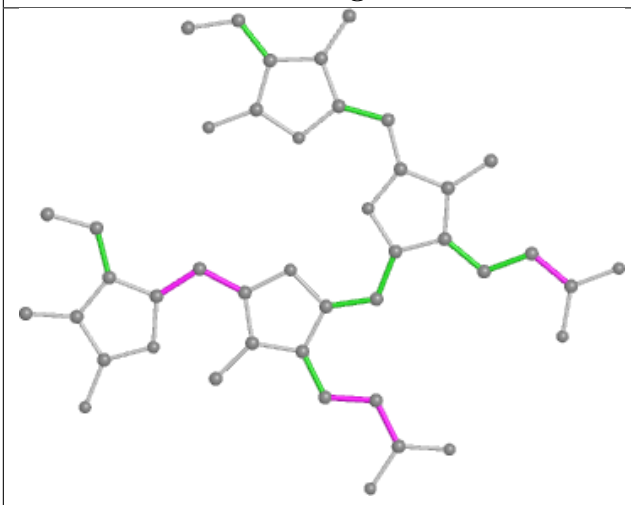

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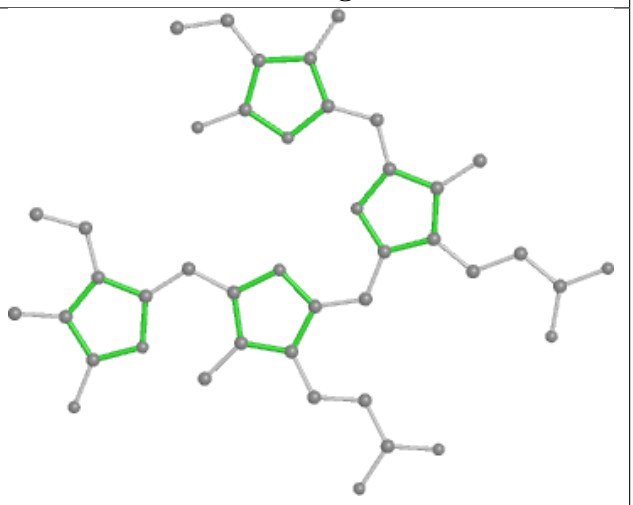

Rings

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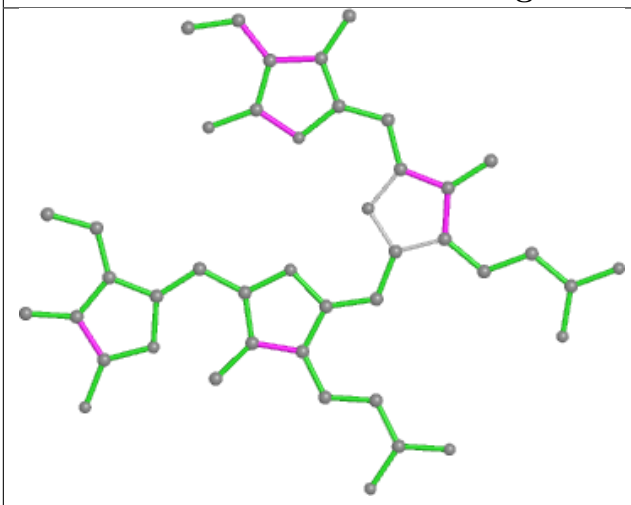

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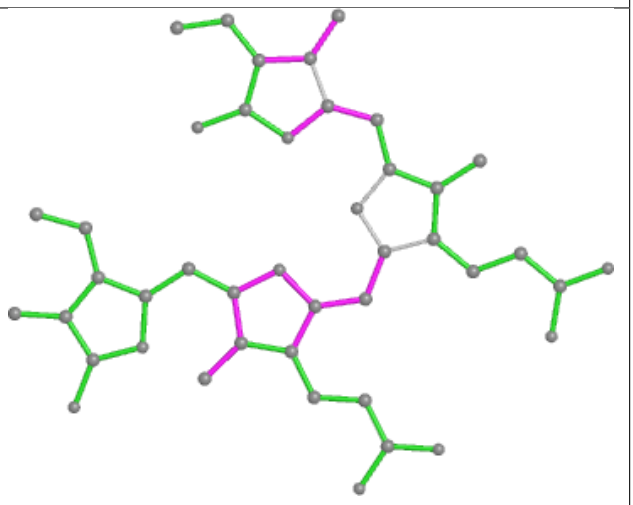

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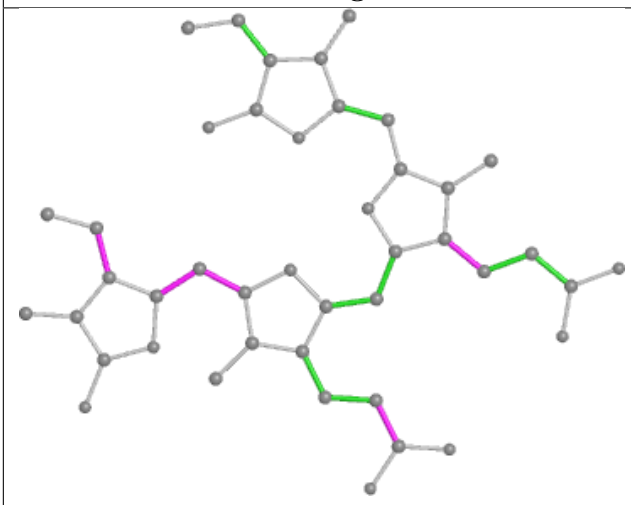

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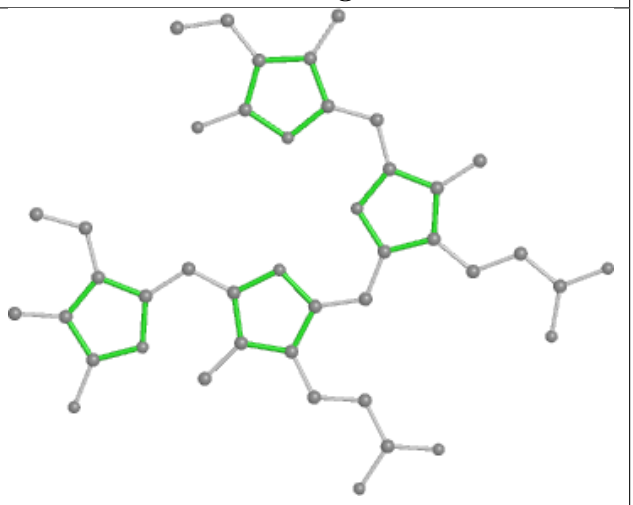
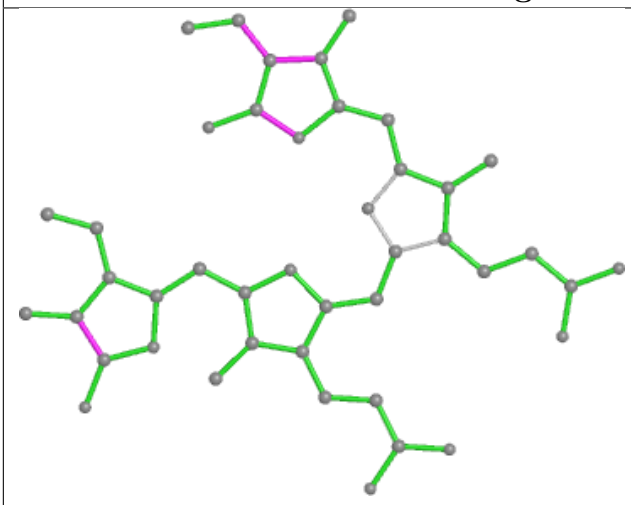


Rings

Ligand PEB H7 201



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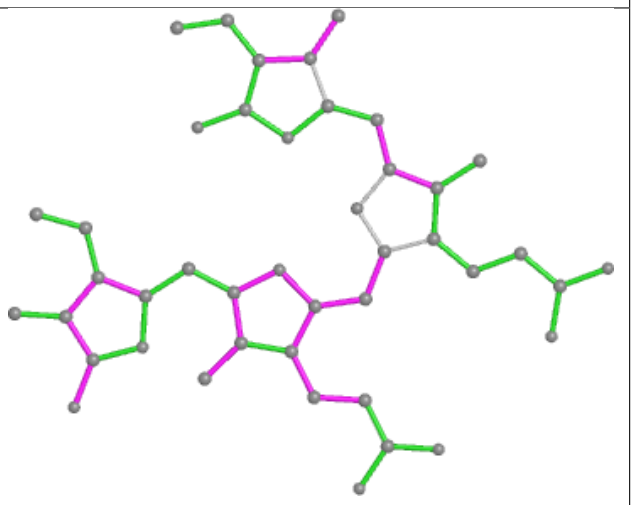

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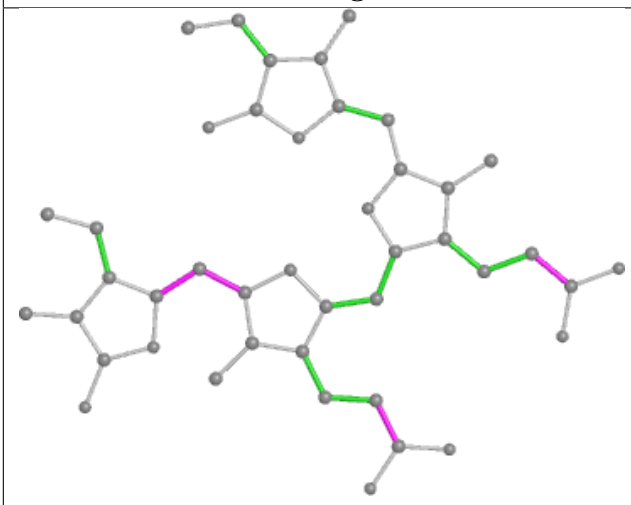

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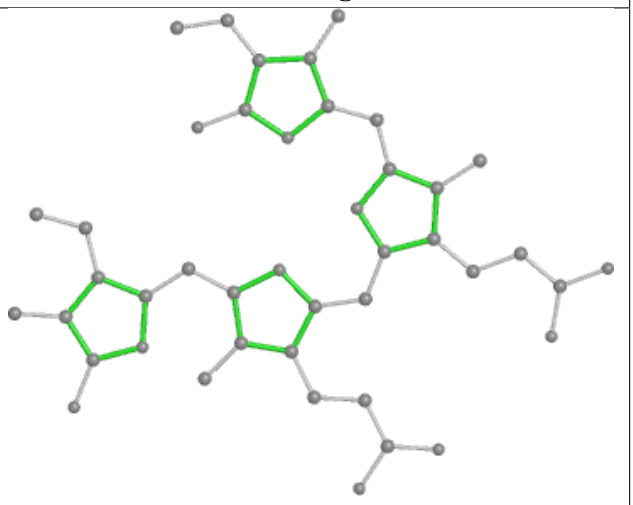
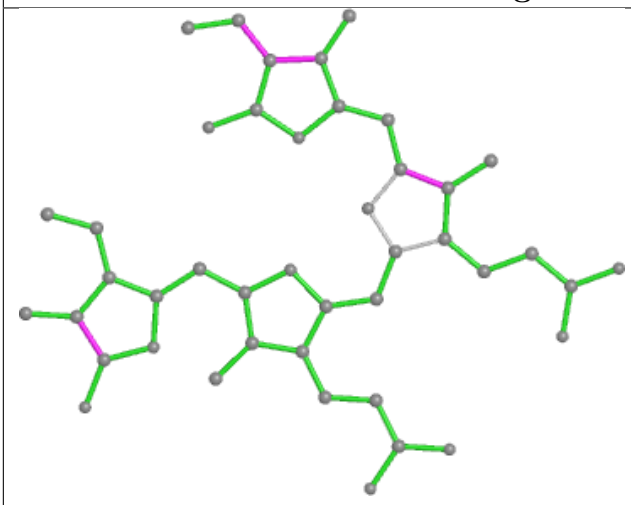


Rings

Ligand PEB m7 202



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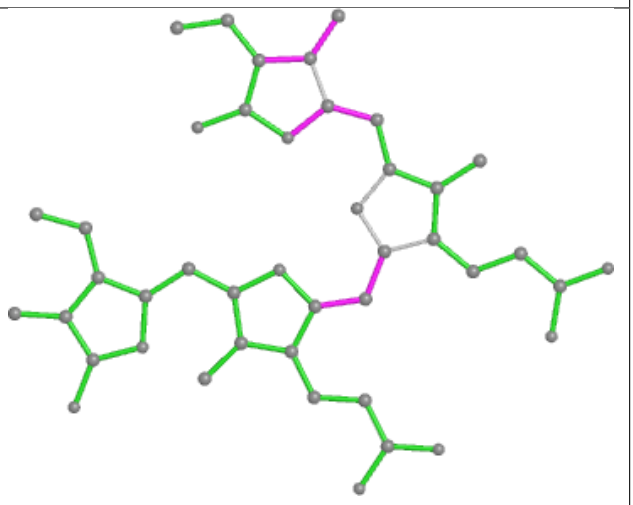

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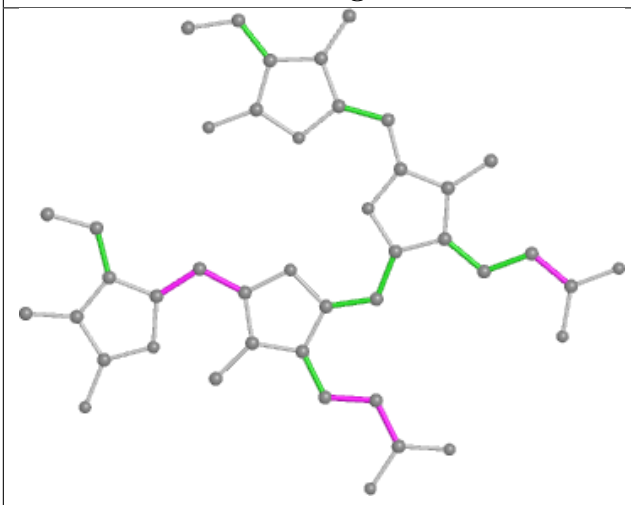

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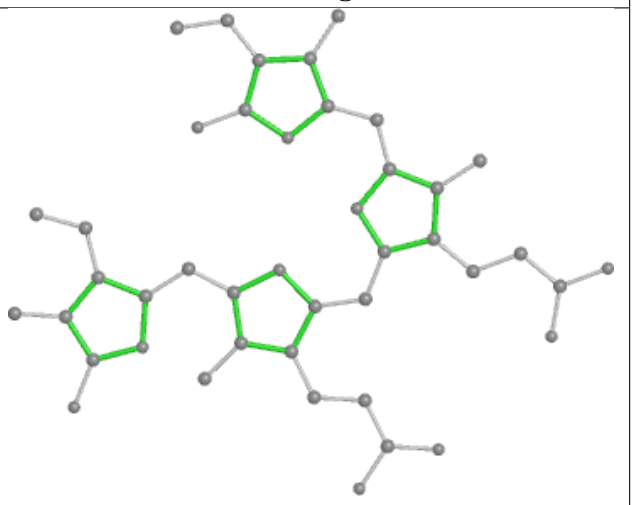
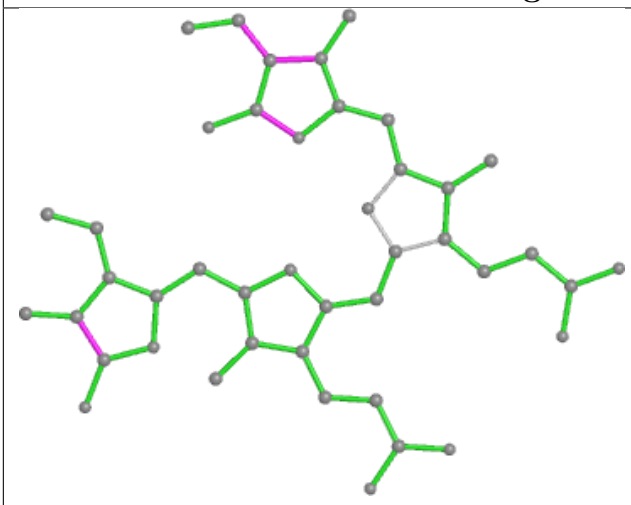
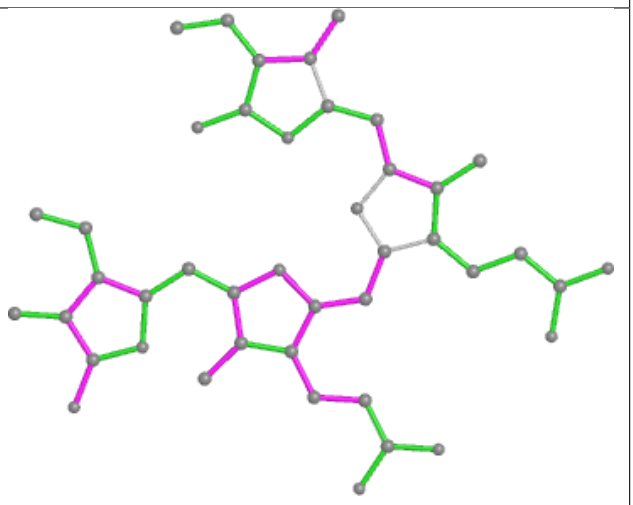


Rings

Ligand PEB f8 201



Bond lengths



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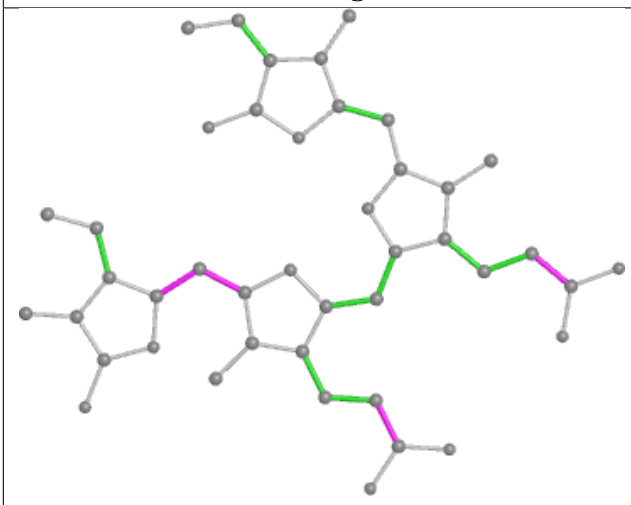
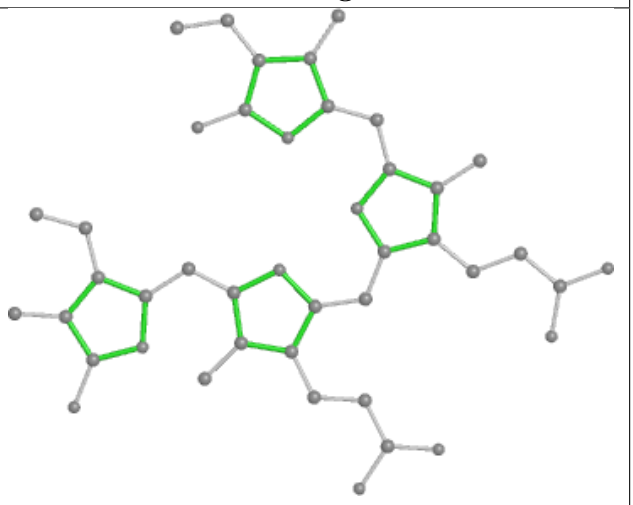
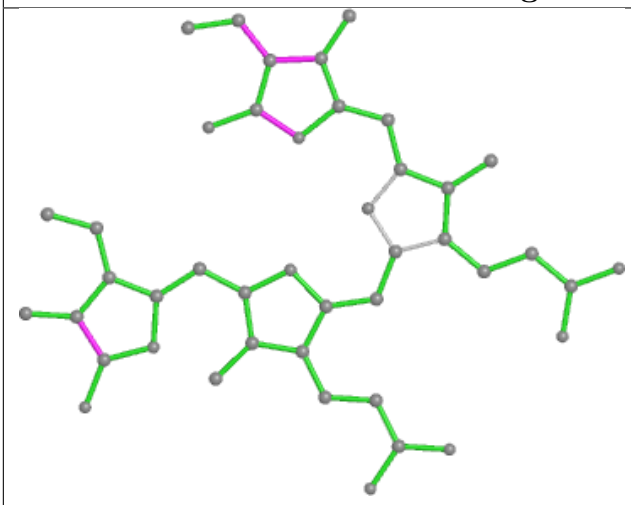


Torsions



Rings

Ligand PEB z9 201



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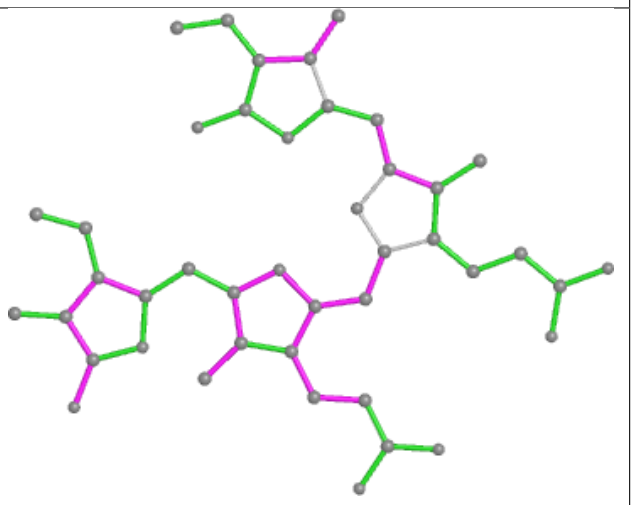

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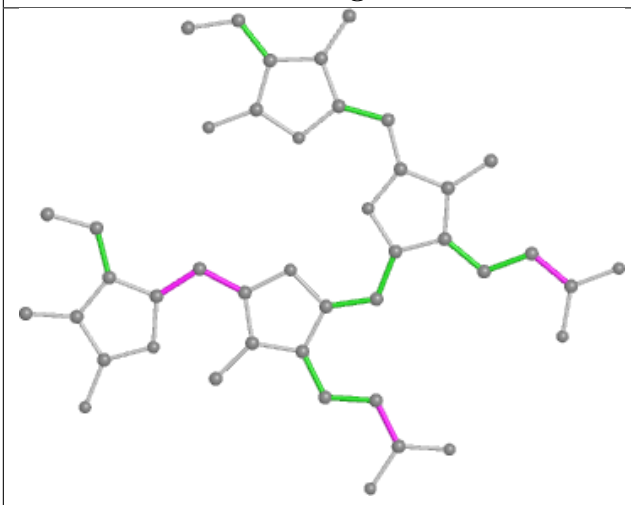

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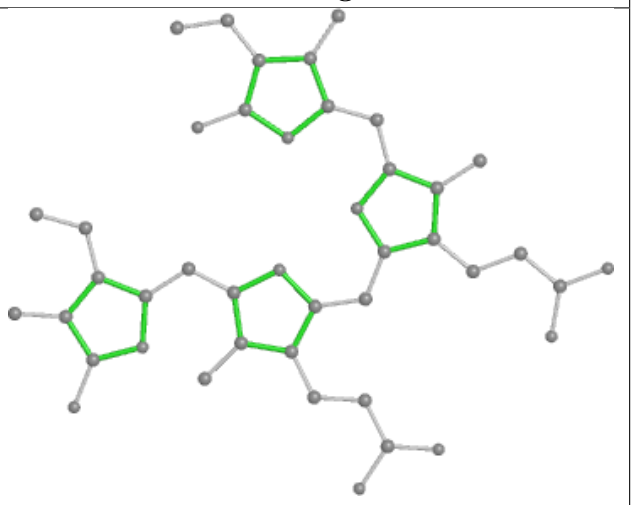
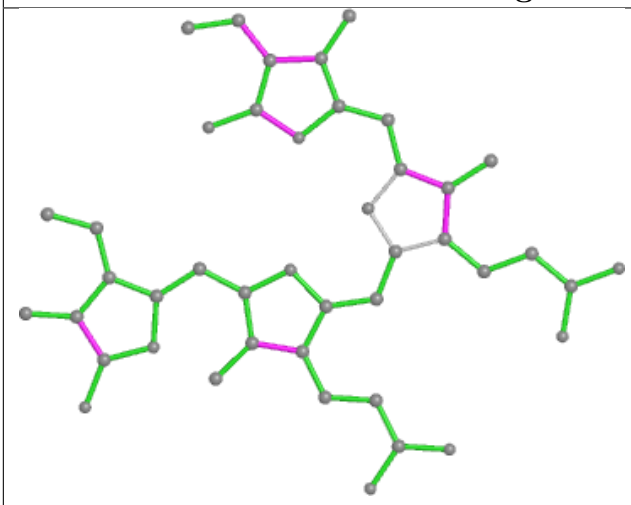


Rings

Ligand PEB X2 202



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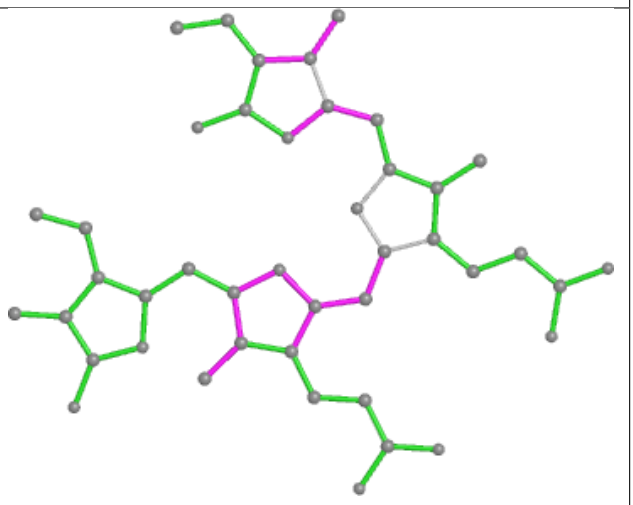

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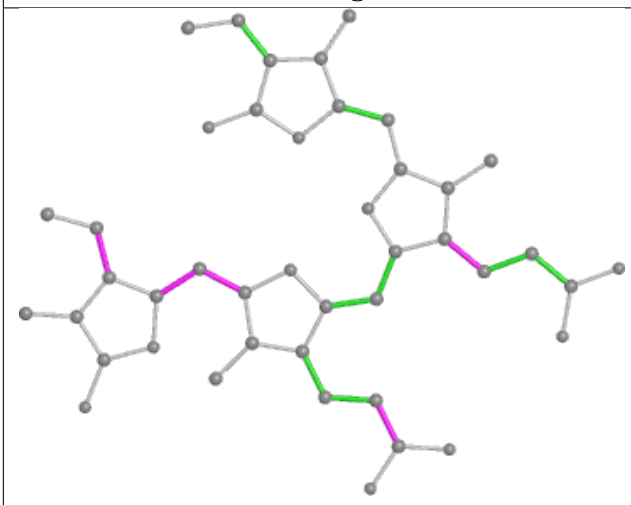

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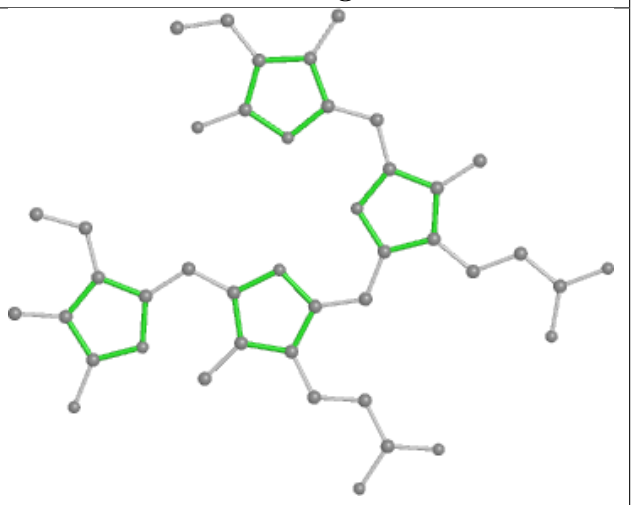

Rings

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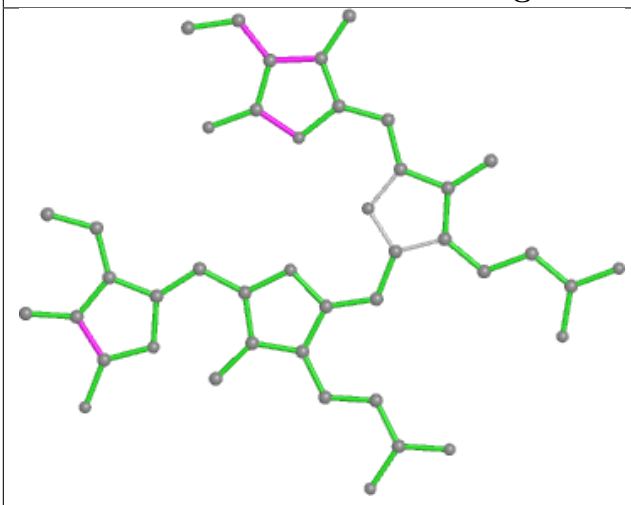

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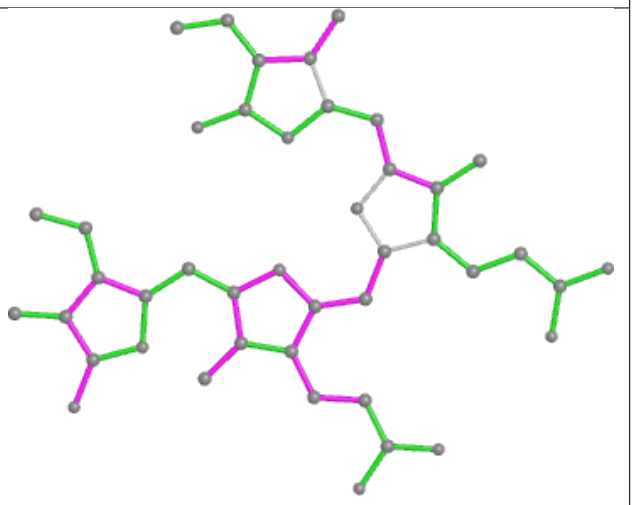

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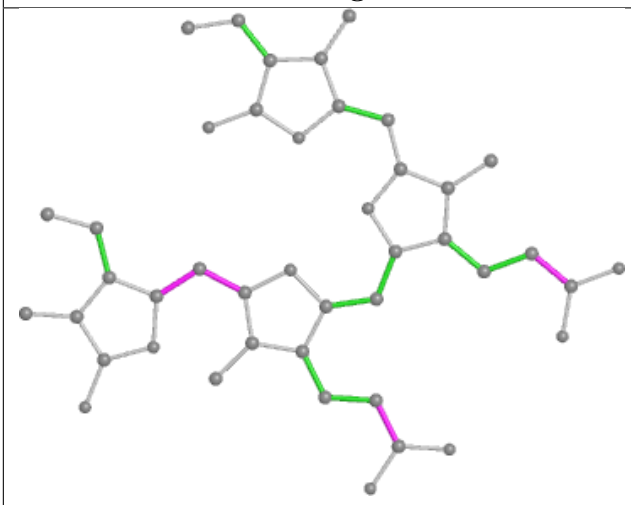

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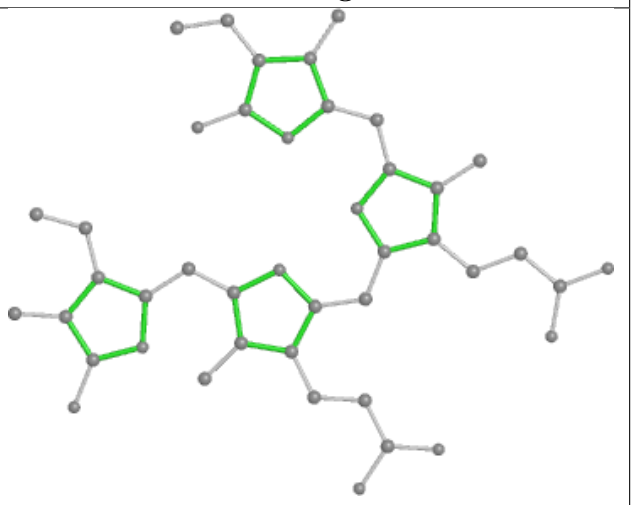

Rings

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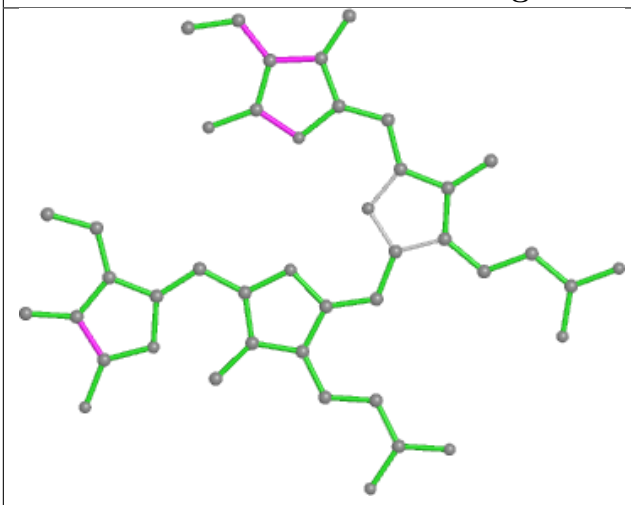

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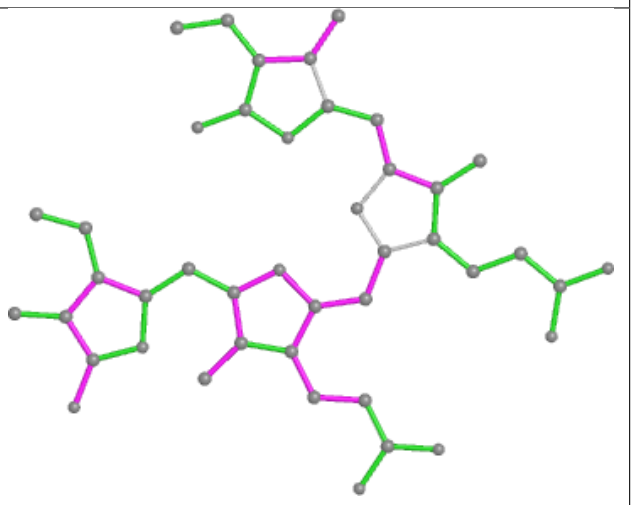

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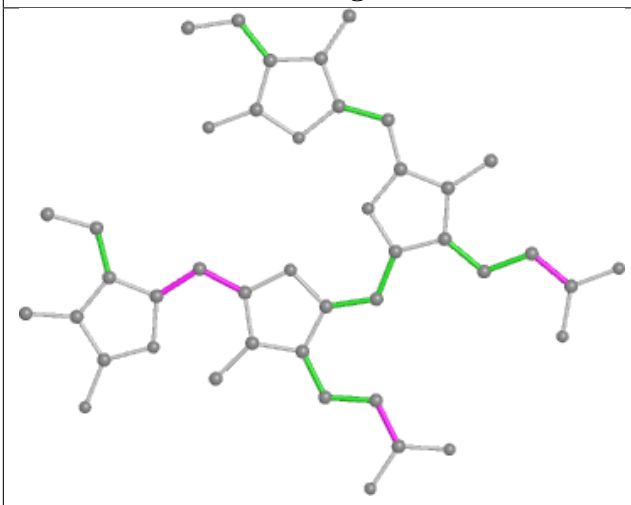

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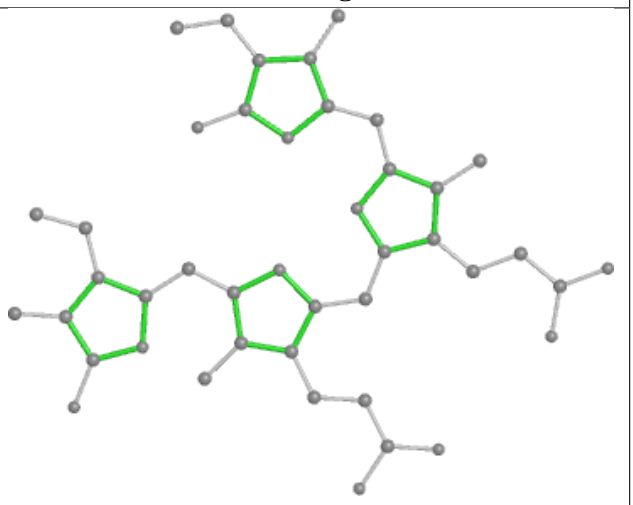
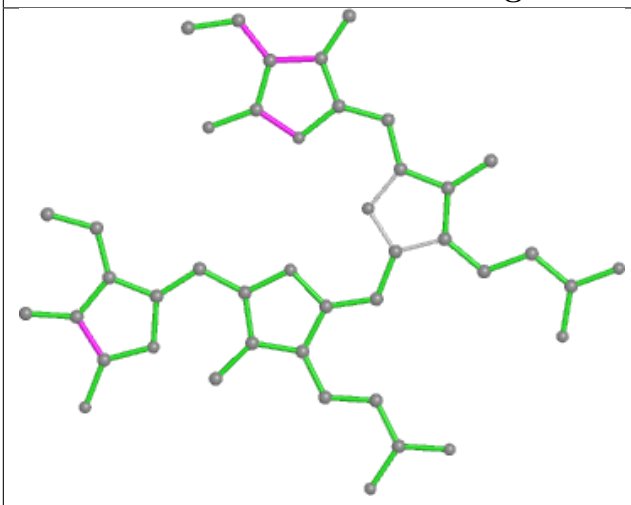


Rings

Ligand PEB m9 1001



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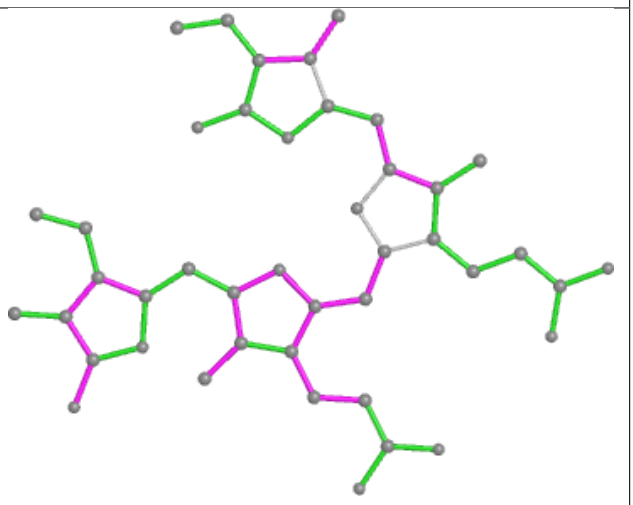

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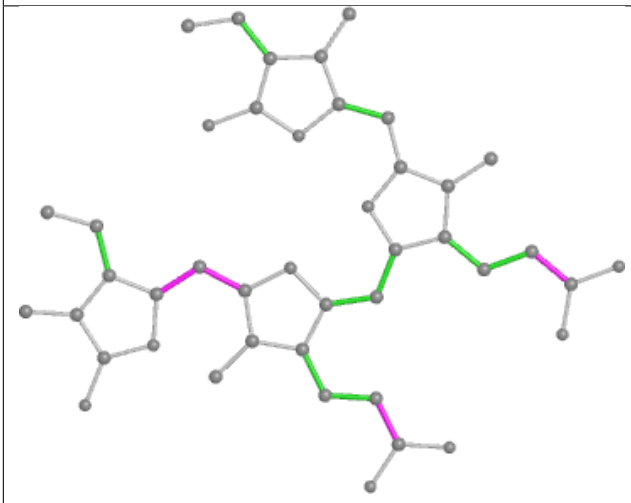

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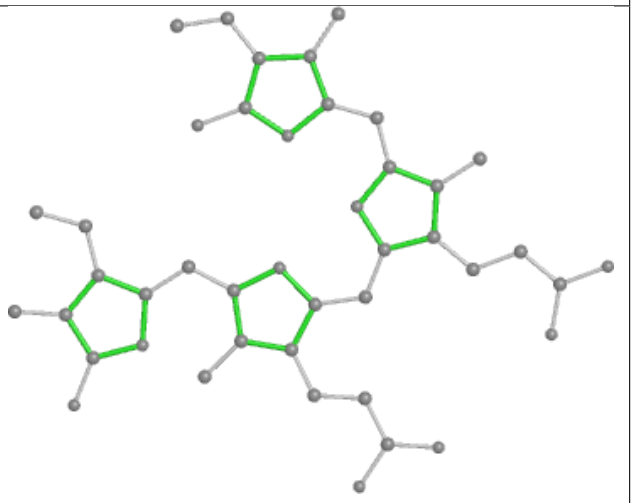

Rings

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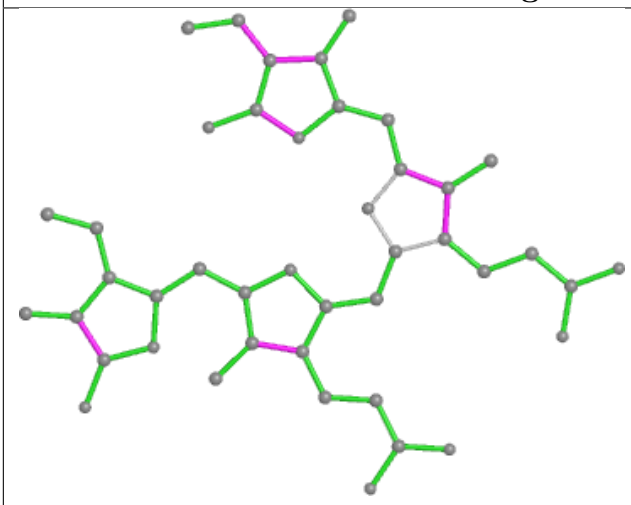

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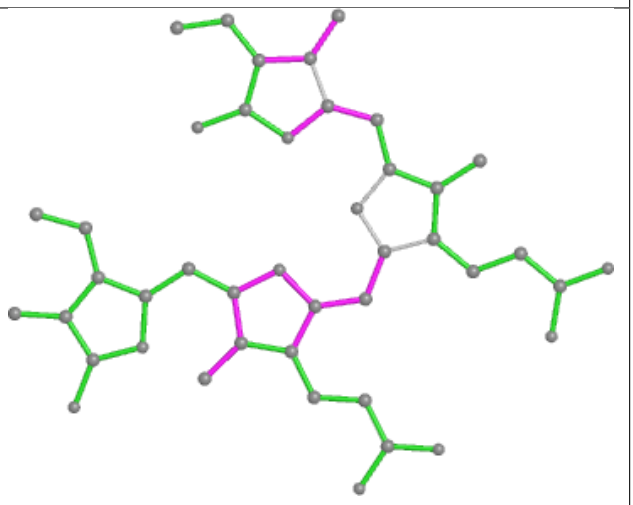

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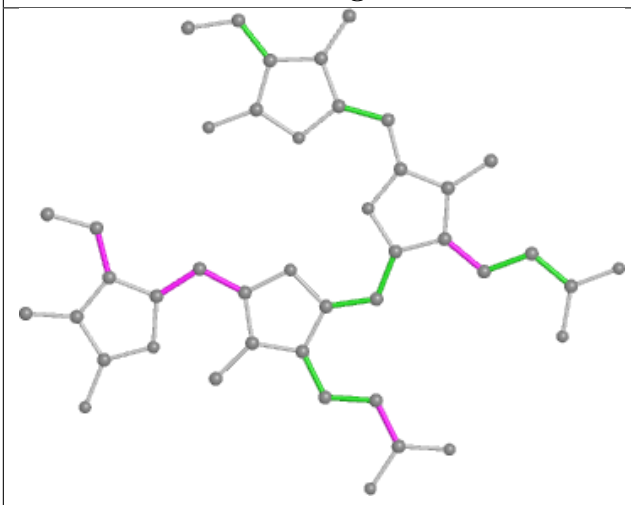

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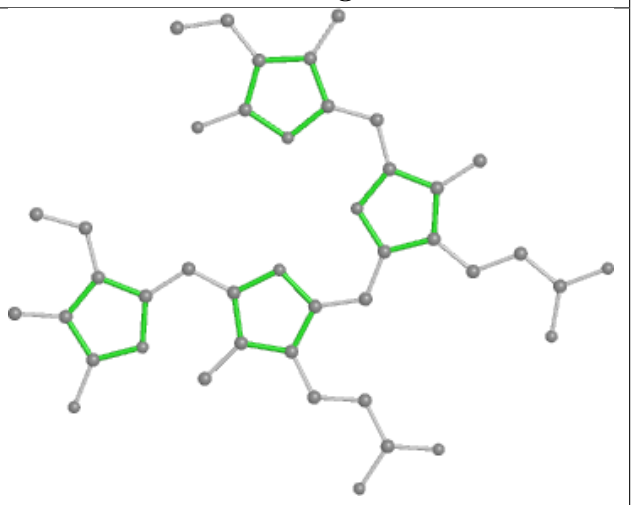

Rings

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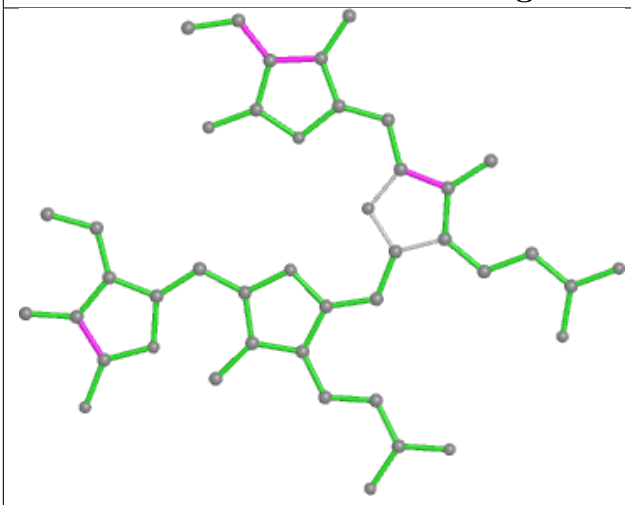

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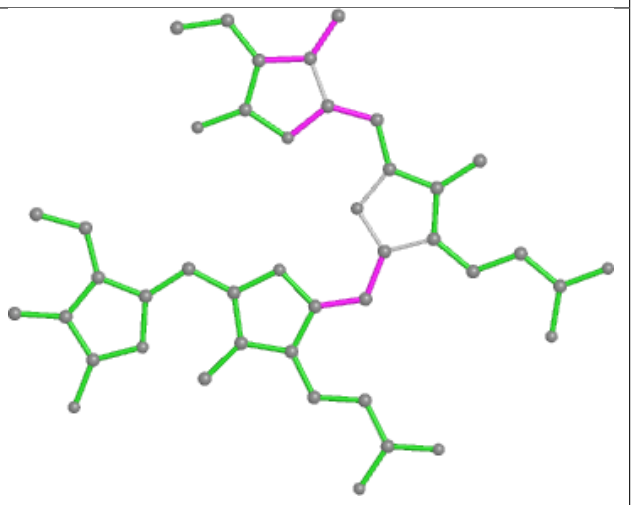

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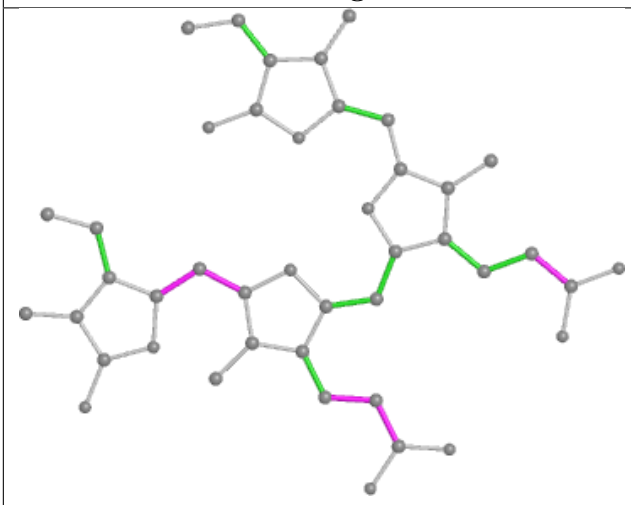

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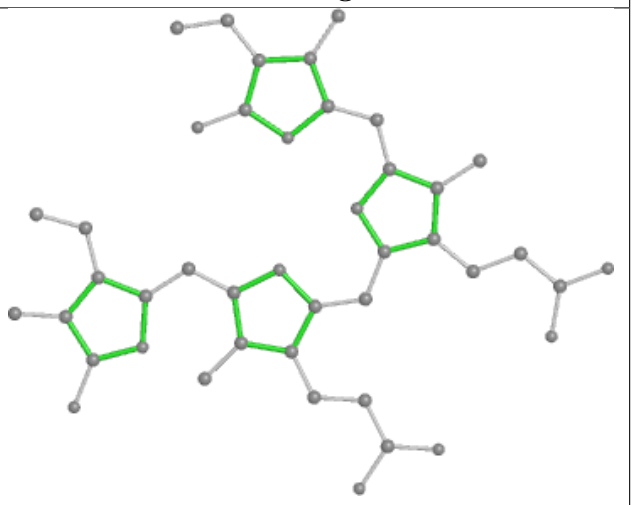

Rings

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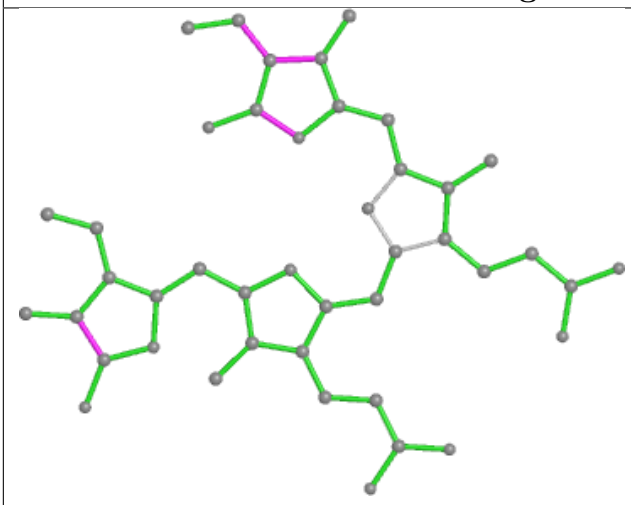

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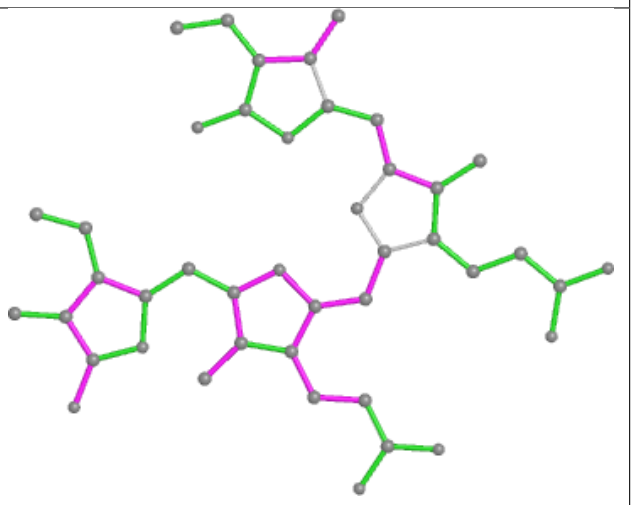

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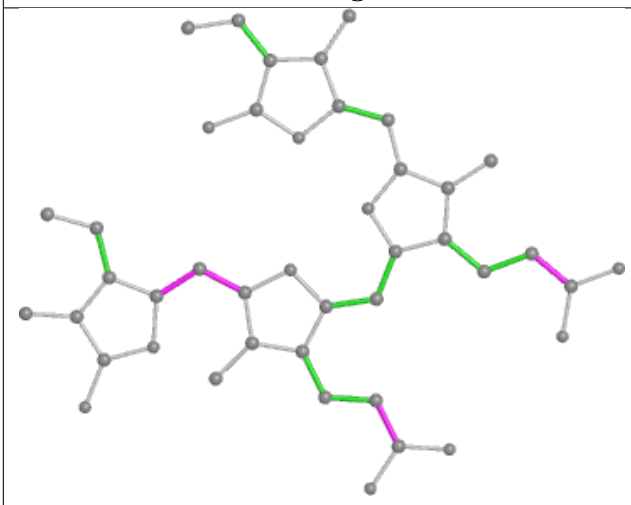

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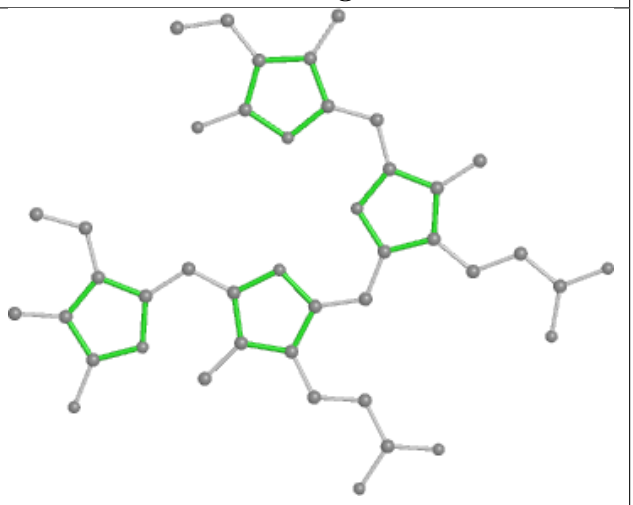

Rings

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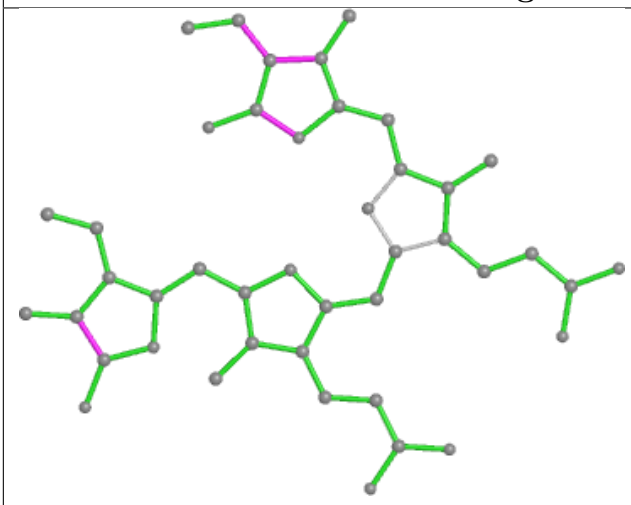

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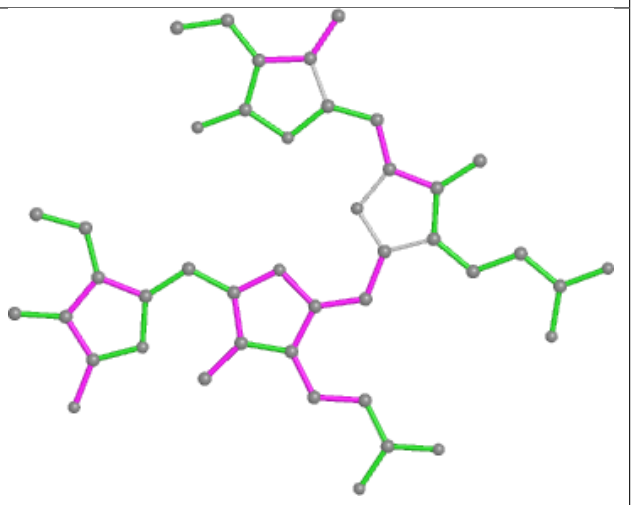

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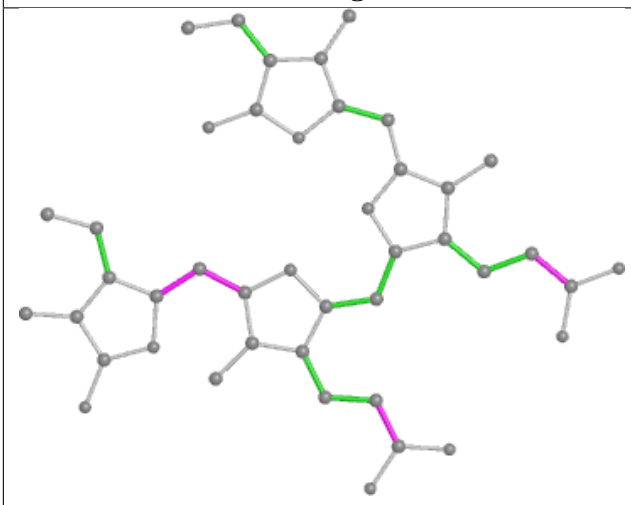

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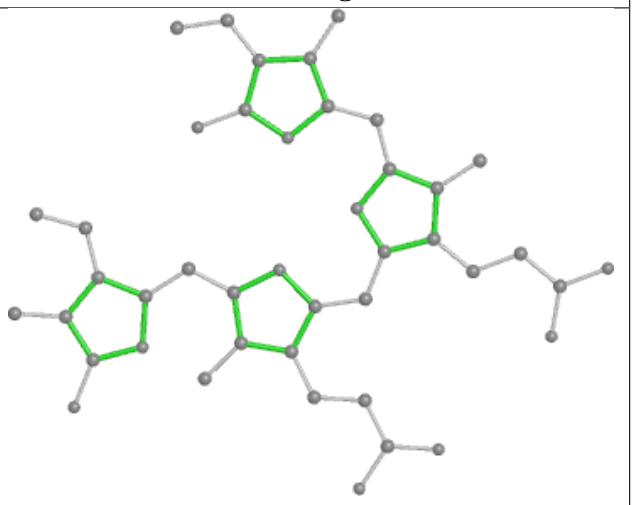
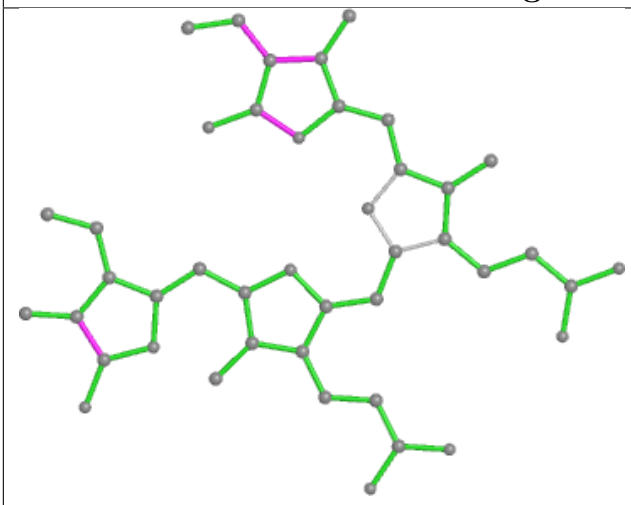


Rings

Ligand PEB j6 201



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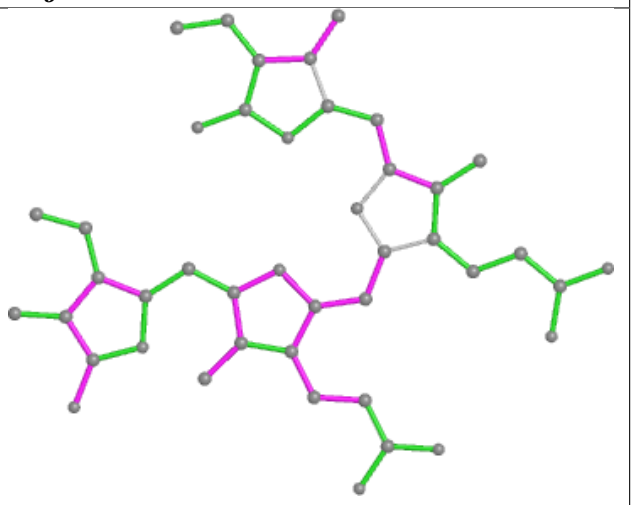

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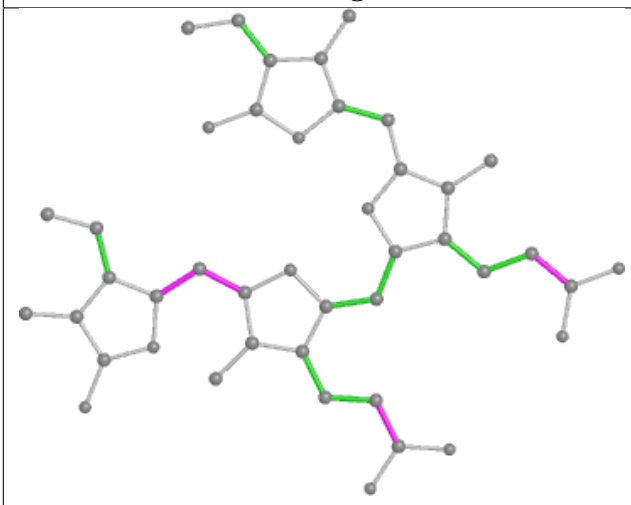

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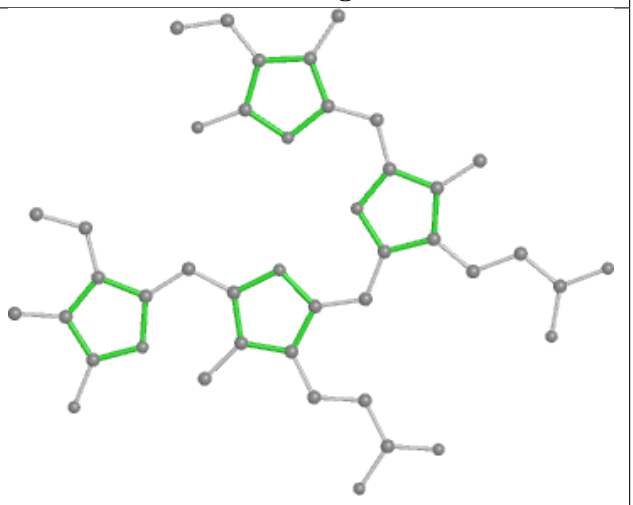
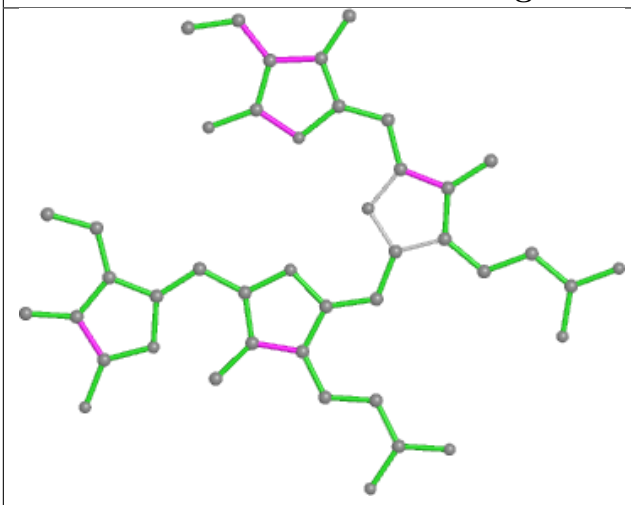


Rings

Ligand PEB D9 202



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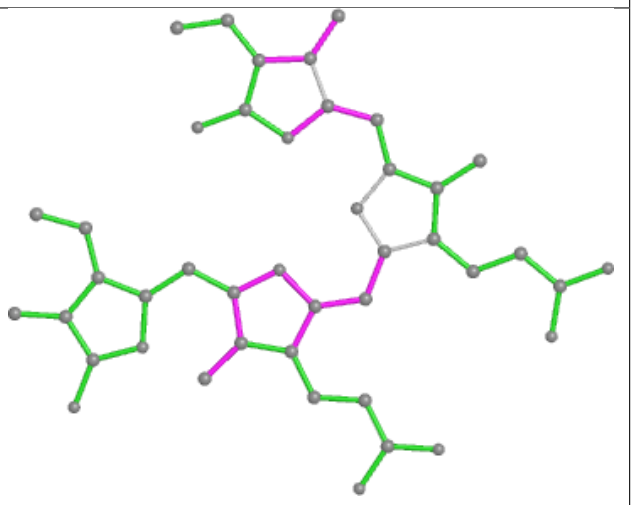

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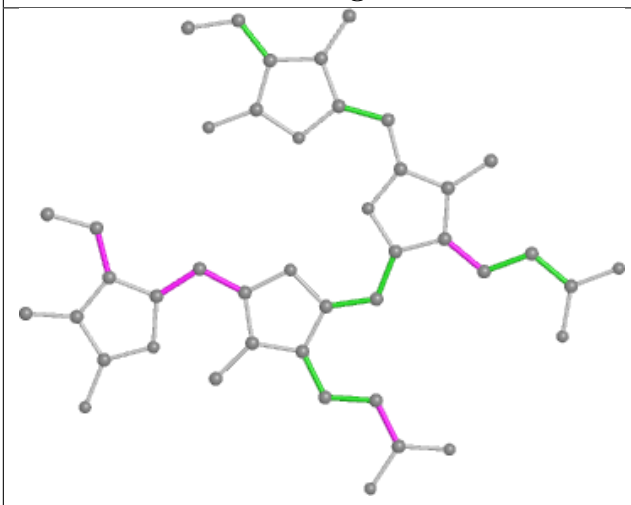

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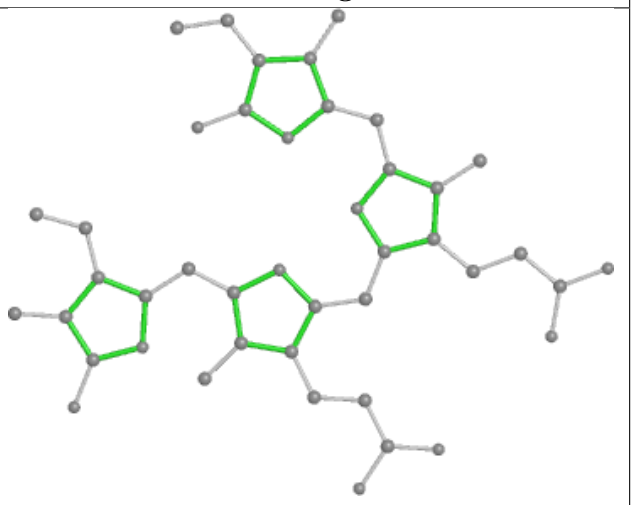
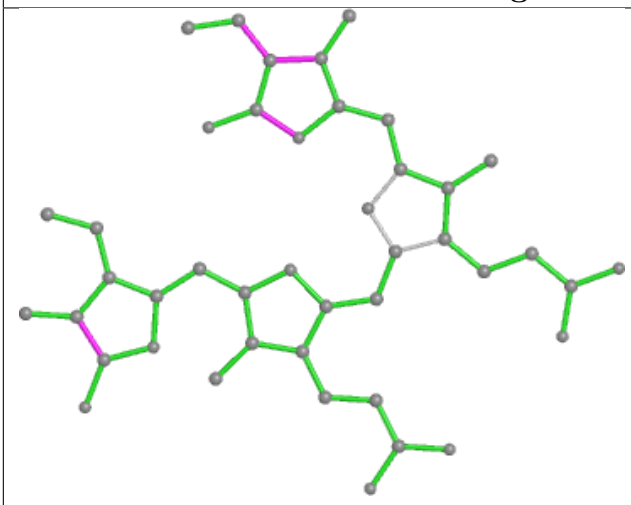


Rings

Ligand PEB y4 1002



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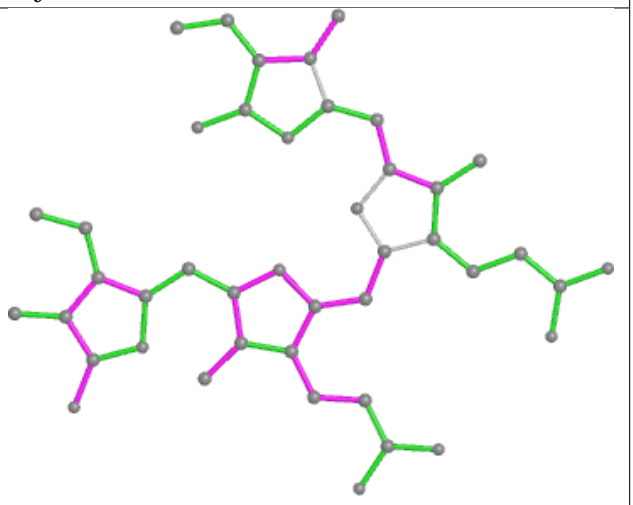

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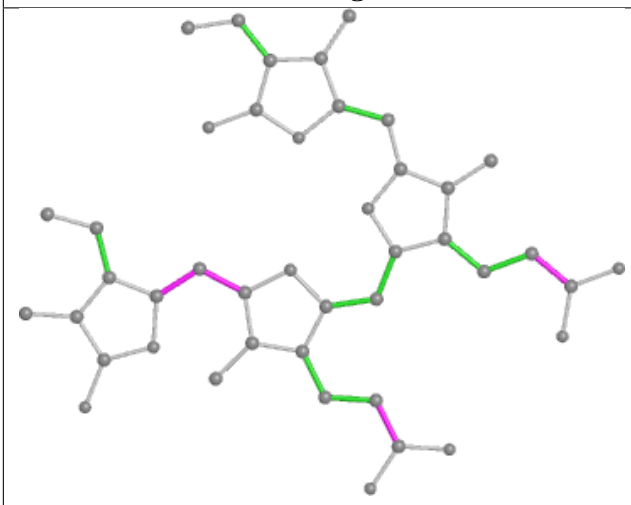

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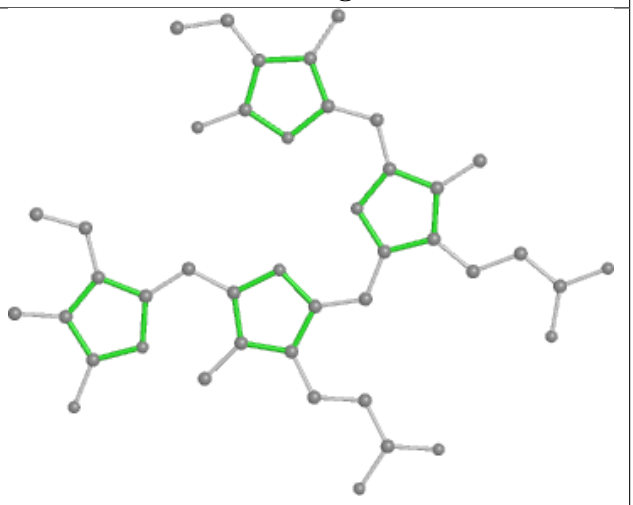
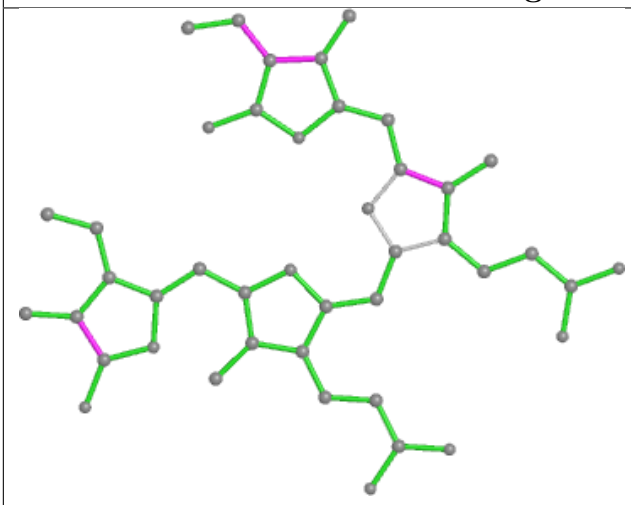


Rings

Ligand PEB ei 201



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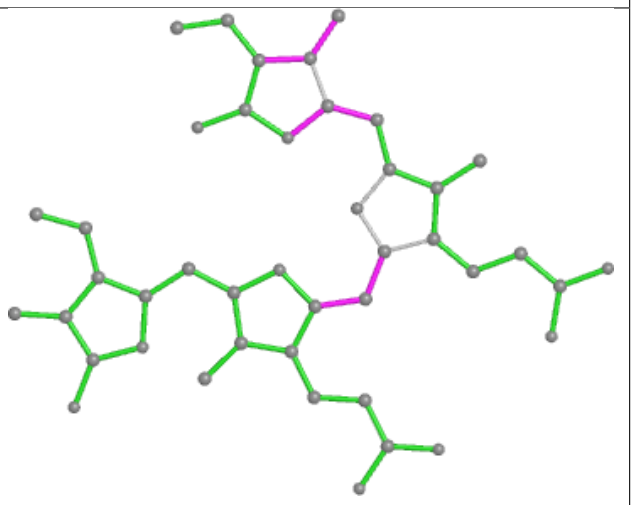
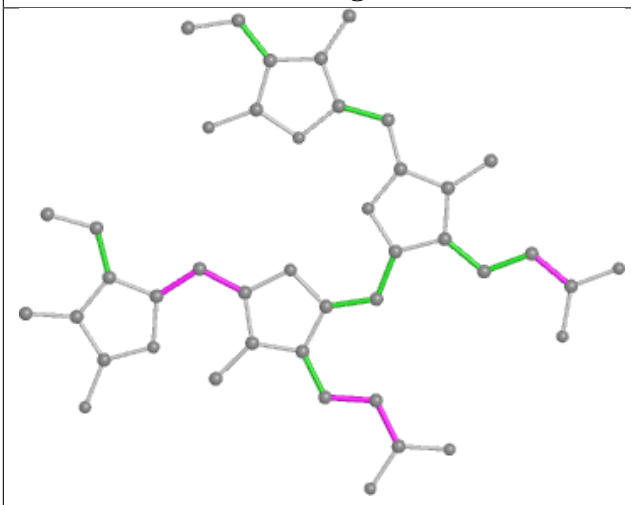
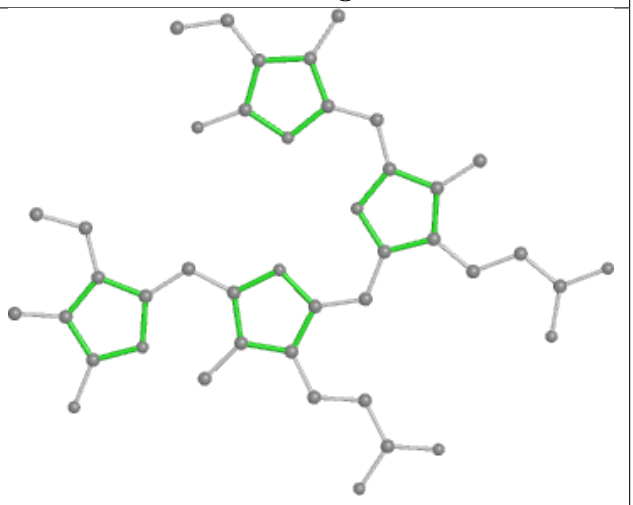


Bond angles

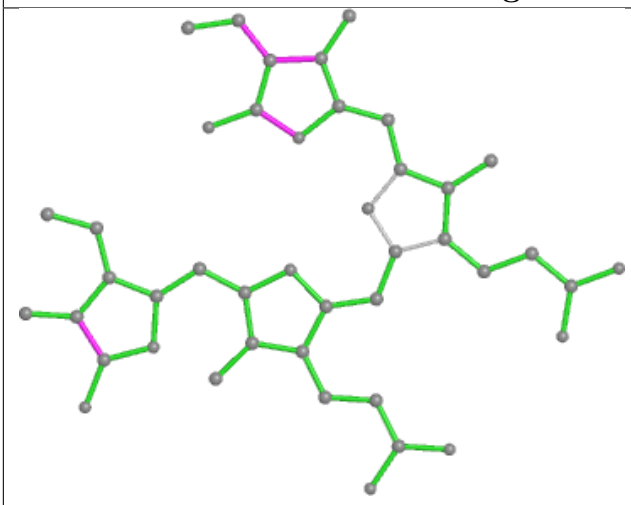


Torsions



Rings

Ligand PEB M6 1001



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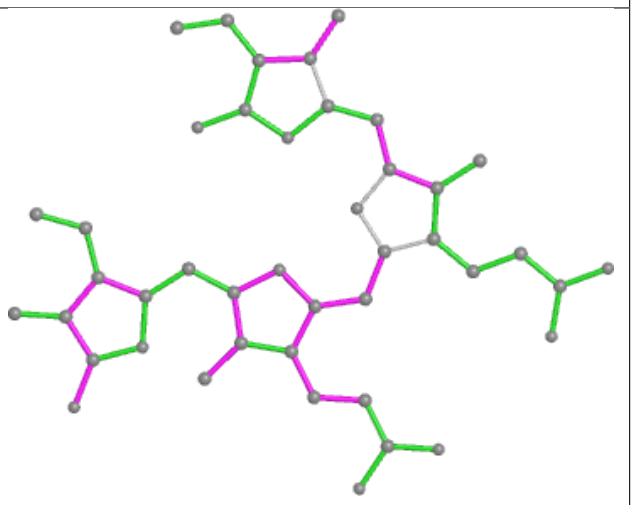

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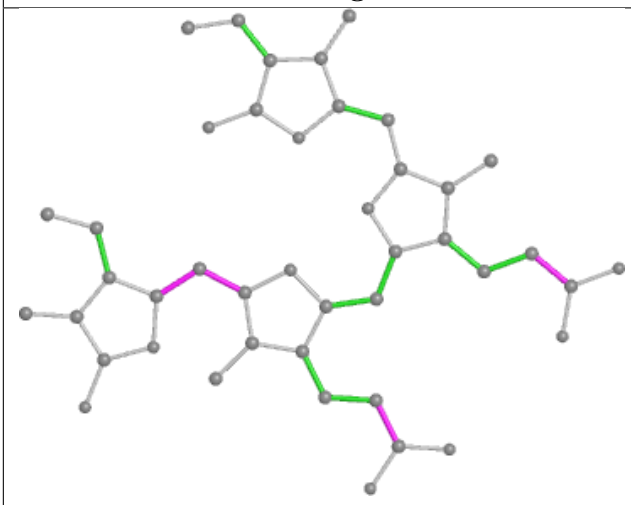

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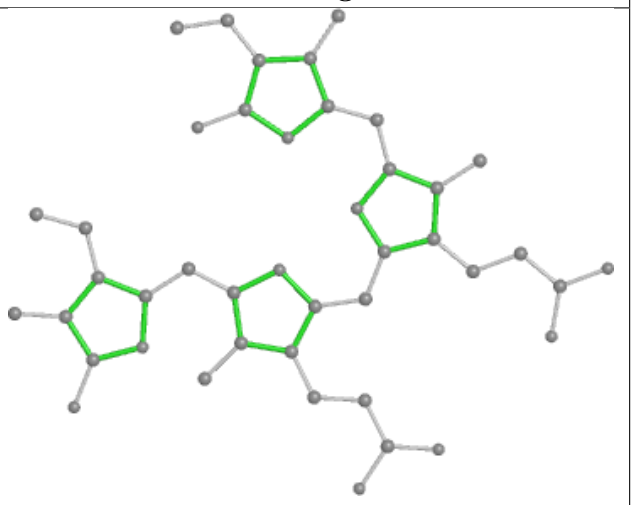
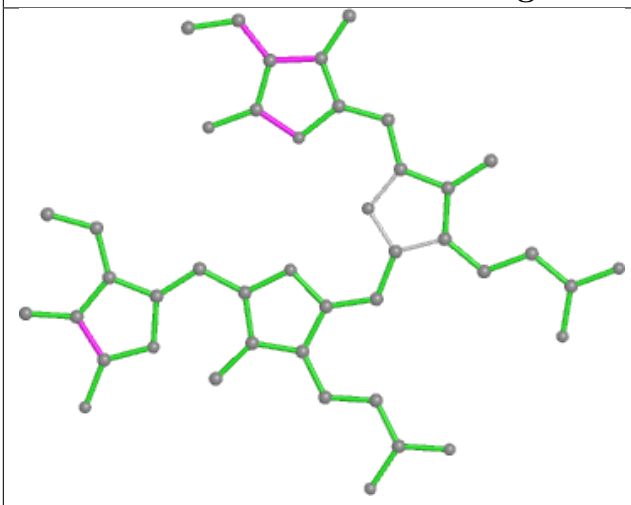


Rings

Ligand PEB F6 202



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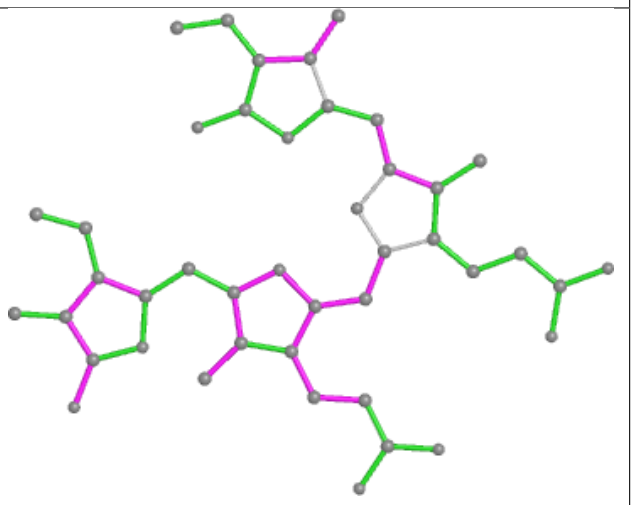

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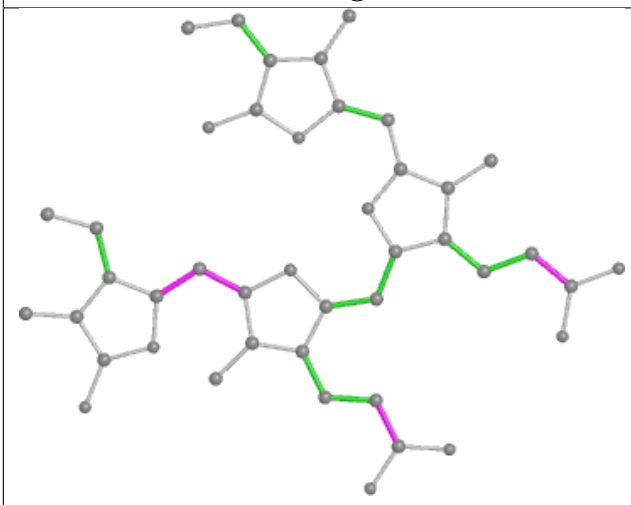

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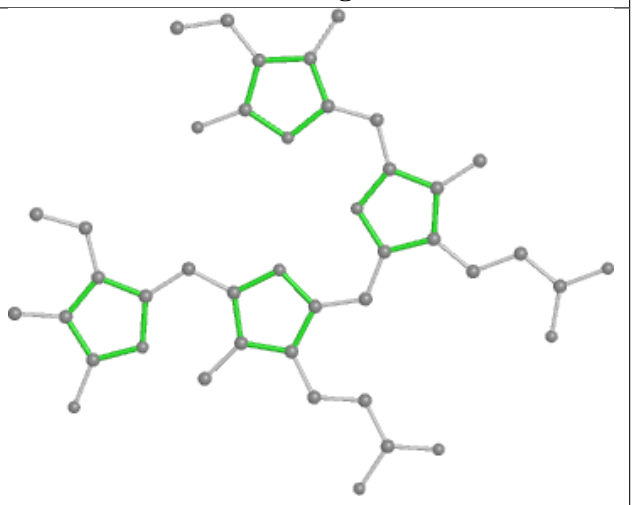
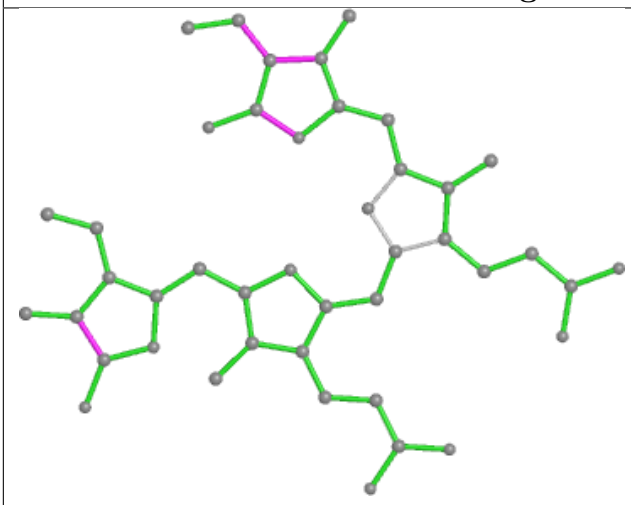


Rings

Ligand PEB cS 202



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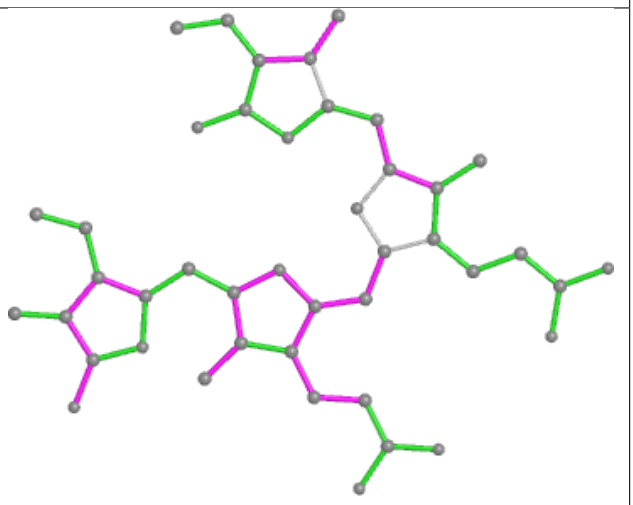
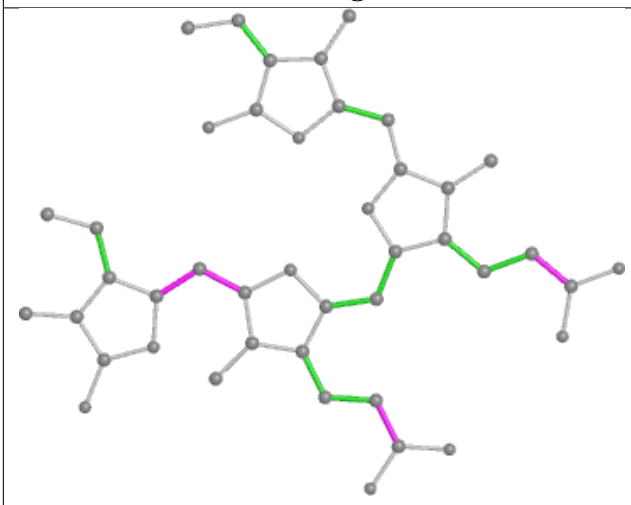


Bond angles



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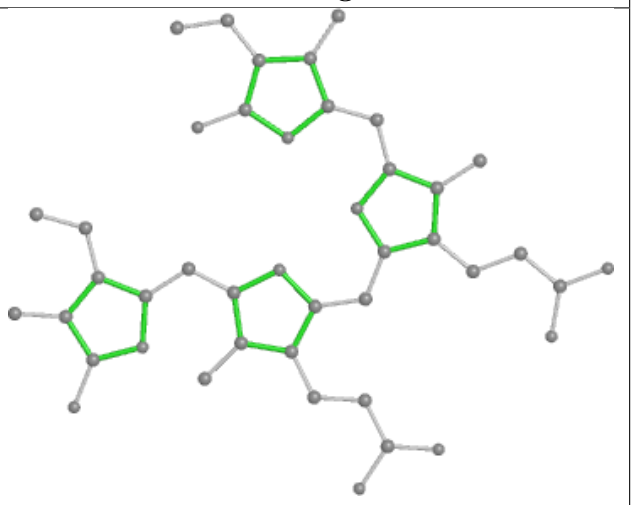
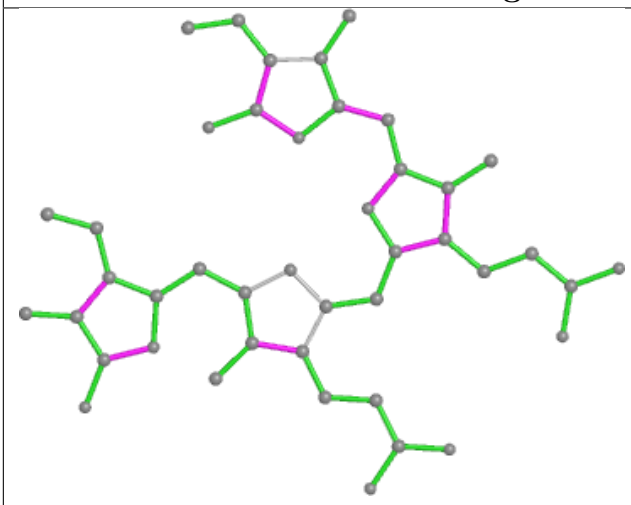


Rings

Ligand PUB bY 1005



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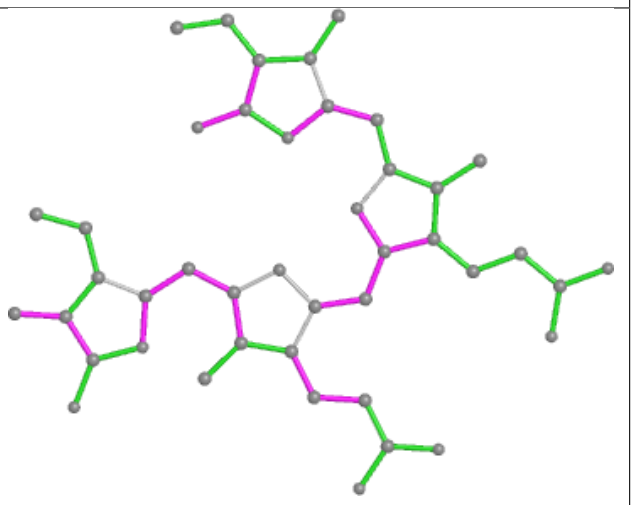

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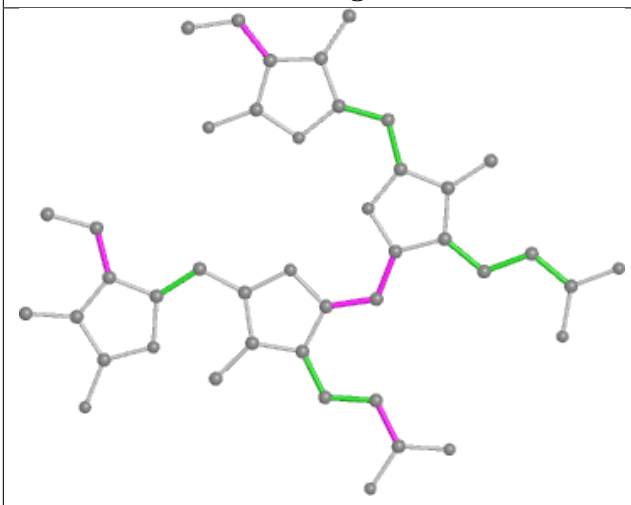

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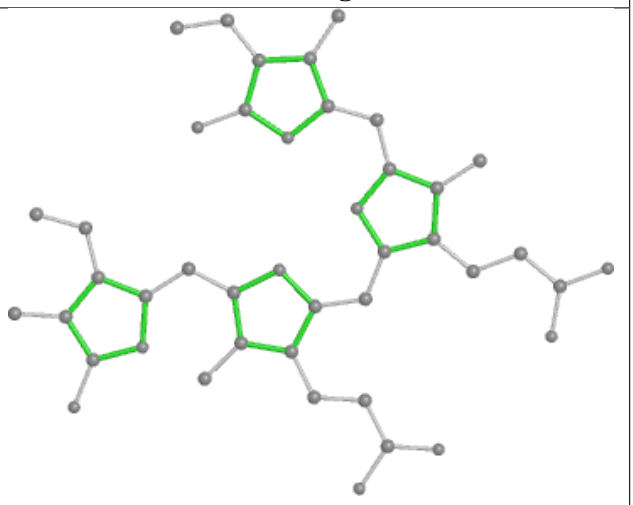

Rings

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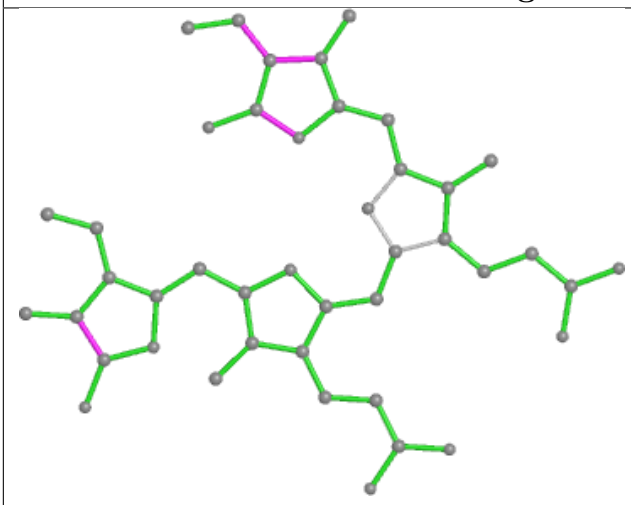

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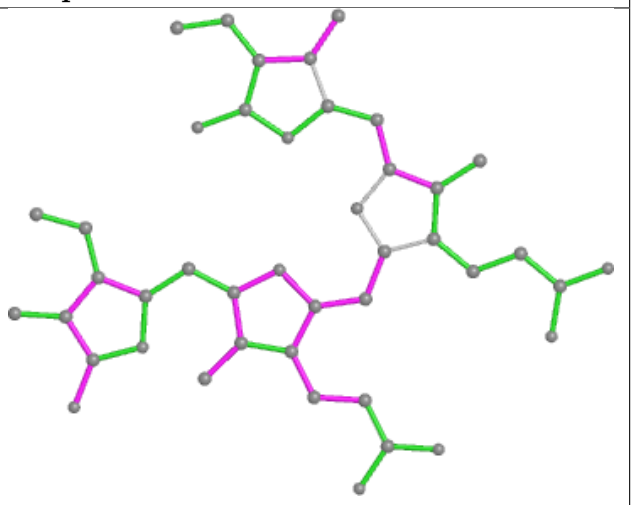

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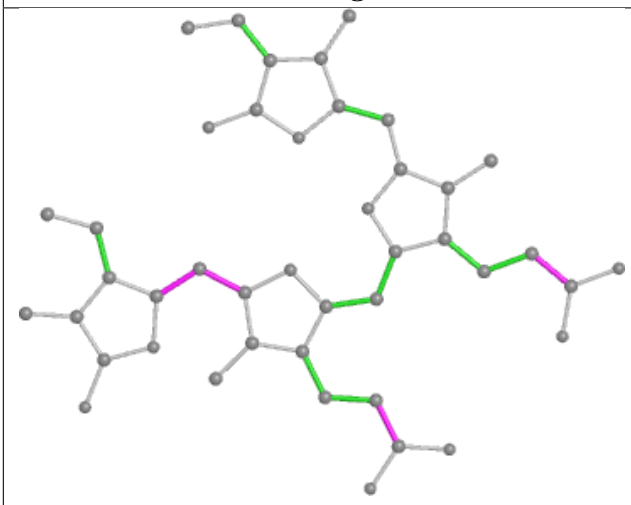

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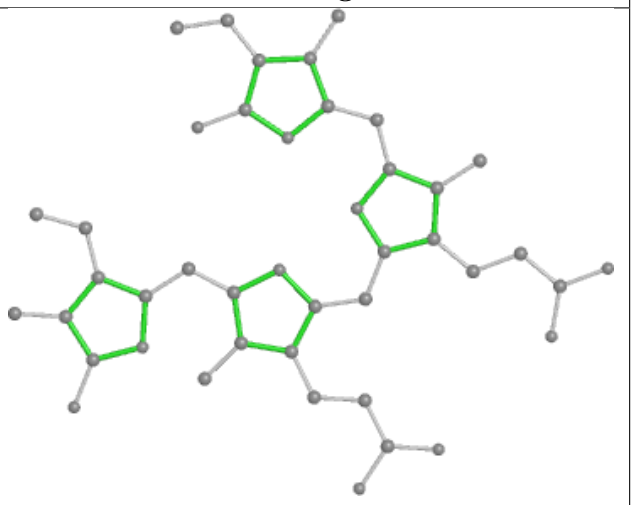
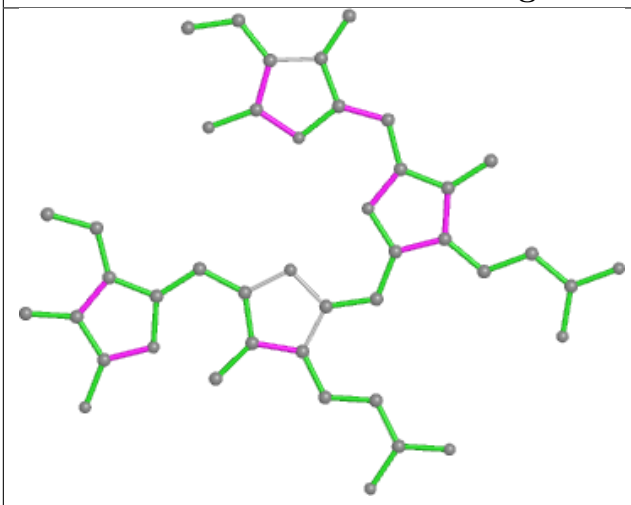


Rings

Ligand PUB c3 305



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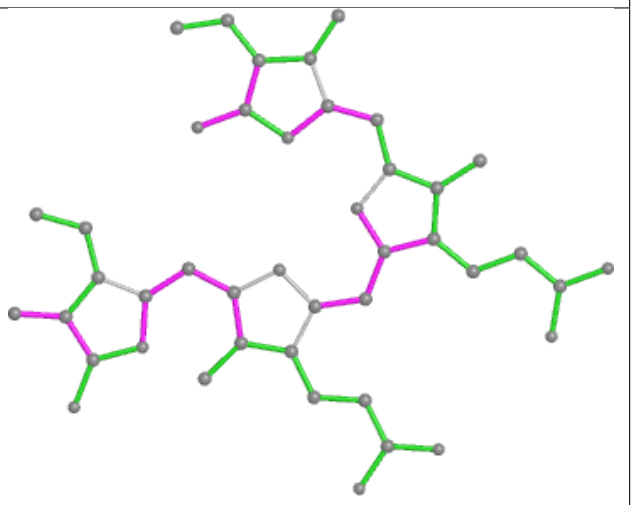

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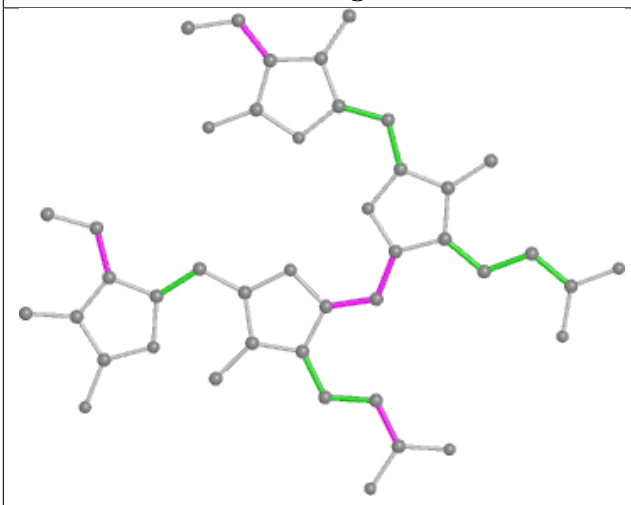

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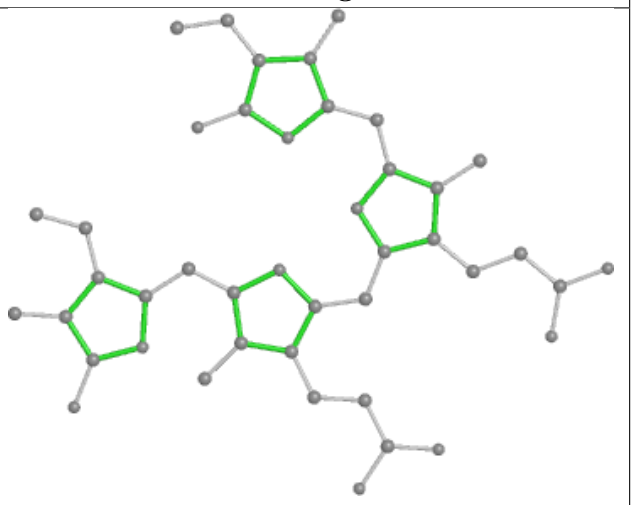

Rings

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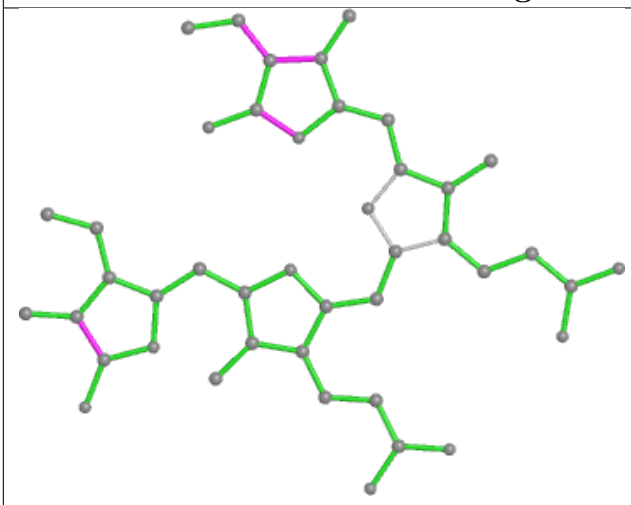

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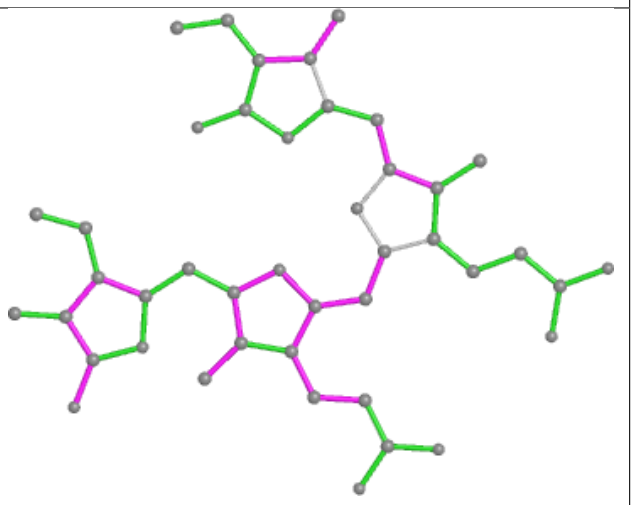

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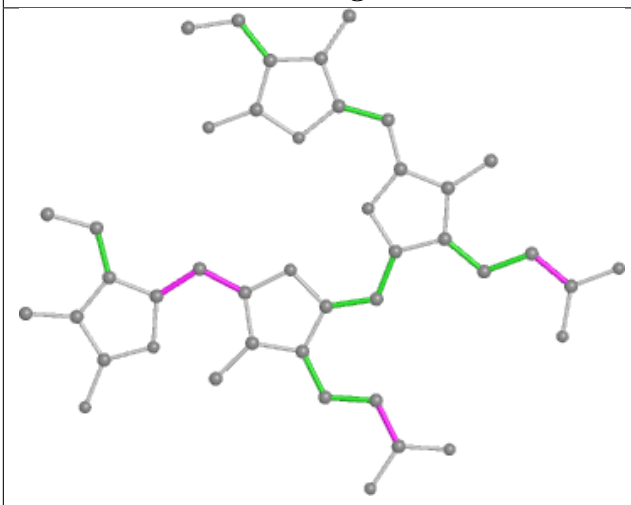

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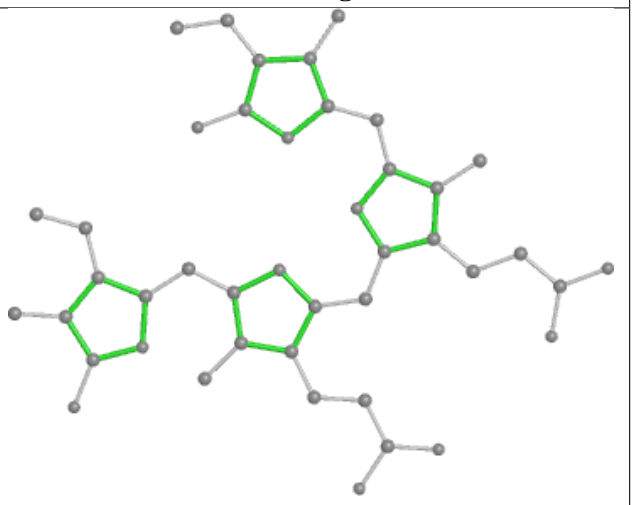

Rings

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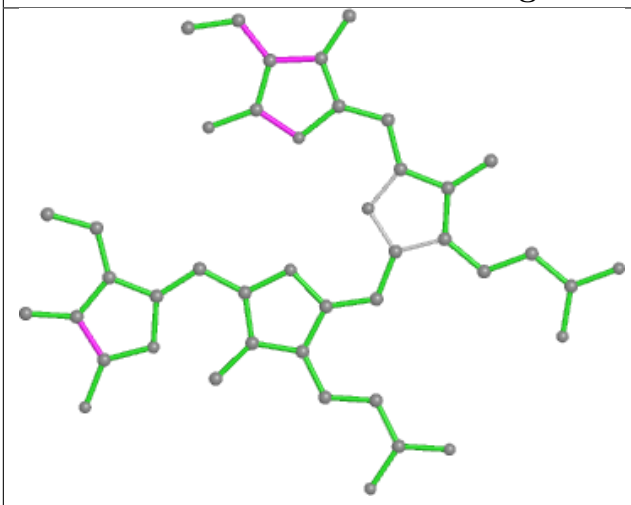

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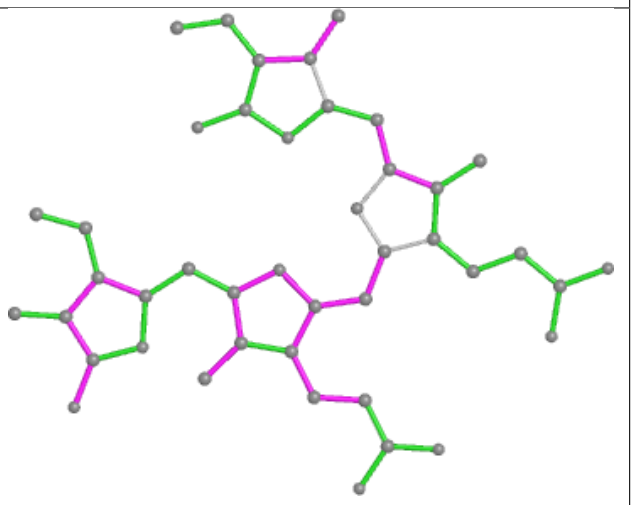

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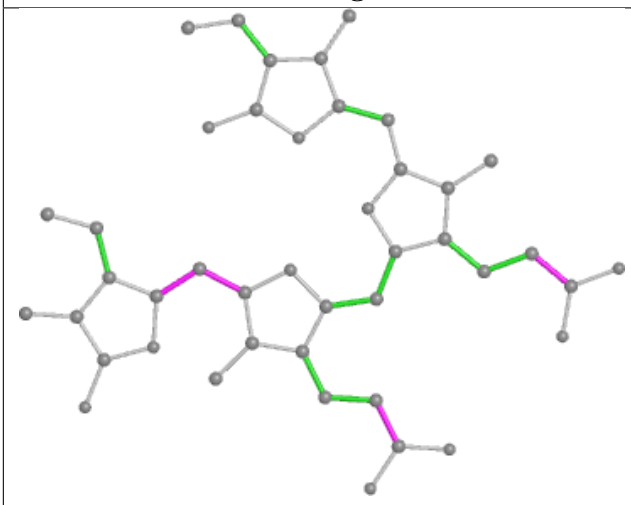

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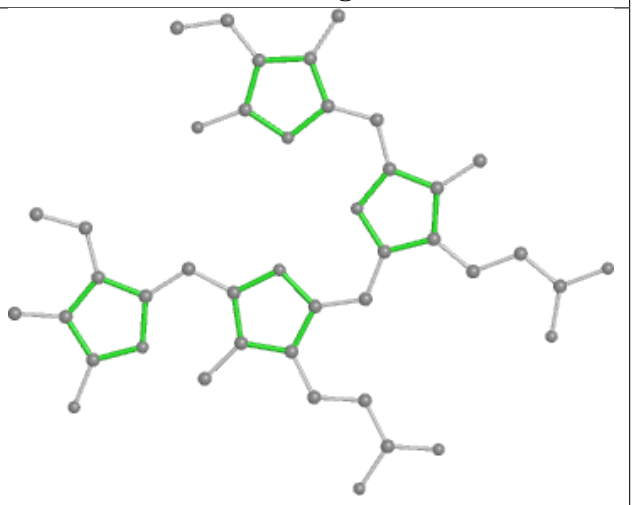
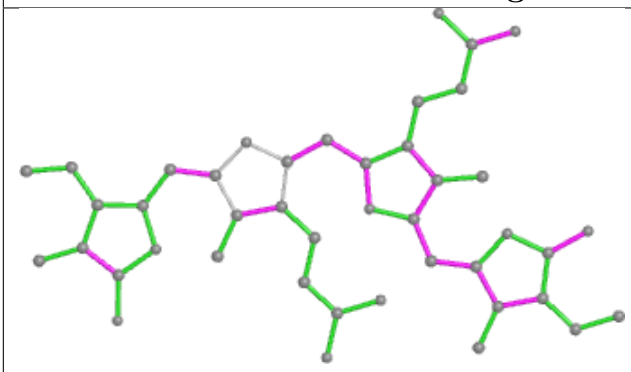


Rings

Ligand CYC d1 1001



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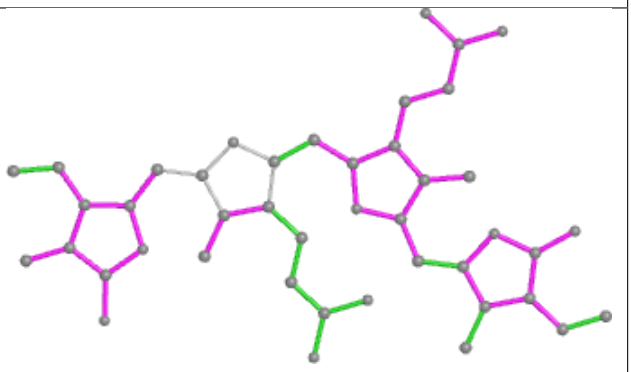

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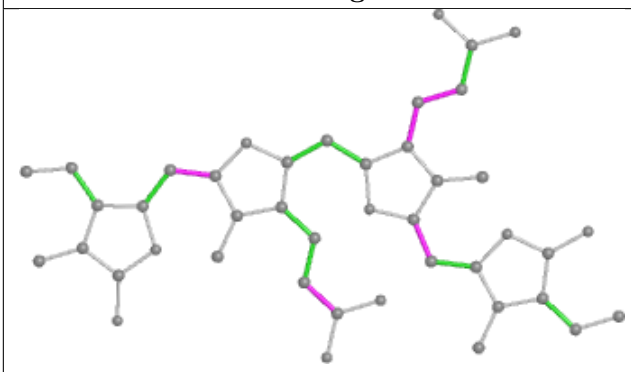

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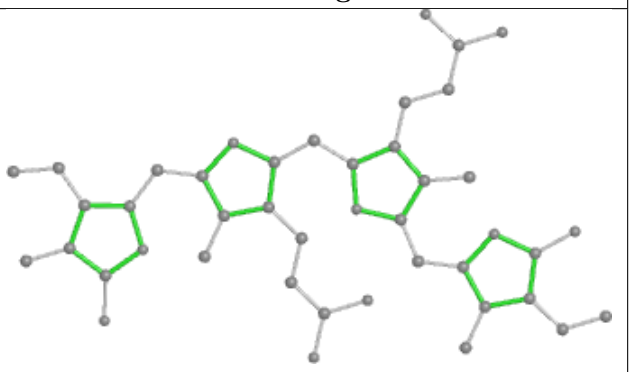
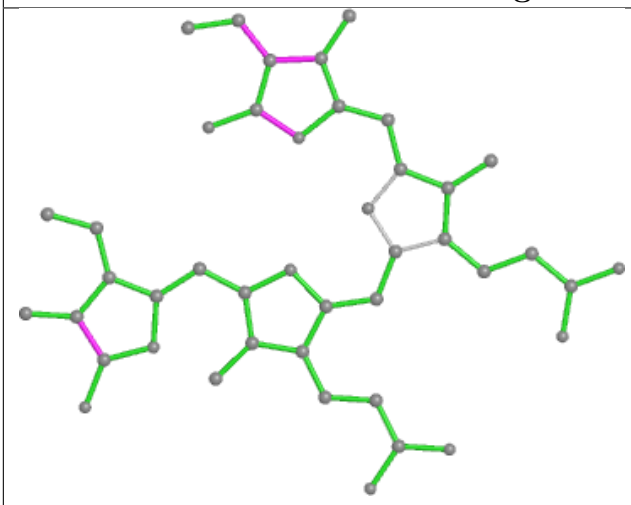


Rings

Ligand PEB m2 201



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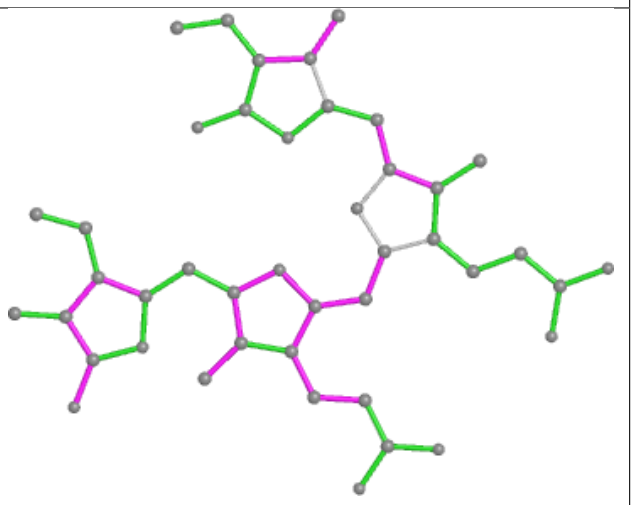

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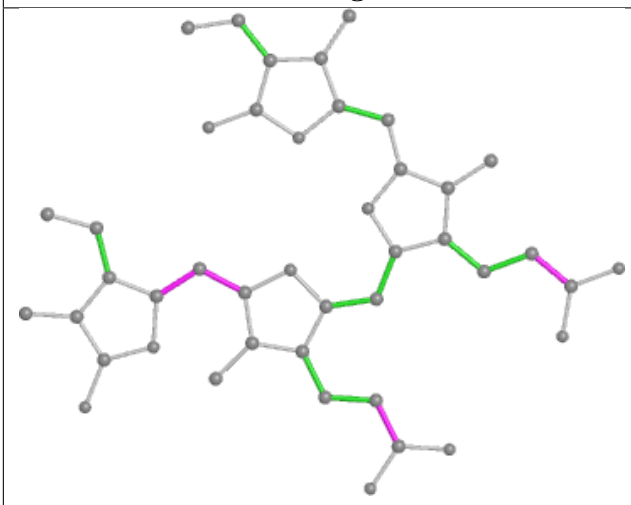

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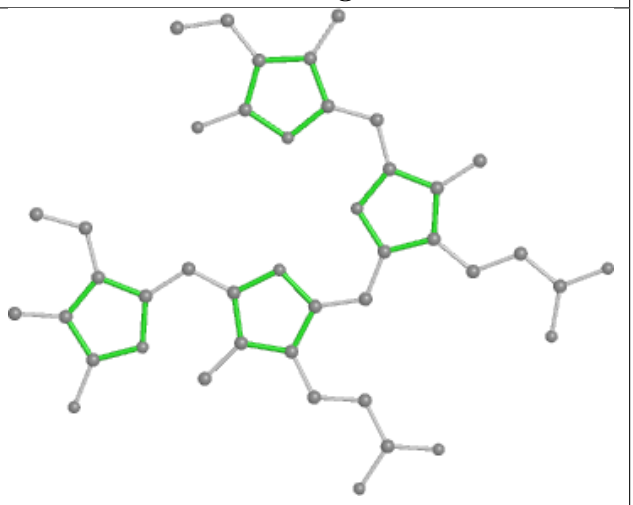

Rings

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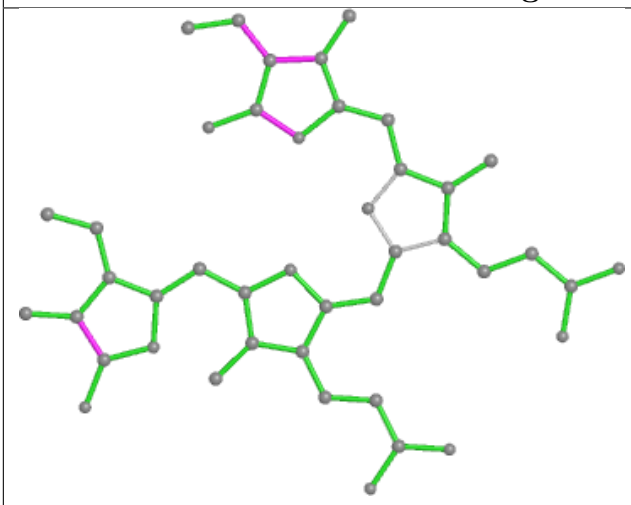

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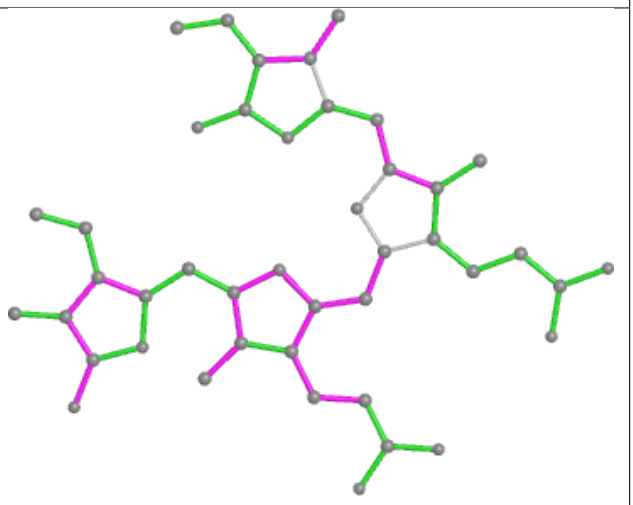

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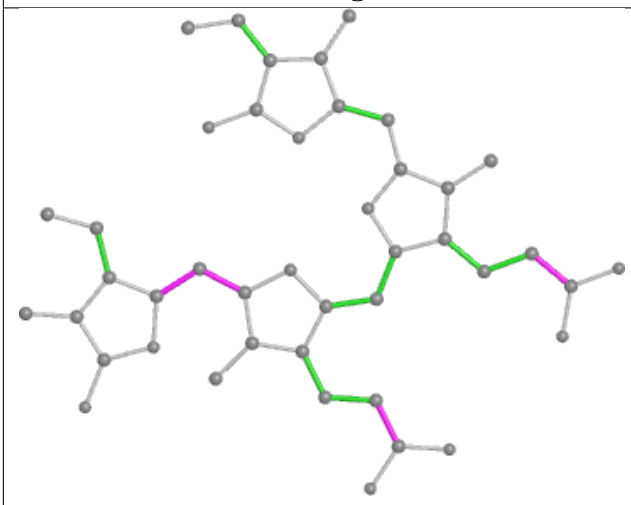

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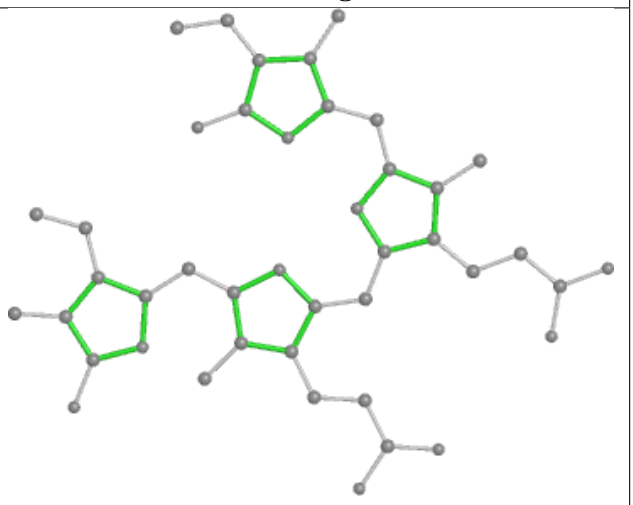
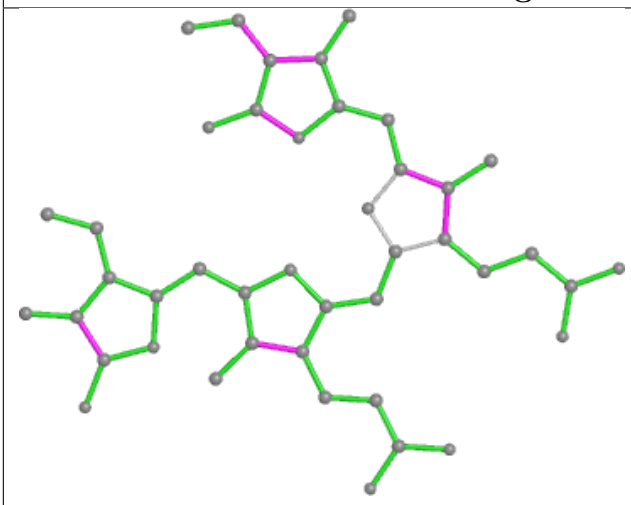


Rings

Ligand PEB N5 202



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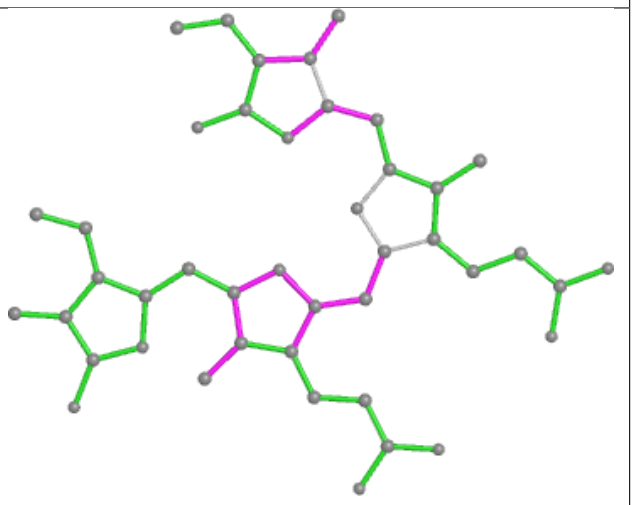

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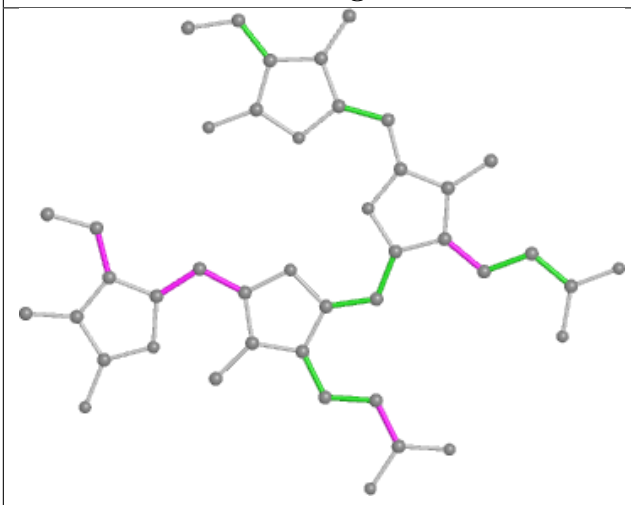

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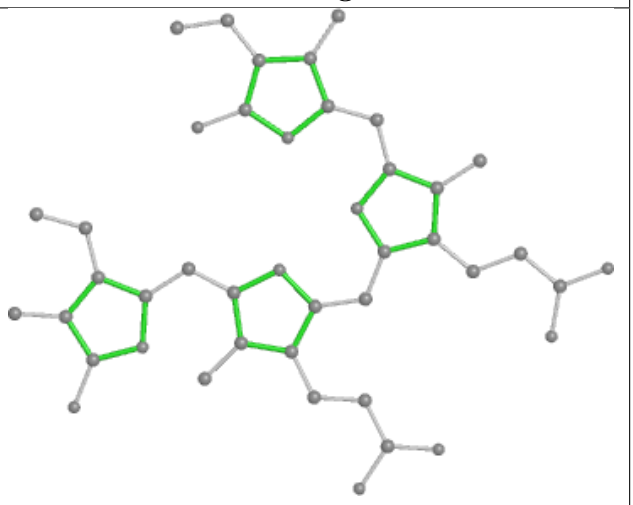
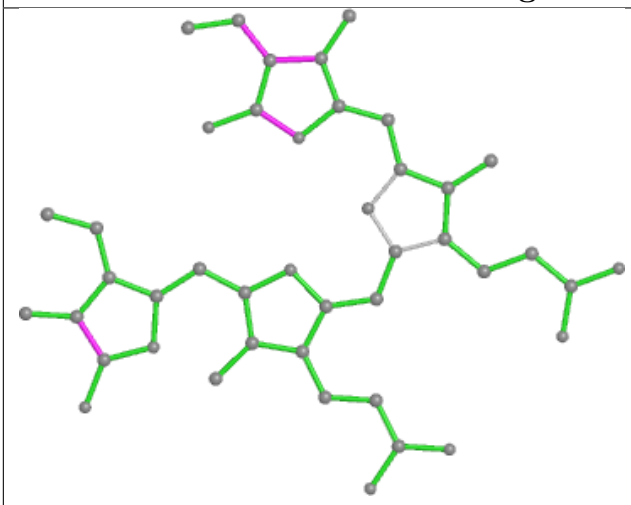


Rings

Ligand PEB bv 202



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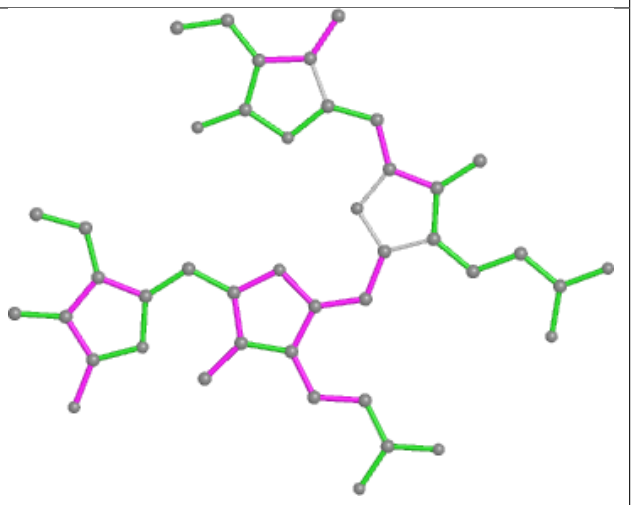
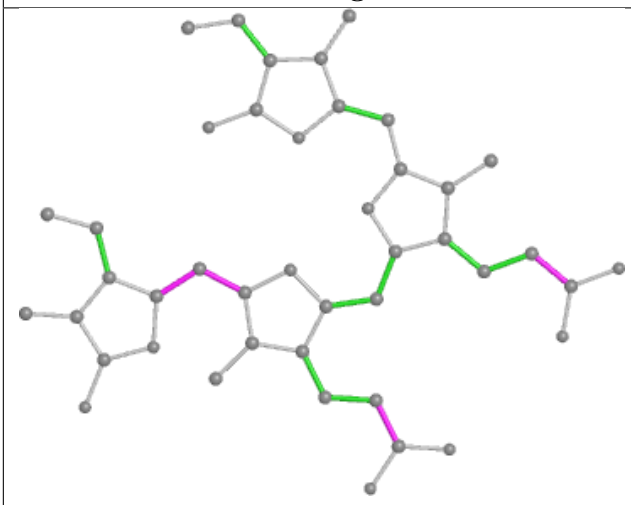
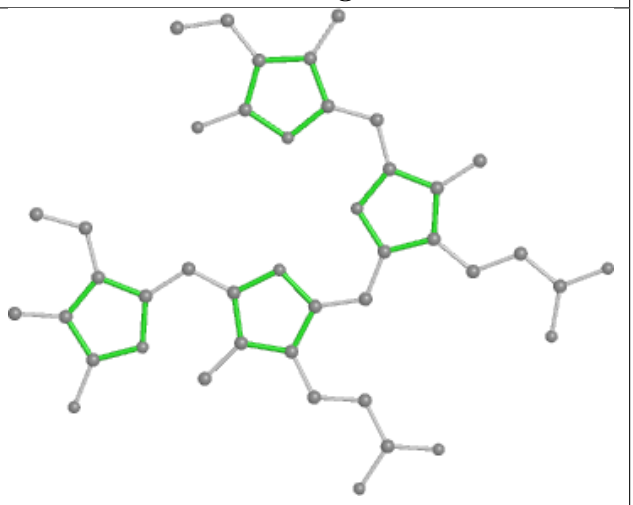


Bond angles

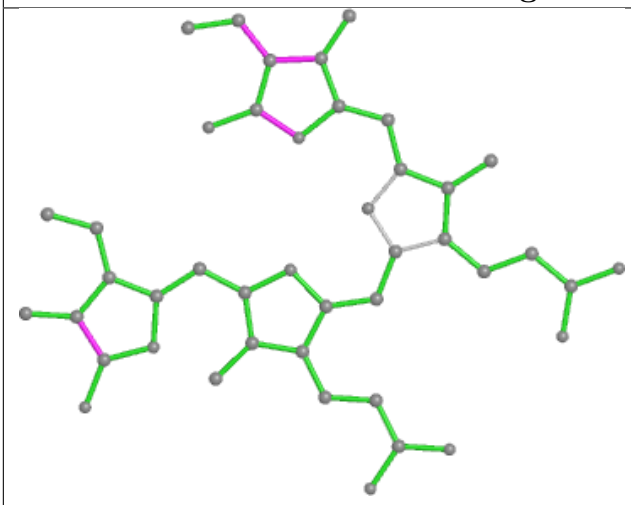


Torsions



Rings

Ligand PEB eS 202



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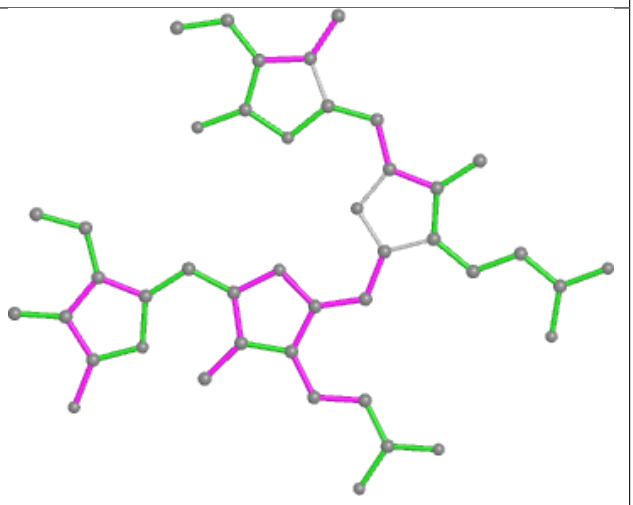

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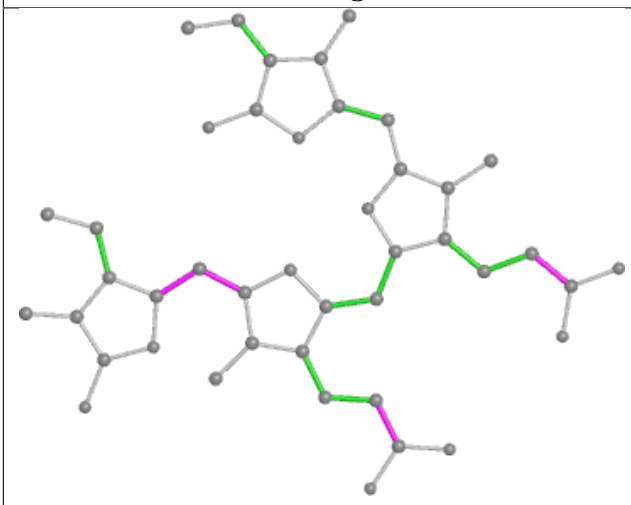

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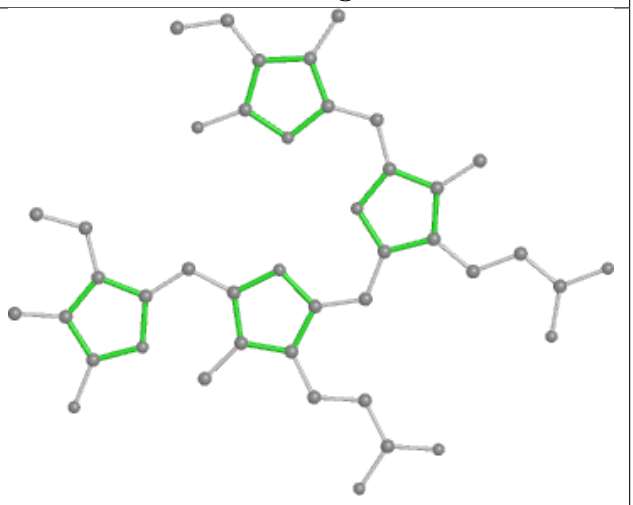
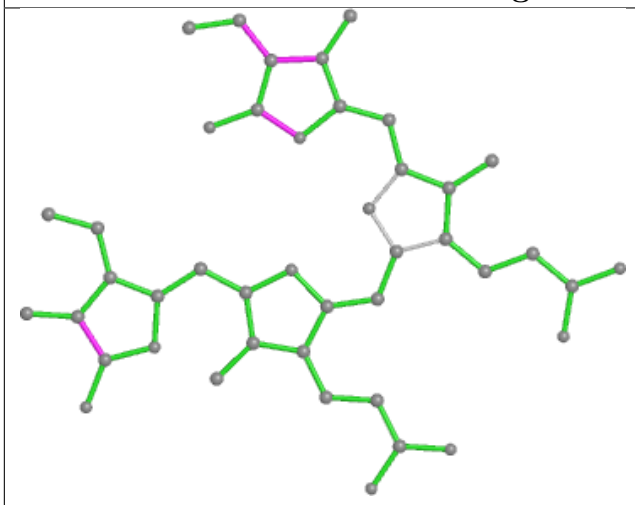


Rings

Ligand PEB ek 1001



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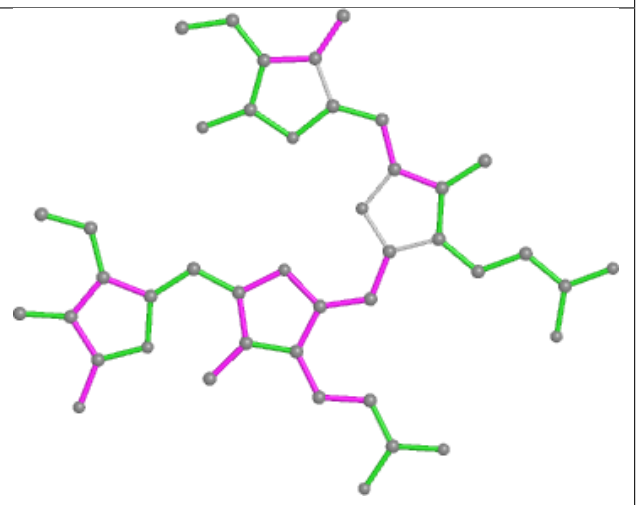

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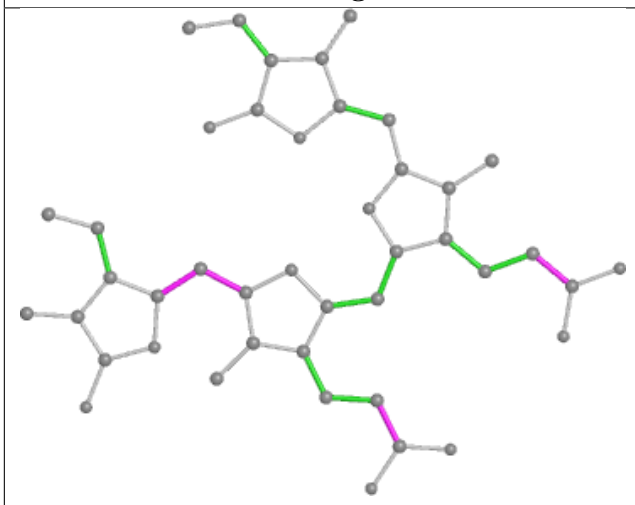

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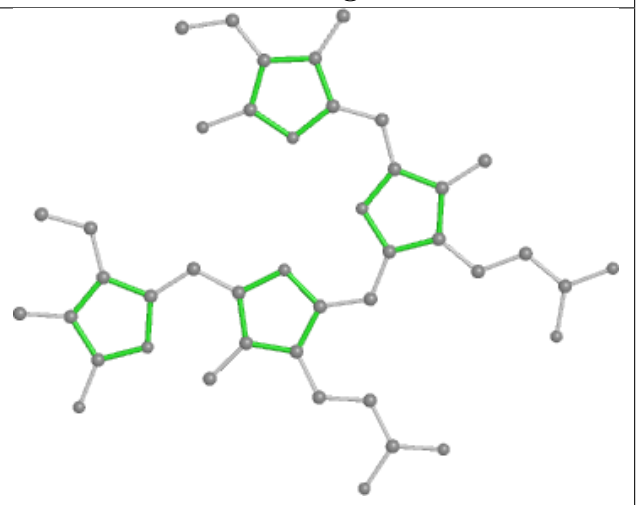

Rings

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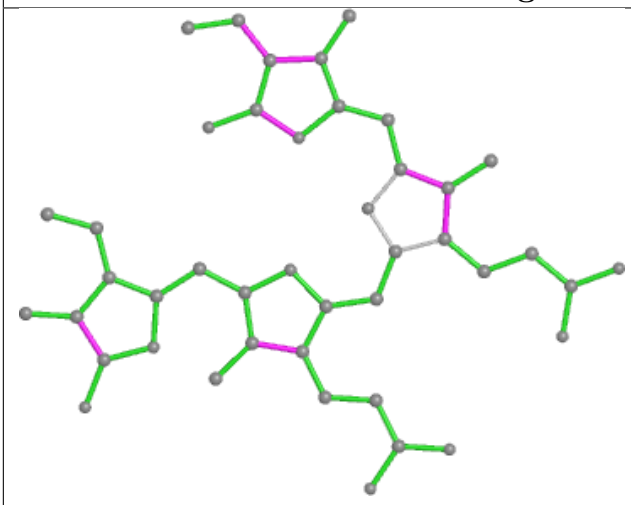

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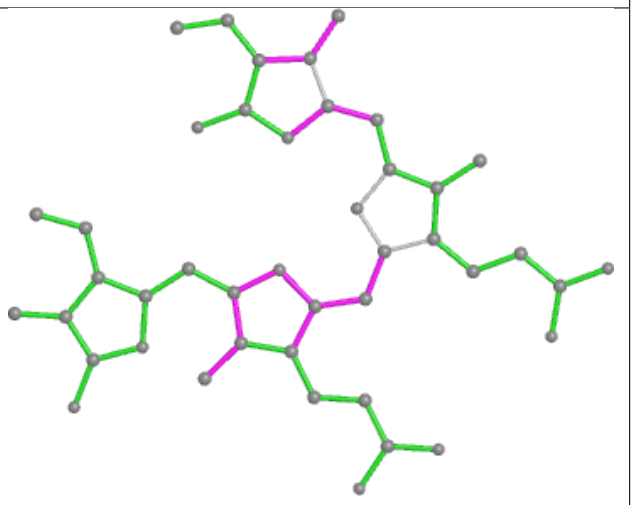

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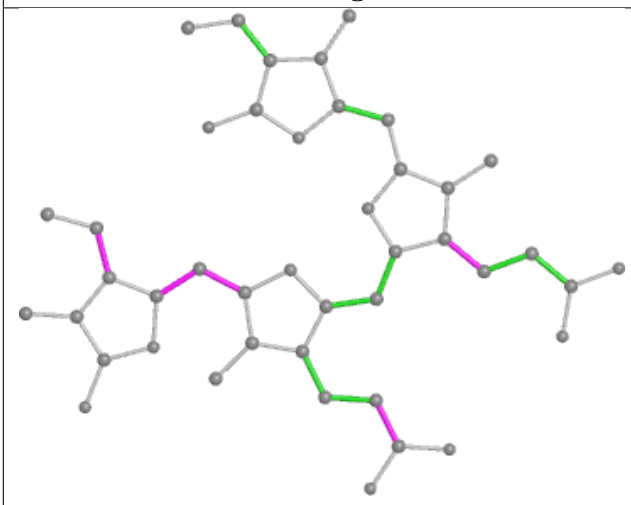

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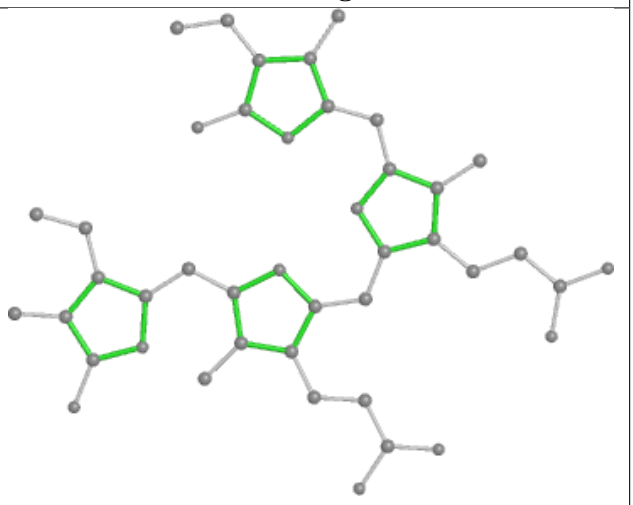
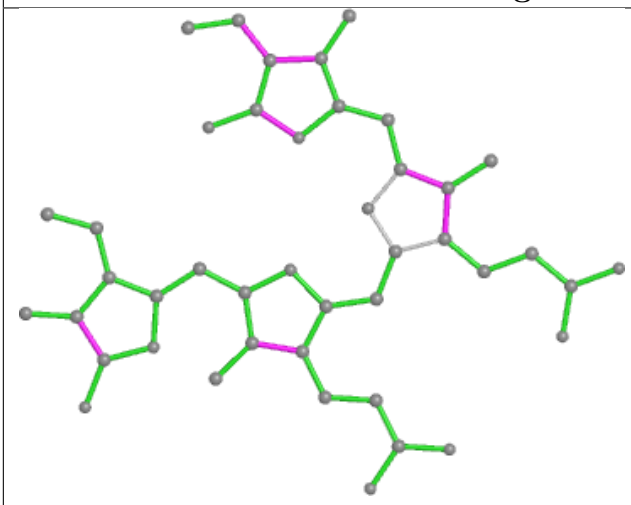


Rings

Ligand PEB hG 201



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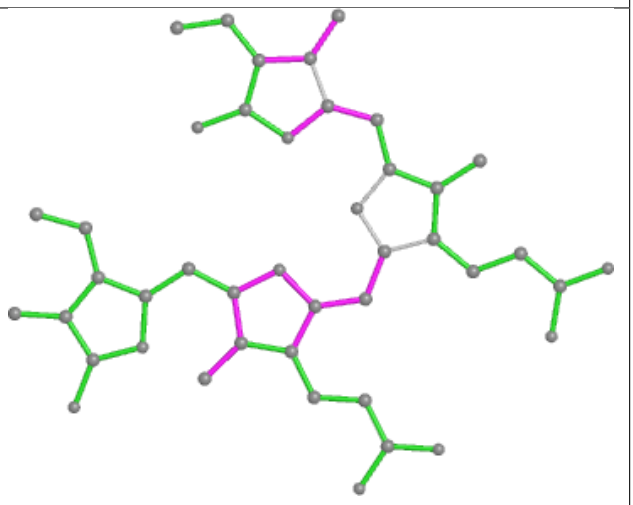

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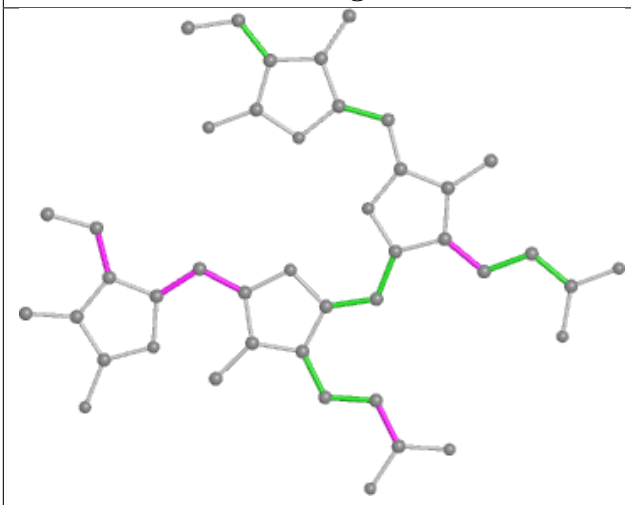

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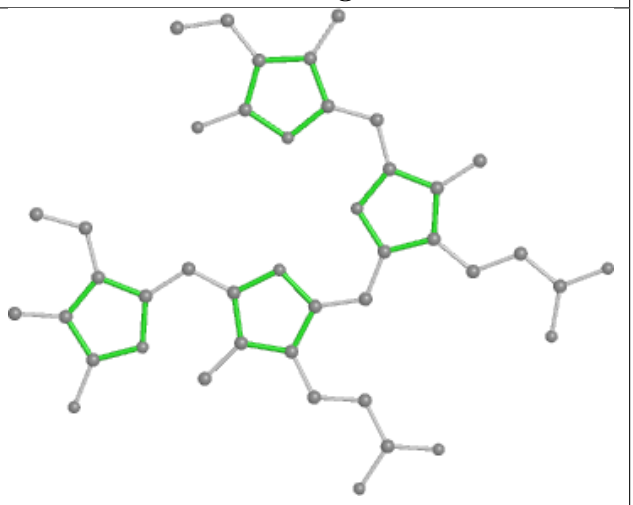
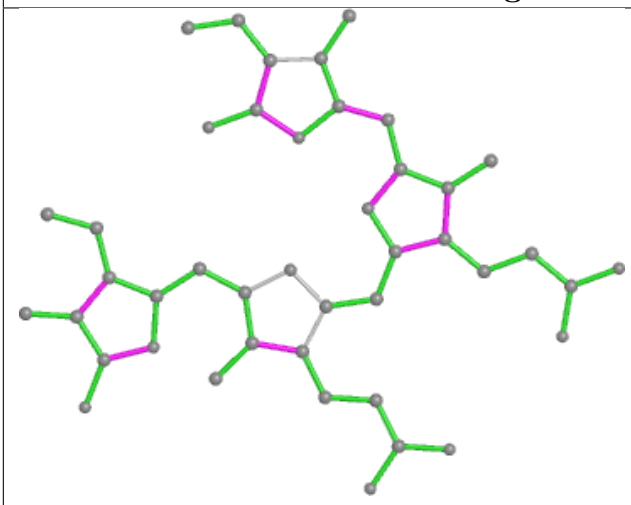


Rings

Ligand PUB kR 1003



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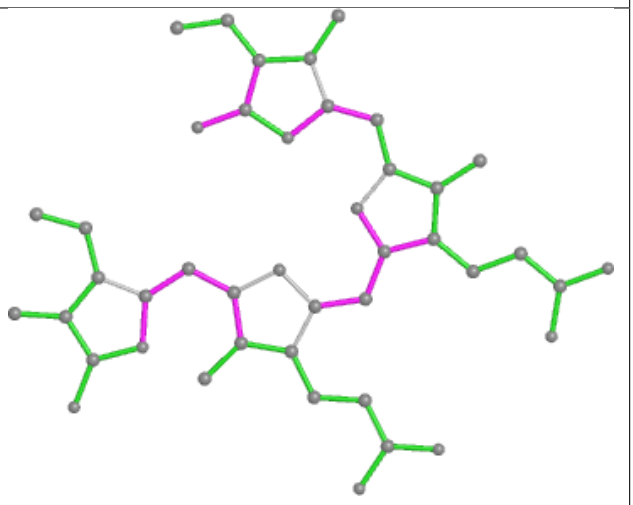

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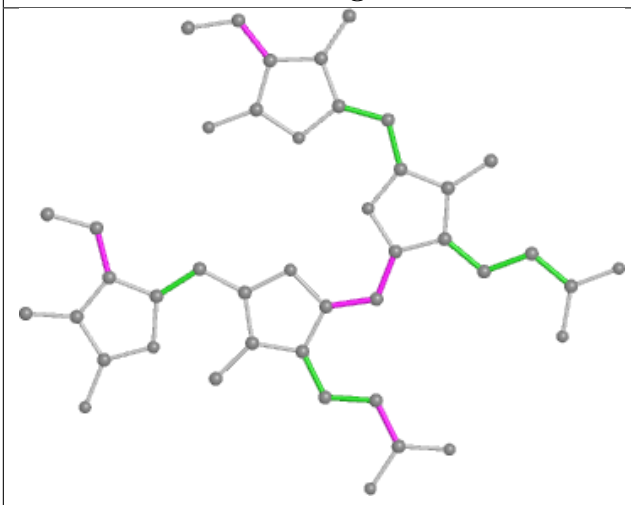

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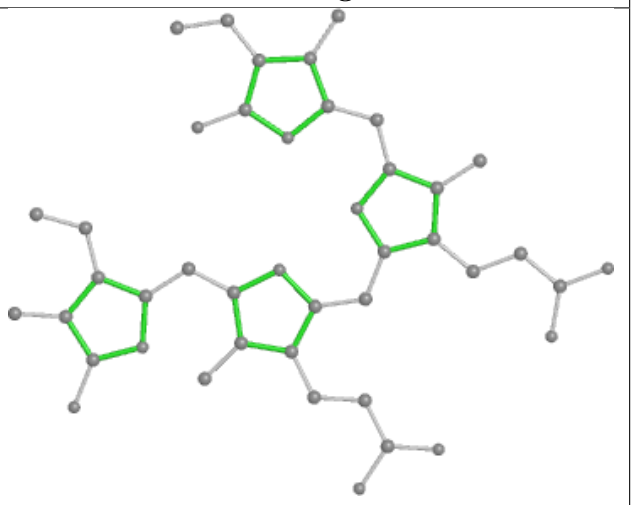

Rings

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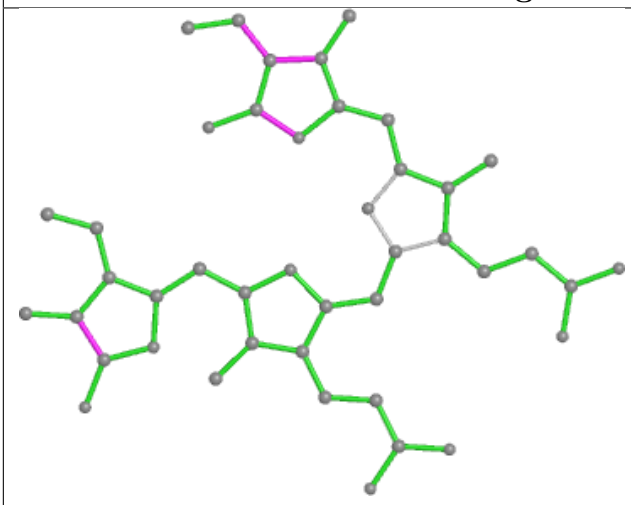

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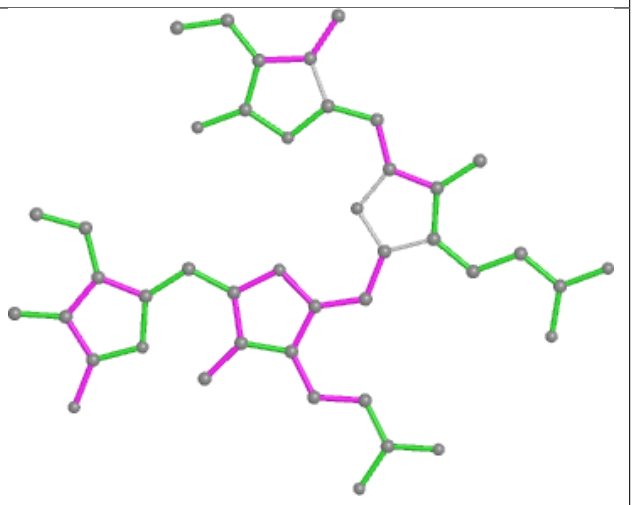

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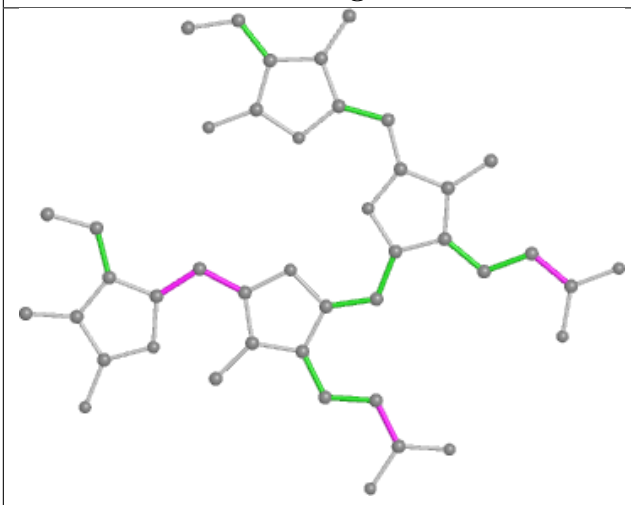

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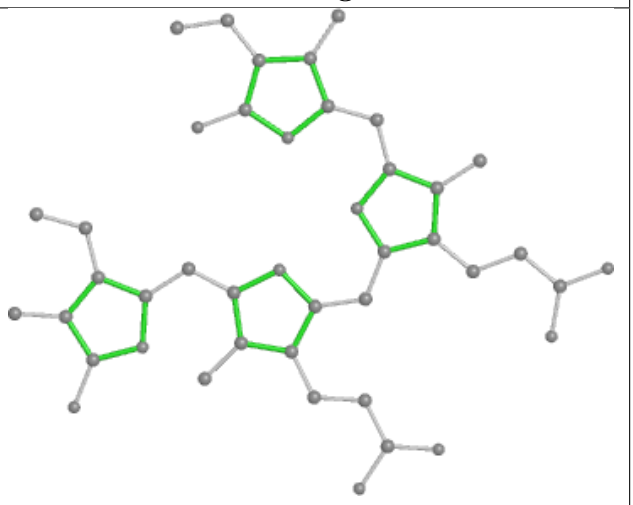

Rings

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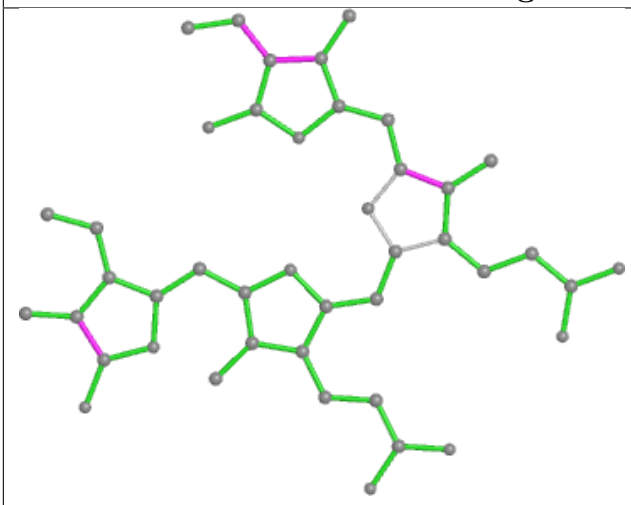

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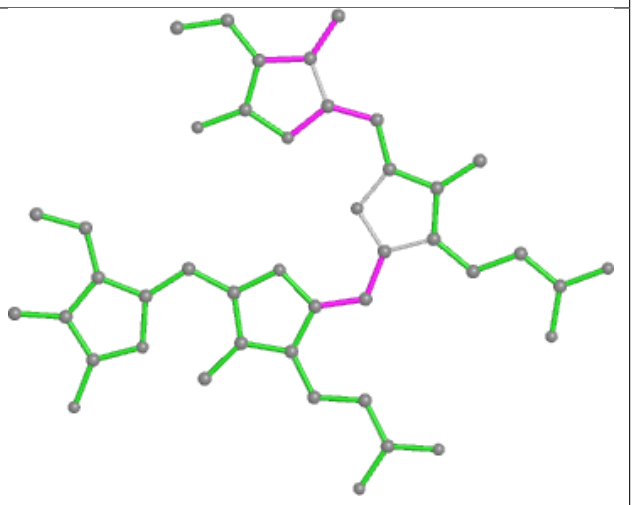

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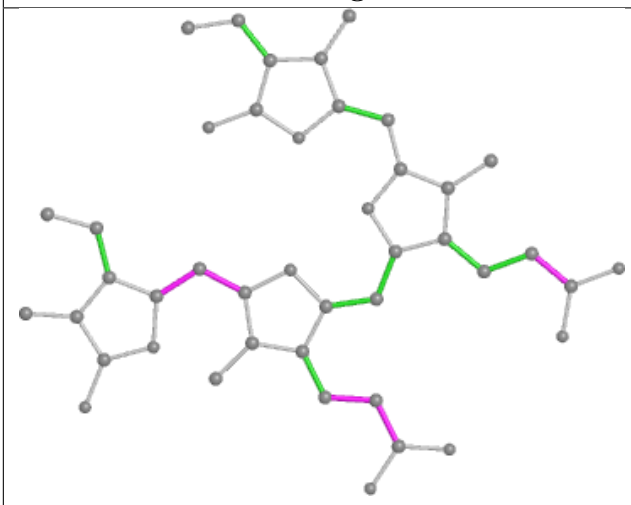

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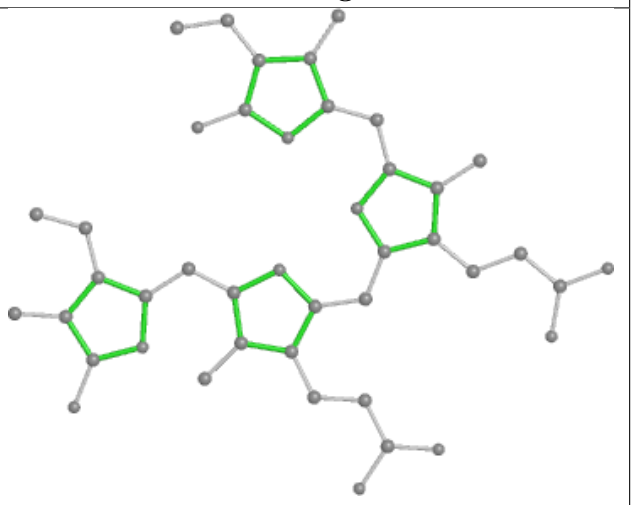
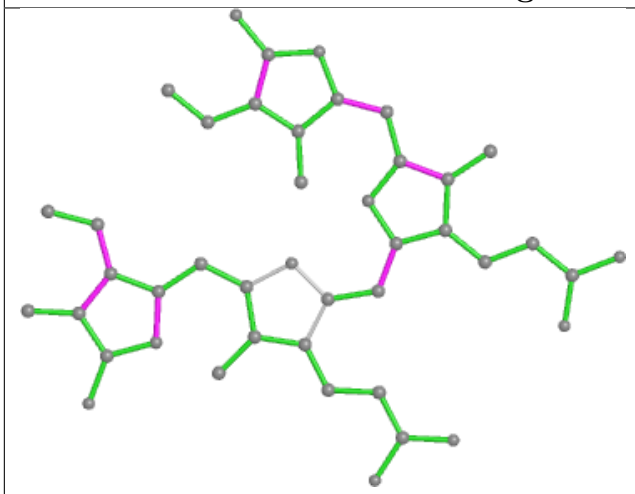


Rings

Ligand PVN d3 302



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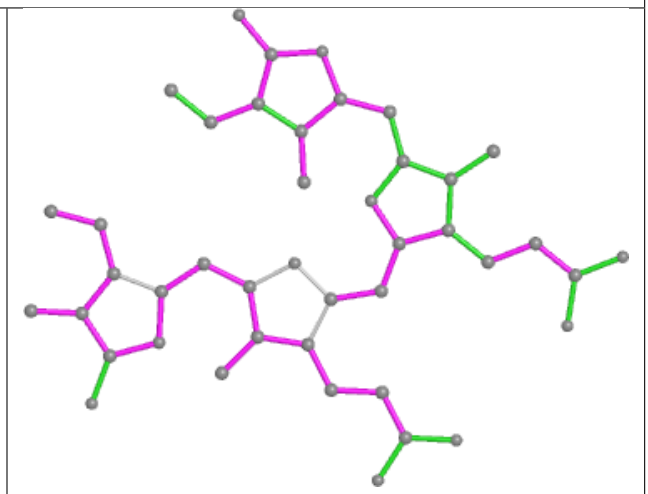

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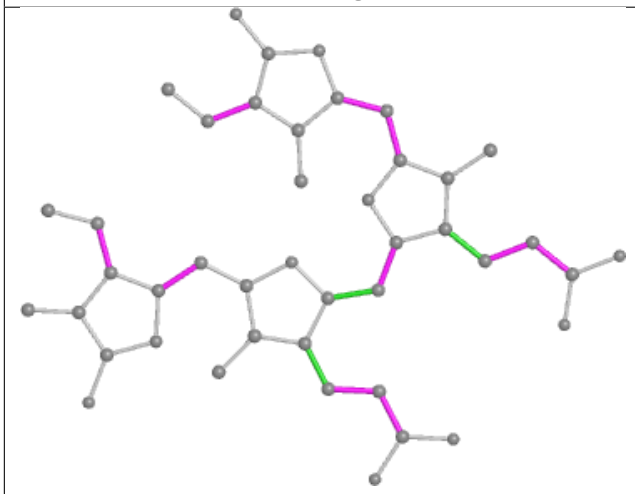

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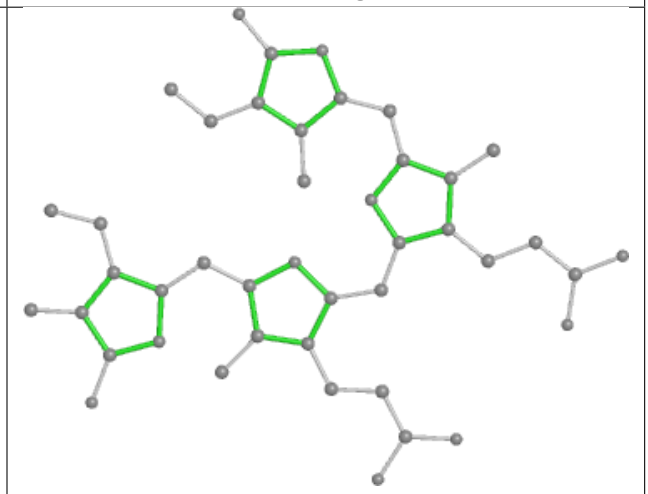
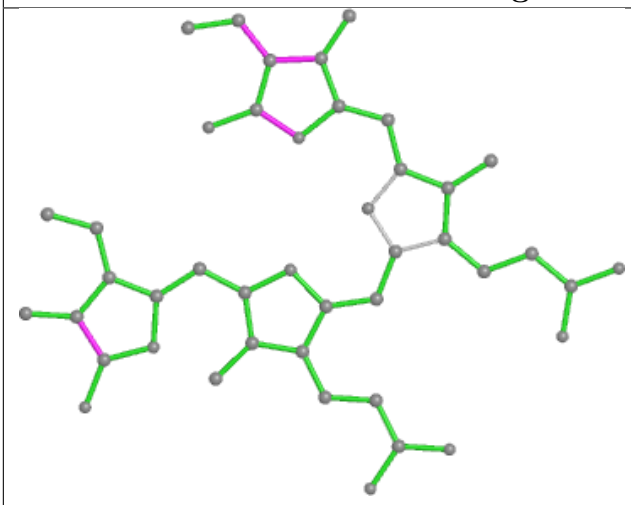


Rings

Ligand PEB c6 1002



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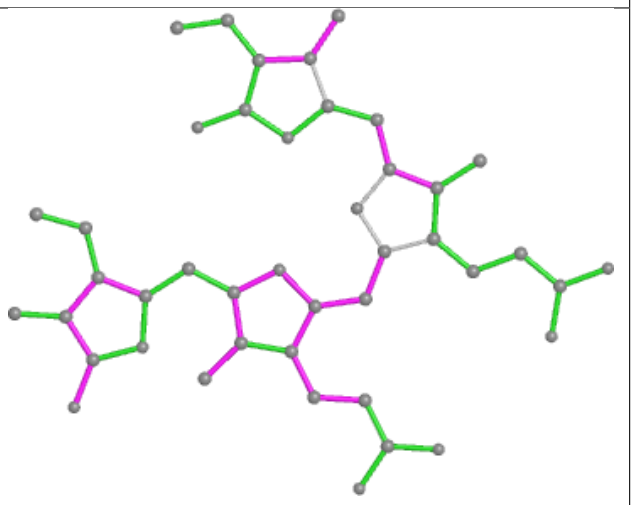

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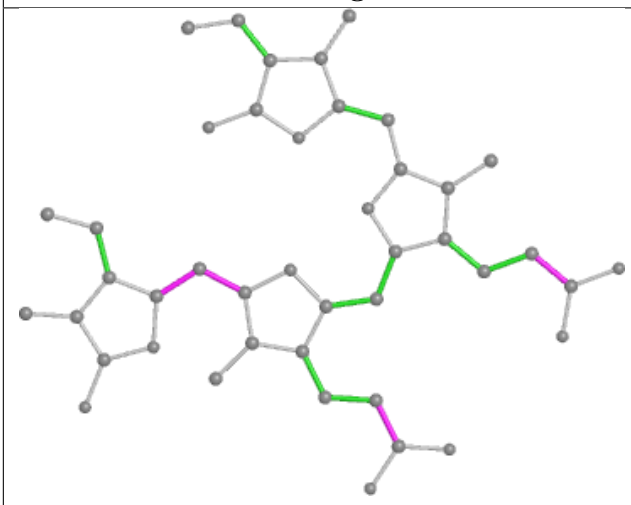

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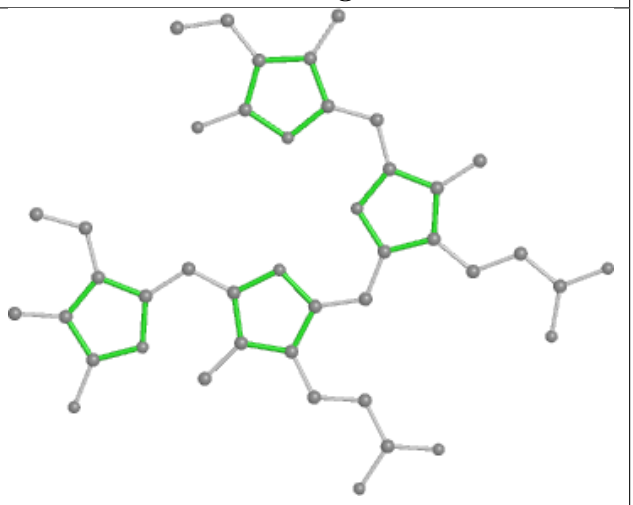
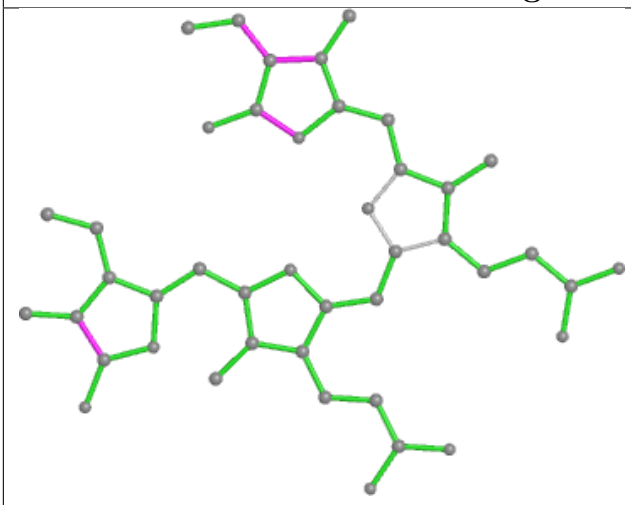


Rings

Ligand PEB j6 202



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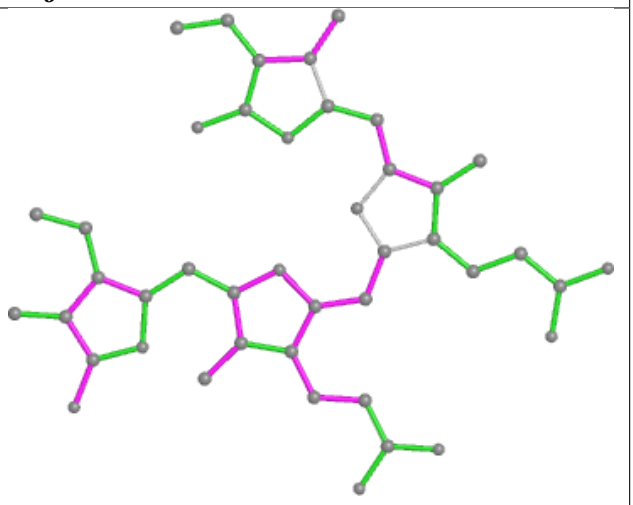

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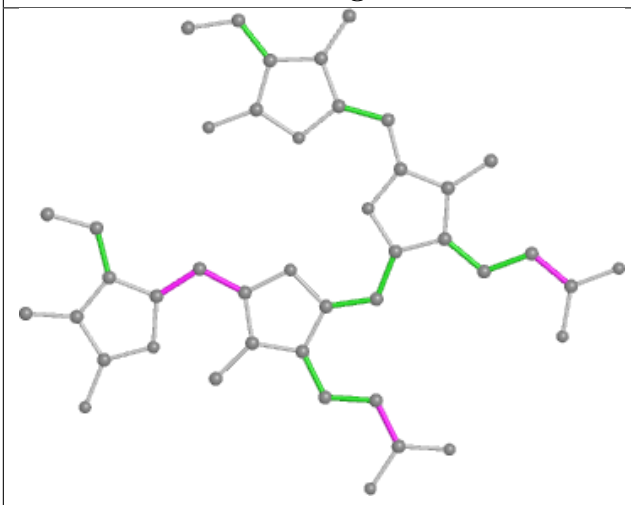

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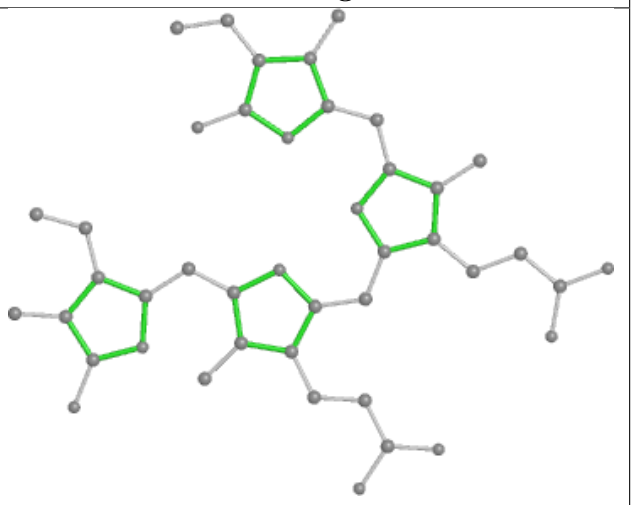

Rings

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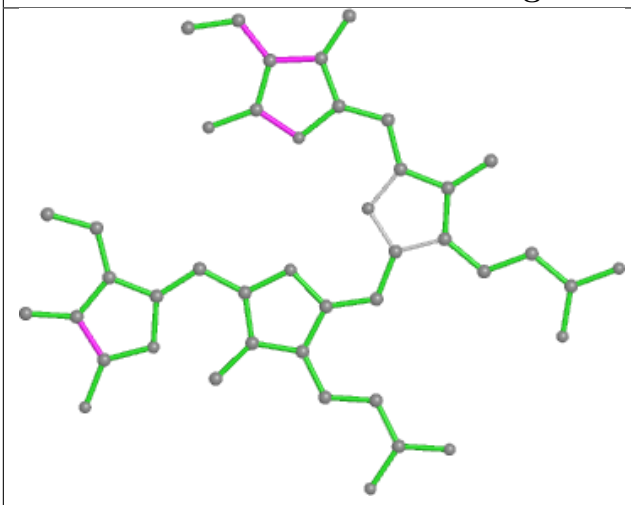

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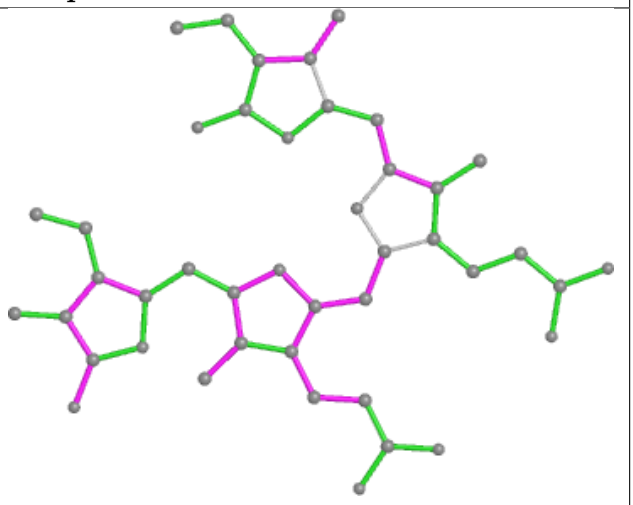
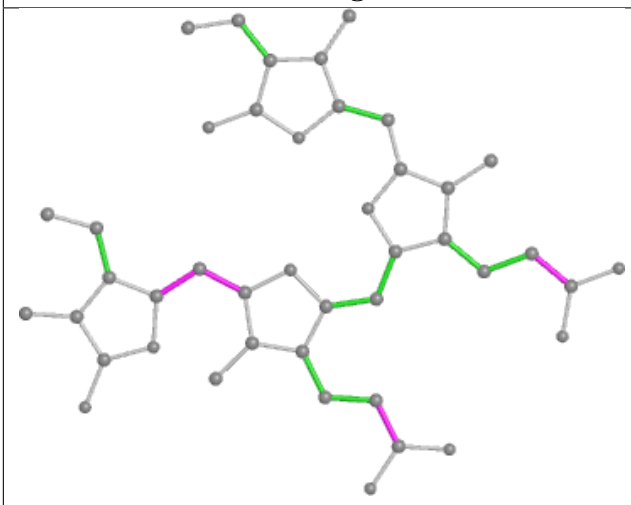


Bond angles



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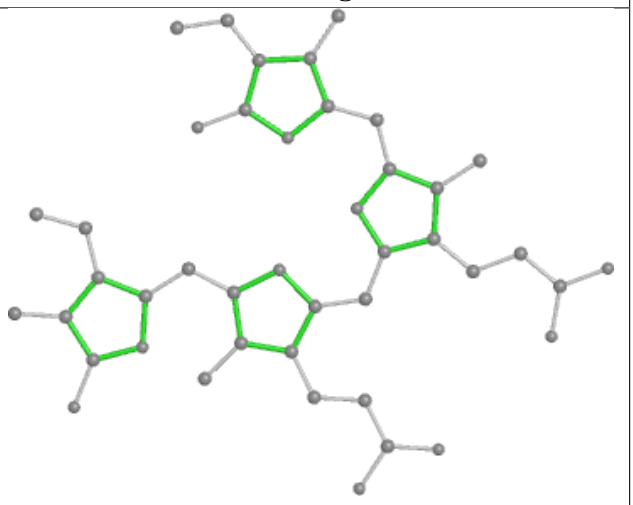
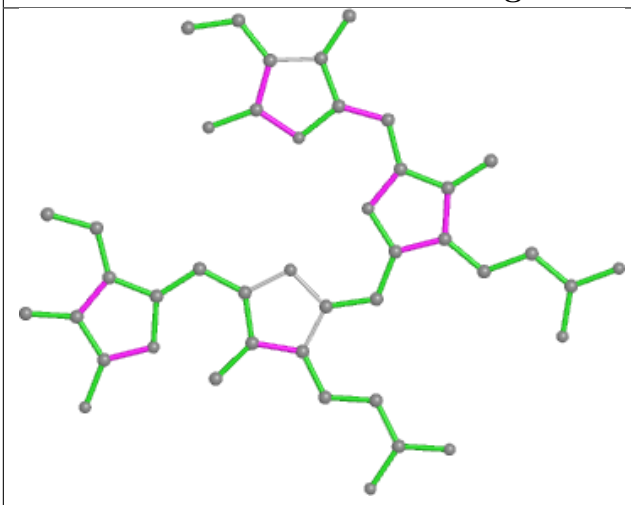


Rings

Ligand PUB jM 1003



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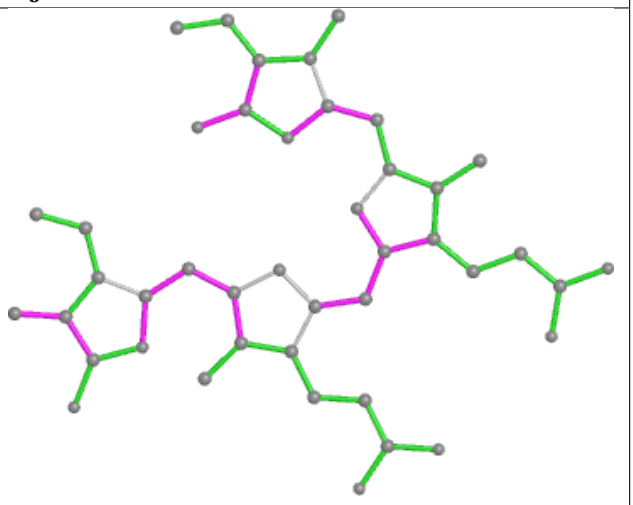

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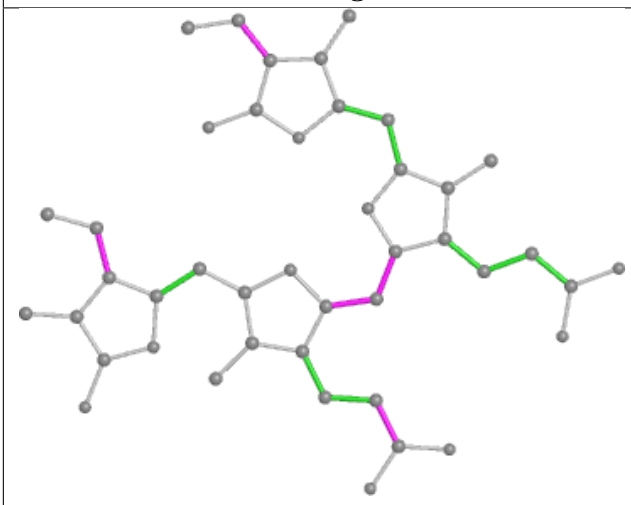

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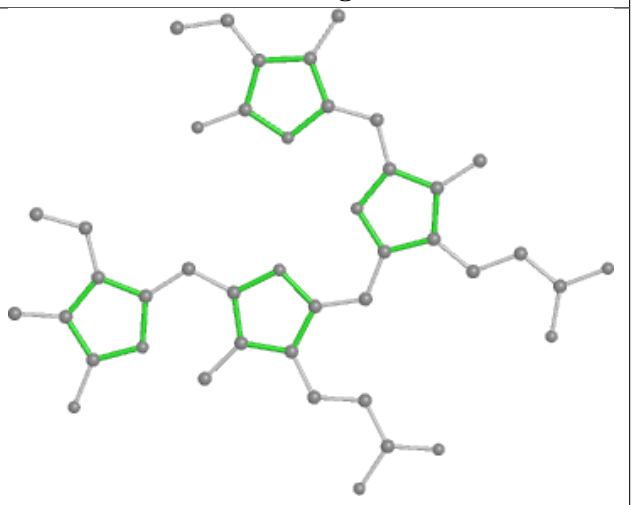
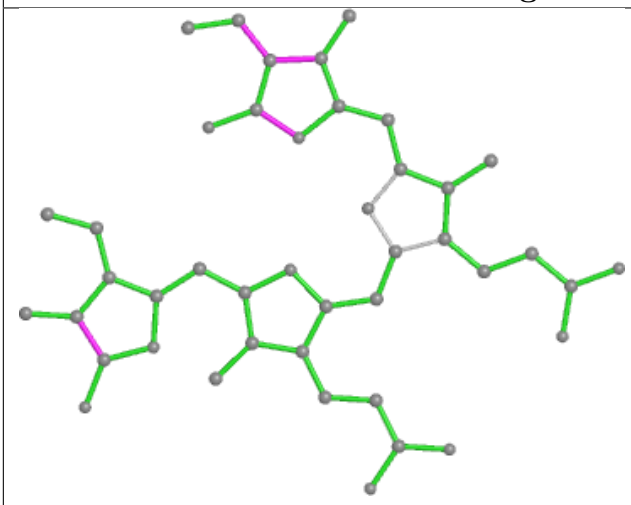


Rings

Ligand PEB cb 201



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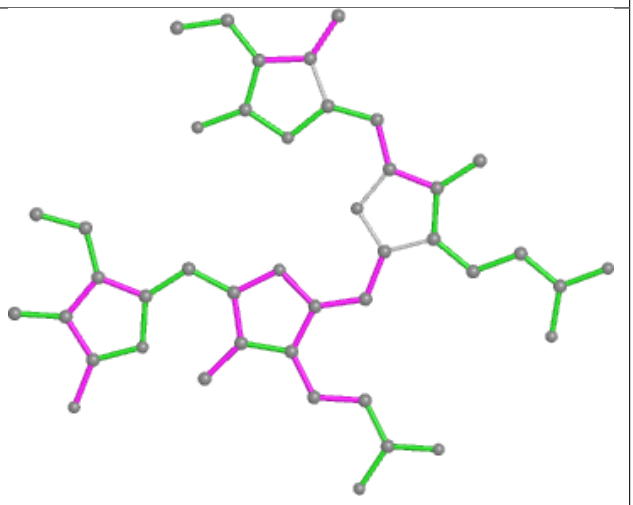
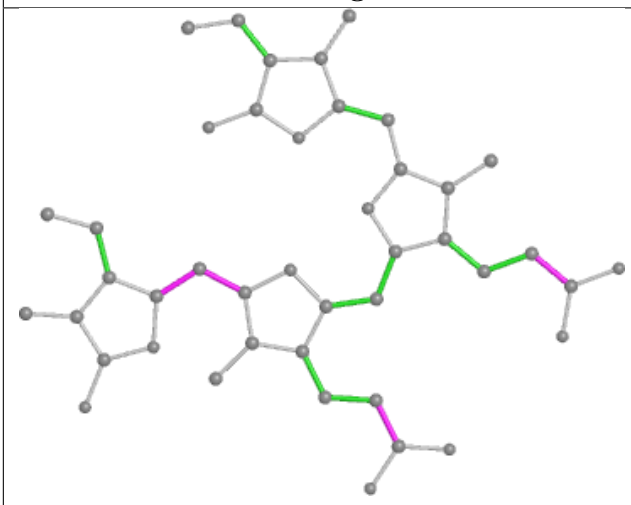


Bond angles



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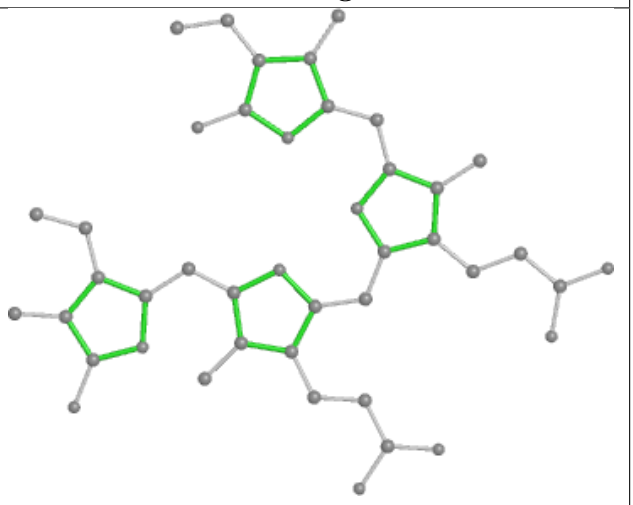
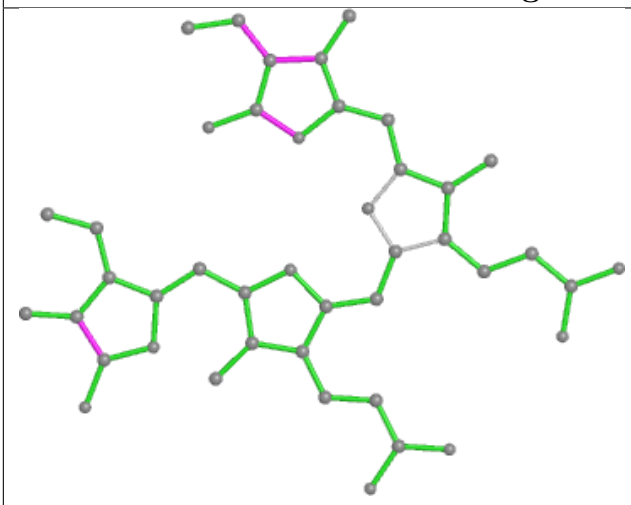
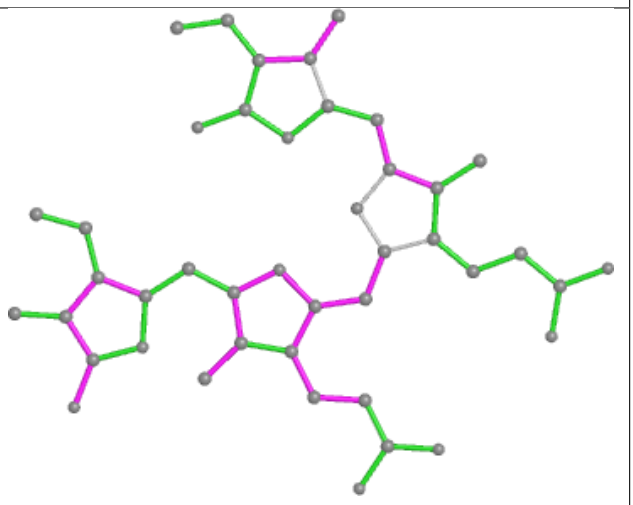


Rings

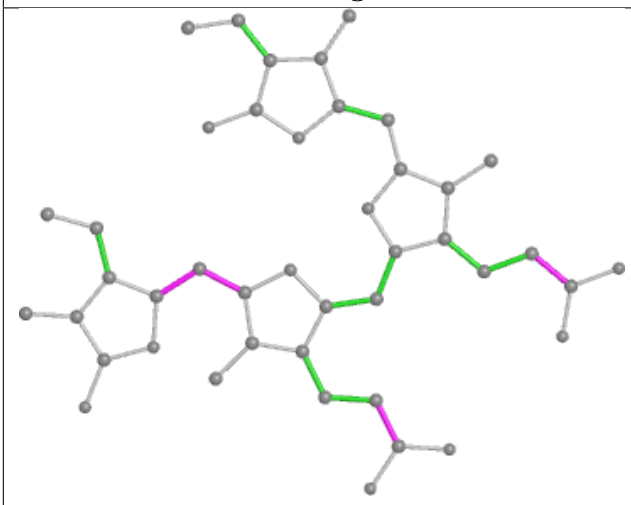
Ligand PEB I7 201



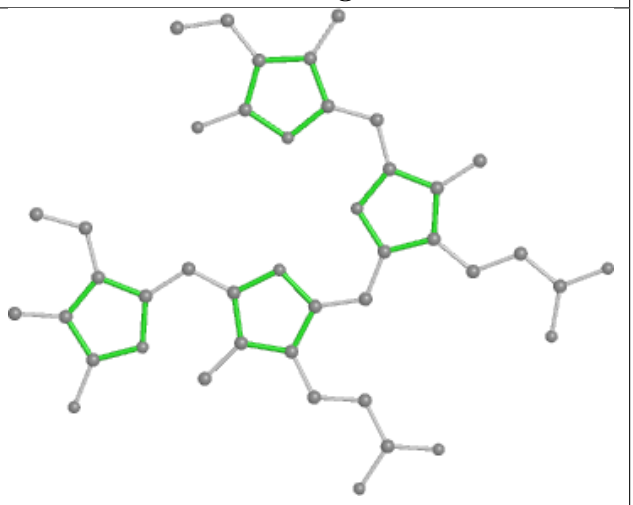
Bond lengths



Bond angles

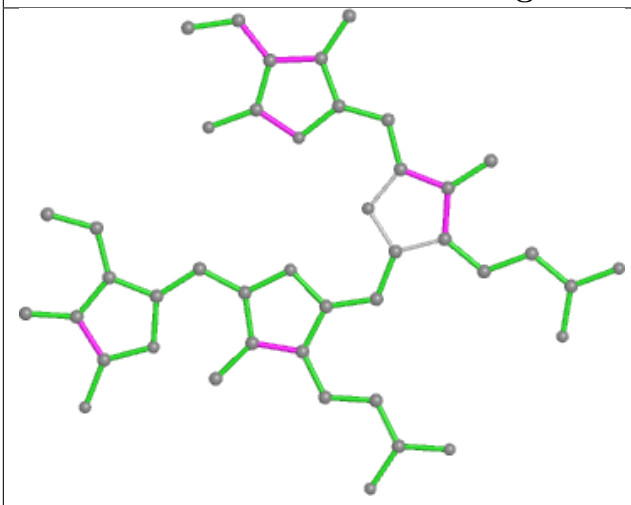


Torsions



Rings

Ligand PEB B1 301



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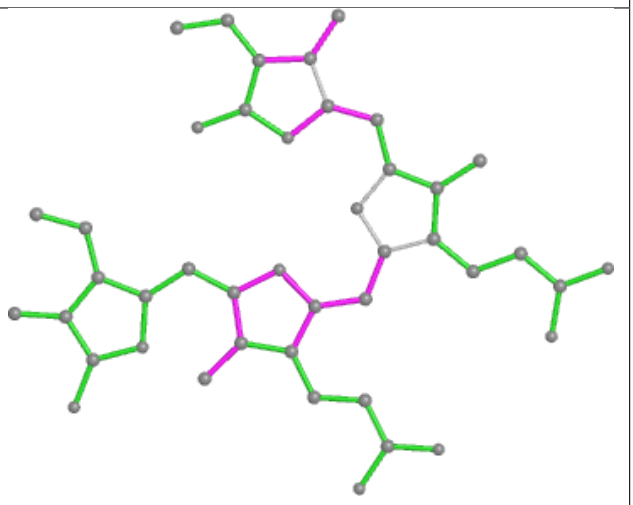

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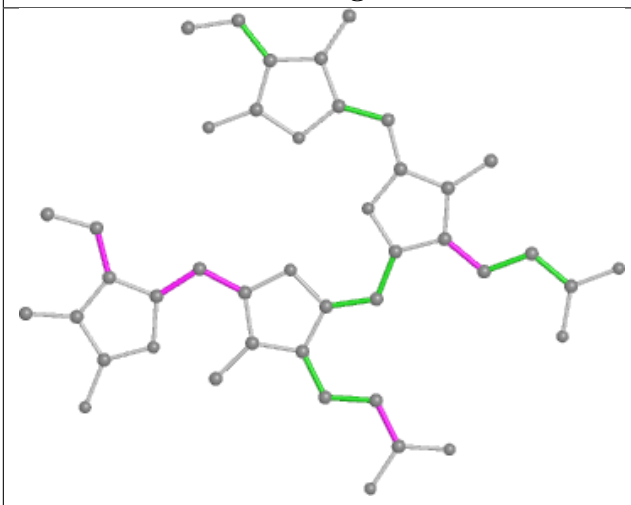

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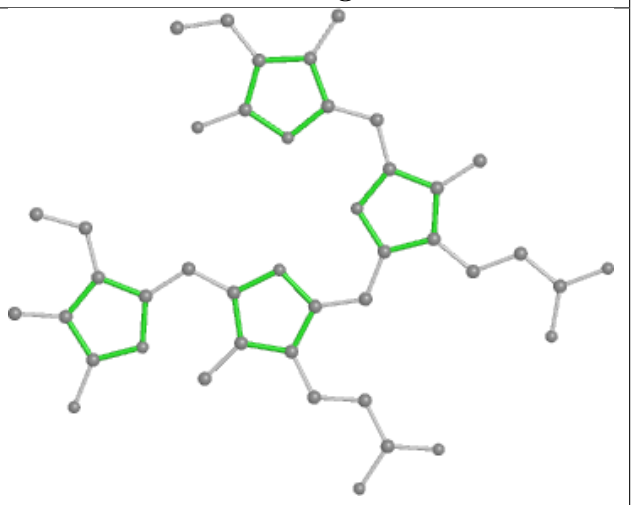
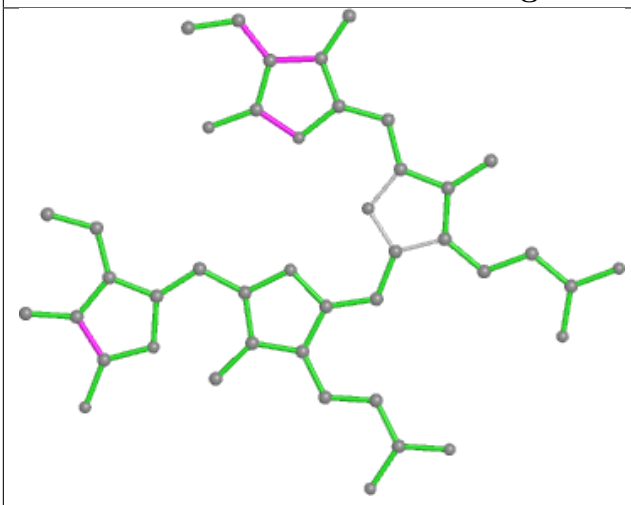


Rings

Ligand PEB ds 202



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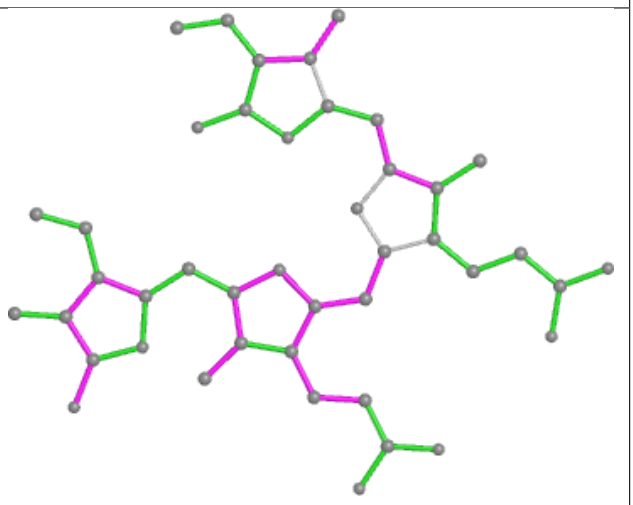

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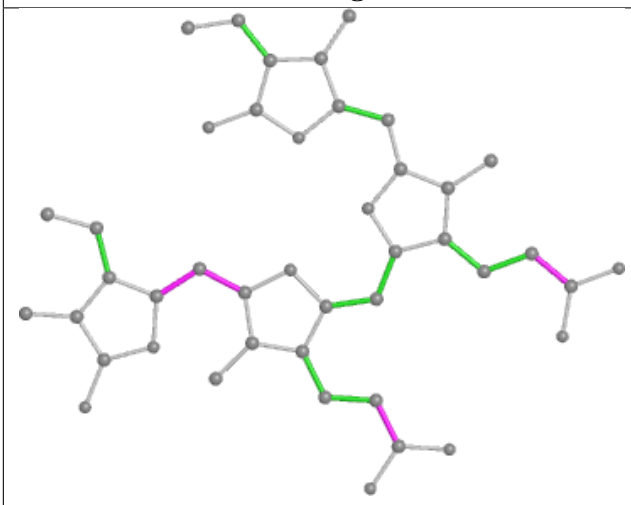

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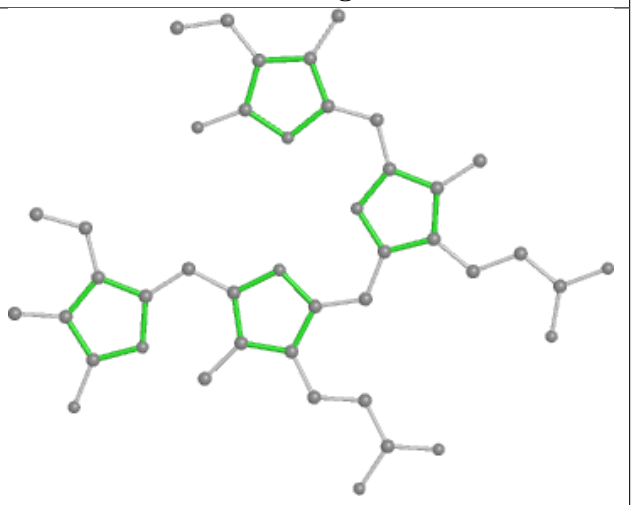

Rings

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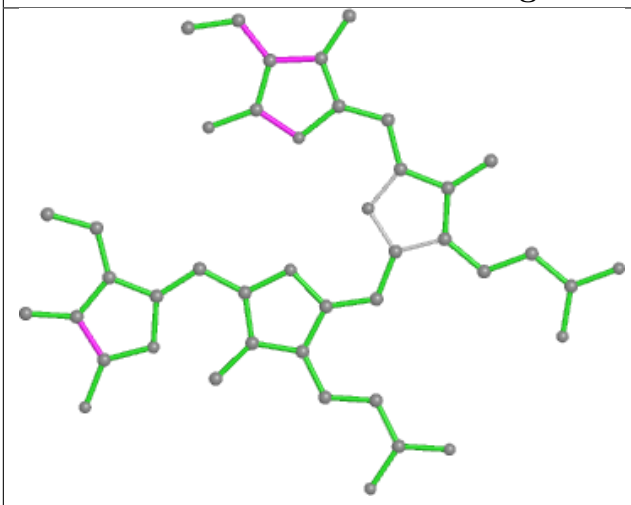

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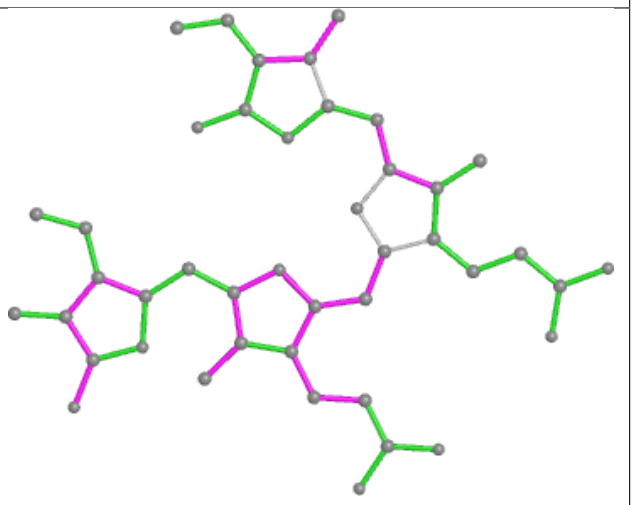

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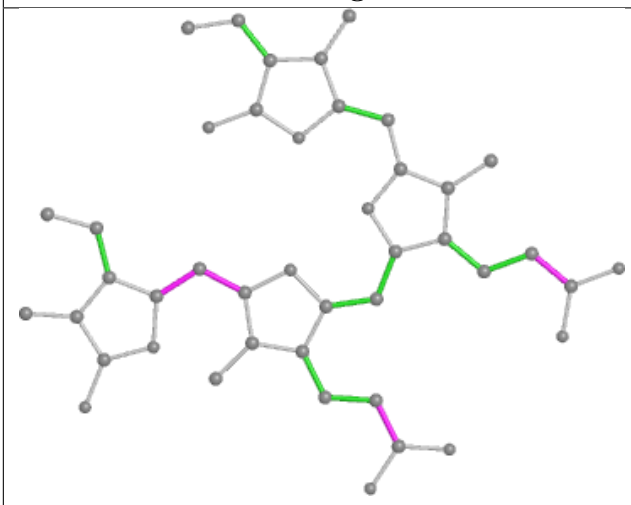

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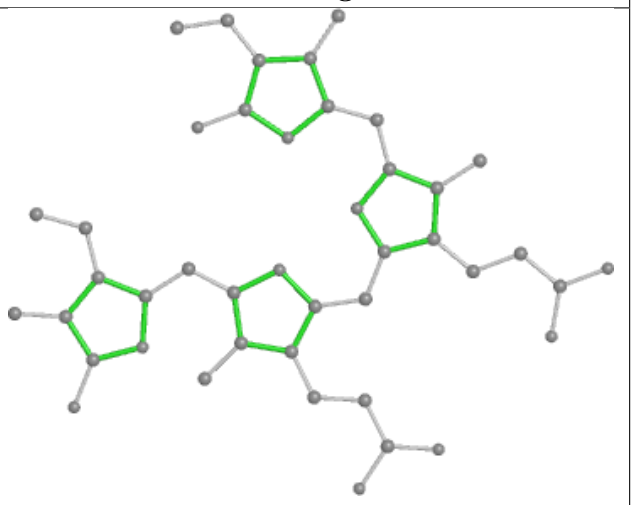

Rings

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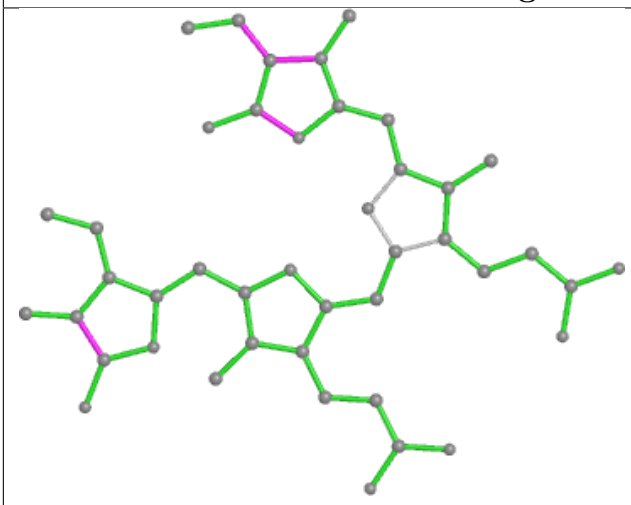

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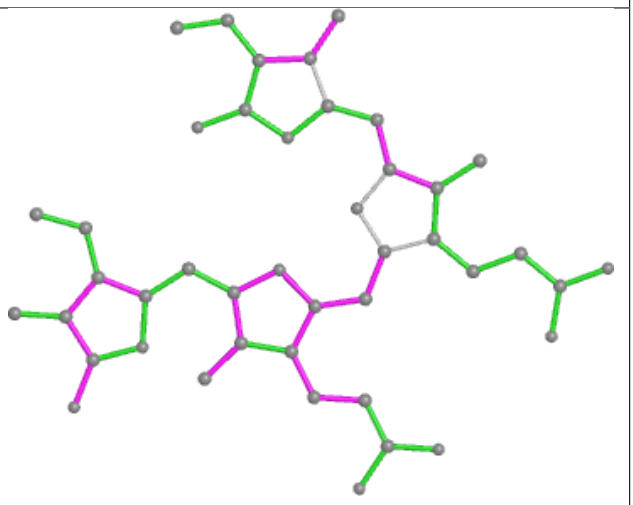

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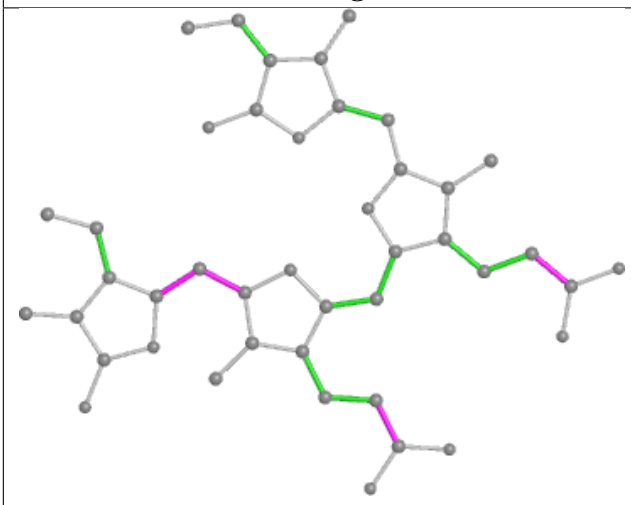

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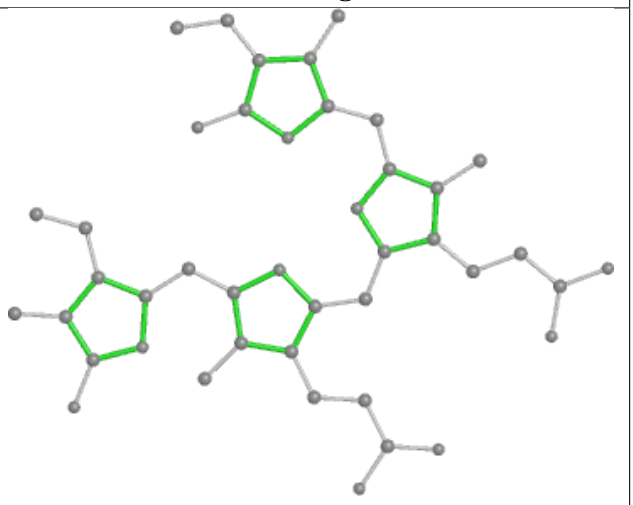

Rings

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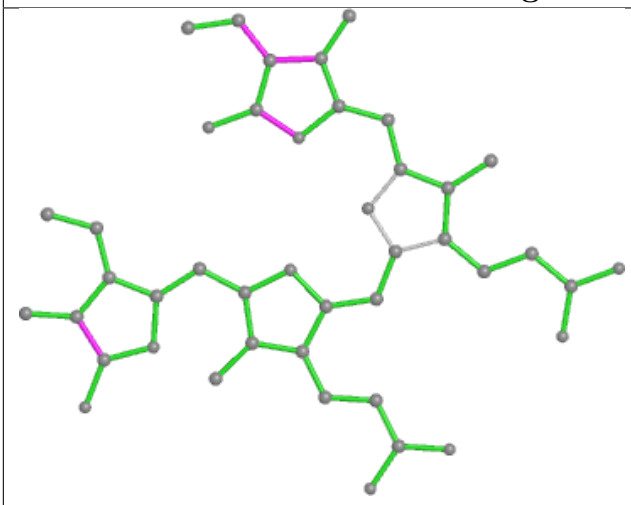

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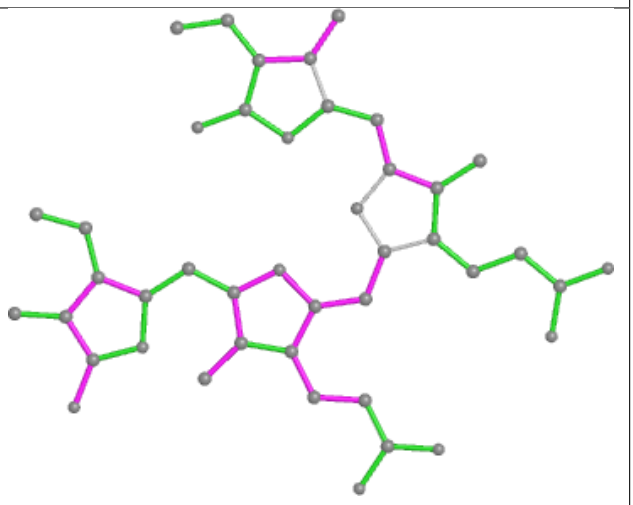

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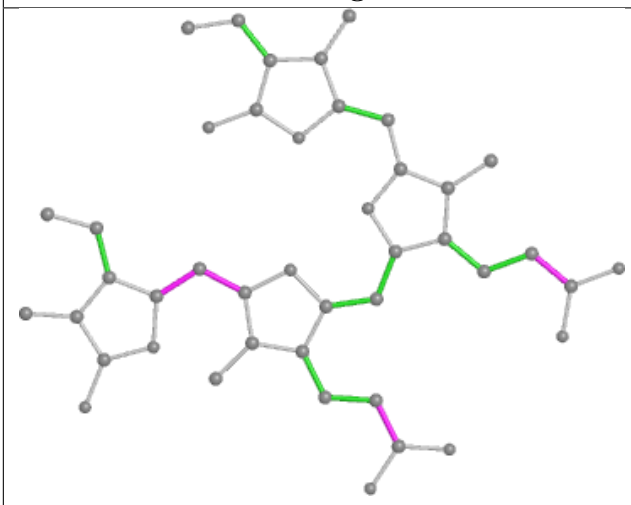

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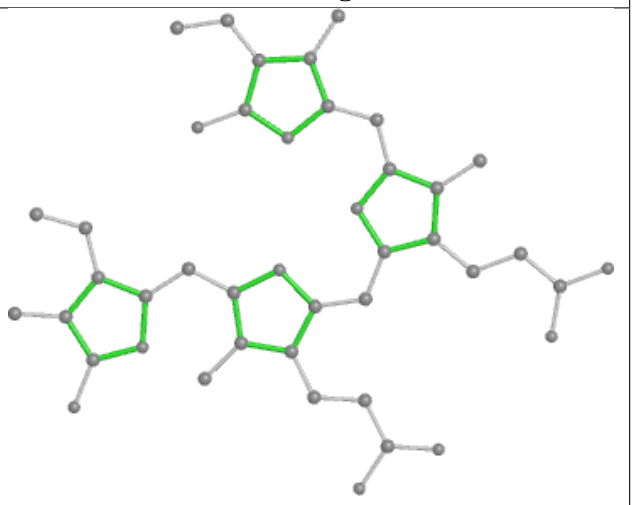
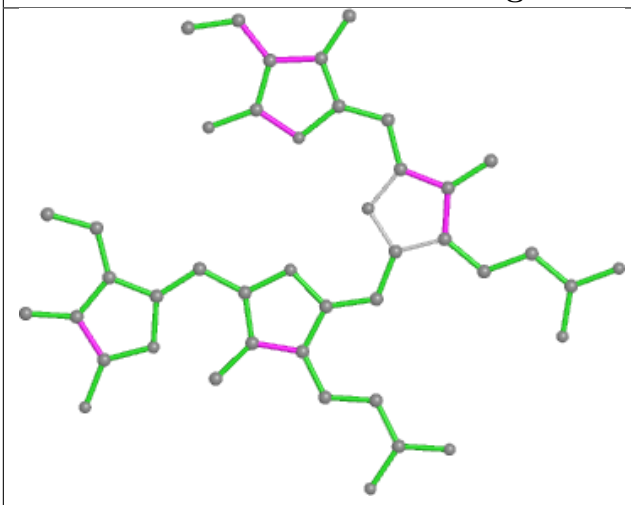


Rings

Ligand PEB jM 1002



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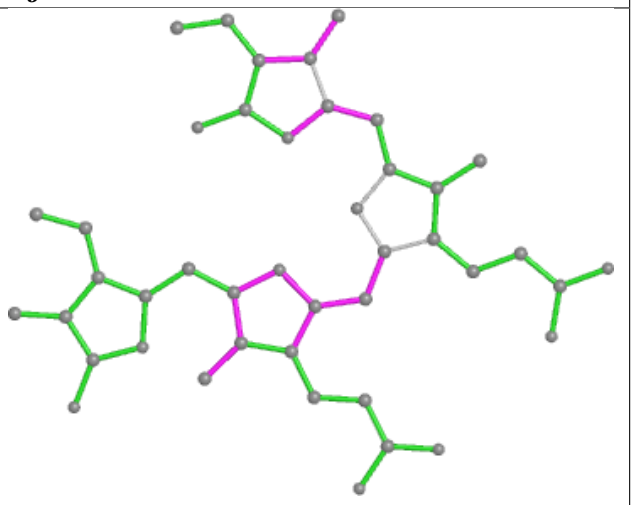

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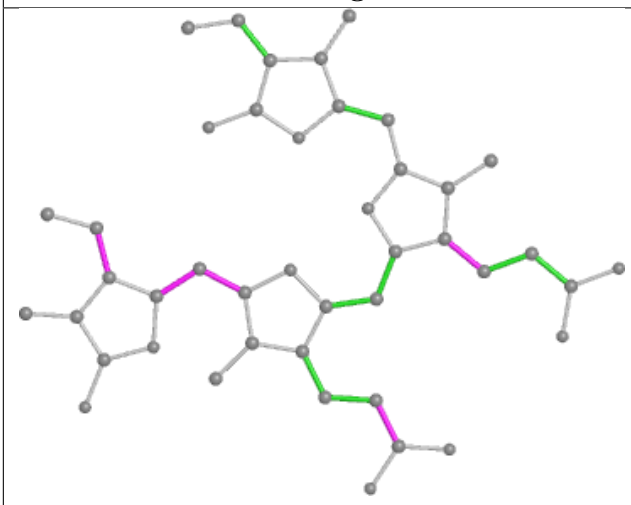

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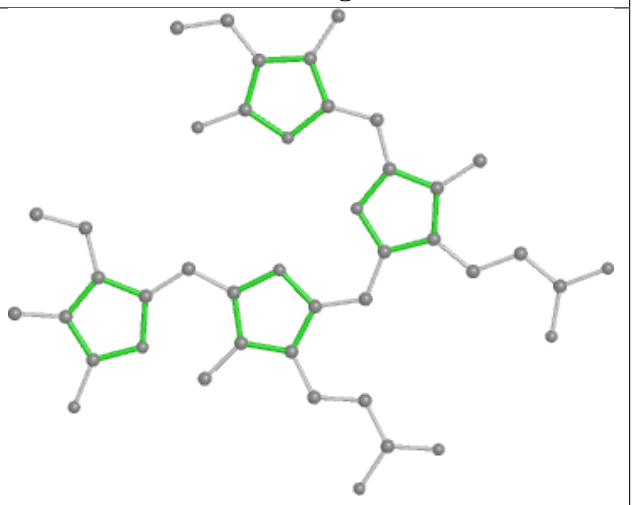

Rings

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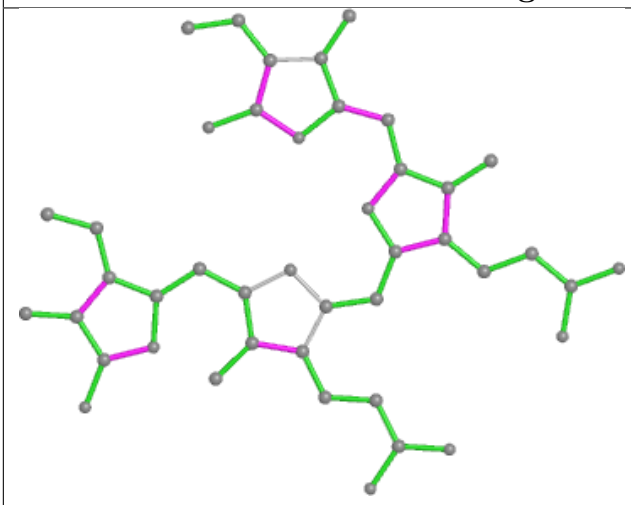

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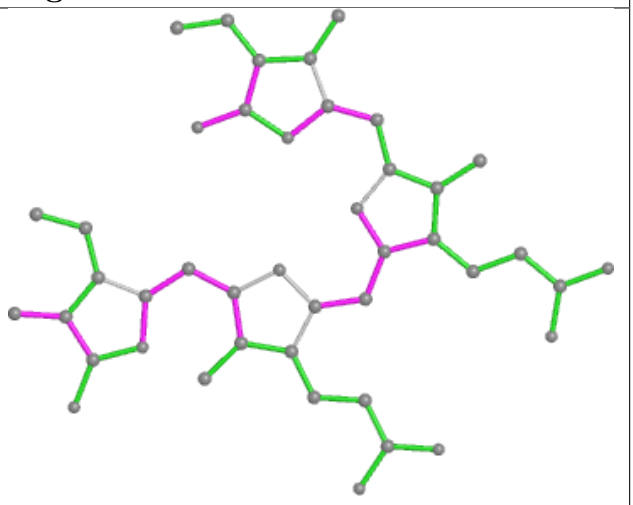

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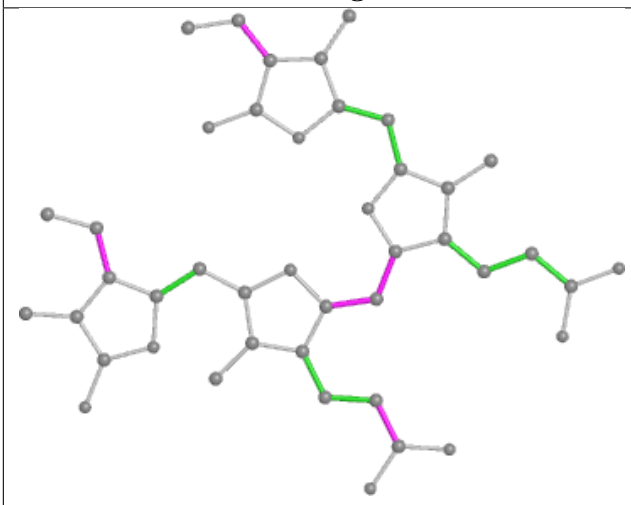

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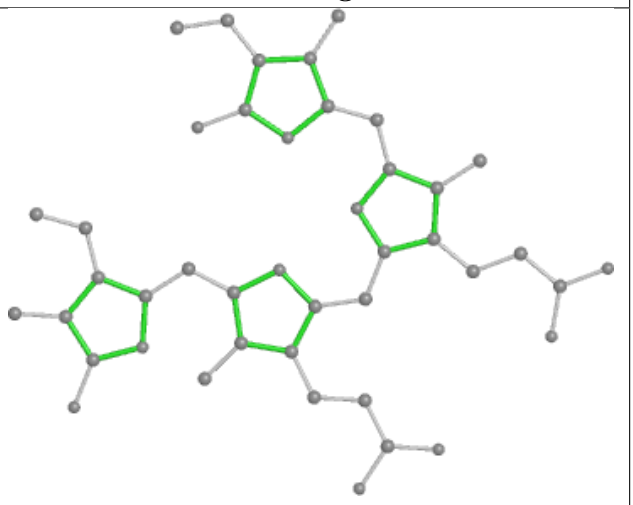

Rings

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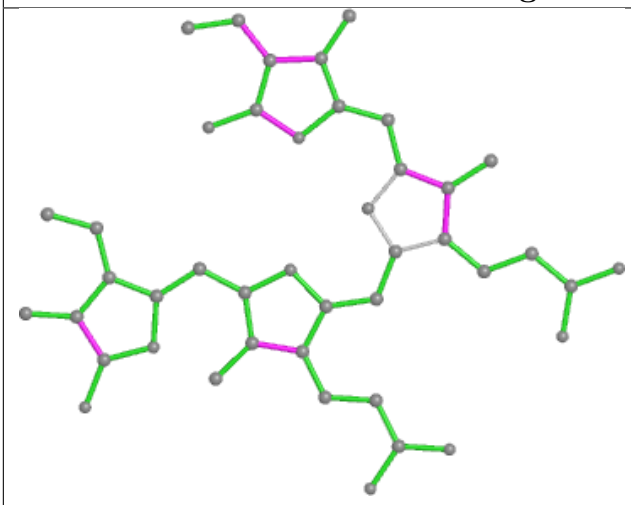

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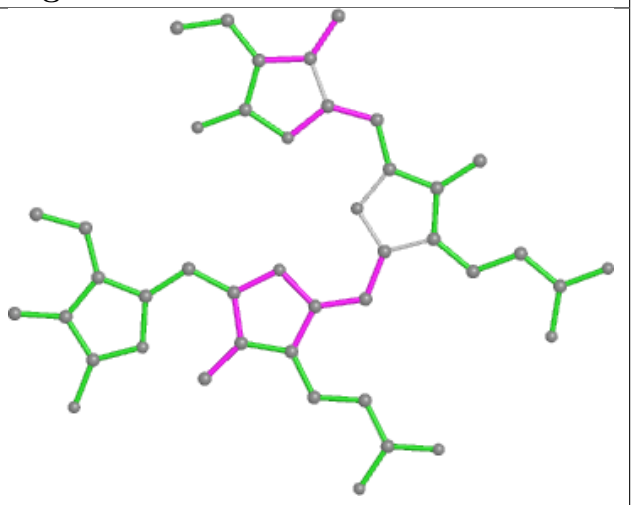

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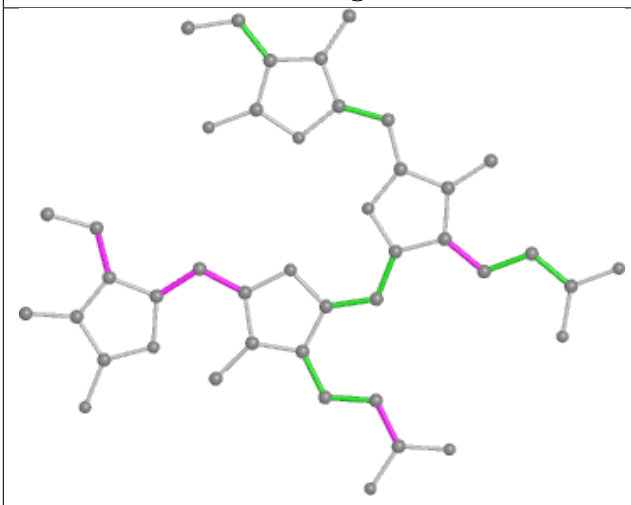

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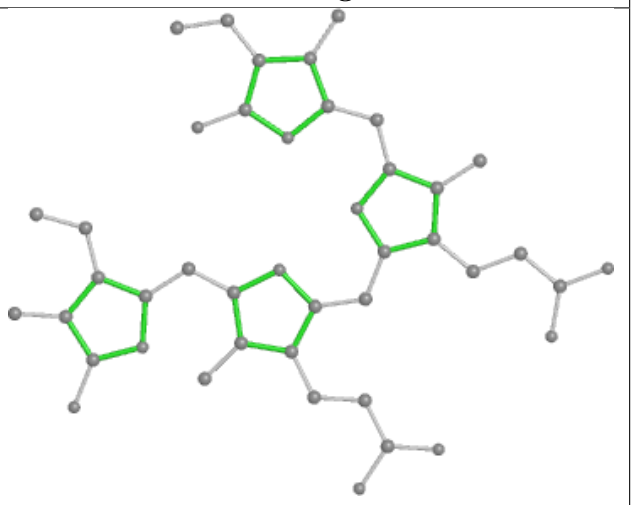
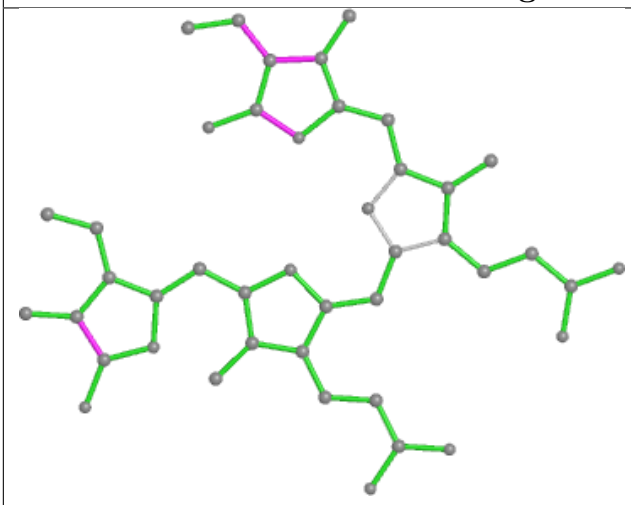


Rings

Ligand PEB h8 201



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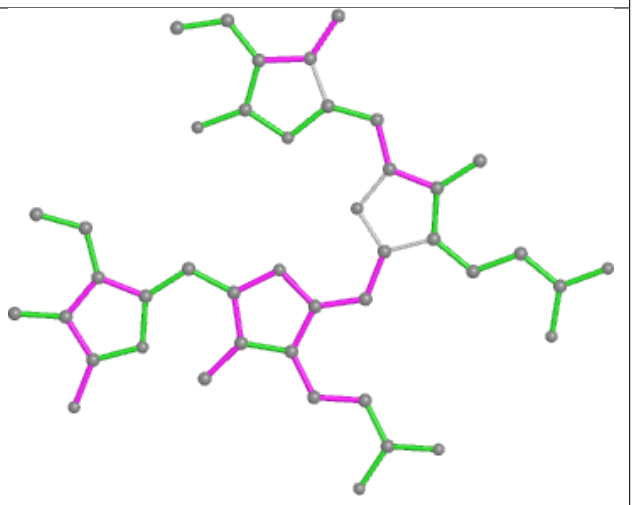

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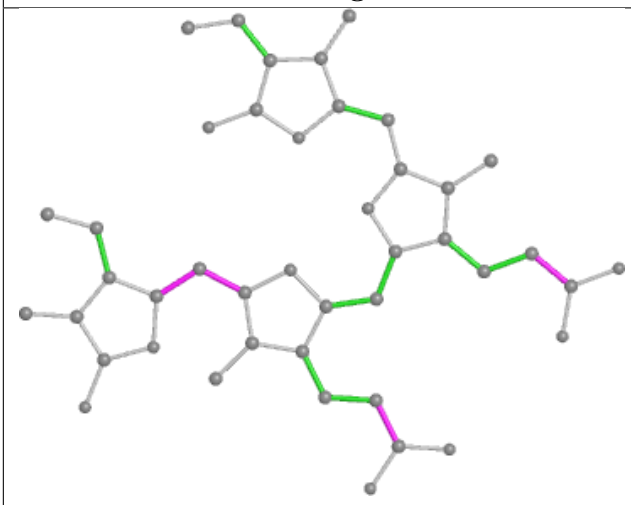

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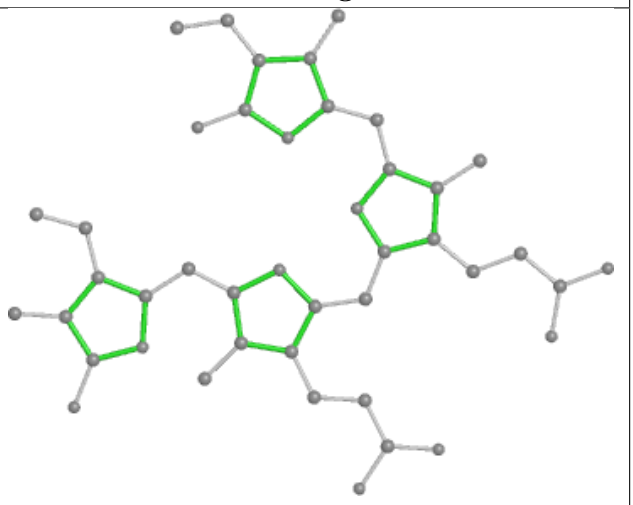

Rings

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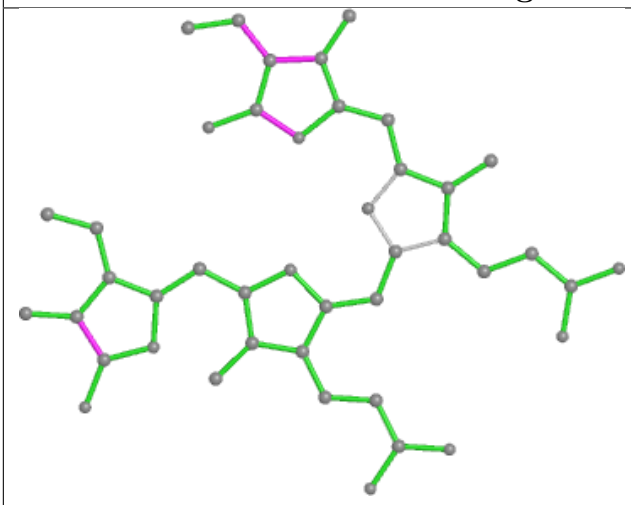

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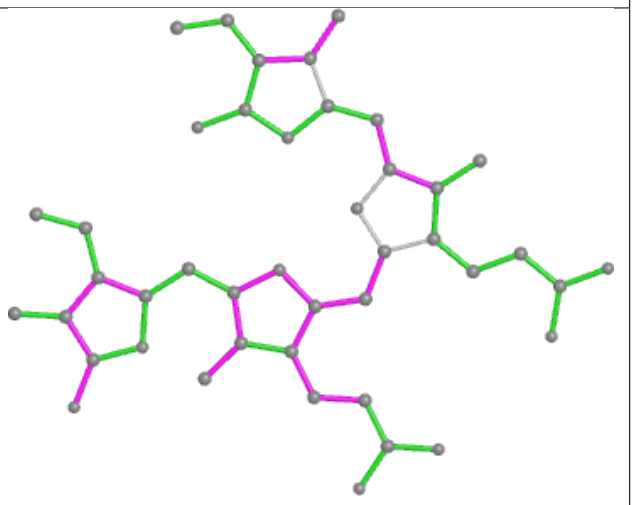

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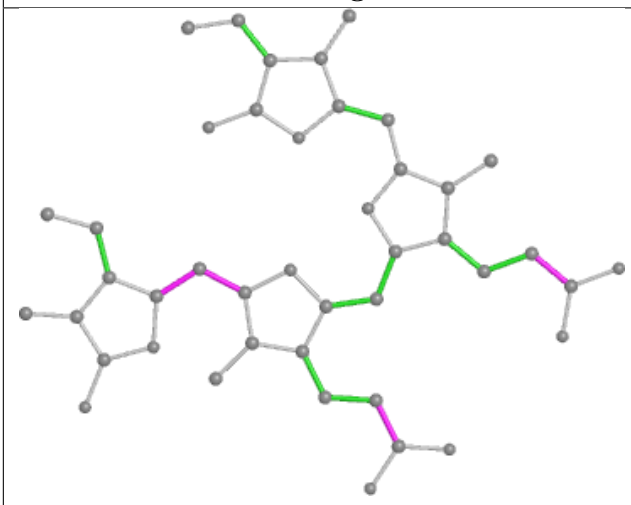

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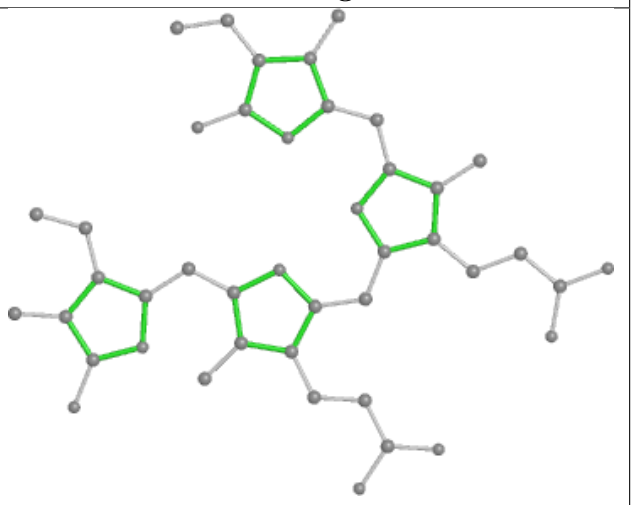
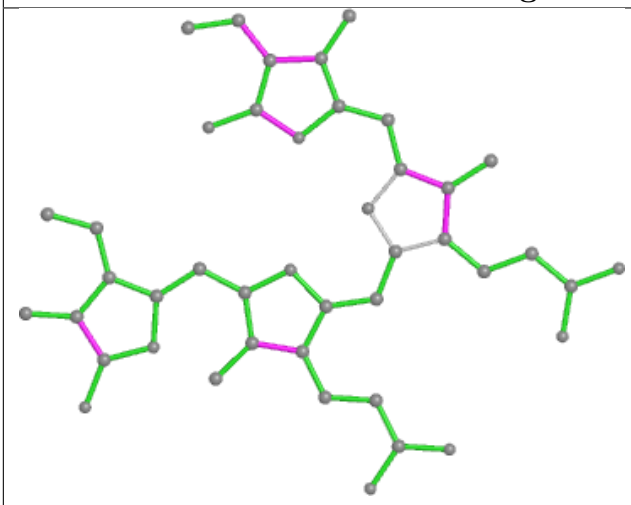


Rings

Ligand PEB gg 202



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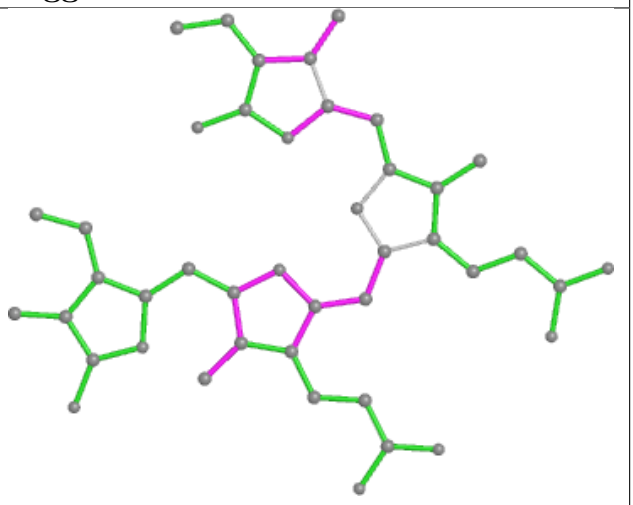

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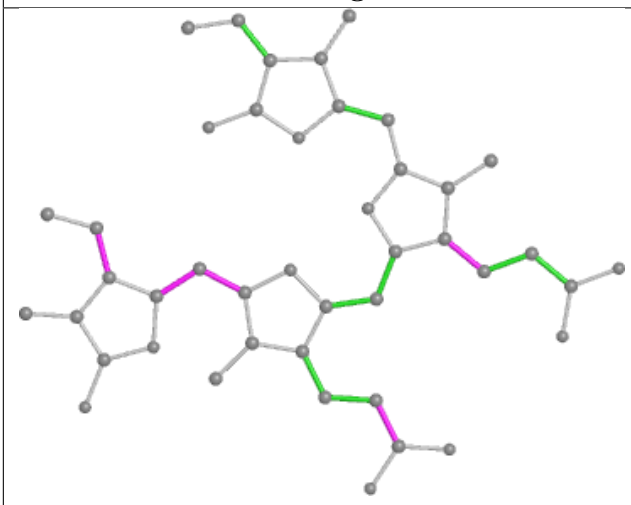

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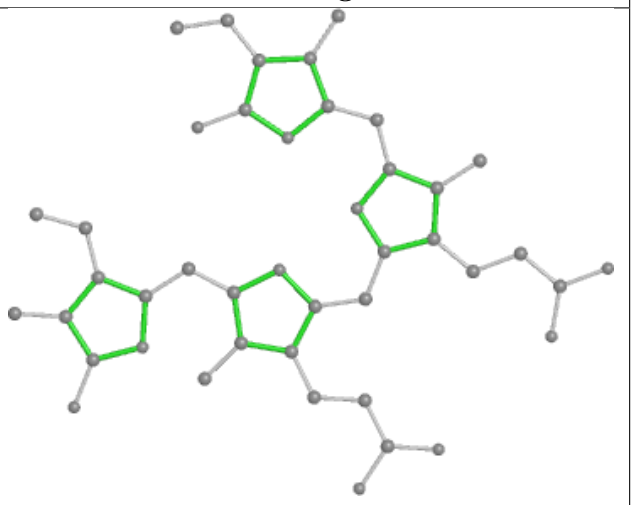

Rings

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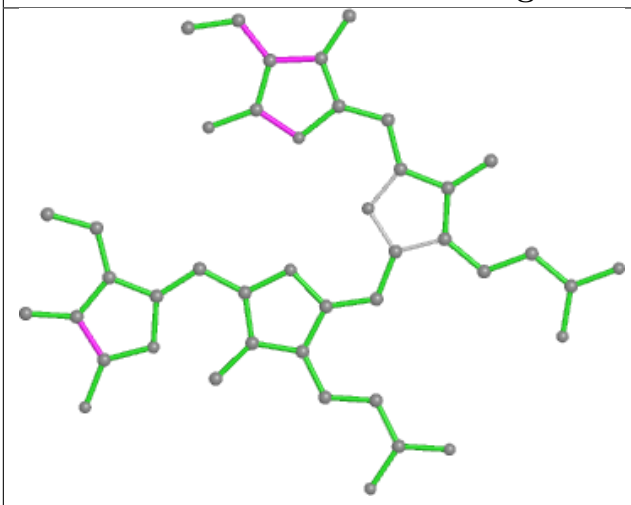

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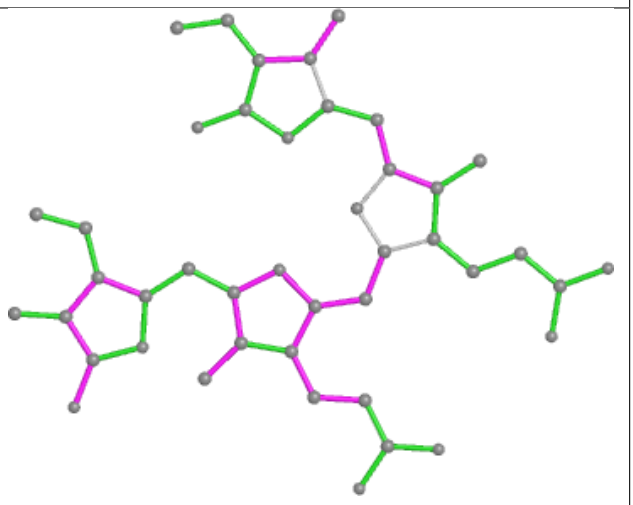

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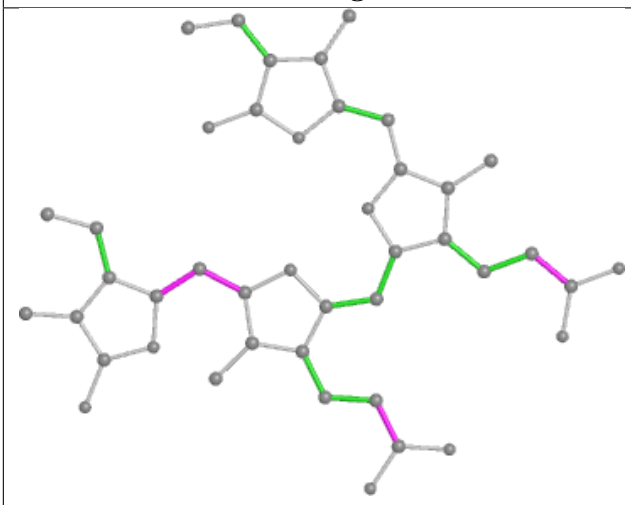

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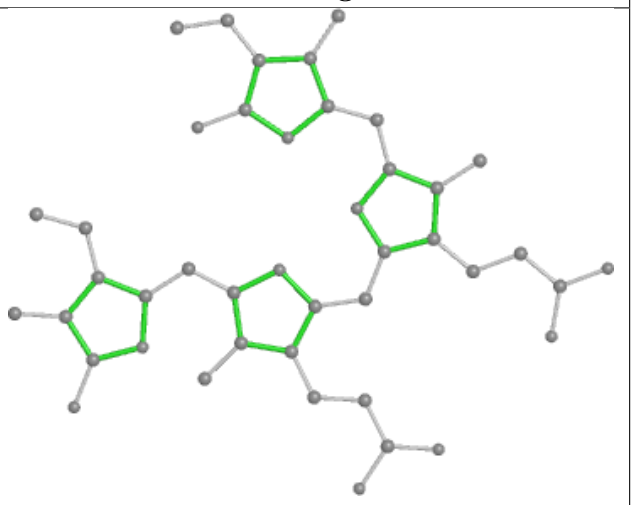
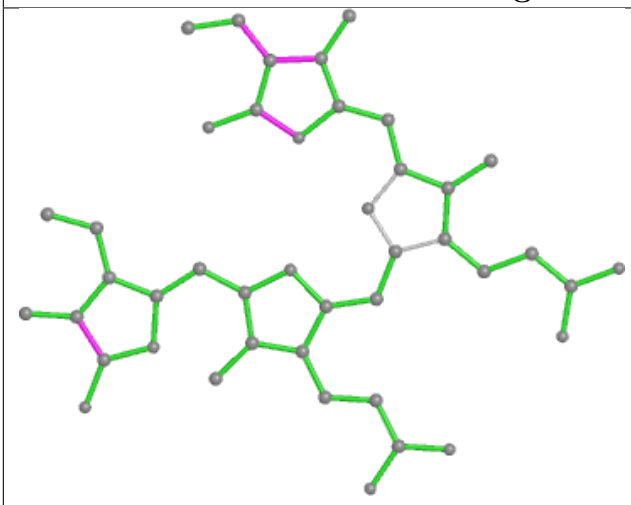


Rings

Ligand PEB dK 201



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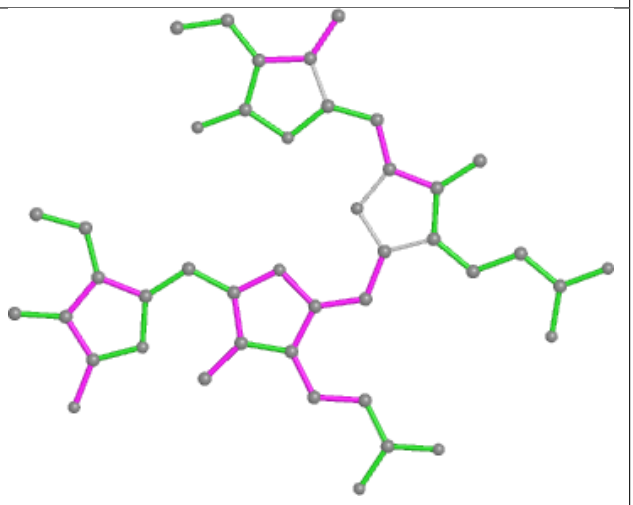
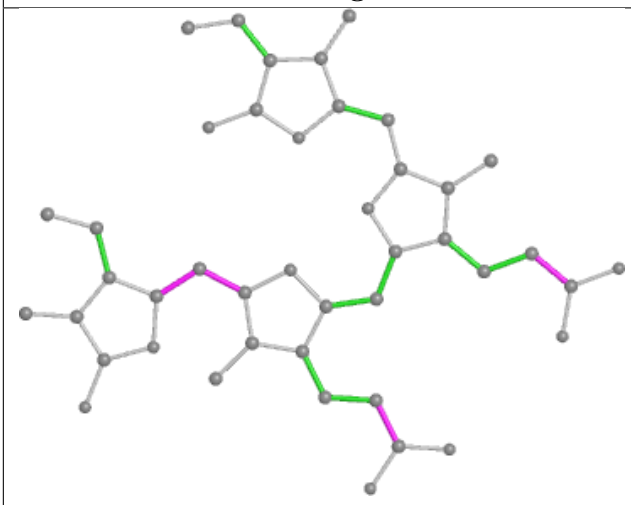
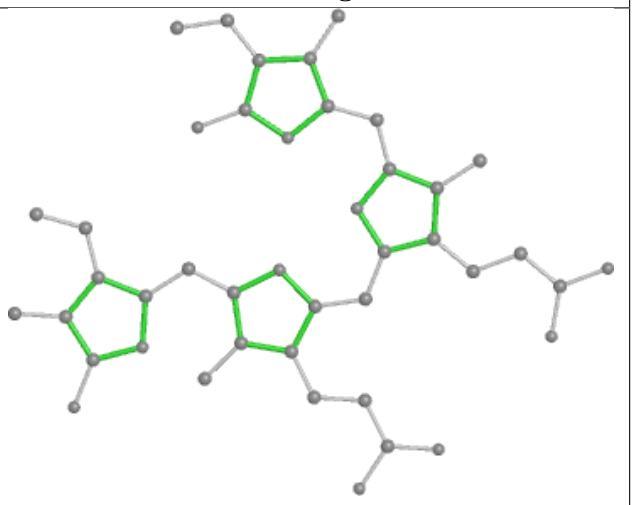


Bond angles

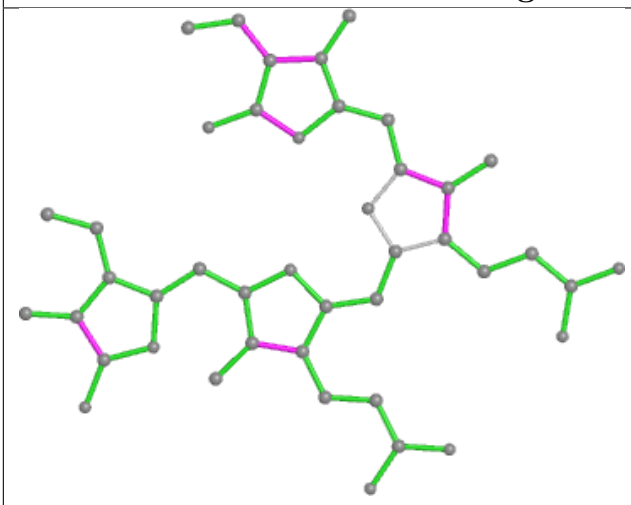


Torsions



Rings

Ligand PEB F7 201



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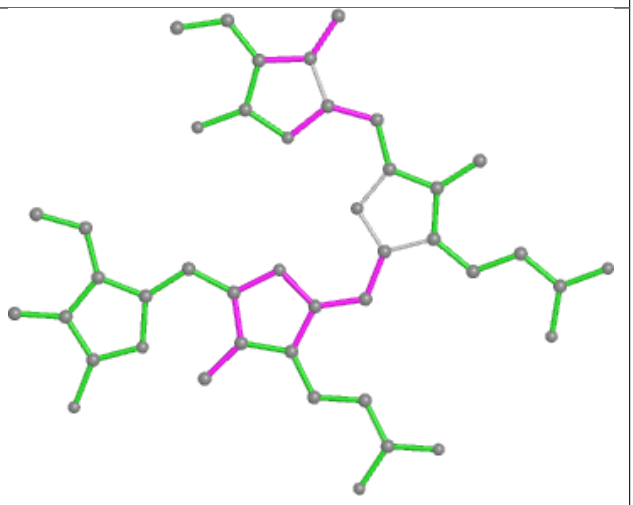

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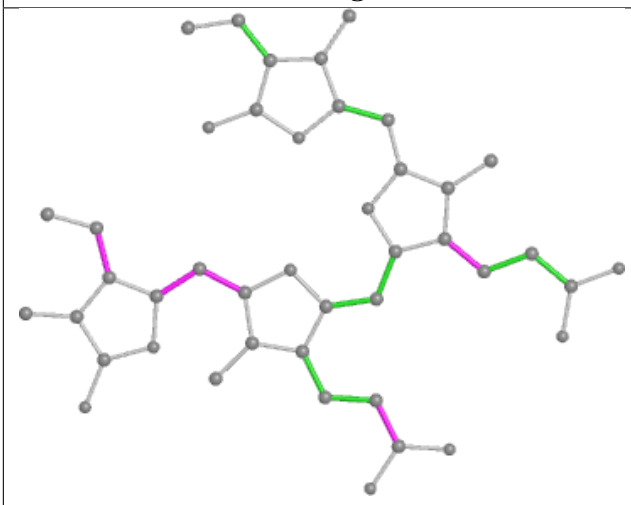

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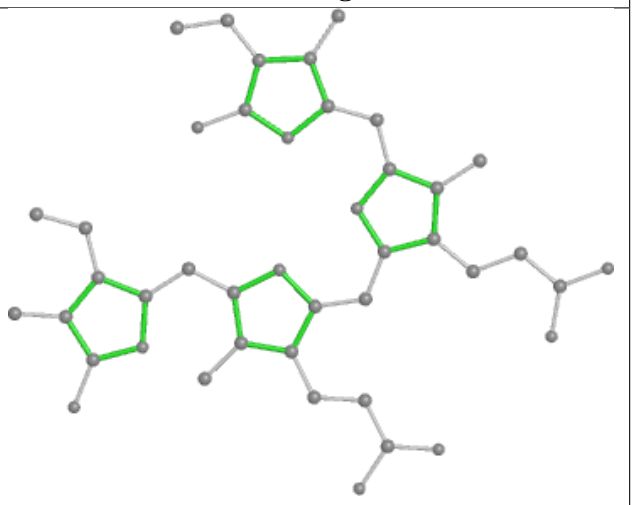
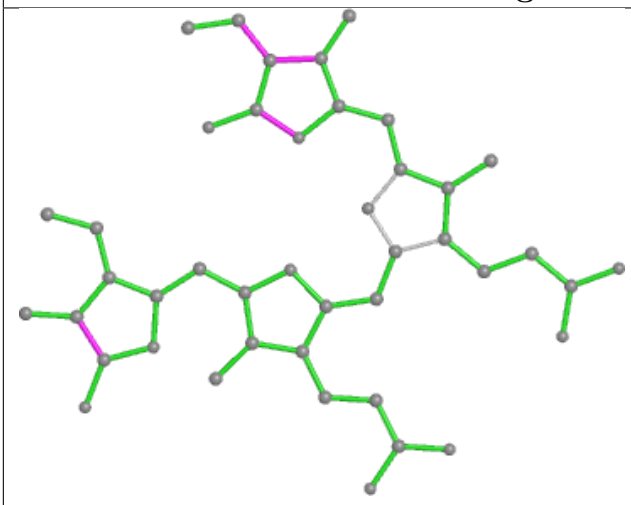


Rings

Ligand PEB cX 201



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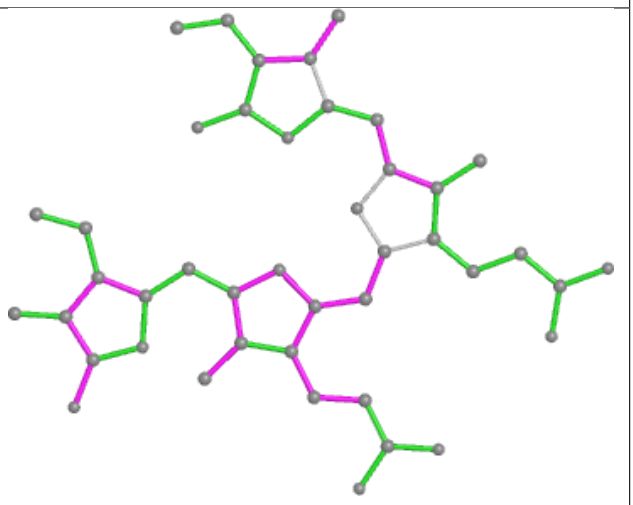

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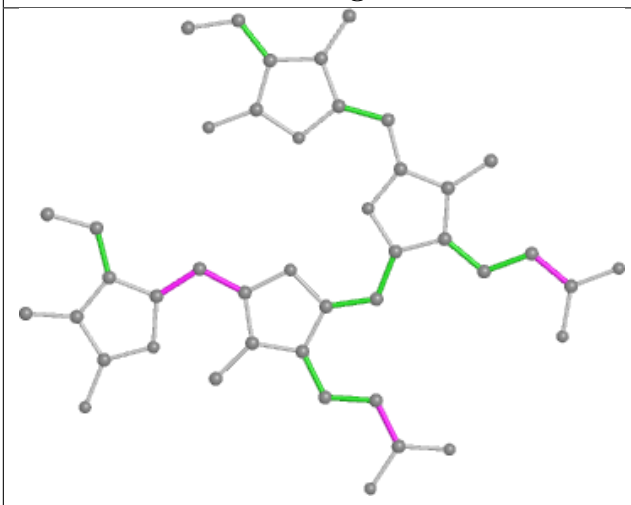

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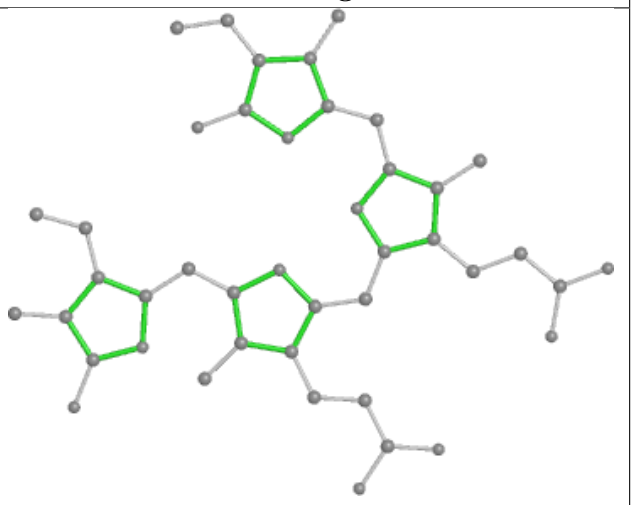

Rings

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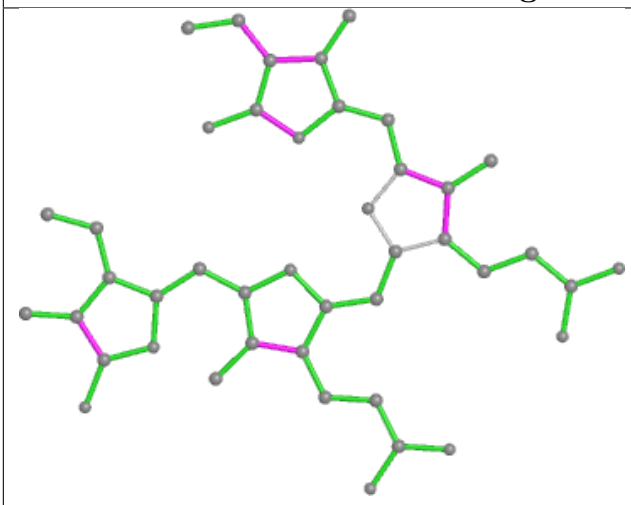

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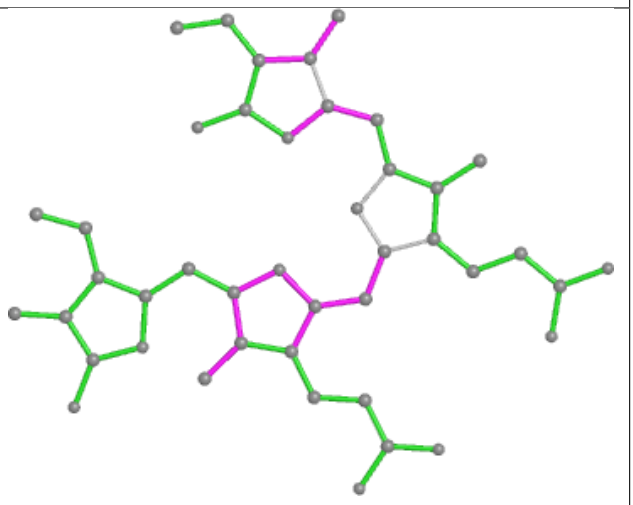

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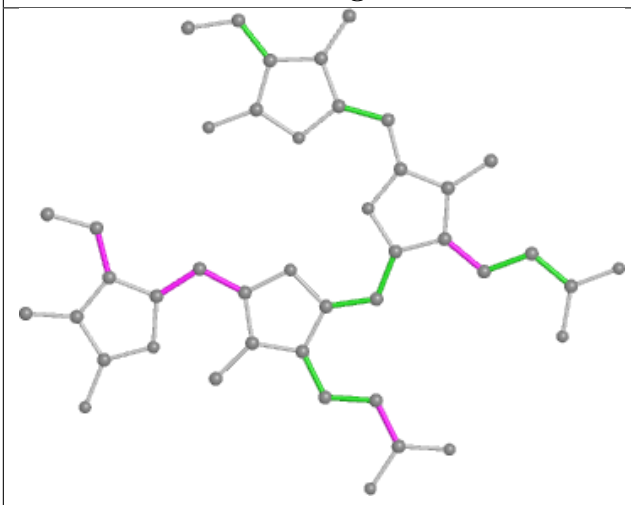

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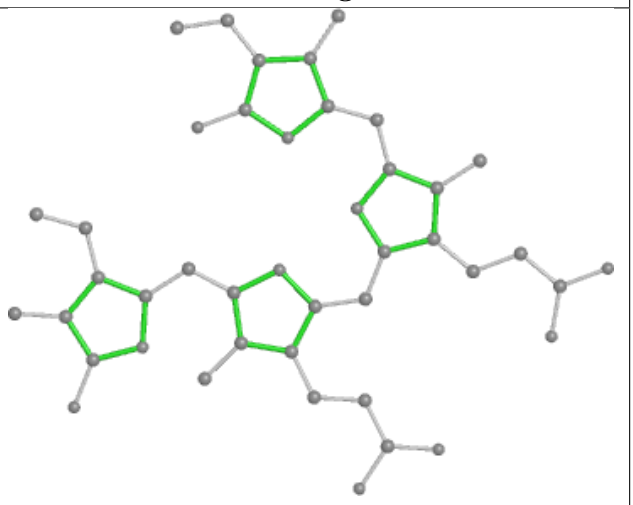
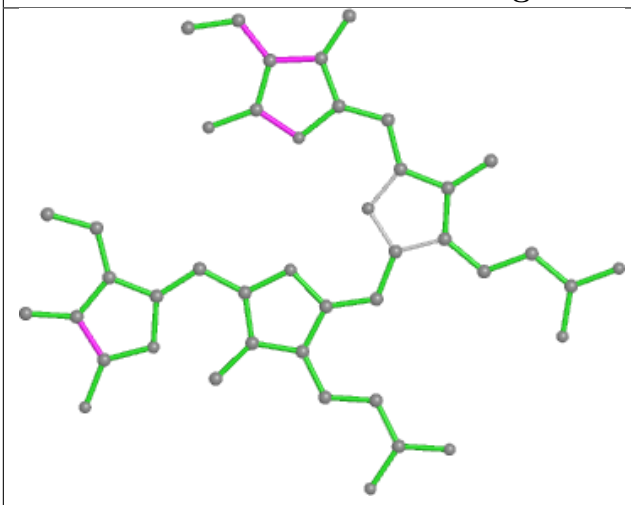


Rings

Ligand PEB cM 202



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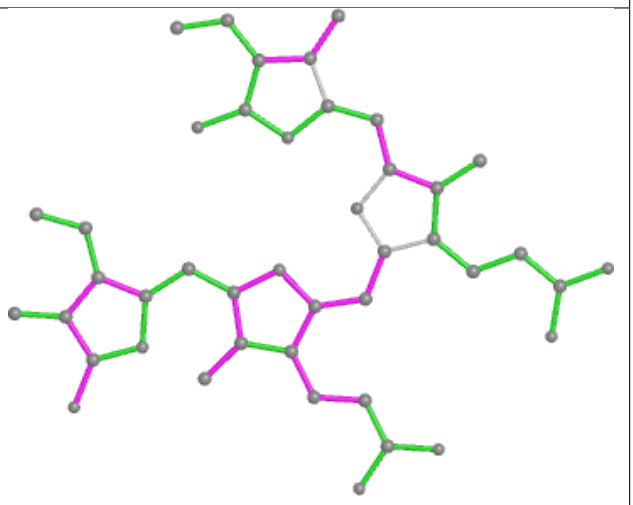

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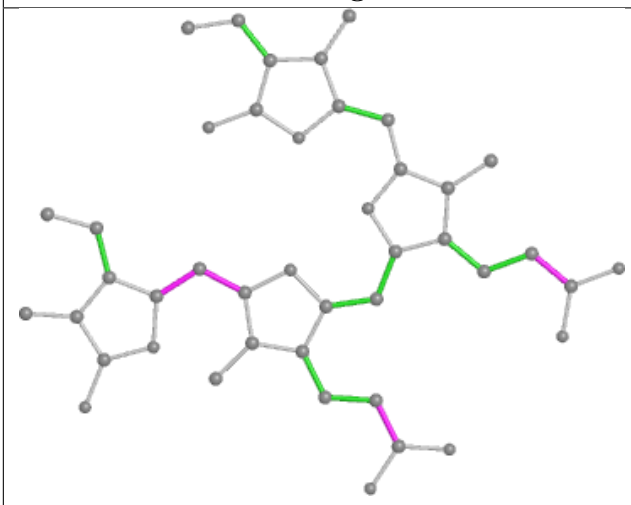

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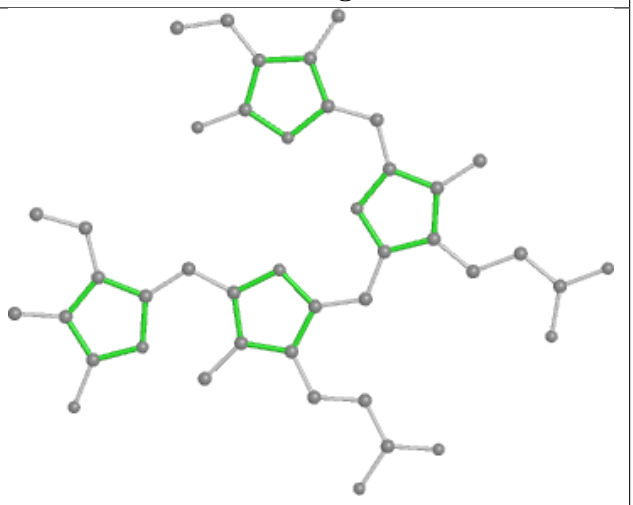
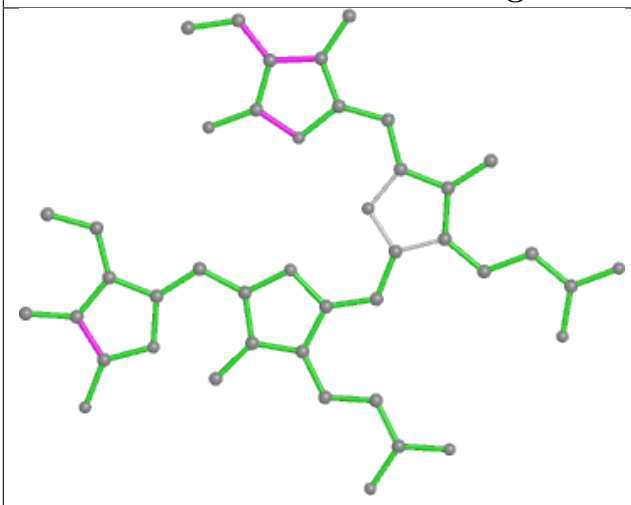


Rings

Ligand PEB C4 1001



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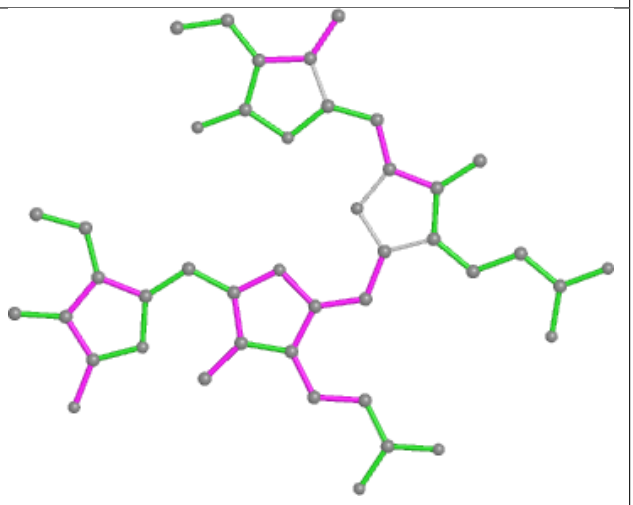

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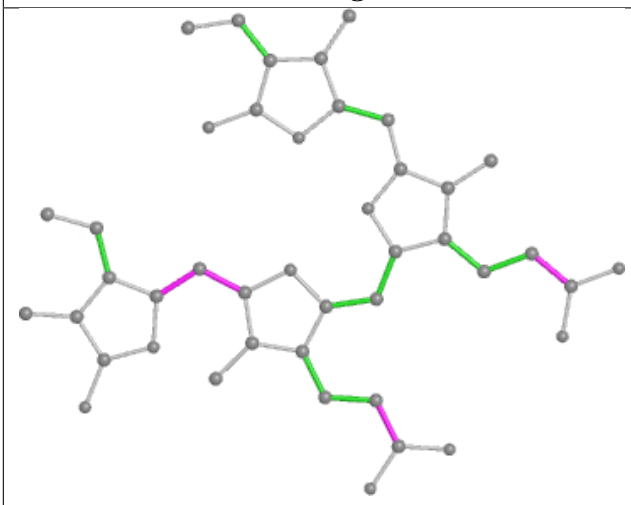

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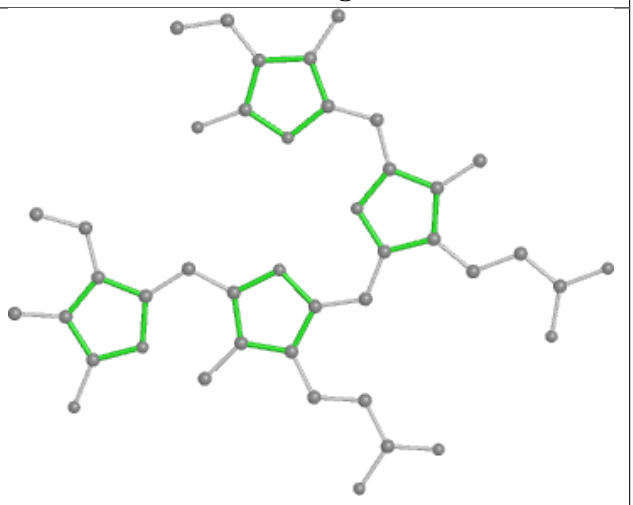
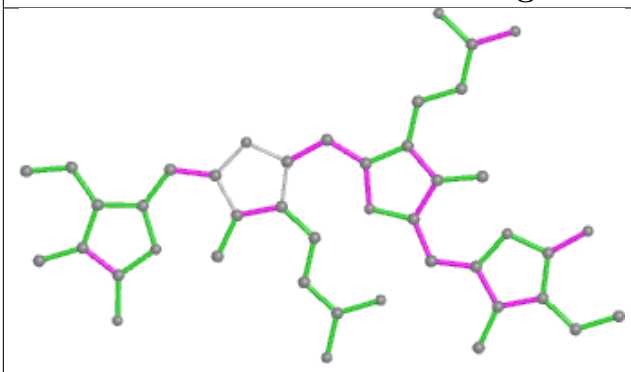


Rings

Ligand CYC g1 201



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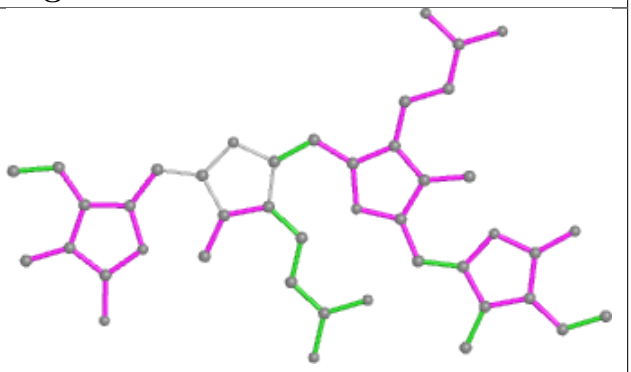

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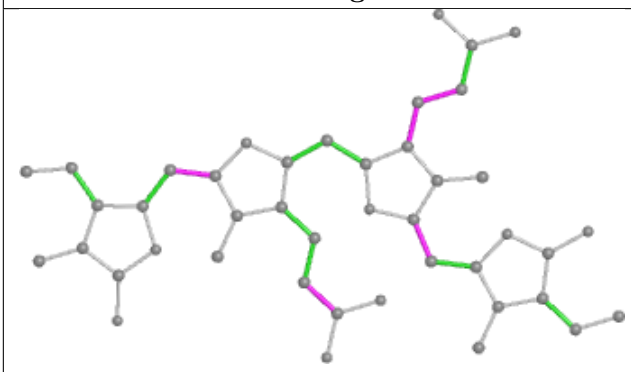

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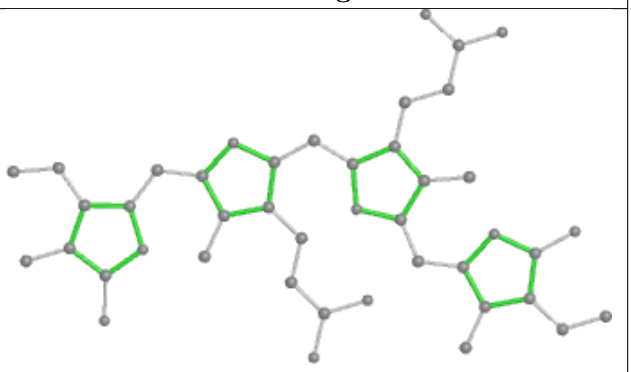

Rings

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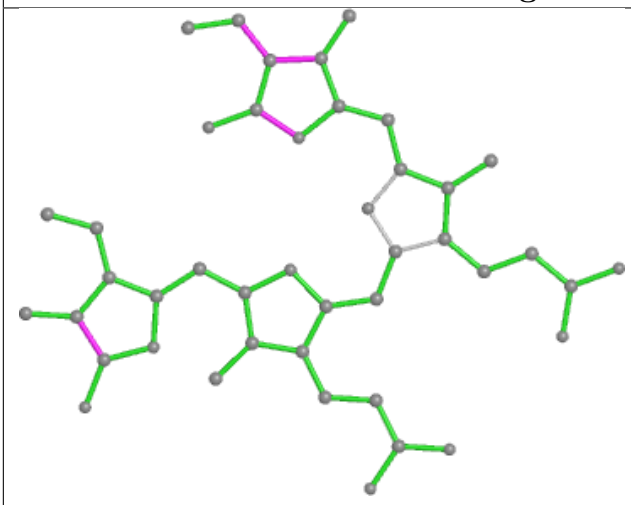

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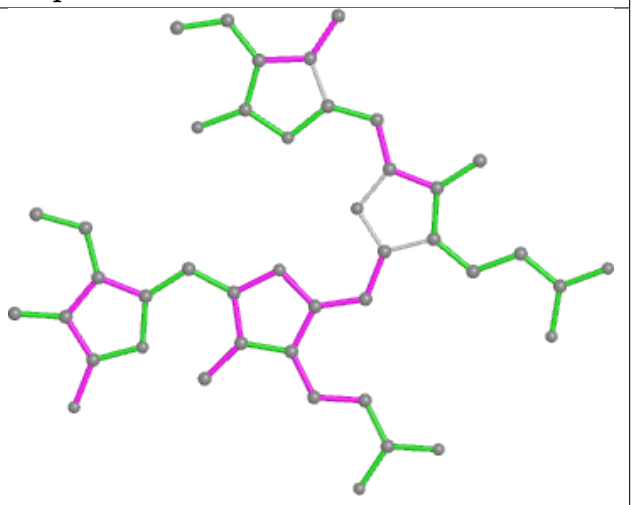

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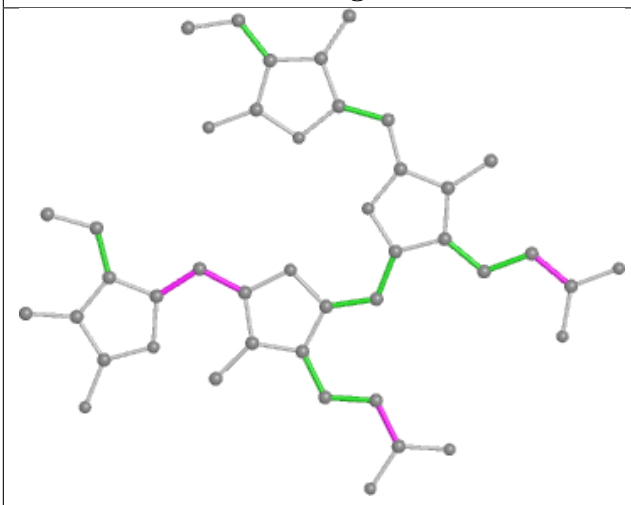

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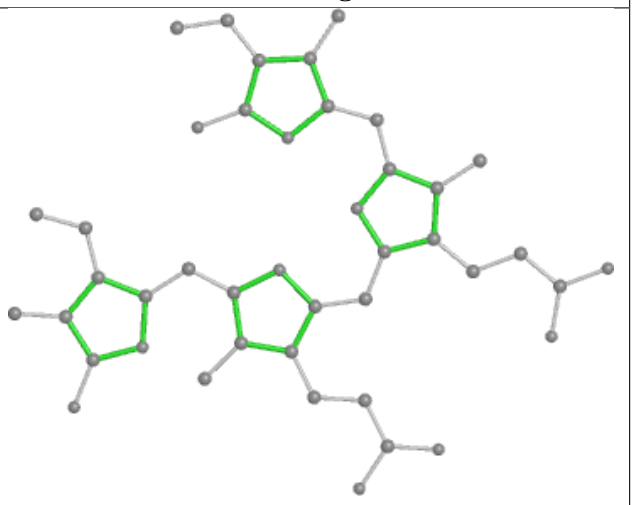
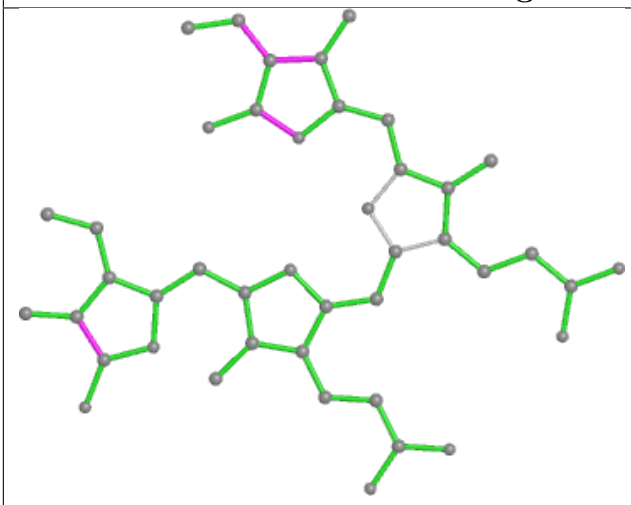


Rings

Ligand PEB aC 201



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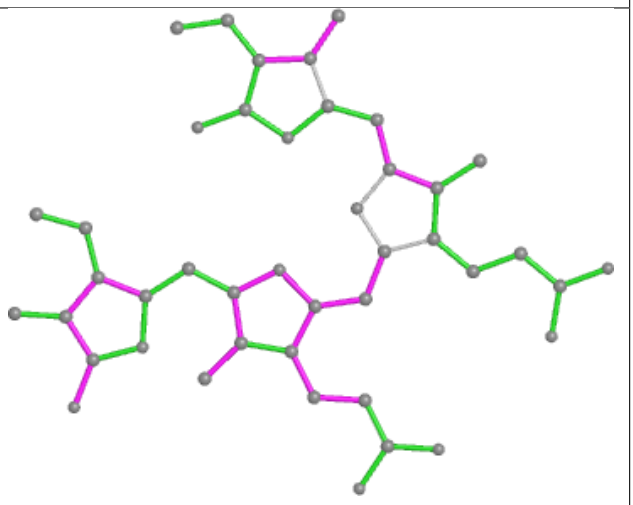

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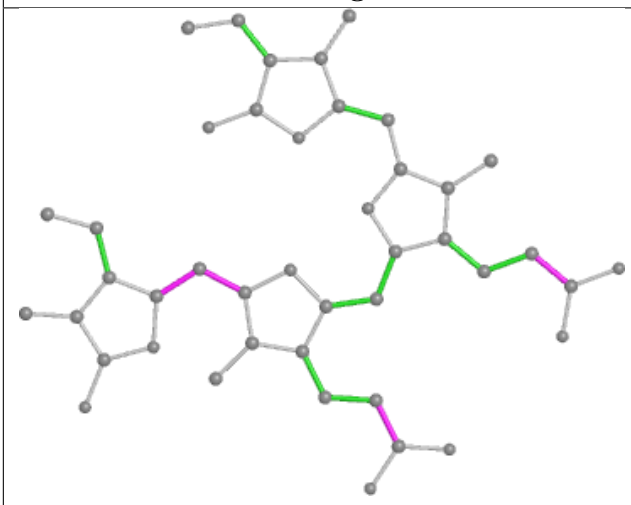

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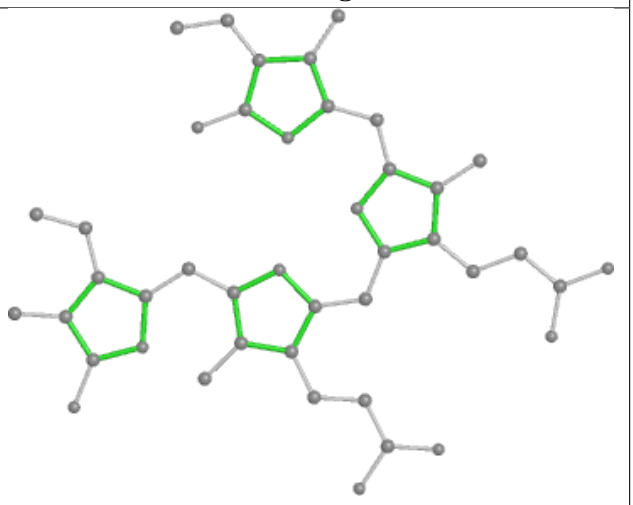

Rings

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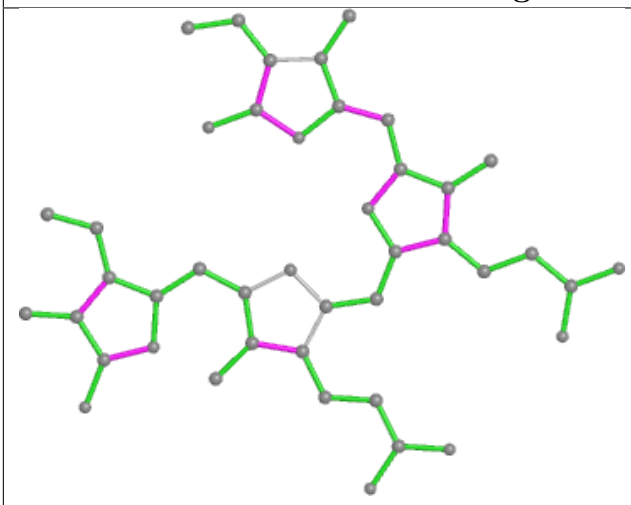

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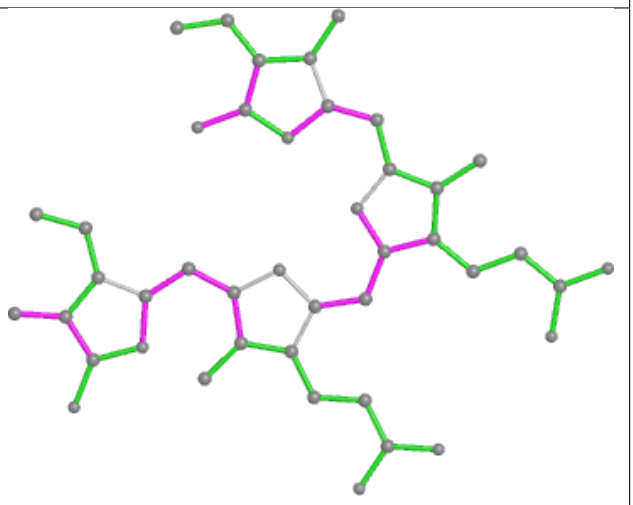

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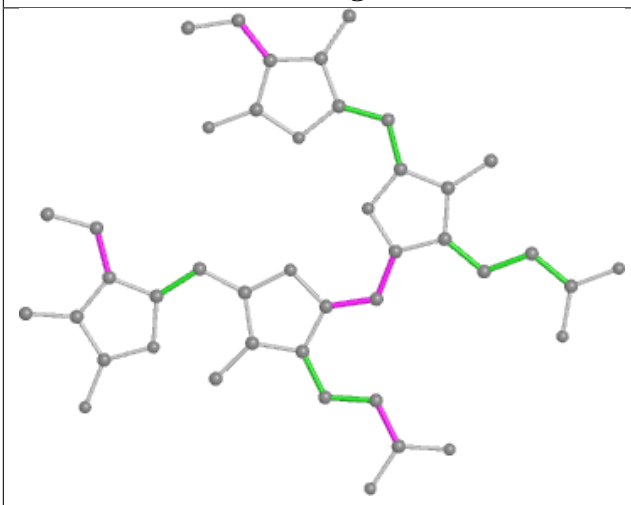

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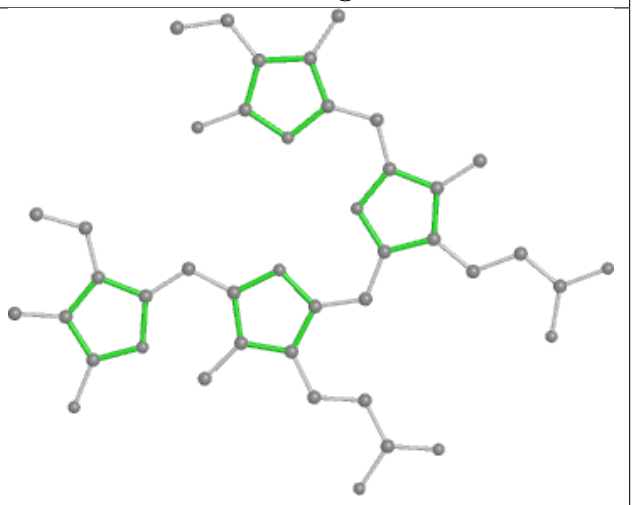
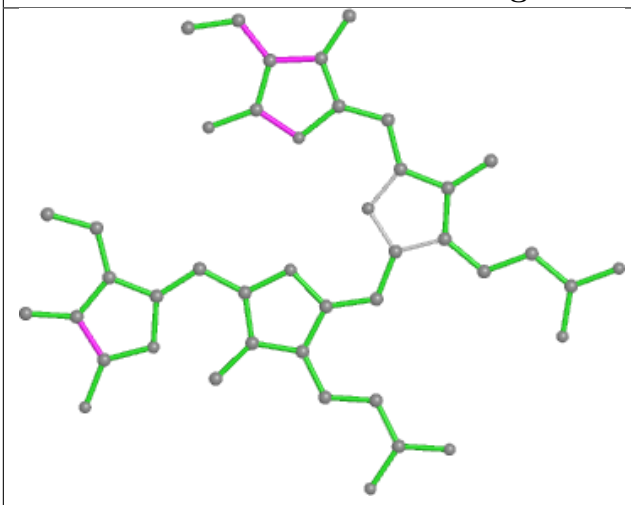


Rings

Ligand PEB iD 1001



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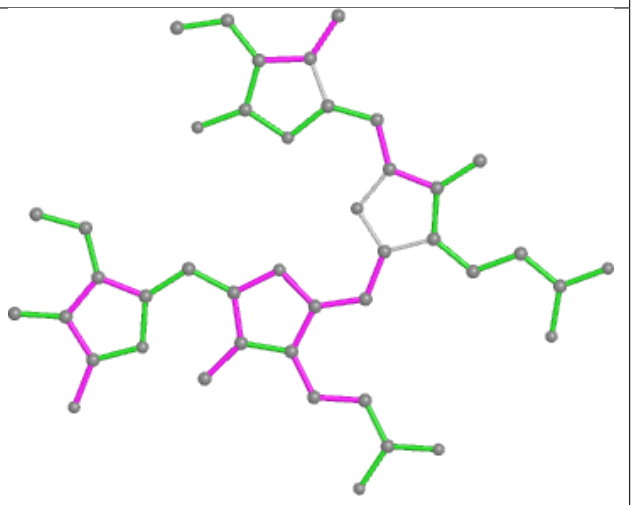

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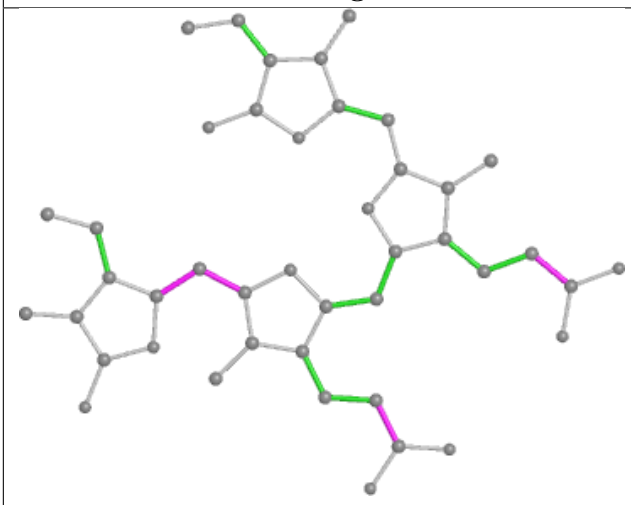

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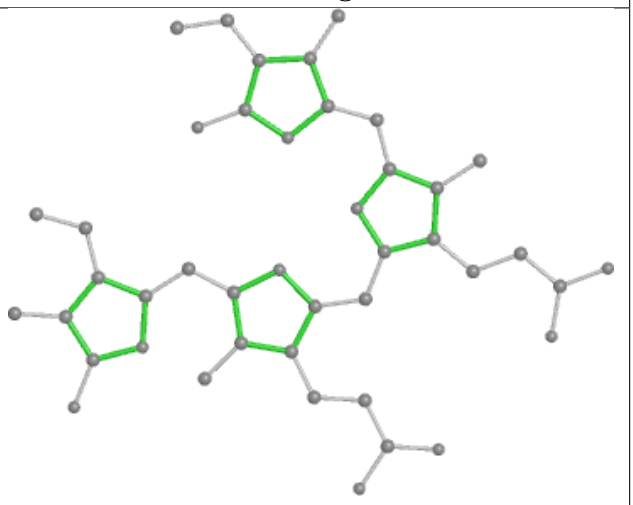

Rings

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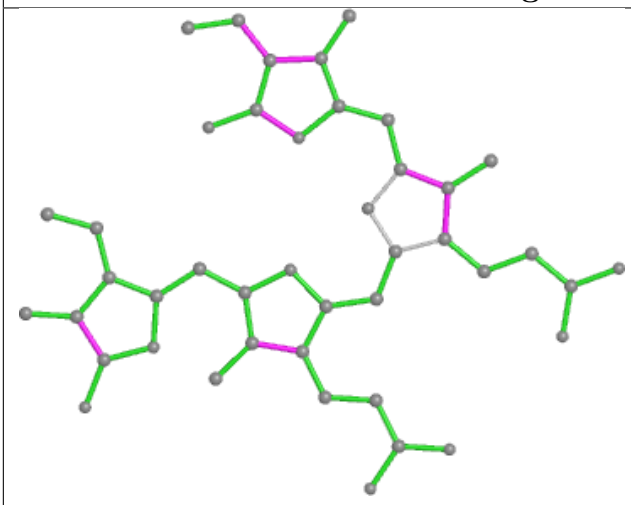

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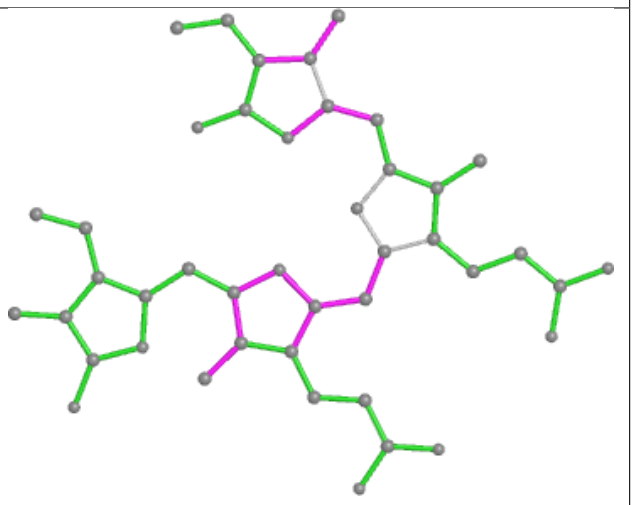

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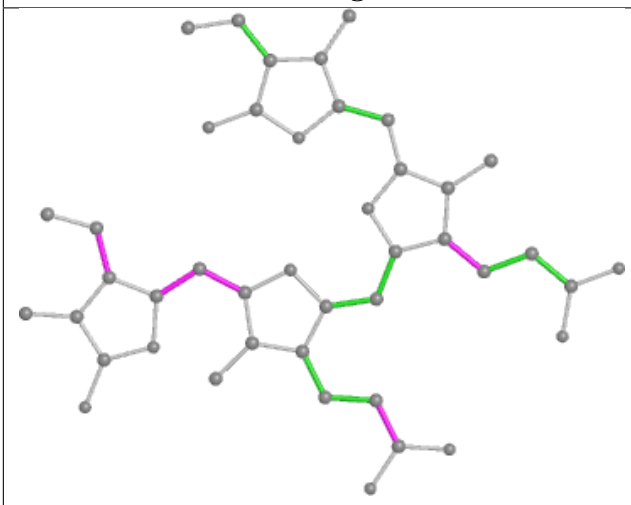

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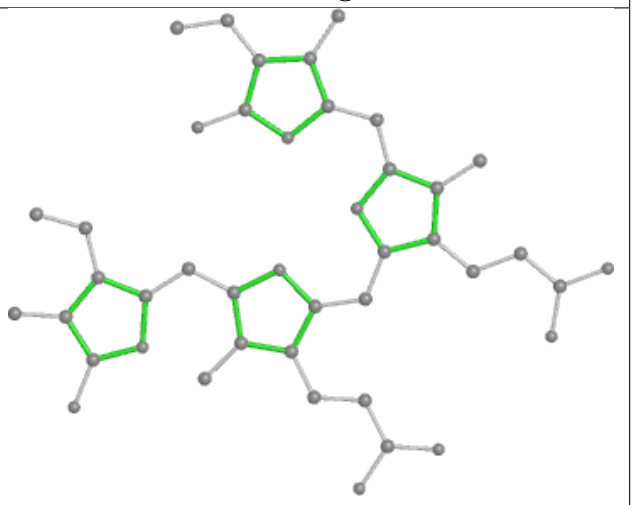
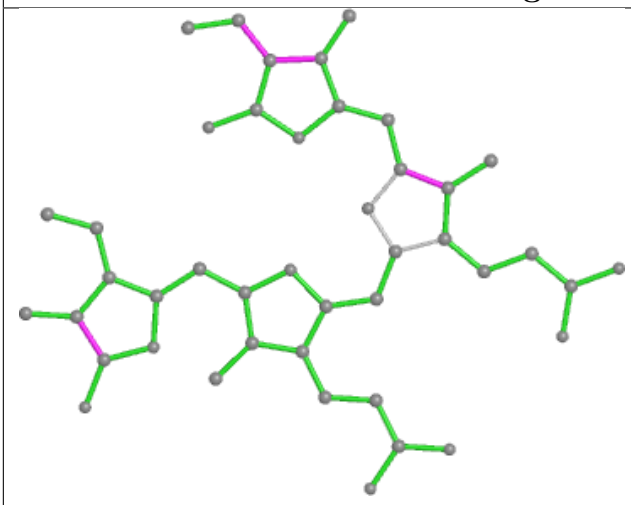


Rings

Ligand PEB j7 202



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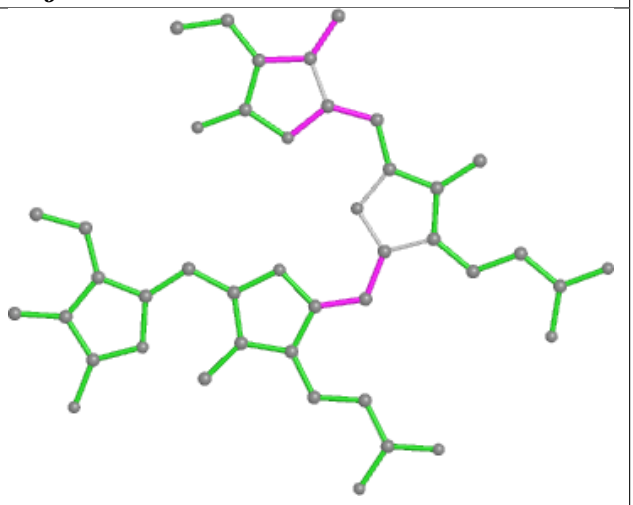

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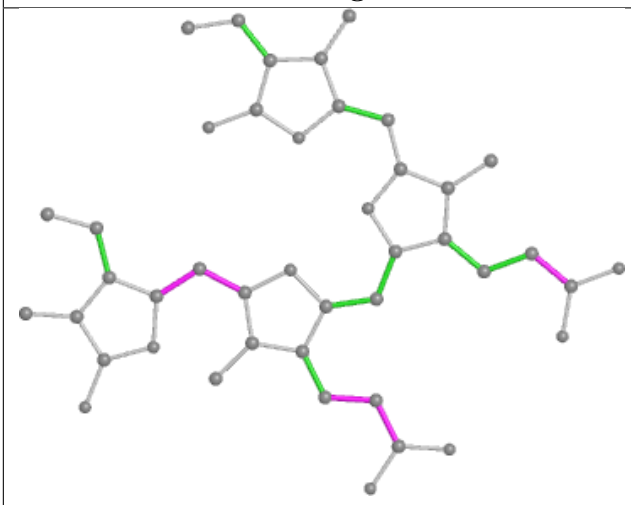

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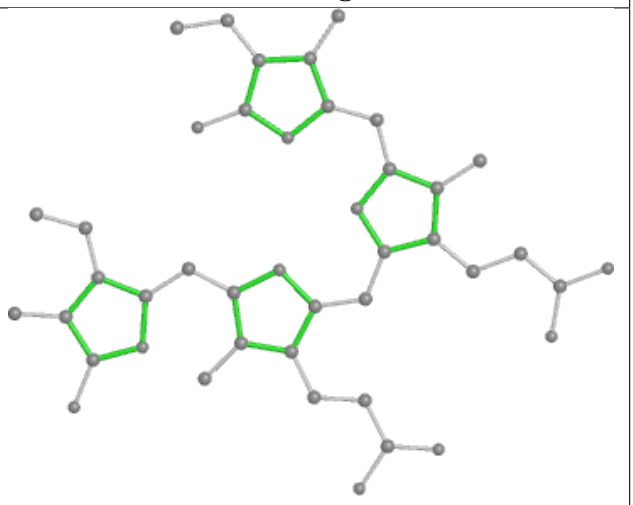
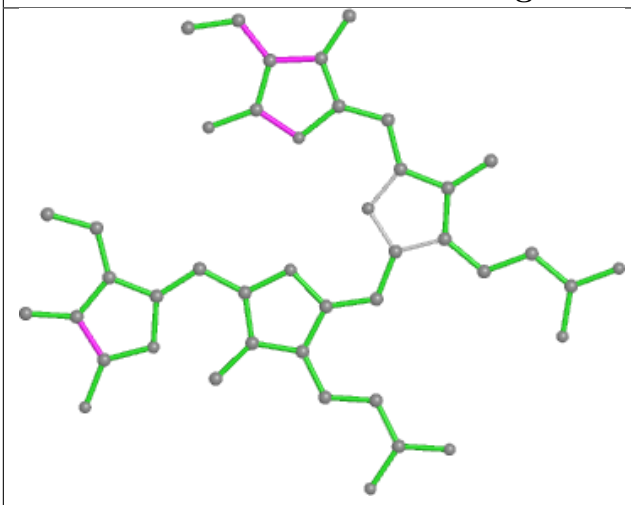


Rings

Ligand PEB Y3 201



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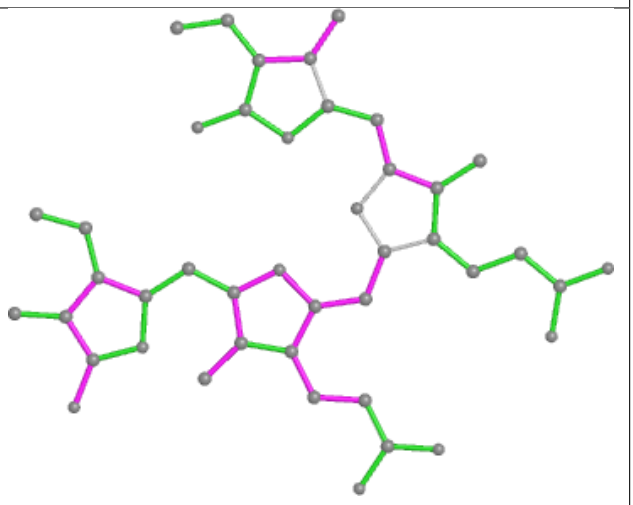
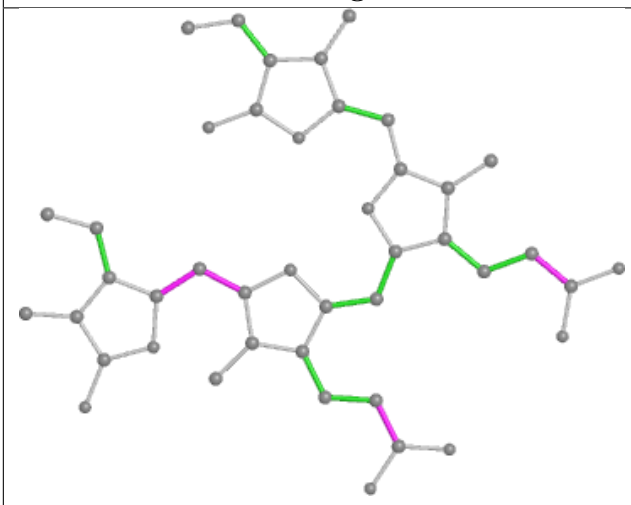
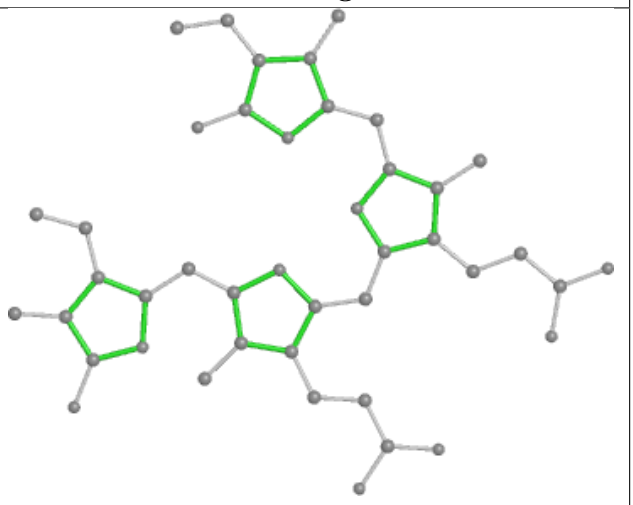


Bond angles

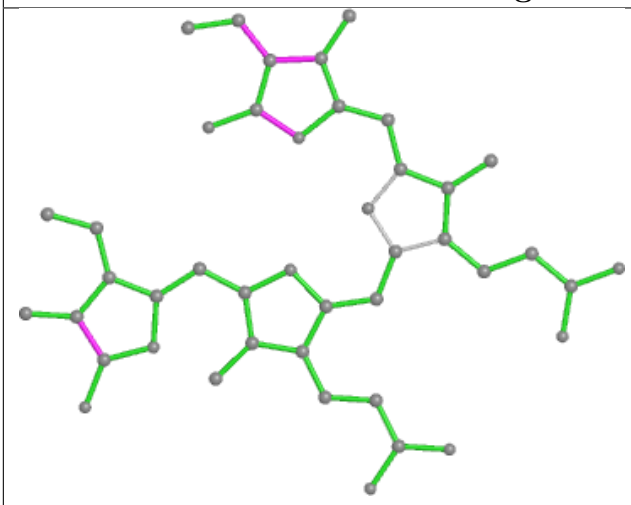


Torsions



Rings

Ligand PEB em 201



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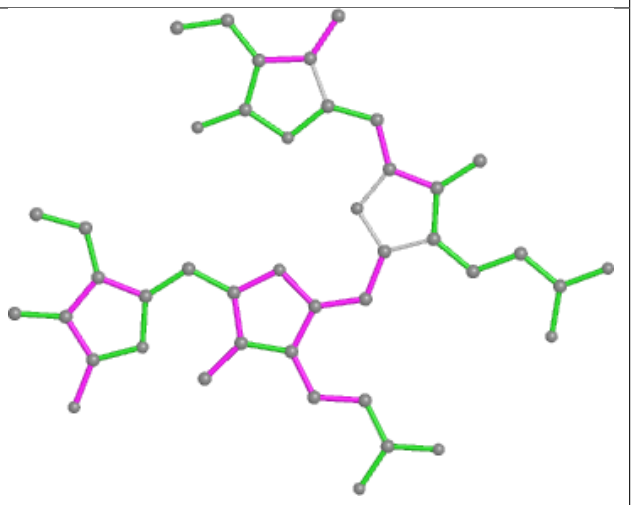
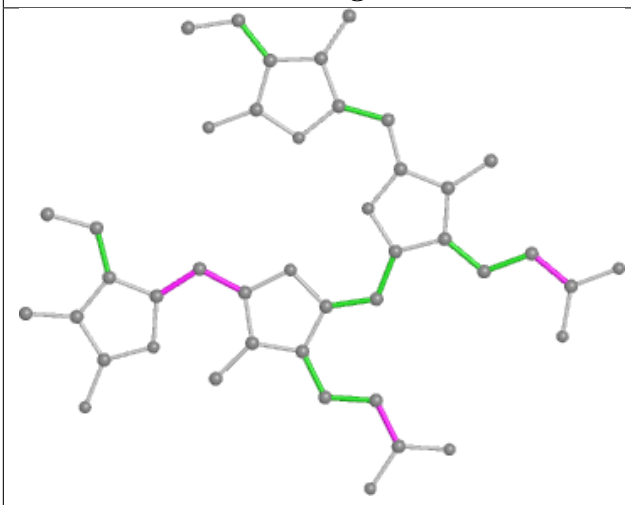


Bond angles



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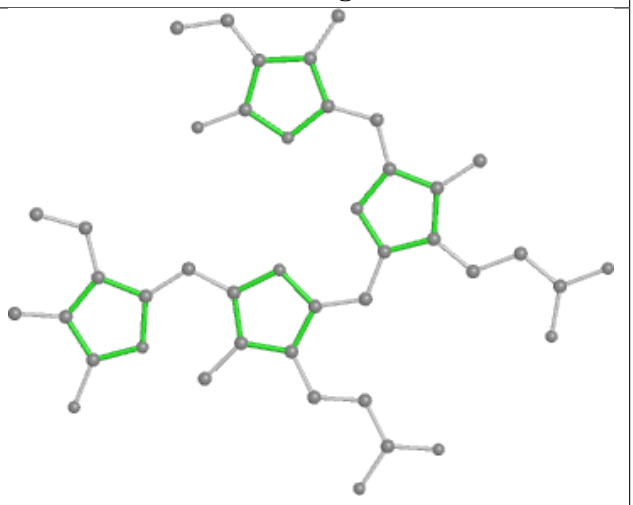
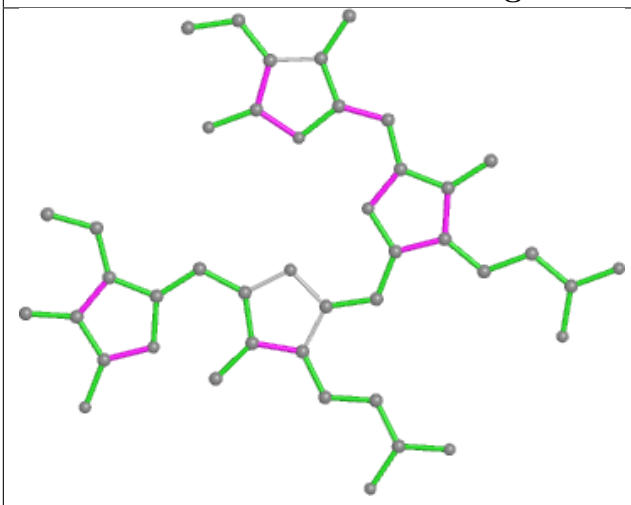


Rings

Ligand PUB Y5 1006



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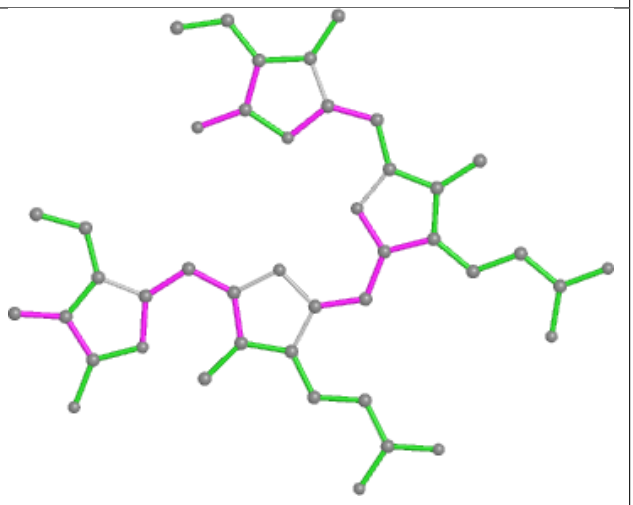

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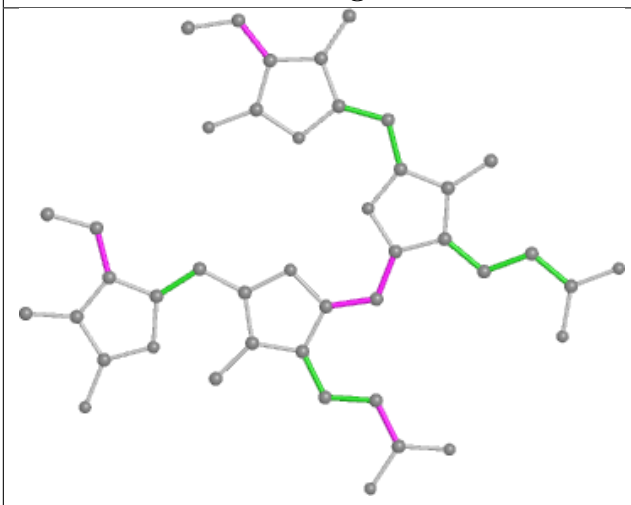

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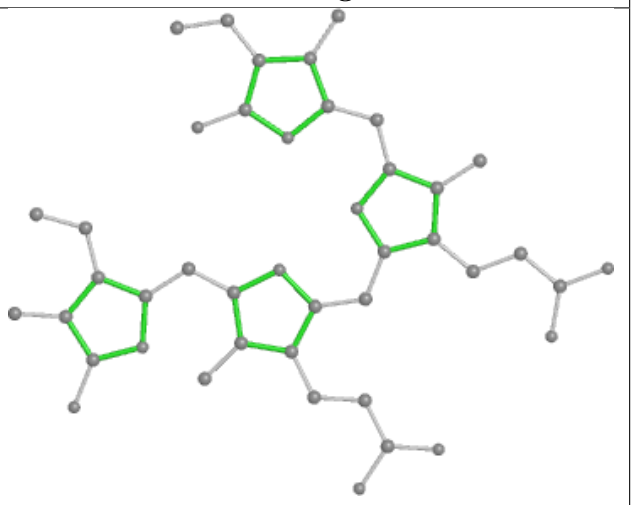

Rings

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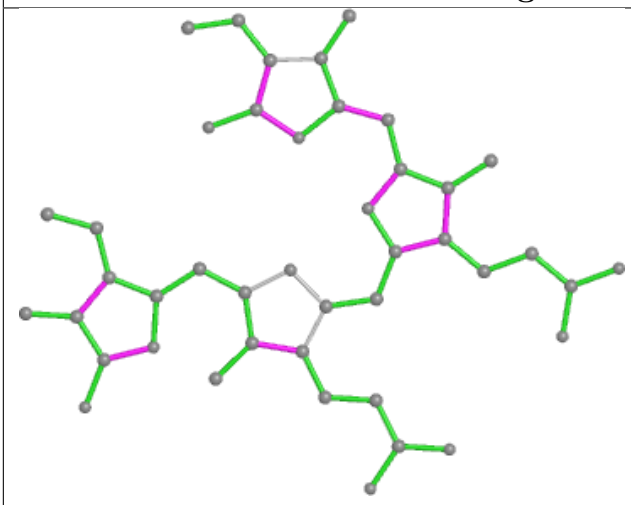

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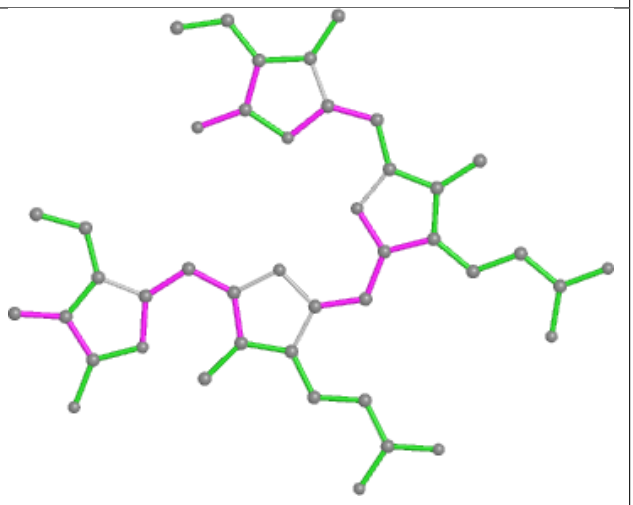

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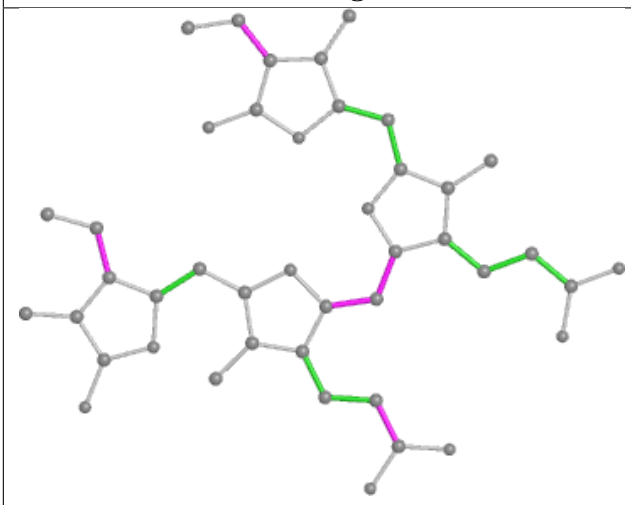

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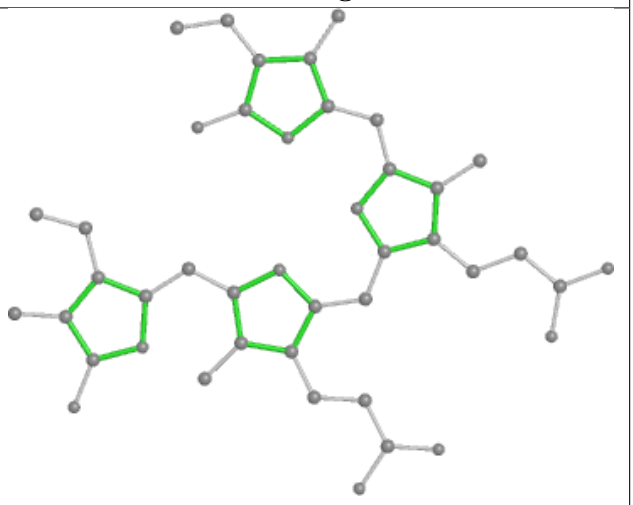
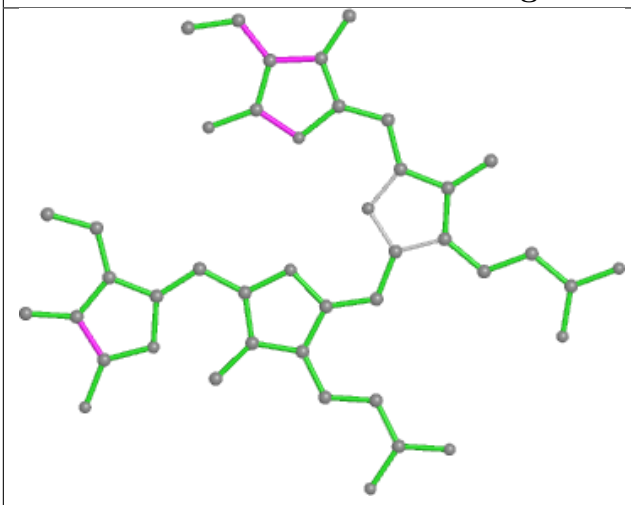


Rings

Ligand PEB cJ 201



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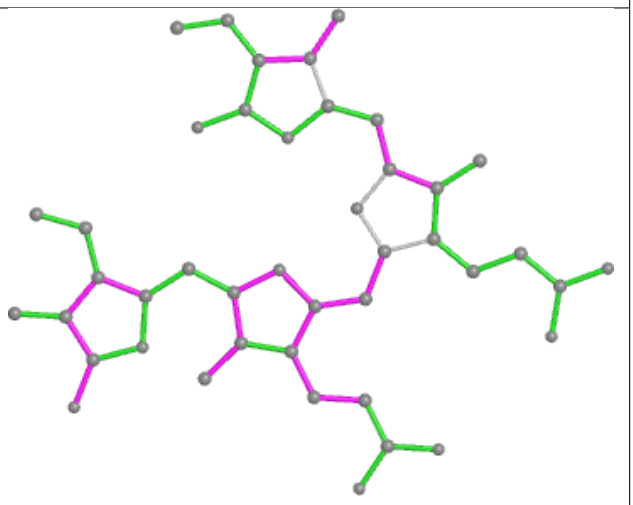

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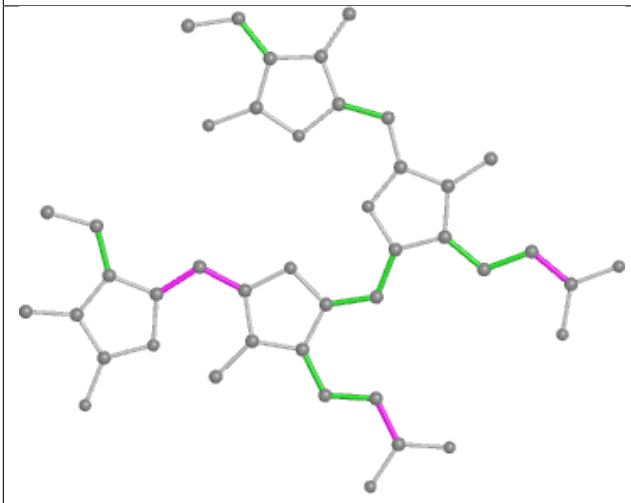

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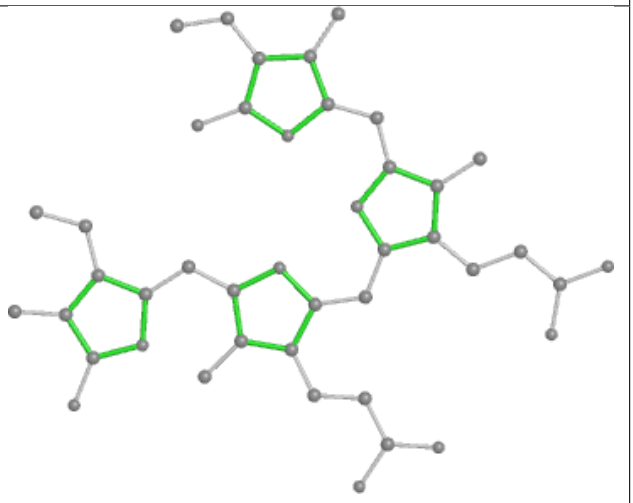
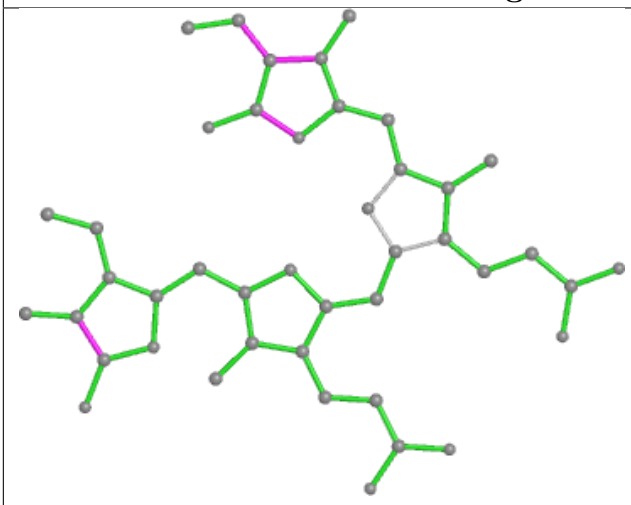


Rings

Ligand PEB kQ 1001



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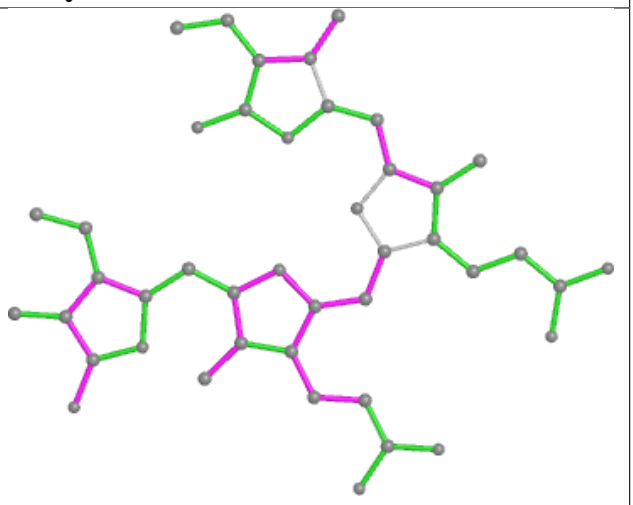

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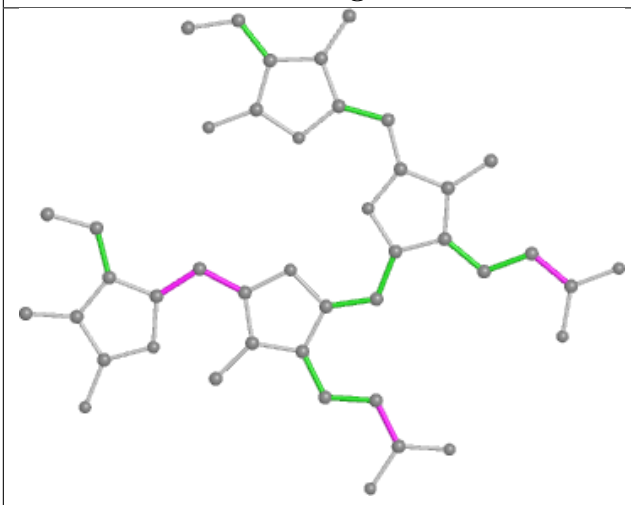

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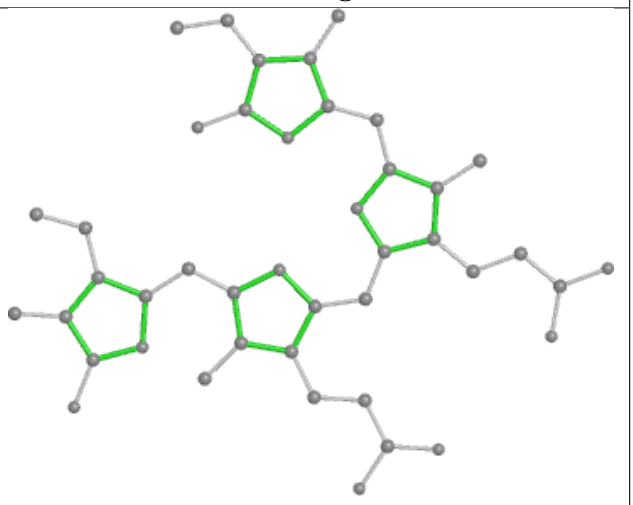

Rings

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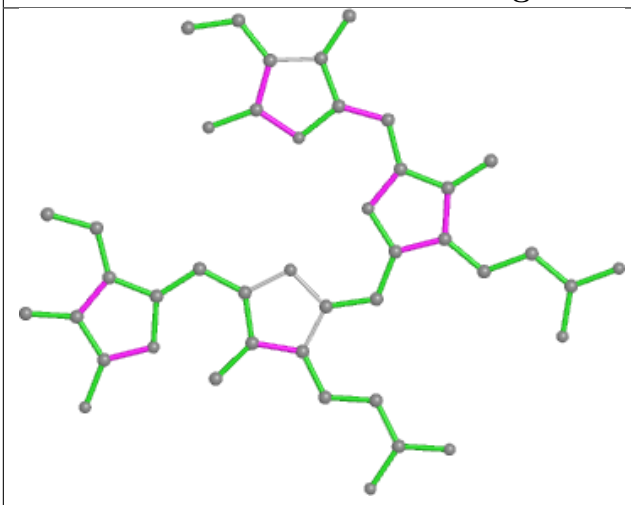

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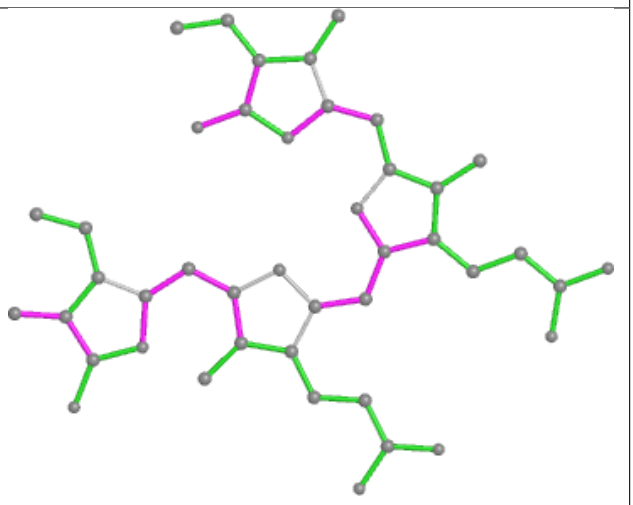

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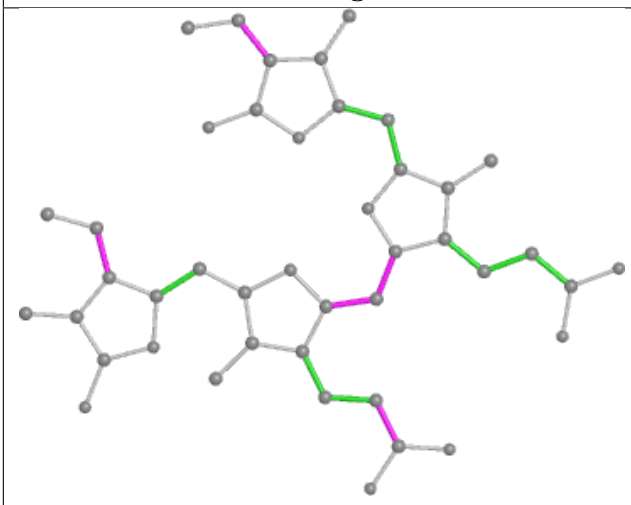

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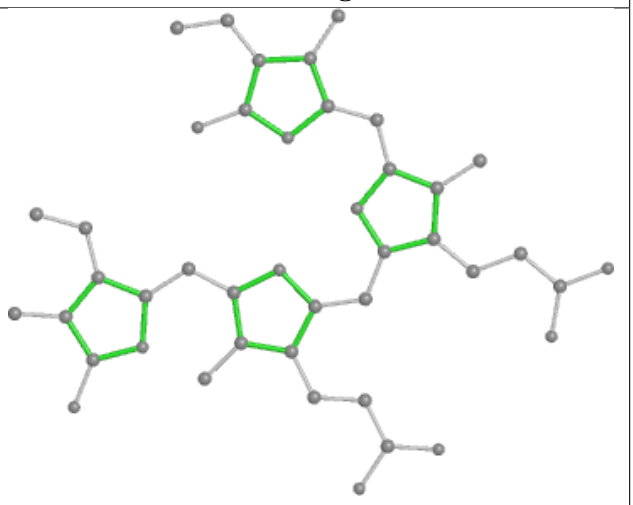

Rings

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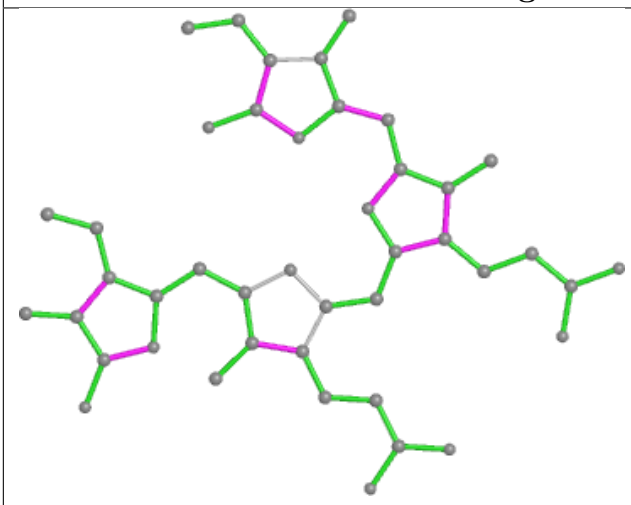

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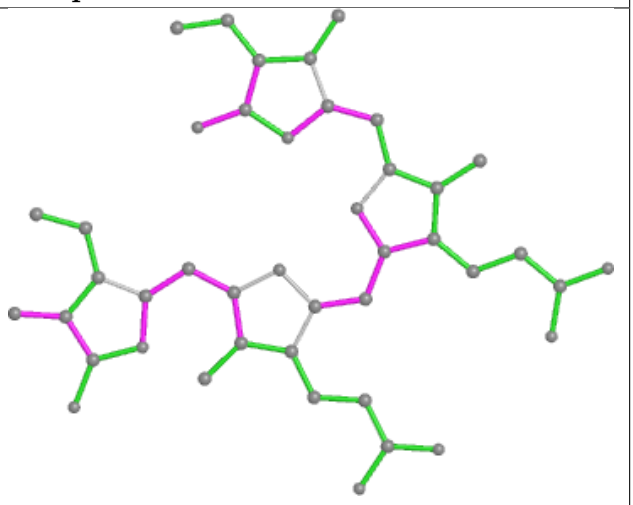

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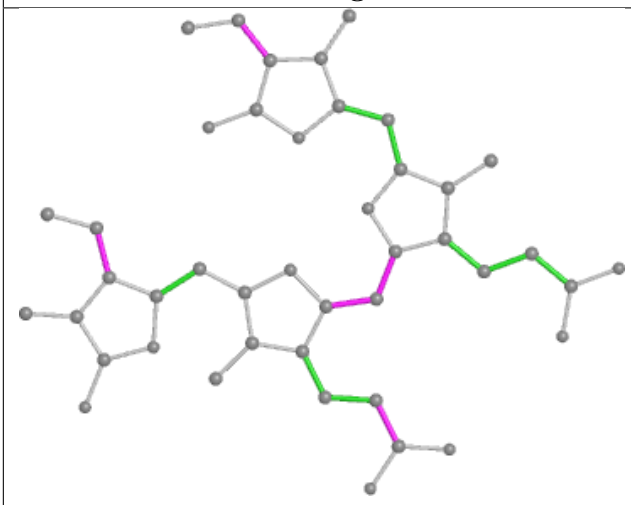

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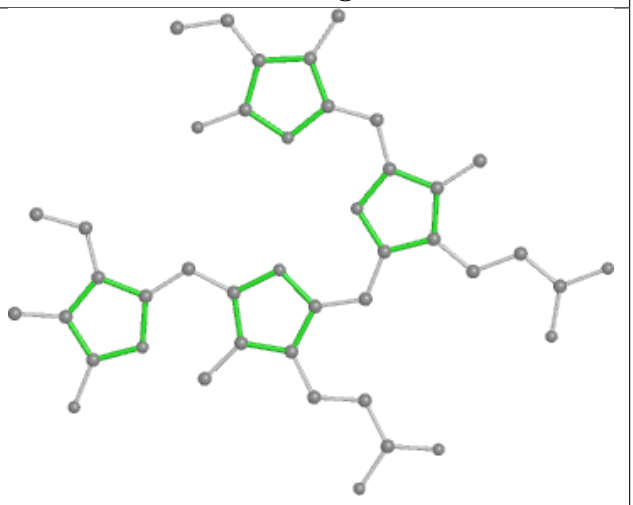

Rings

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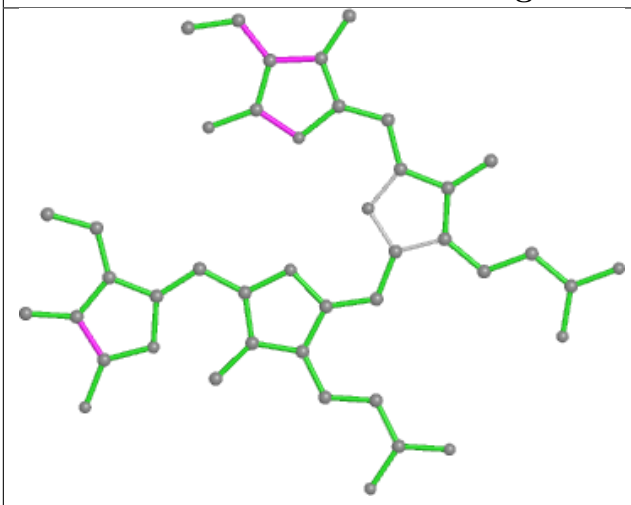

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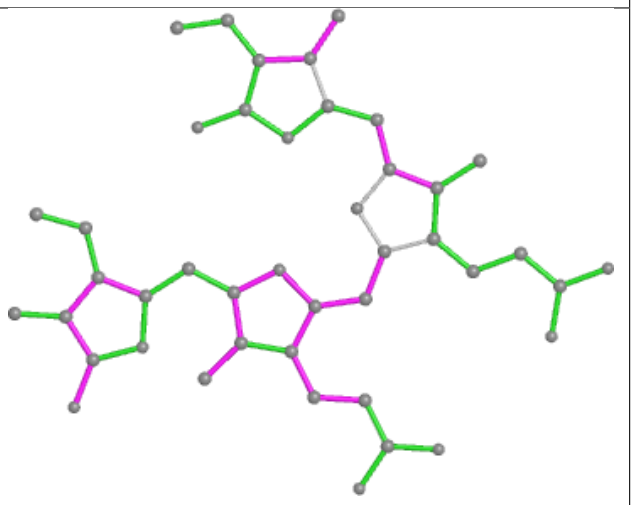

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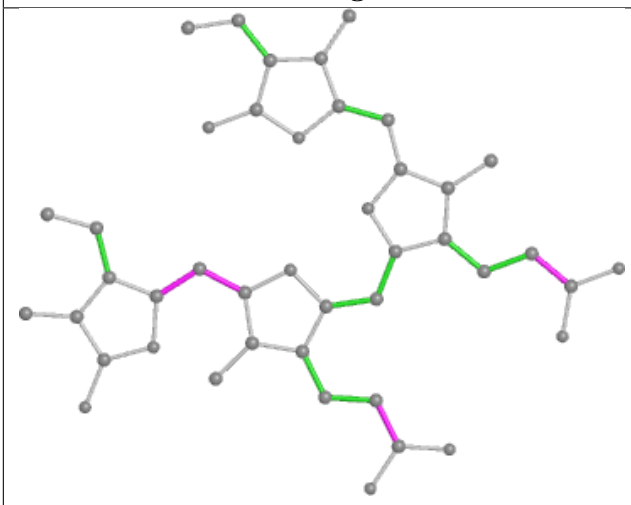

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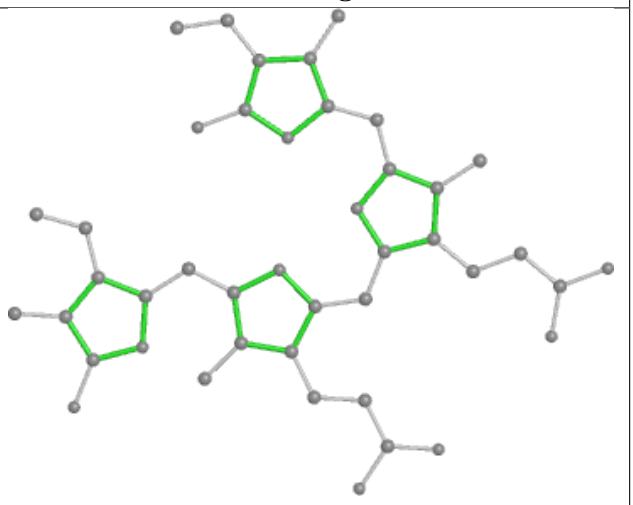

Rings

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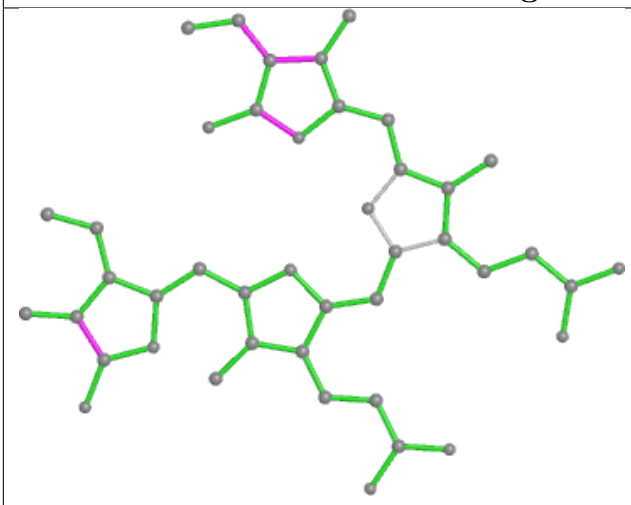

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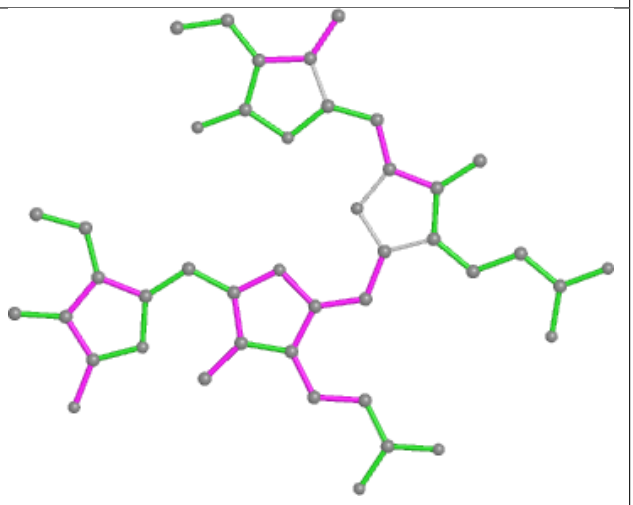

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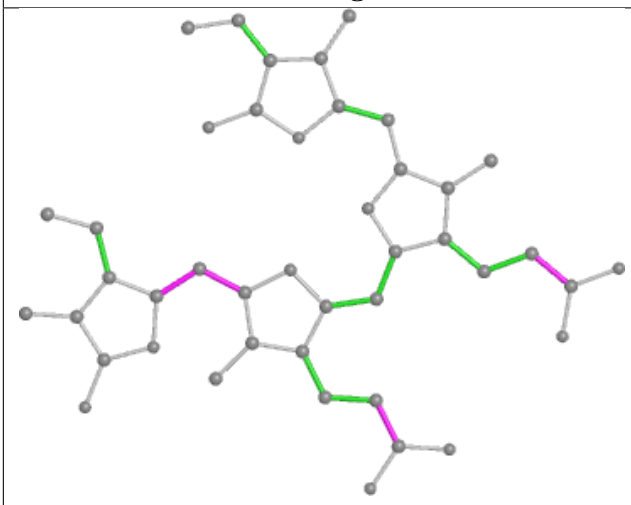

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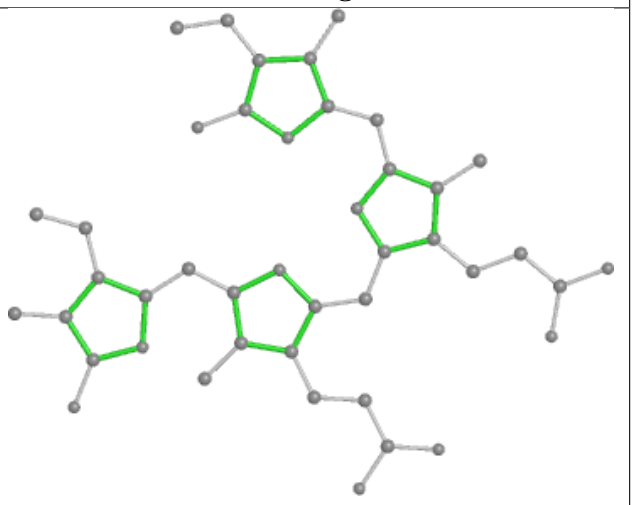

Rings

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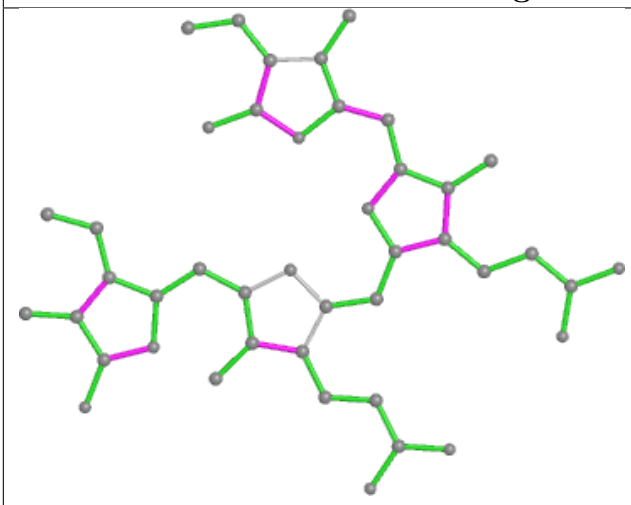

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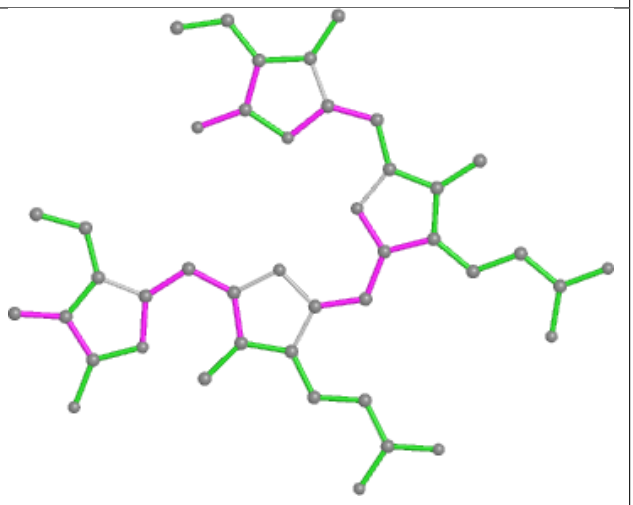

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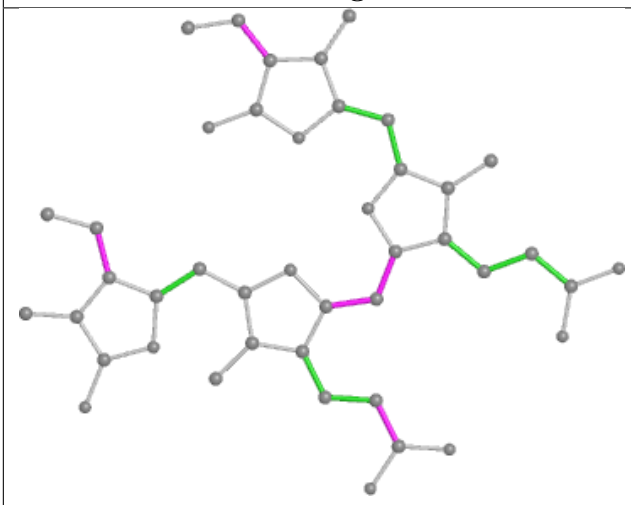

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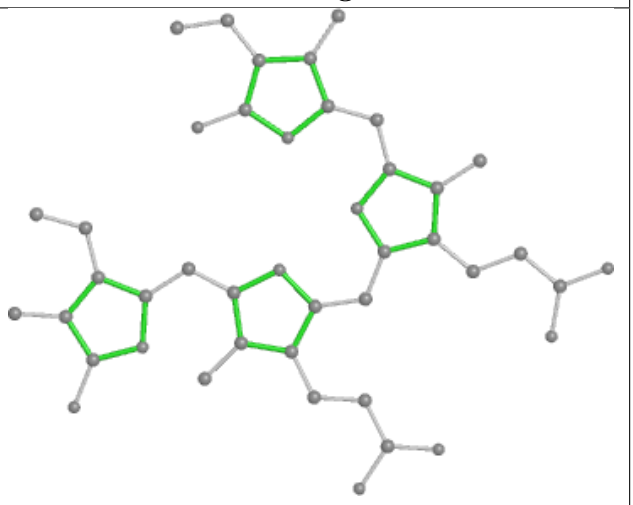

Rings

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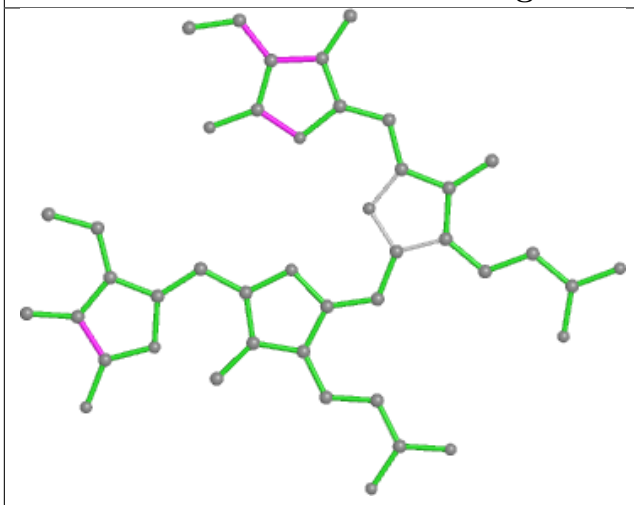

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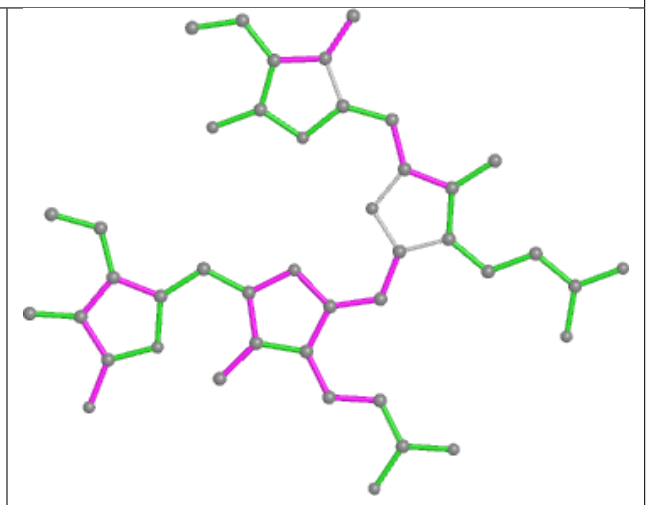

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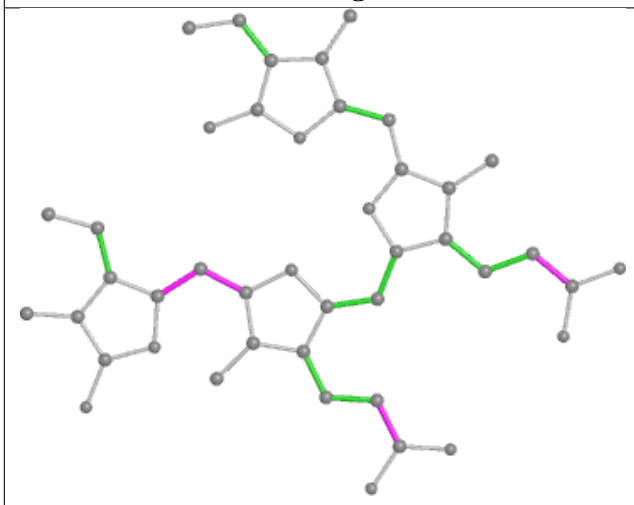

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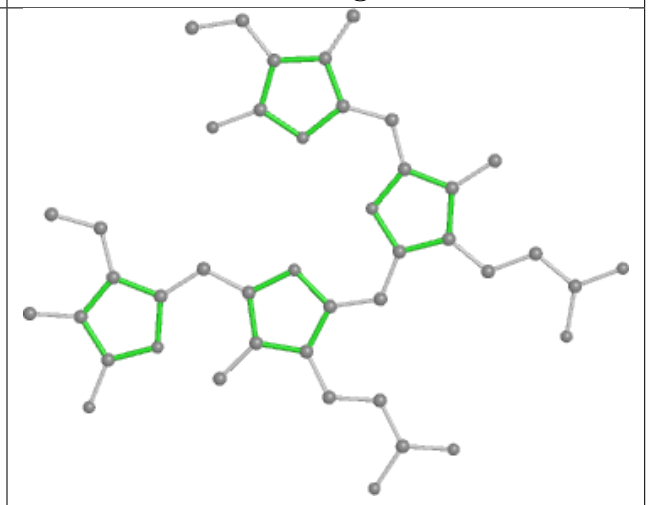

Rings

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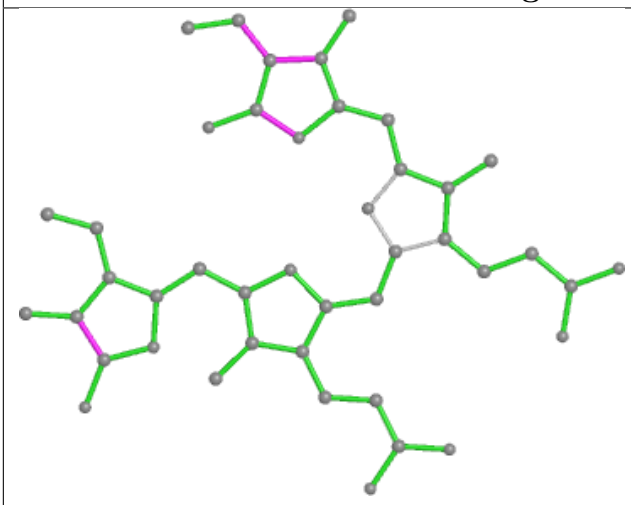

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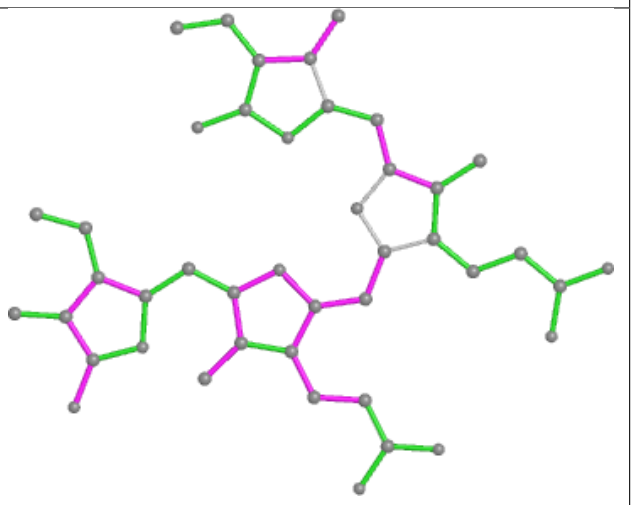
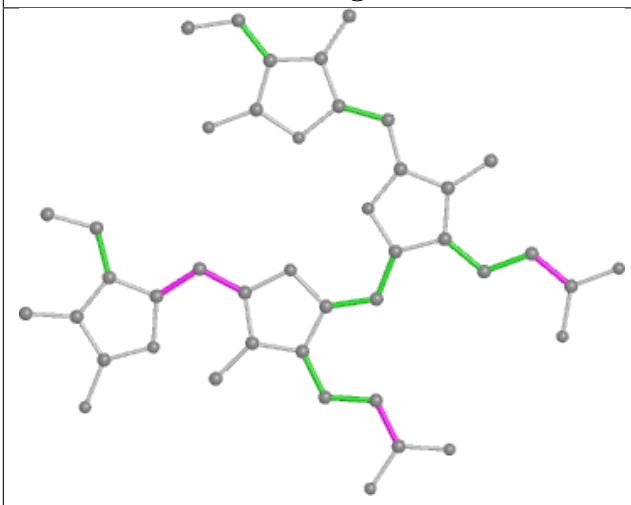


Bond angles



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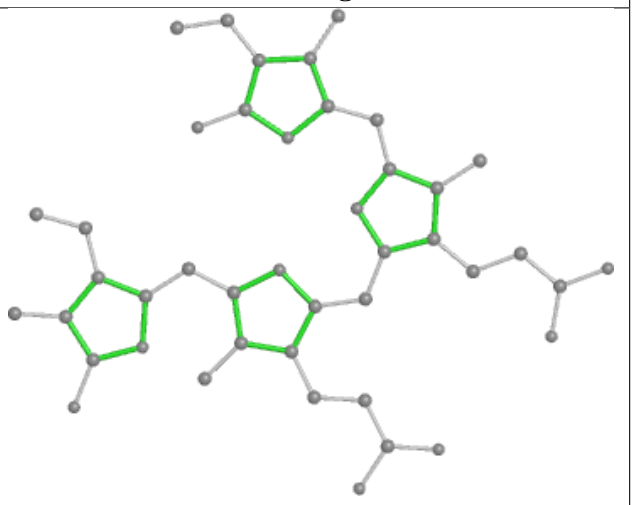
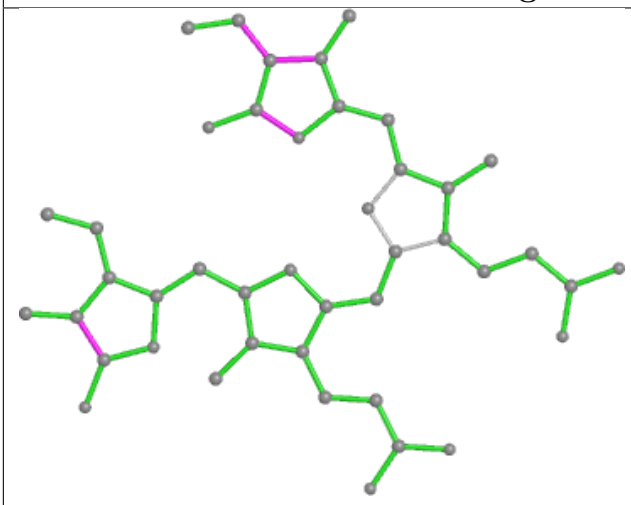


Rings

Ligand PEB gy 303



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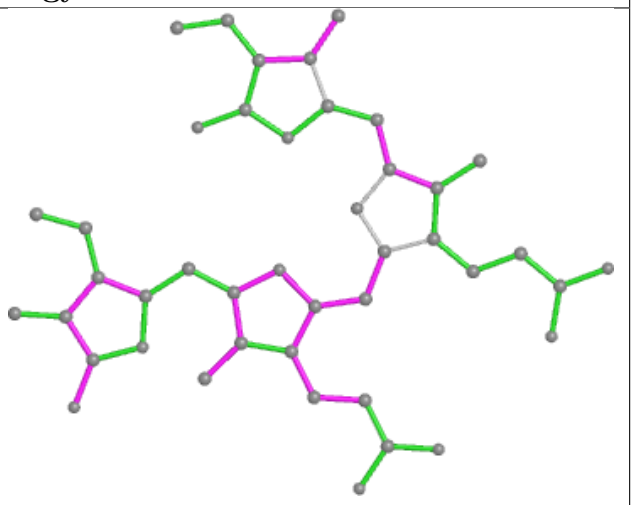

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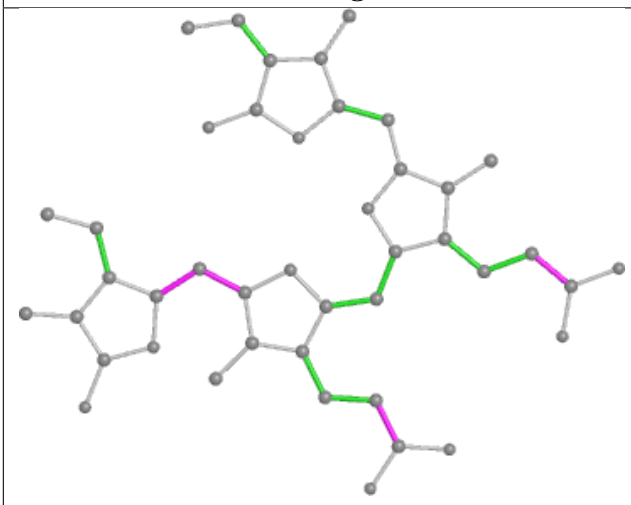

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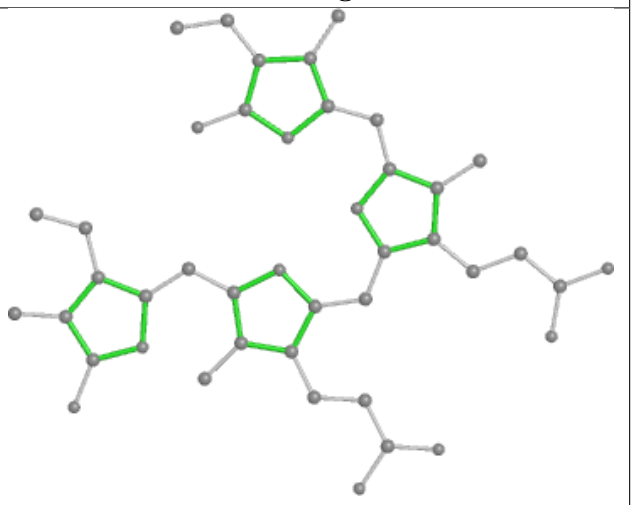
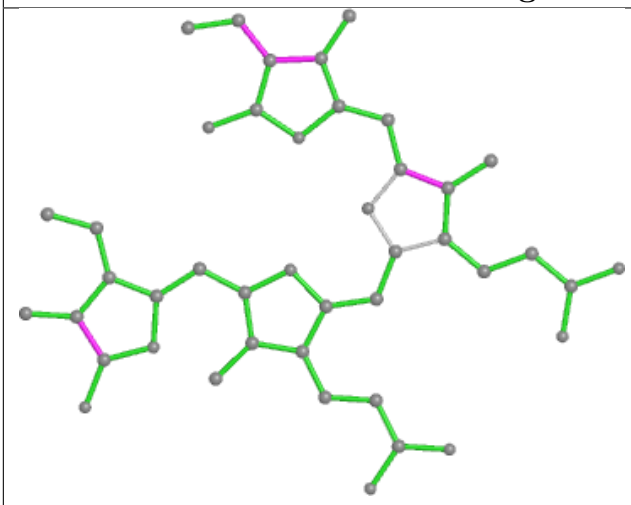


Rings

Ligand PEB d8 301



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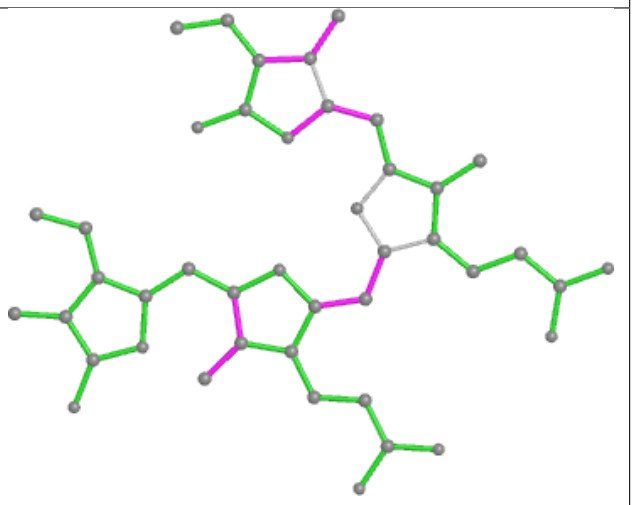

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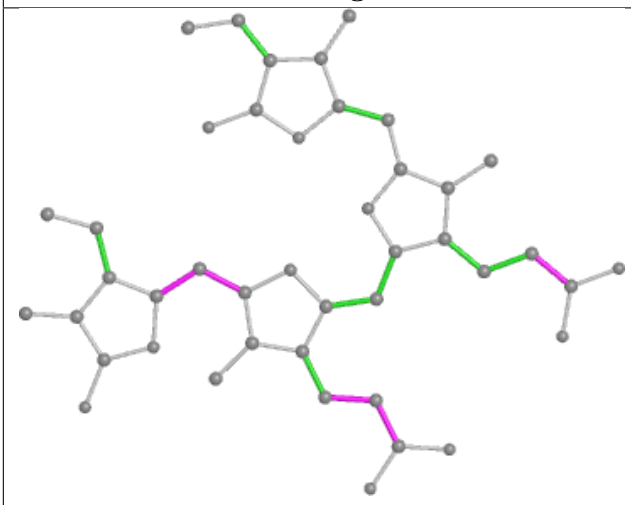
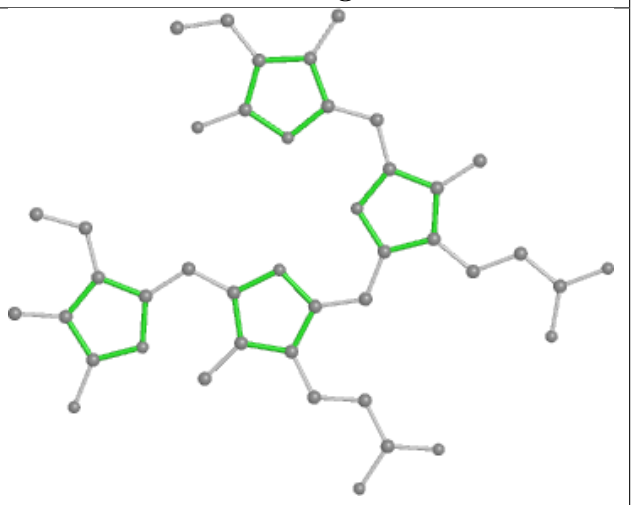


Torsions



Rings

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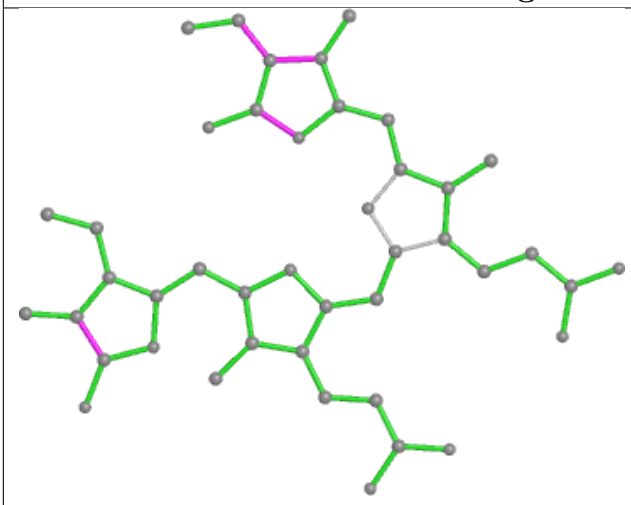

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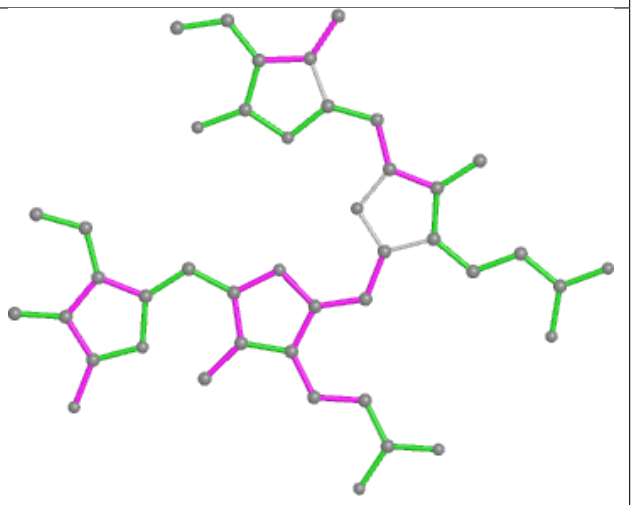

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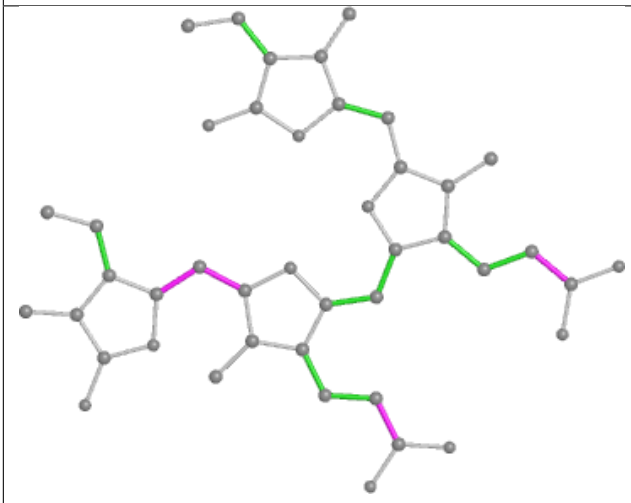

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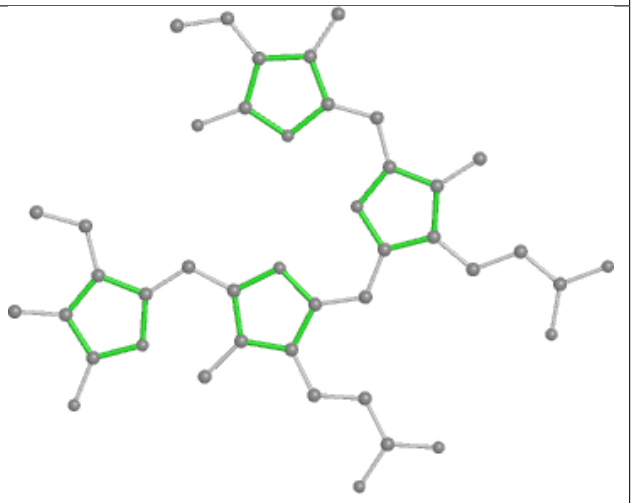
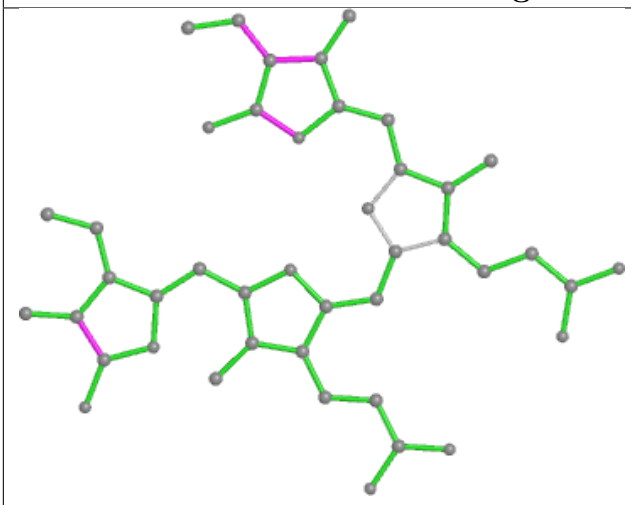


Rings

Ligand PEB dm 201



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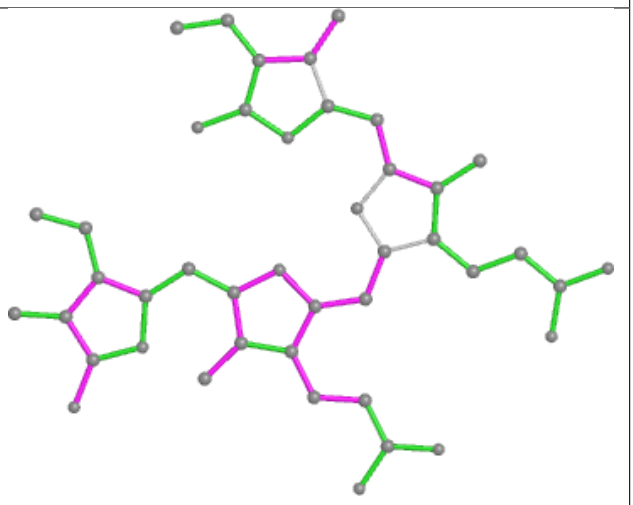

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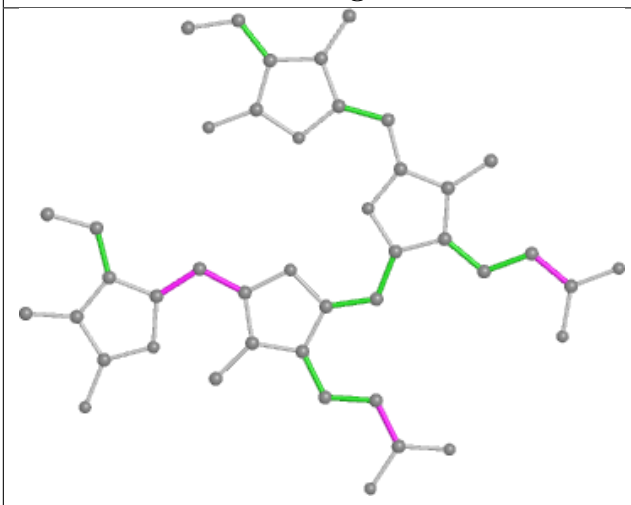

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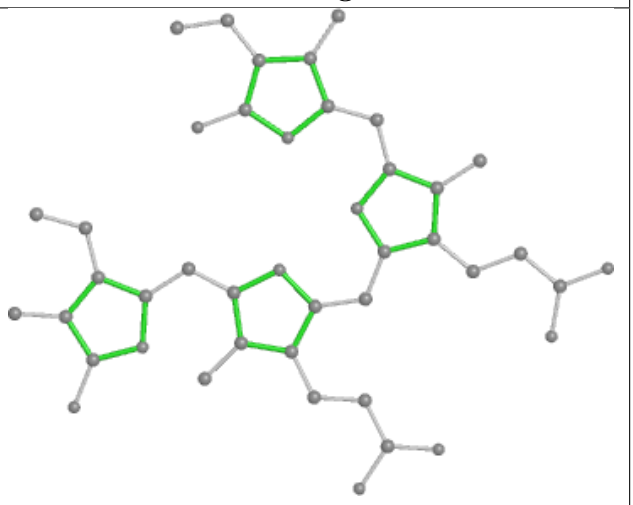

Rings

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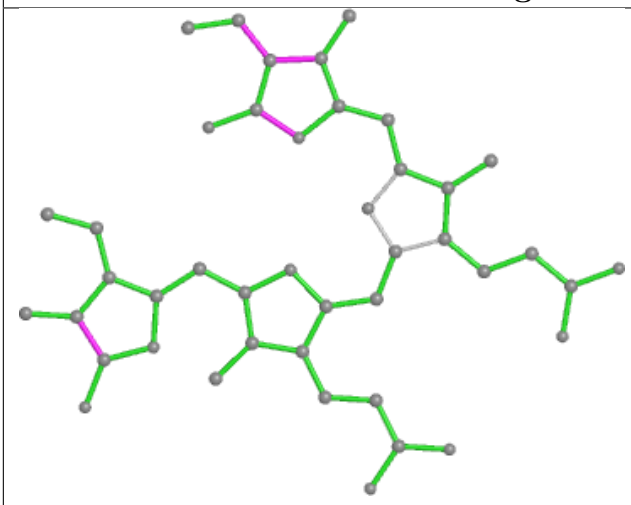

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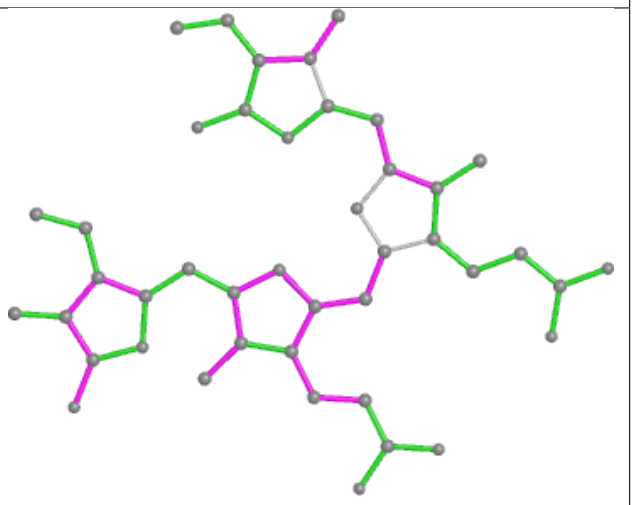

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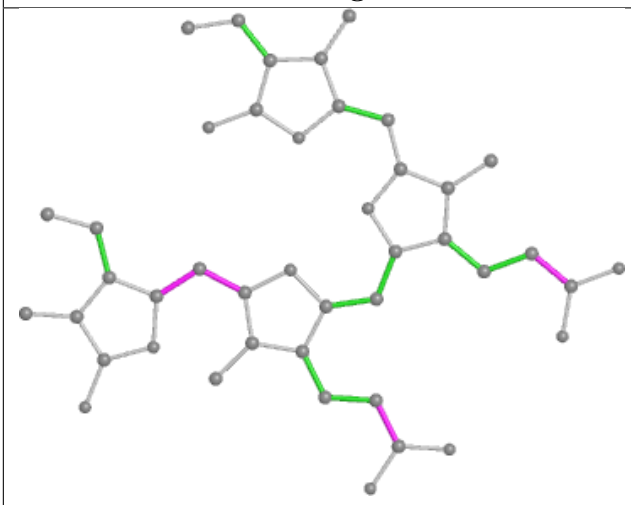

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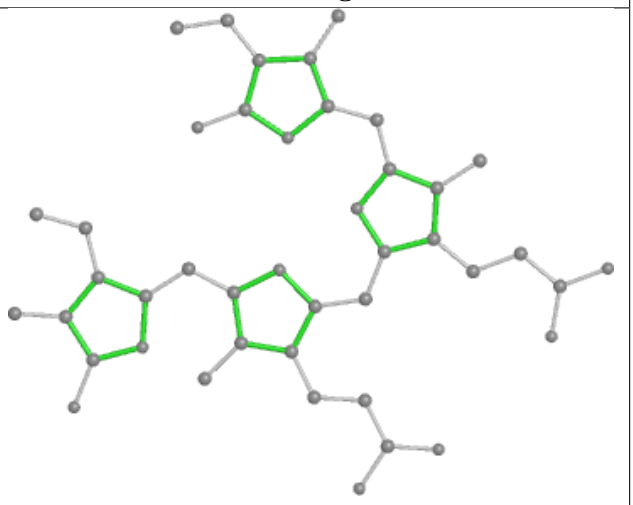

Rings

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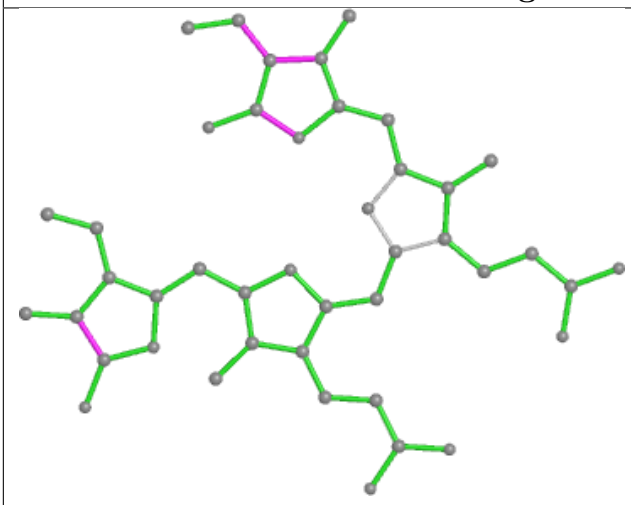

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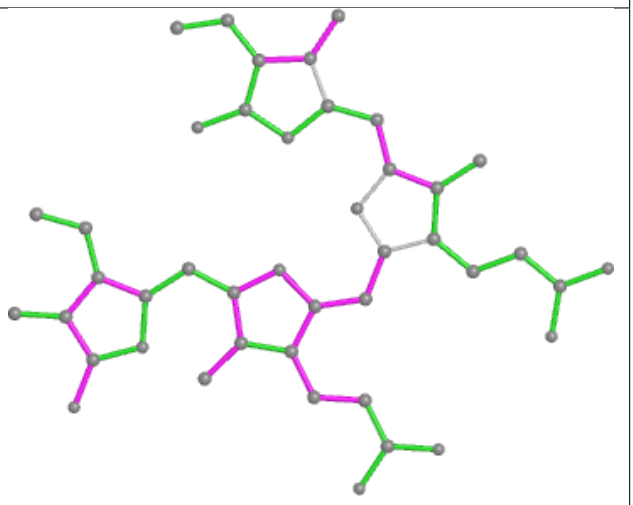

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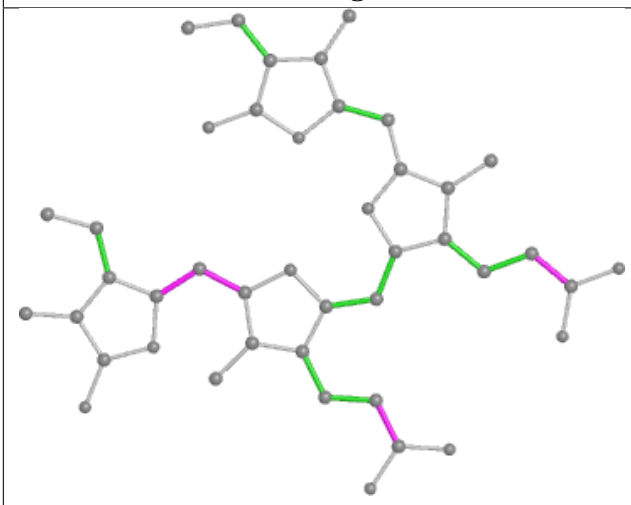

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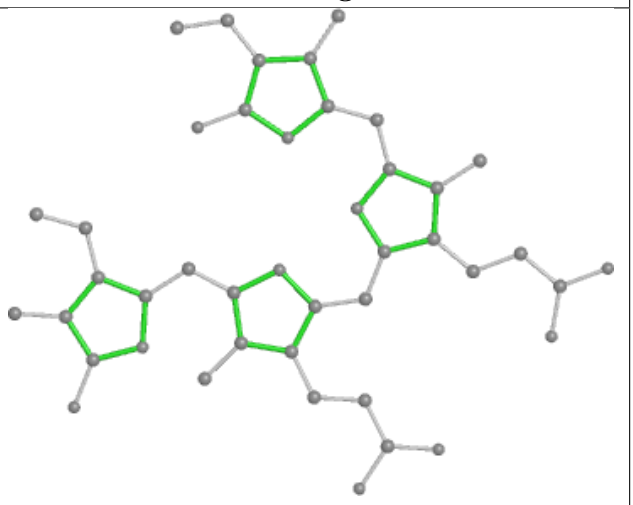

Rings

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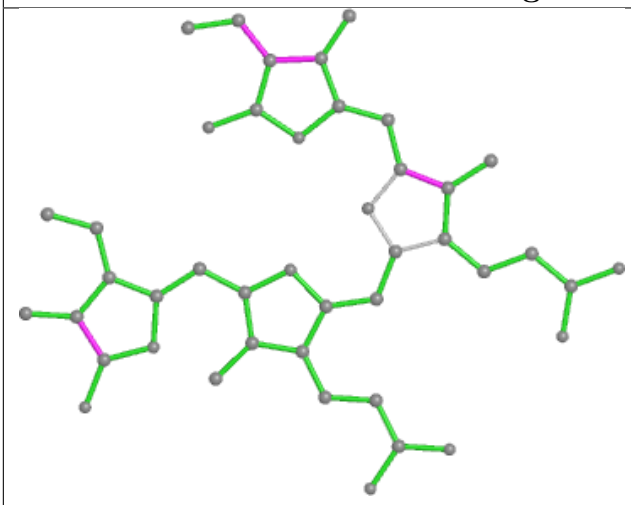

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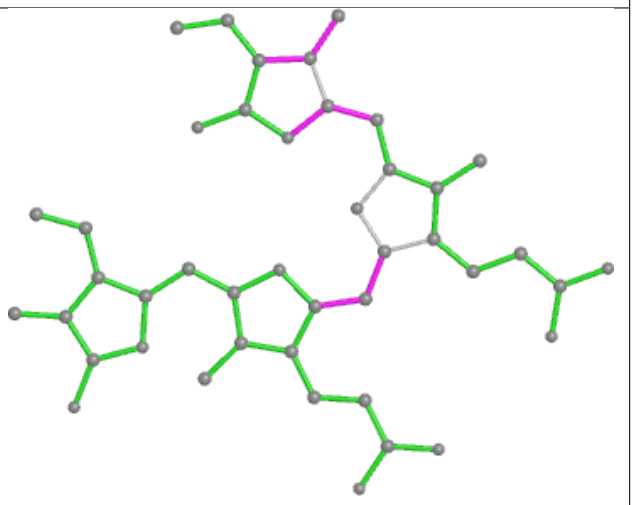

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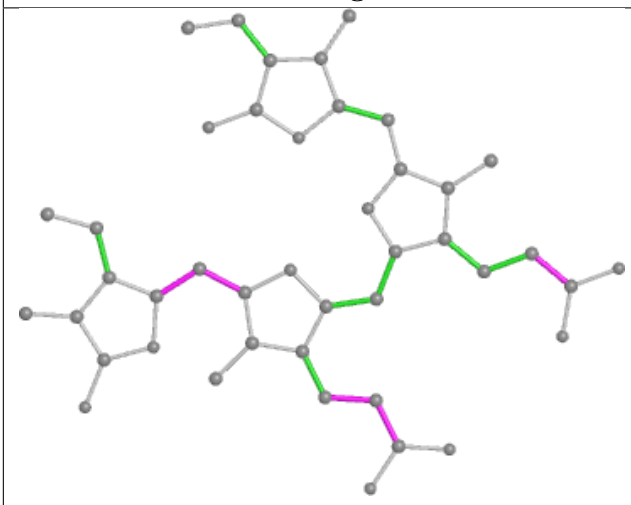

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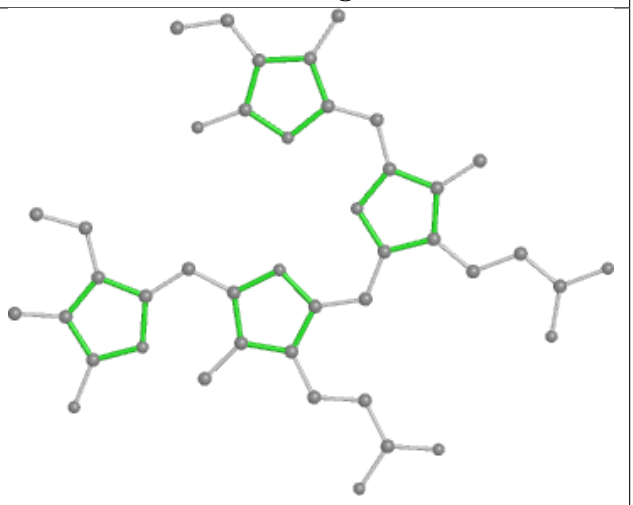

Rings

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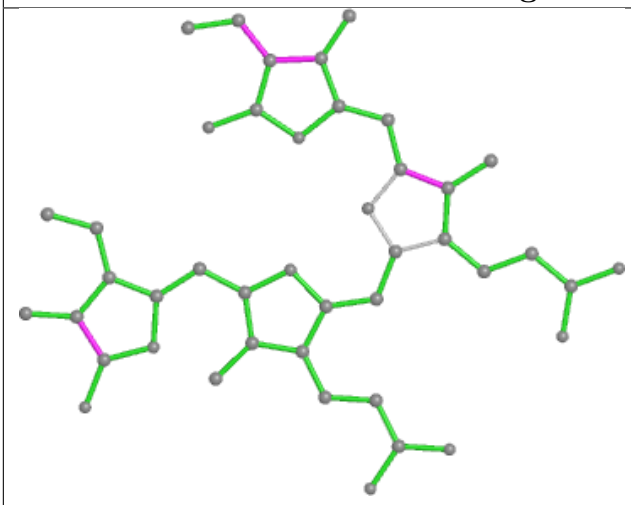

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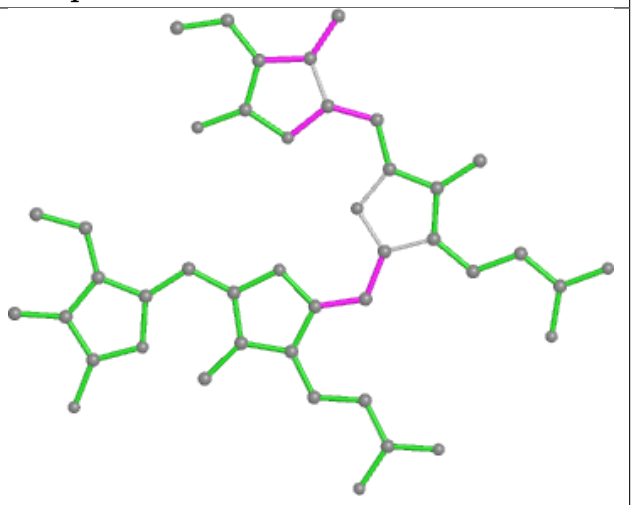

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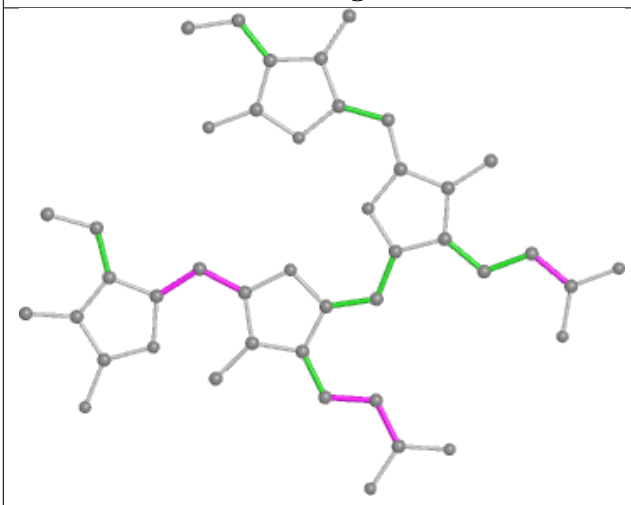

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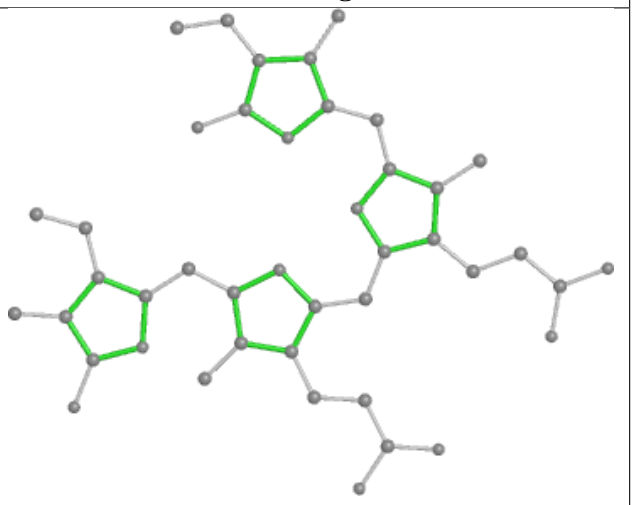

Rings

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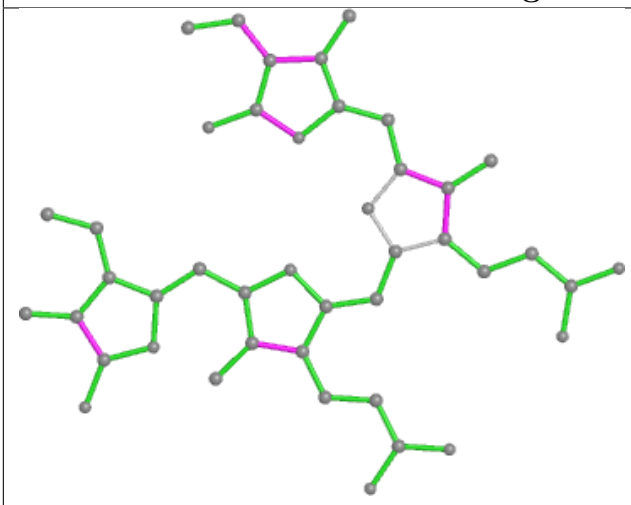

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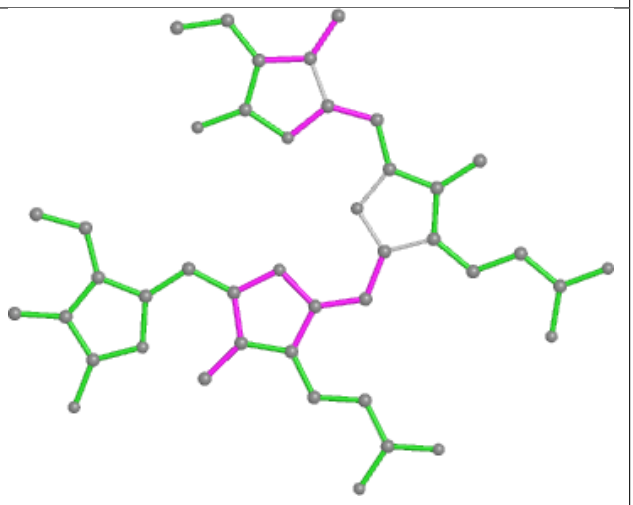

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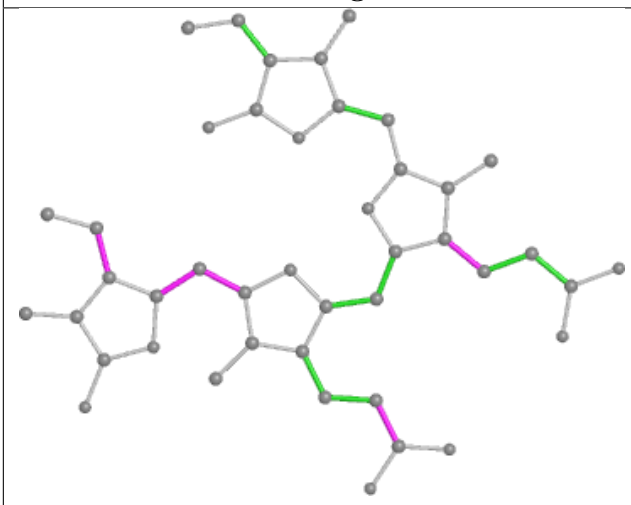

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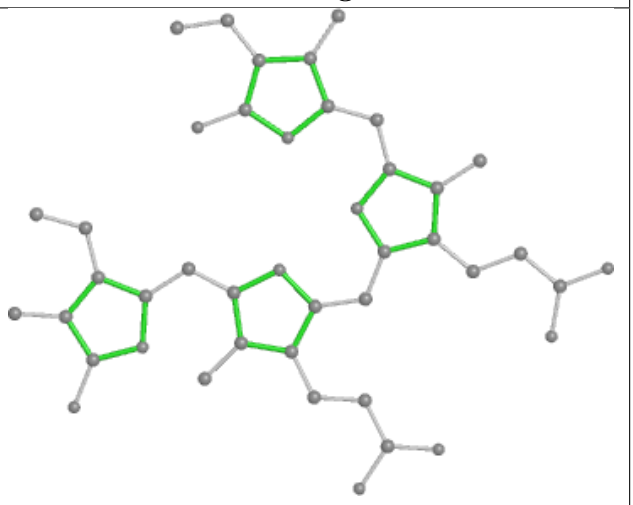

Rings

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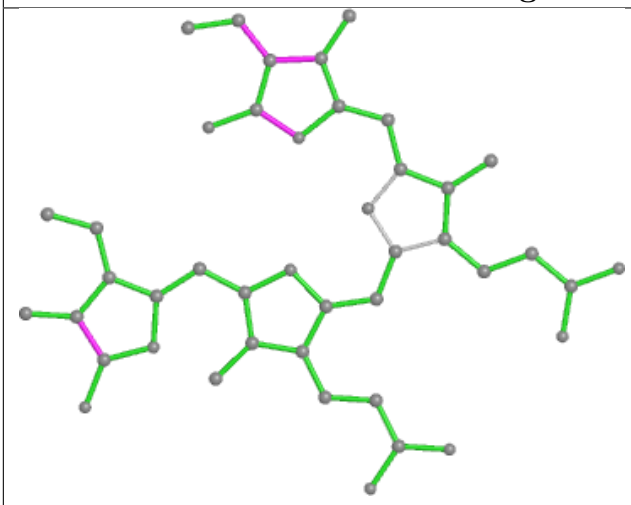

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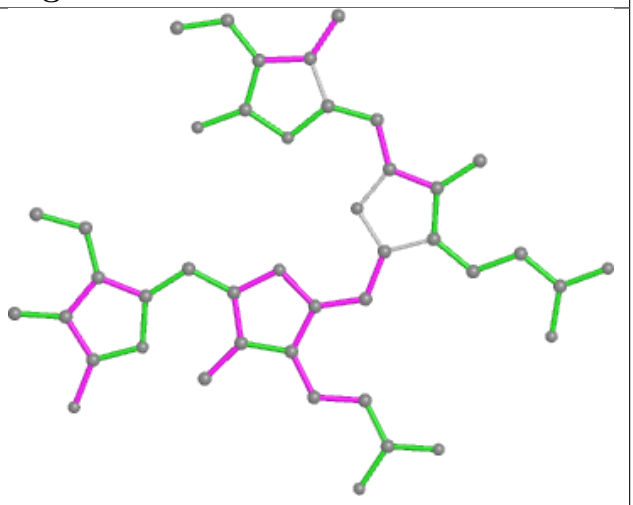

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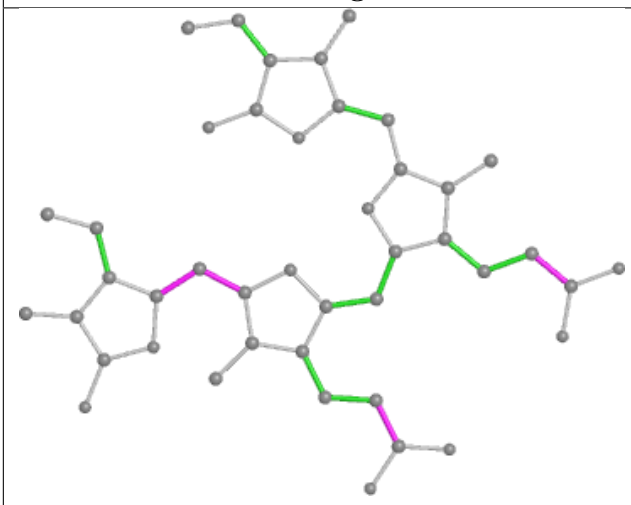

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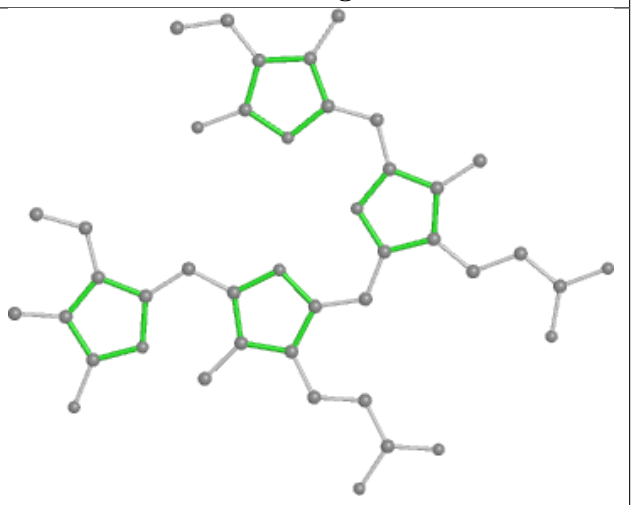

Rings

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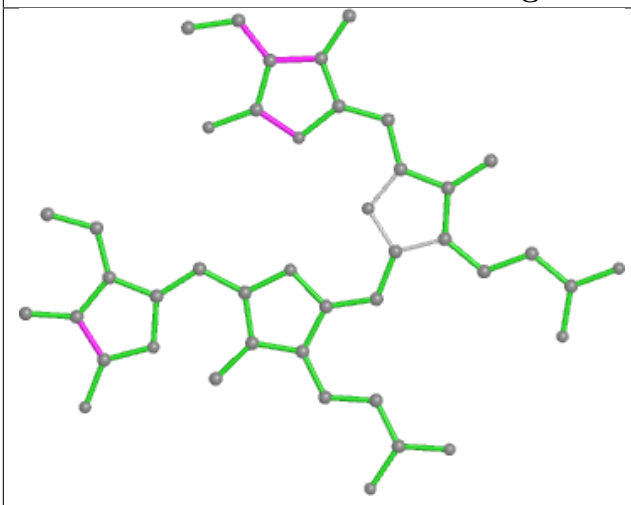

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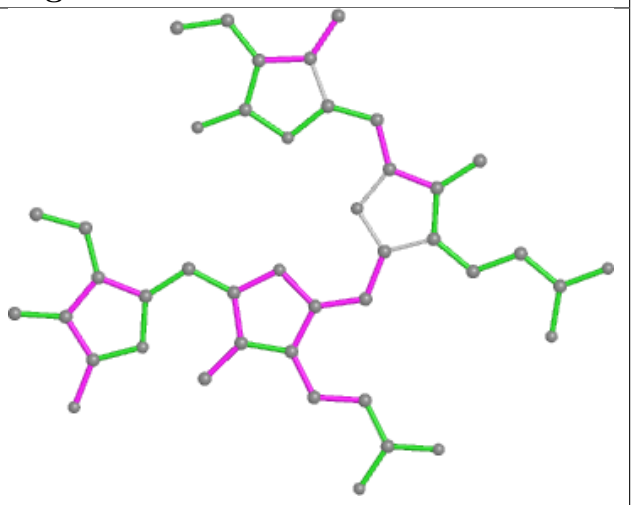

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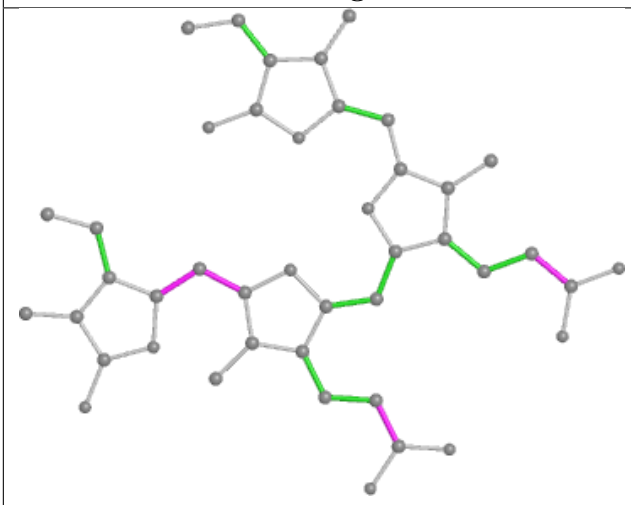

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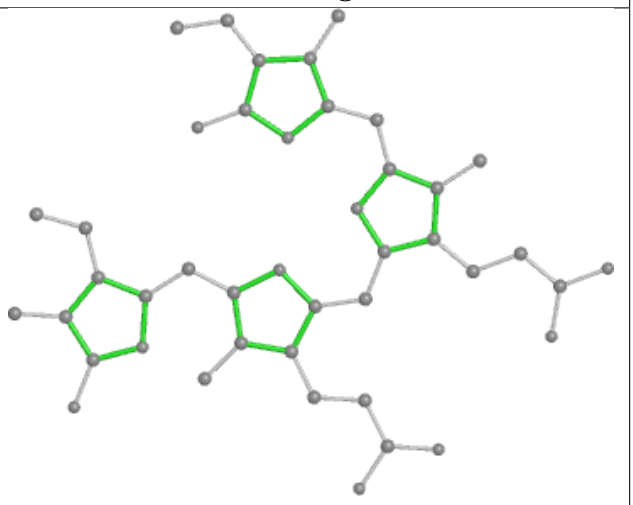
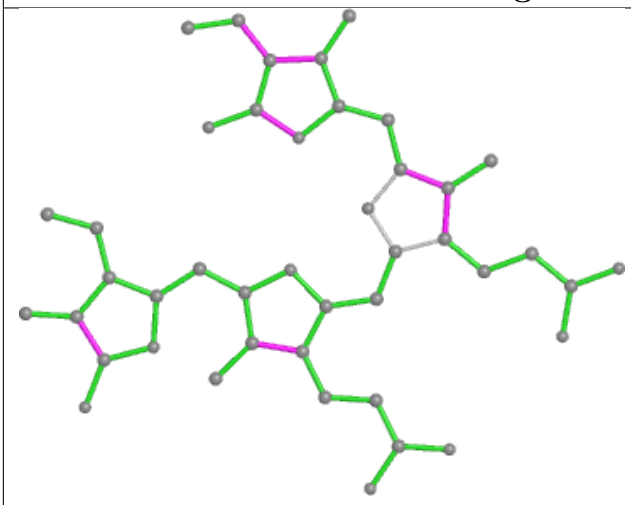


Rings

Ligand PEB jJ 1002



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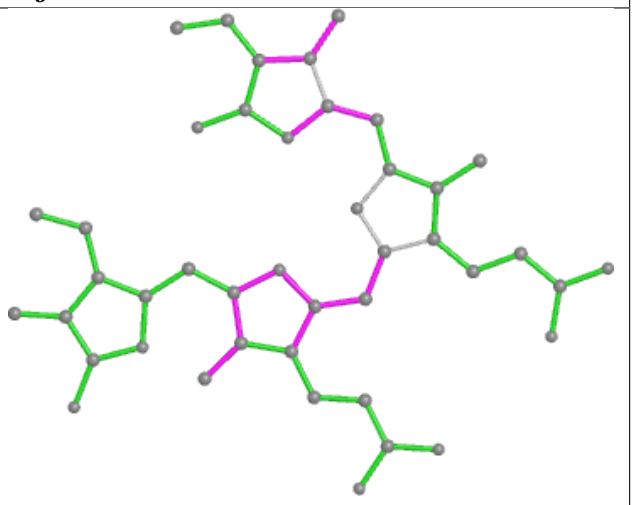

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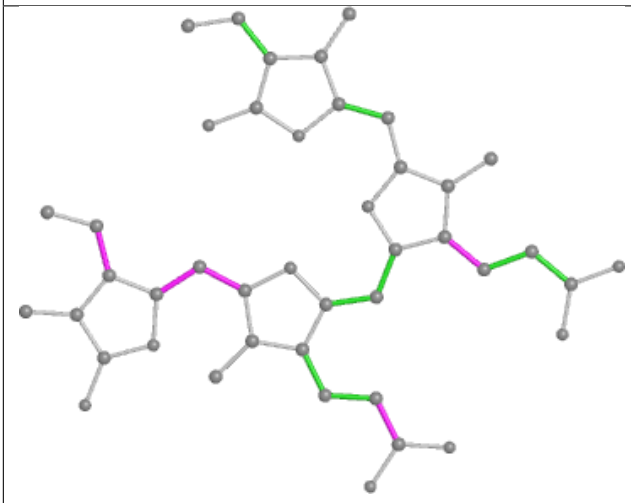

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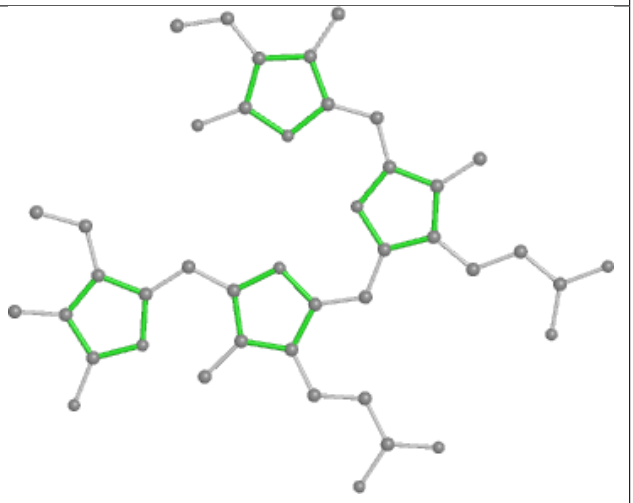

Rings

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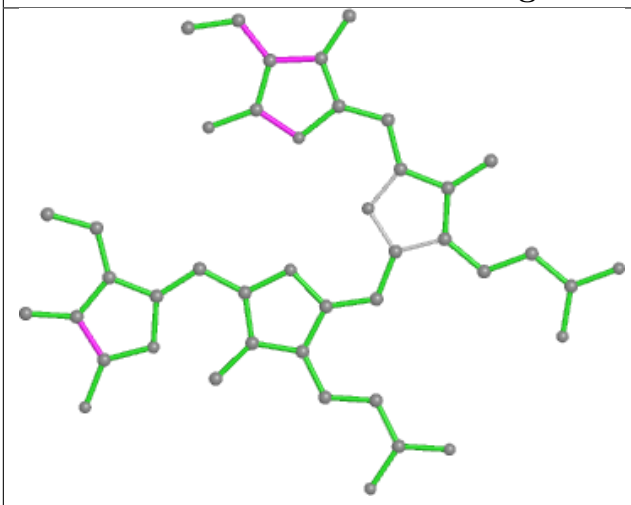

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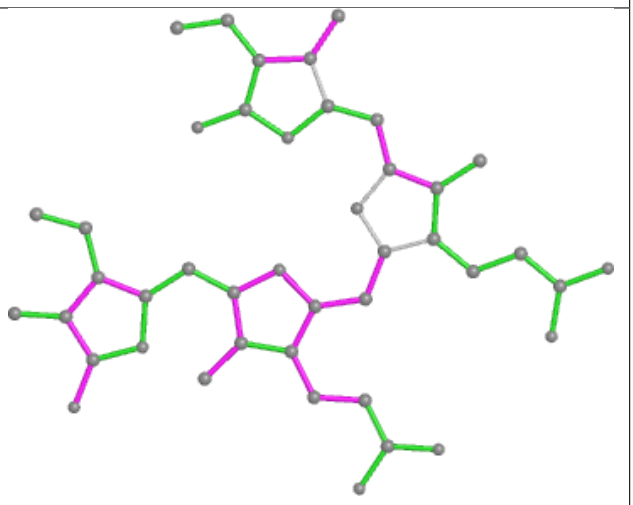

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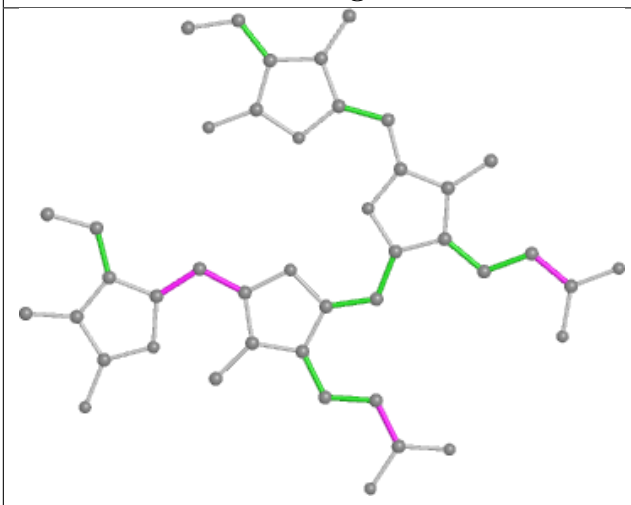

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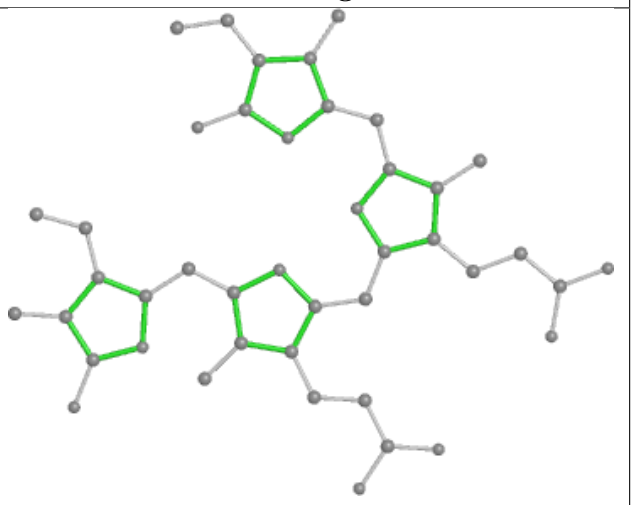

Rings

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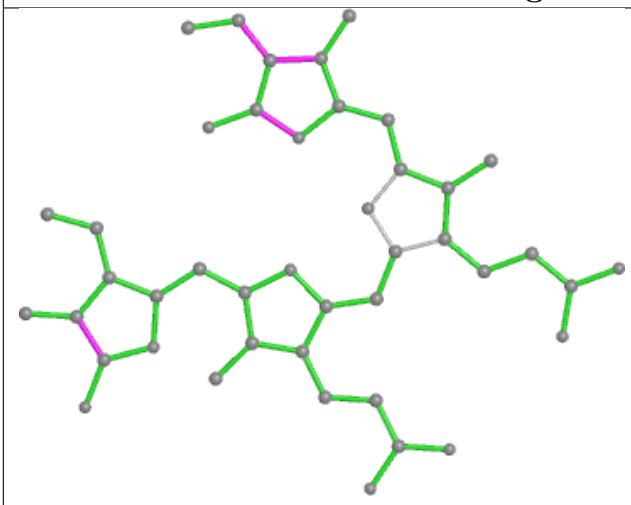

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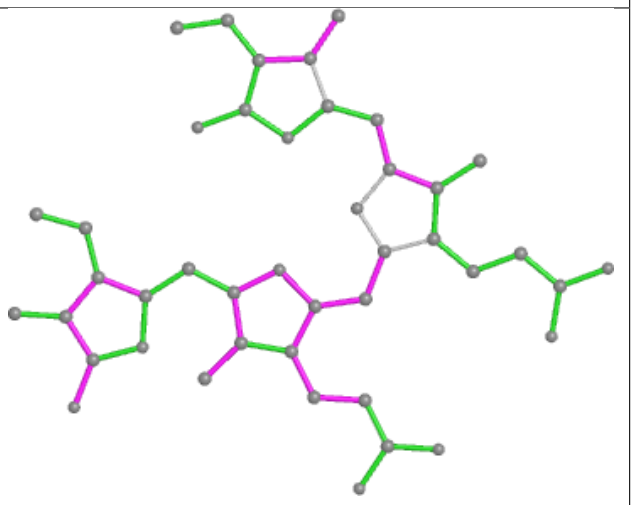

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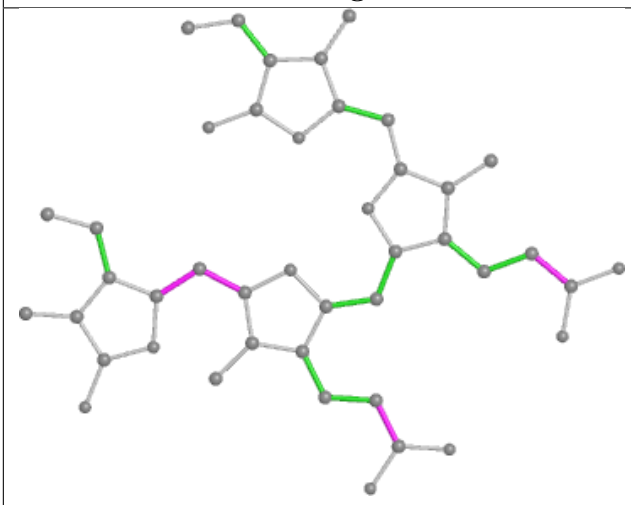

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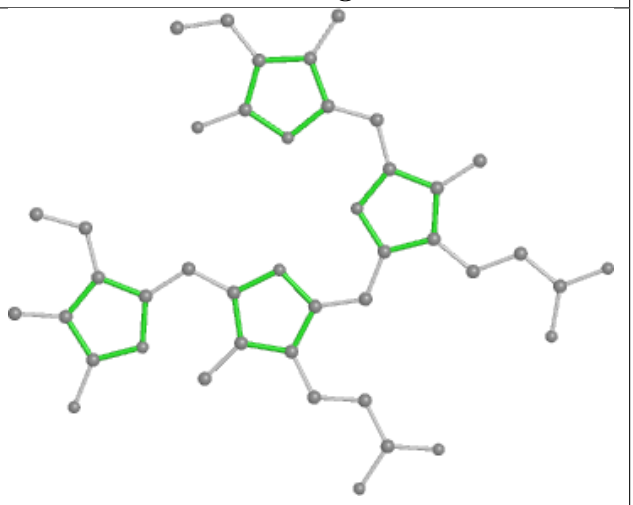
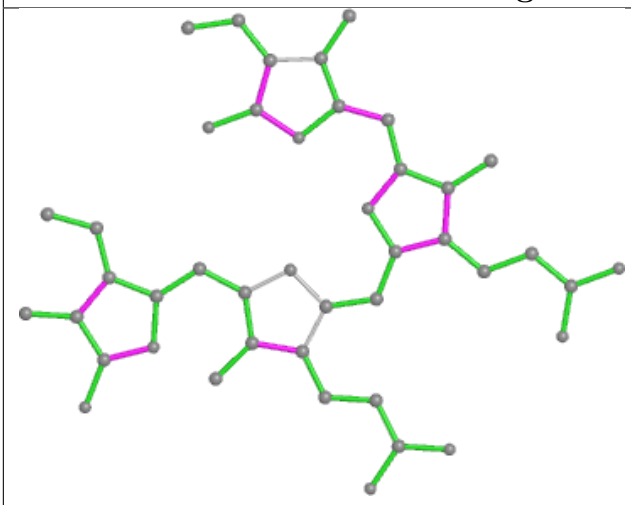


Rings

Ligand PUB dx 406



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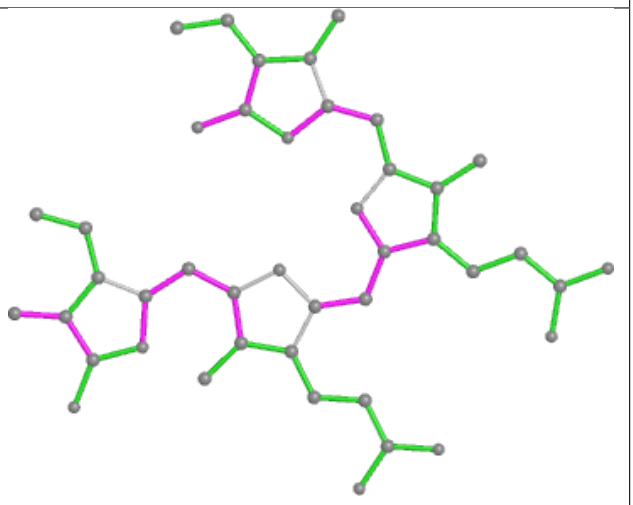
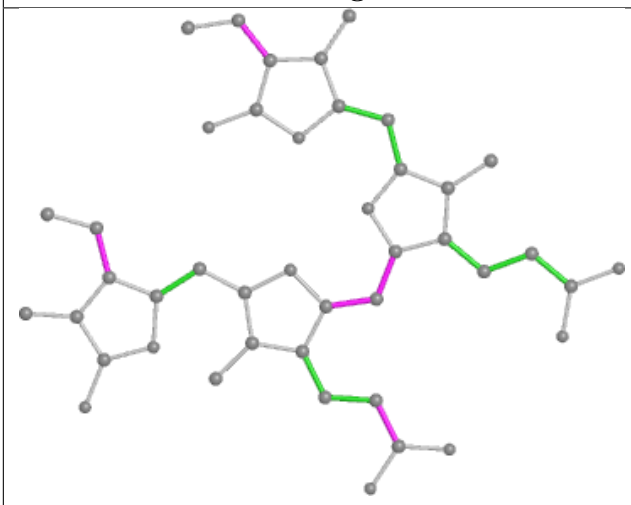
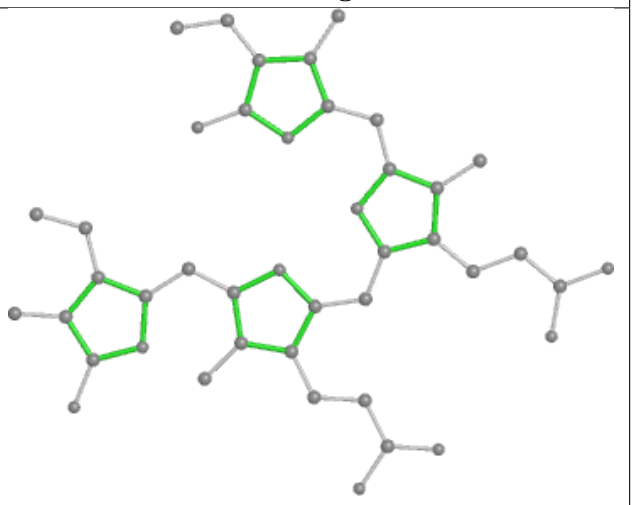


Bond angles

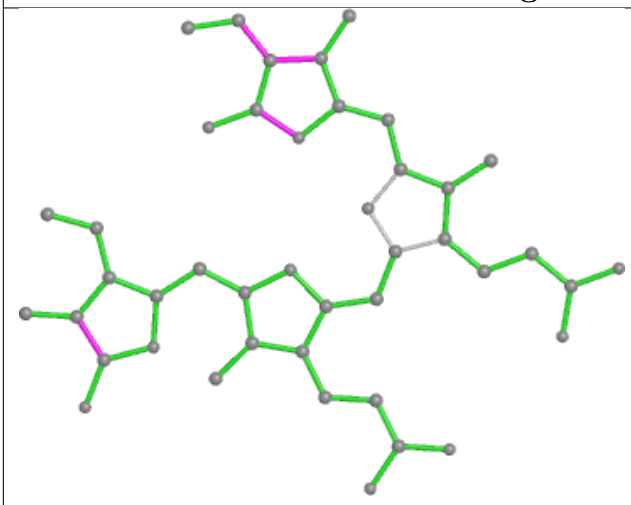


Torsions



Rings

Ligand PEB br 202



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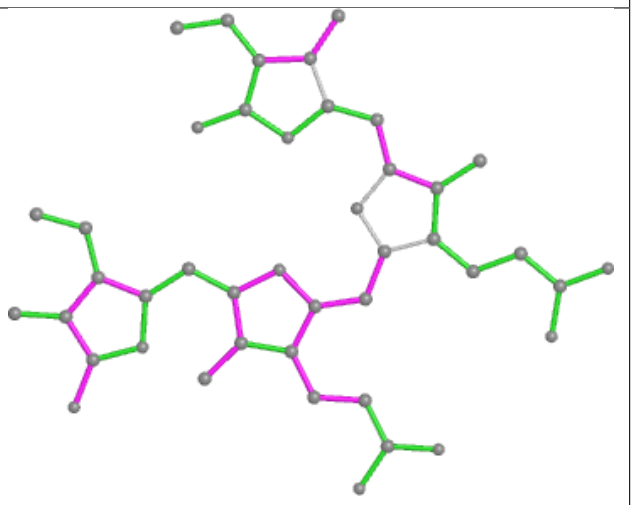

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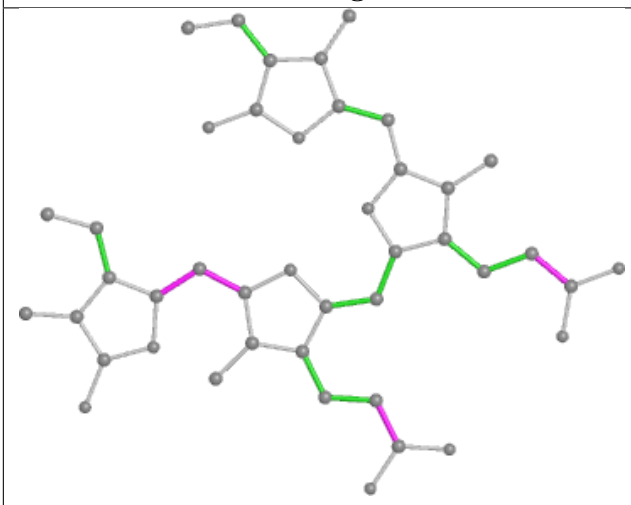

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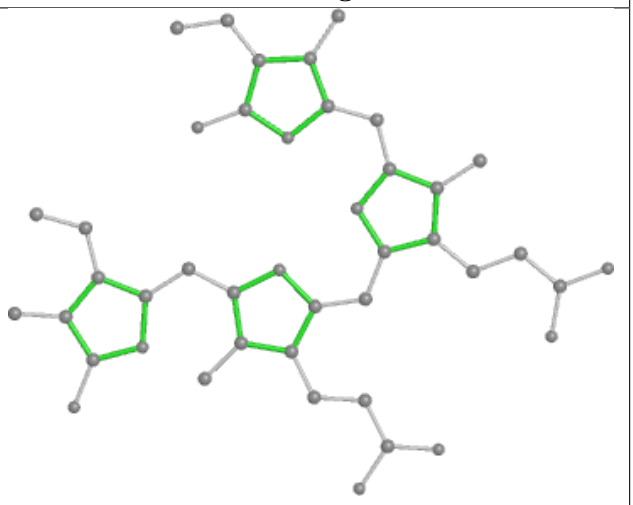
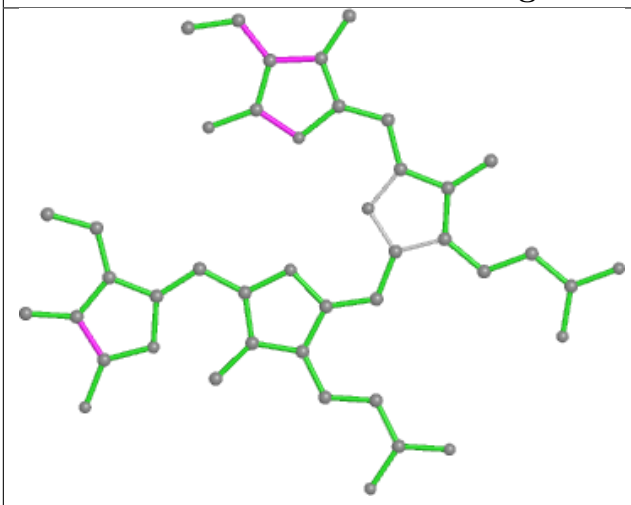


Rings

Ligand PEB b9 403



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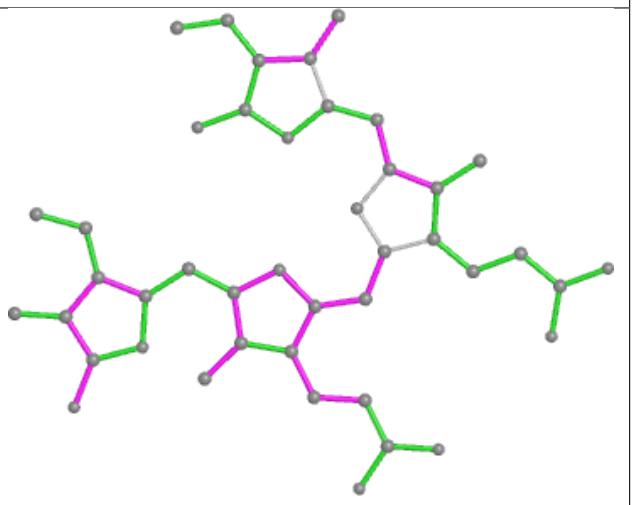

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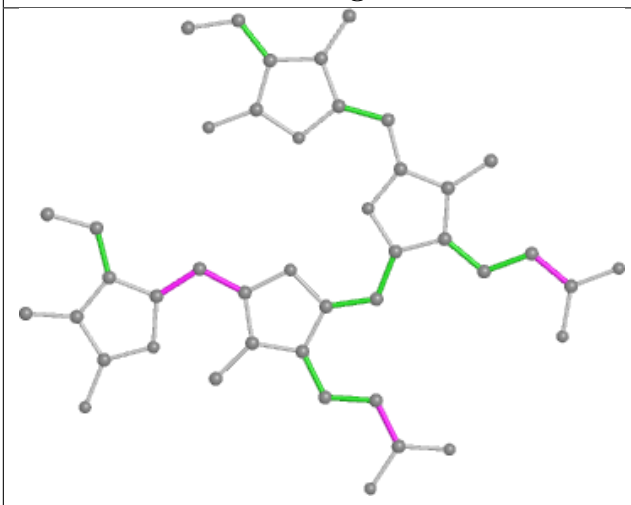

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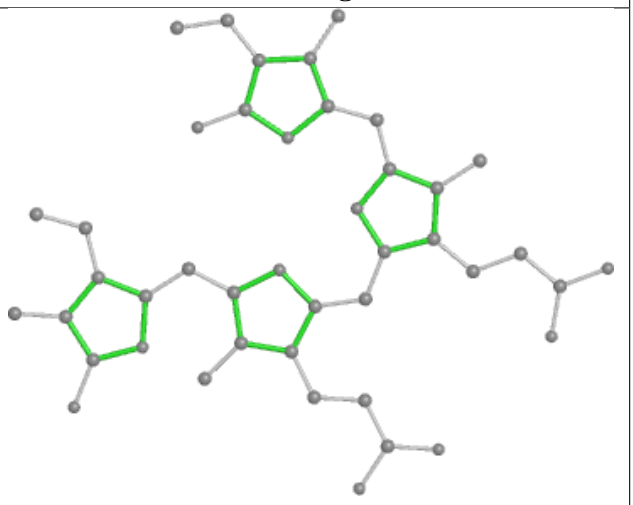
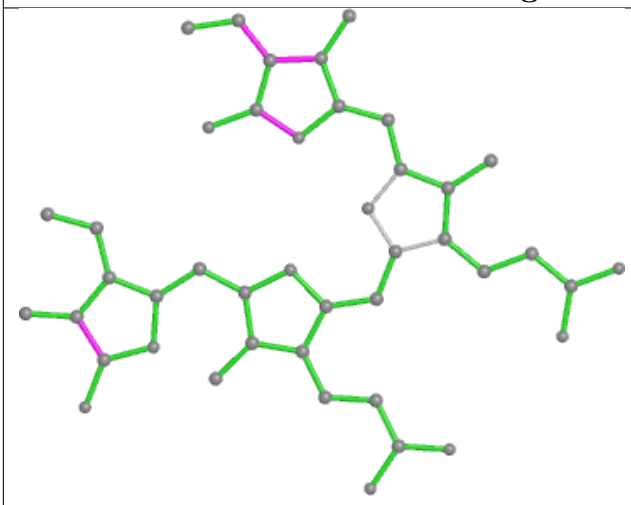


Rings

Ligand PEB z4 202



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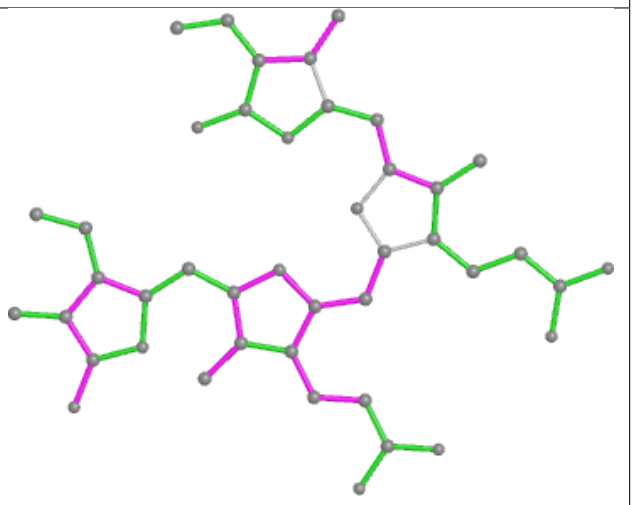

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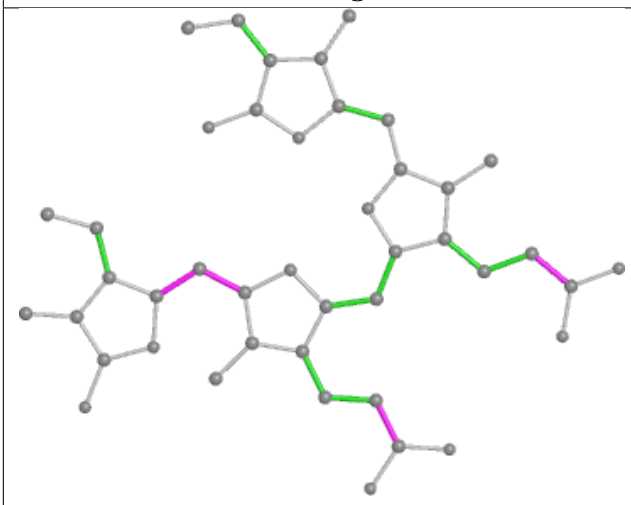

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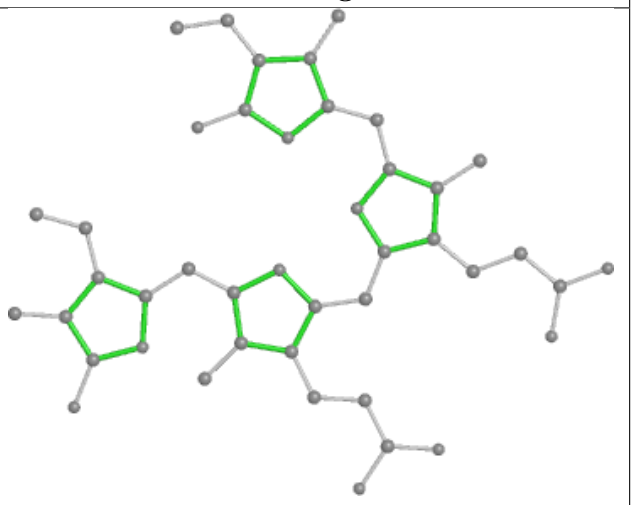
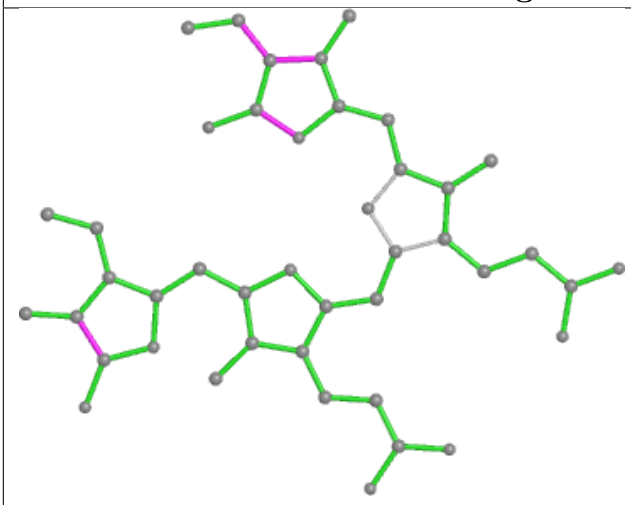


Rings

Ligand PEB w9 201



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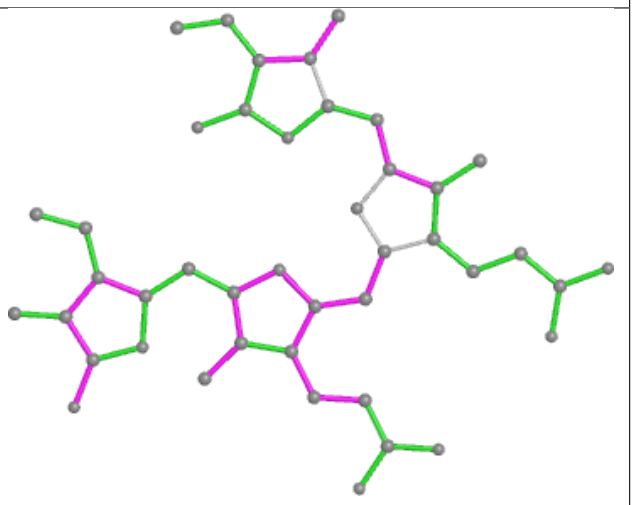

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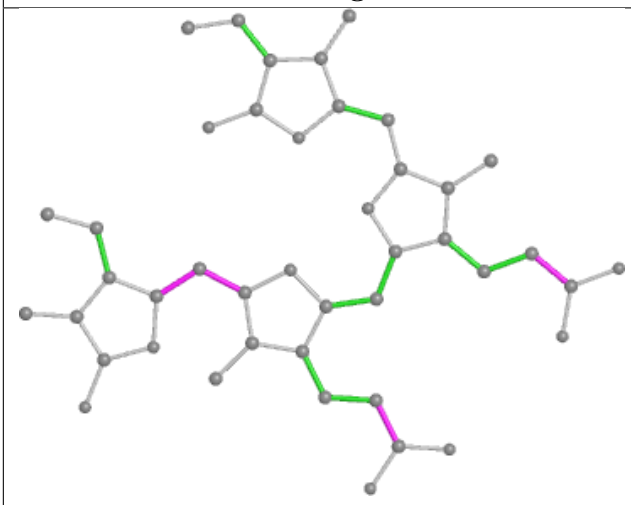

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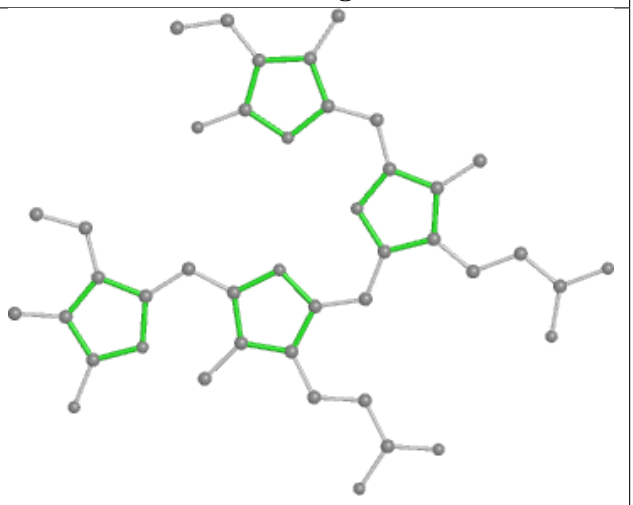
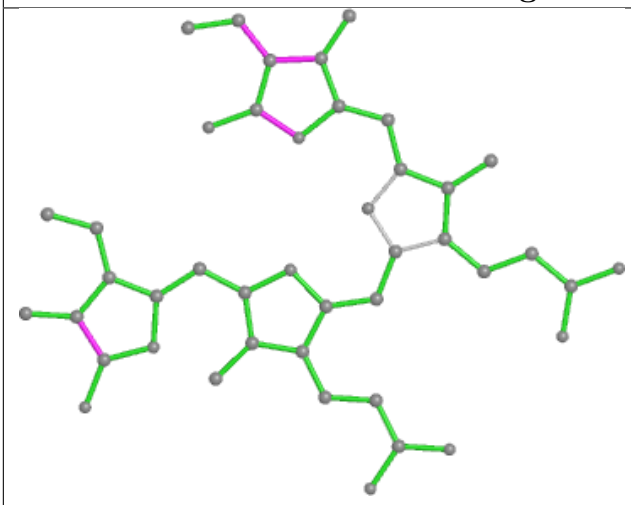


Rings

Ligand PEB v5 201



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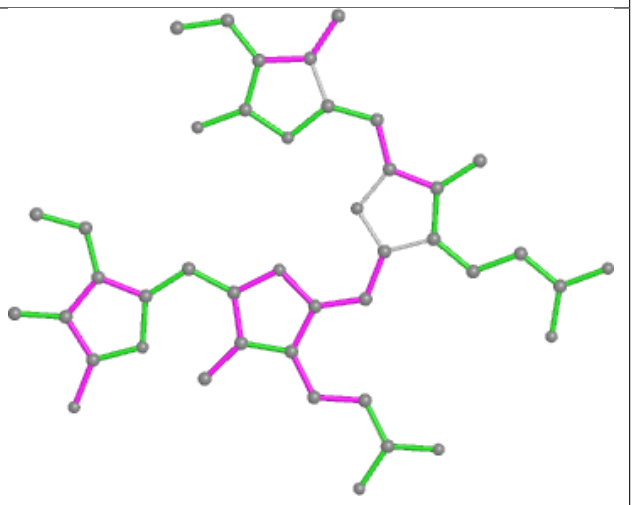

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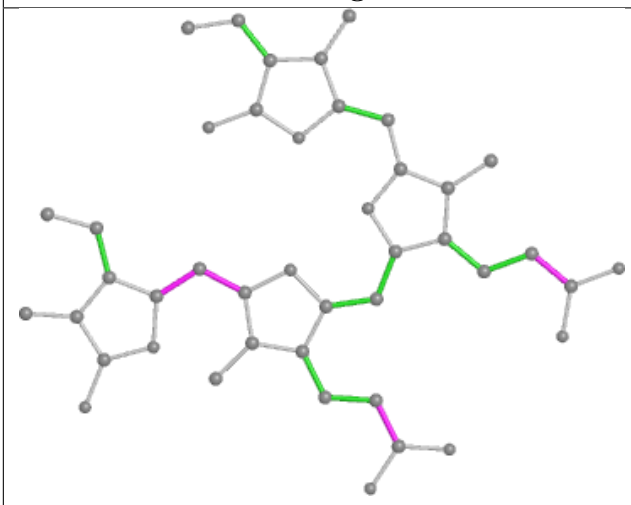

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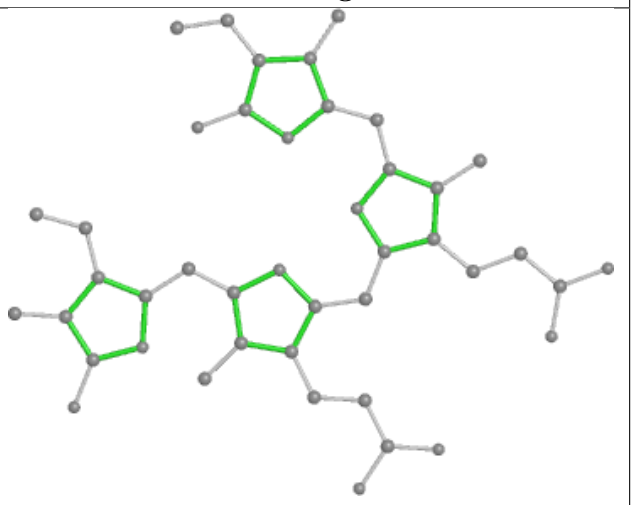

Rings

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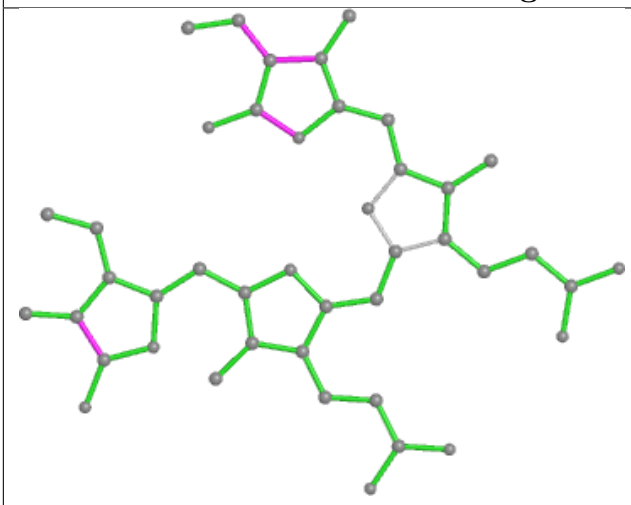

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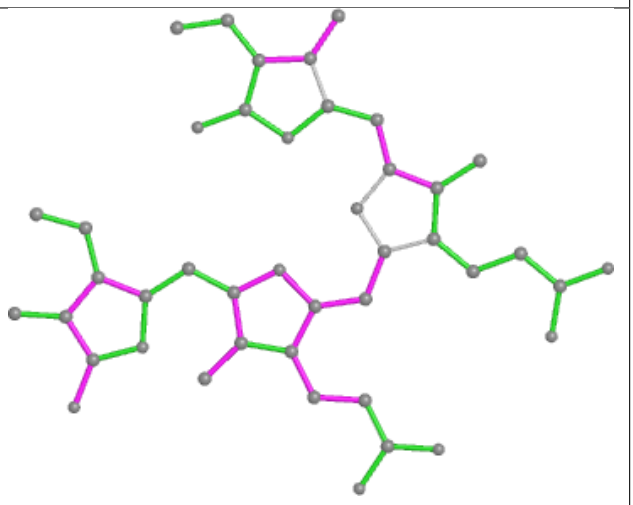

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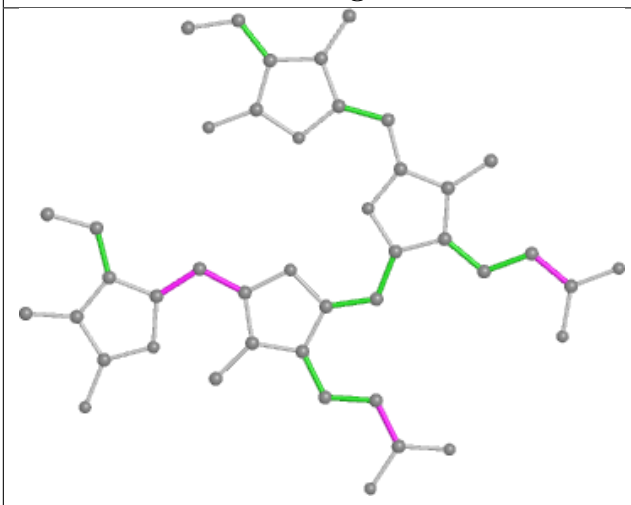

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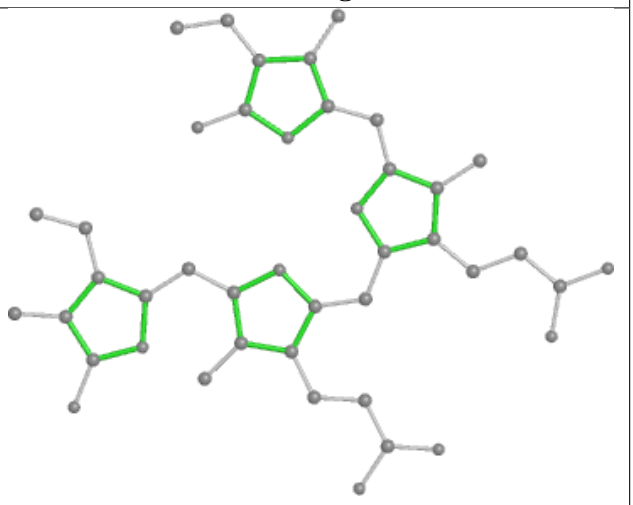
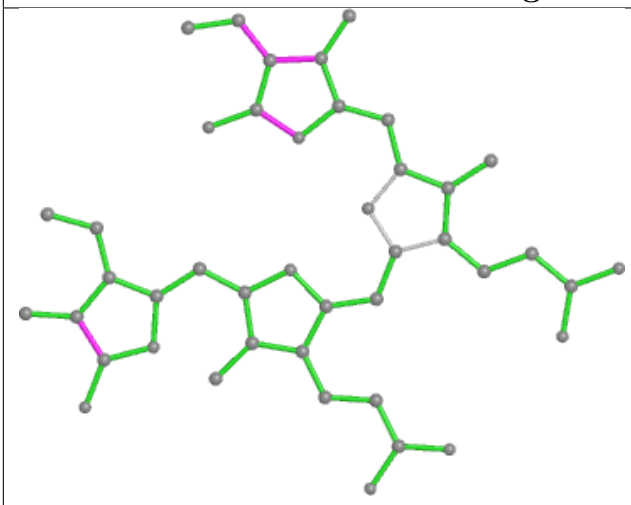


Rings

Ligand PEB lu 201



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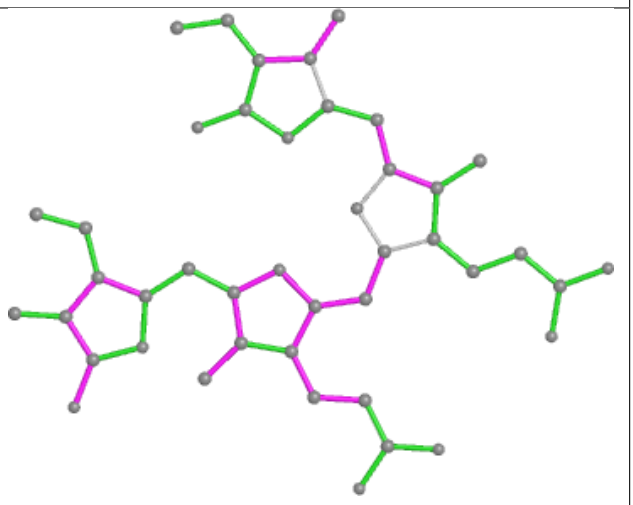

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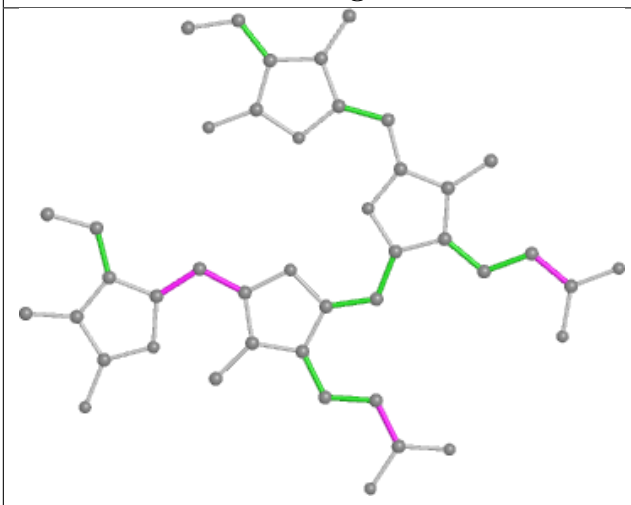

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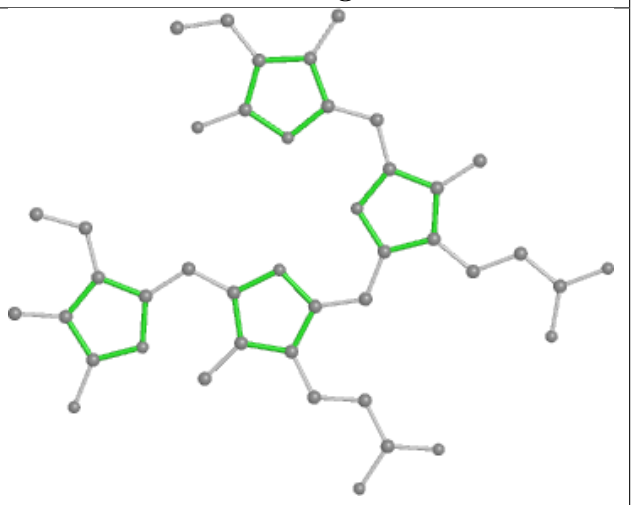
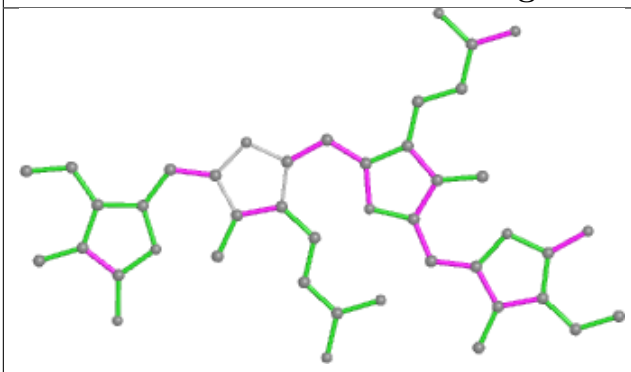


Rings

Ligand CYC e1 201



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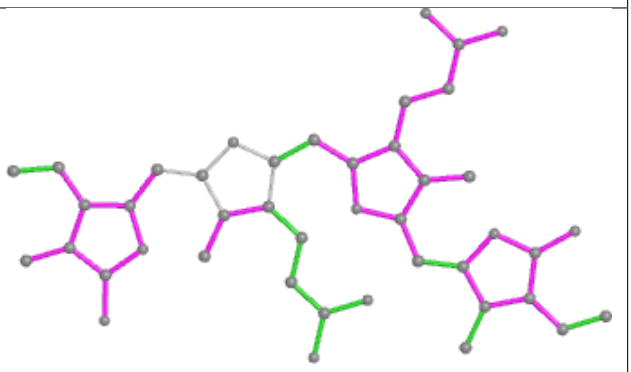

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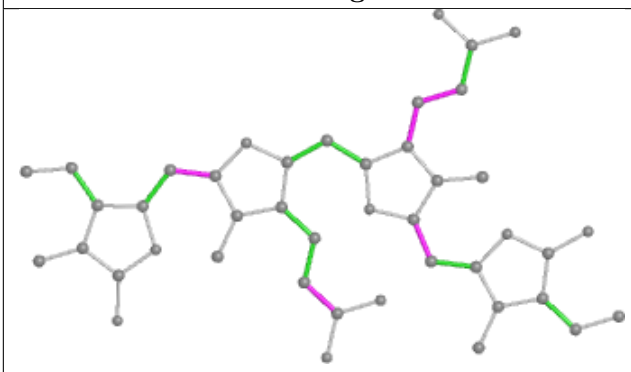

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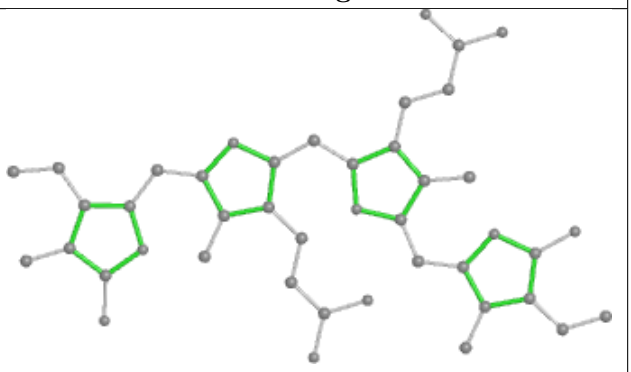
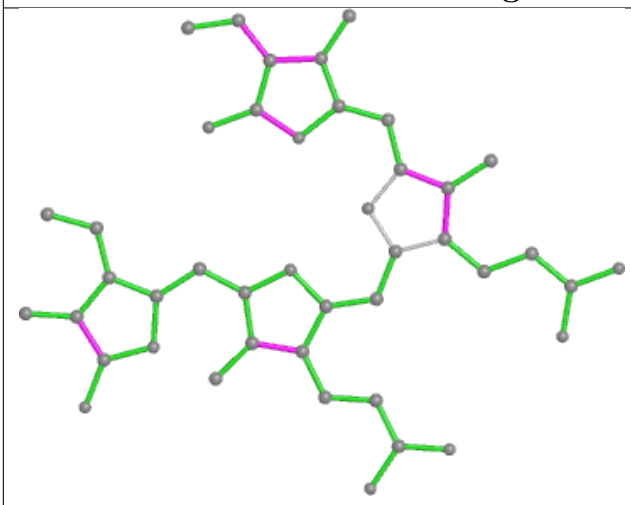


Rings

Ligand PEB kW 1002



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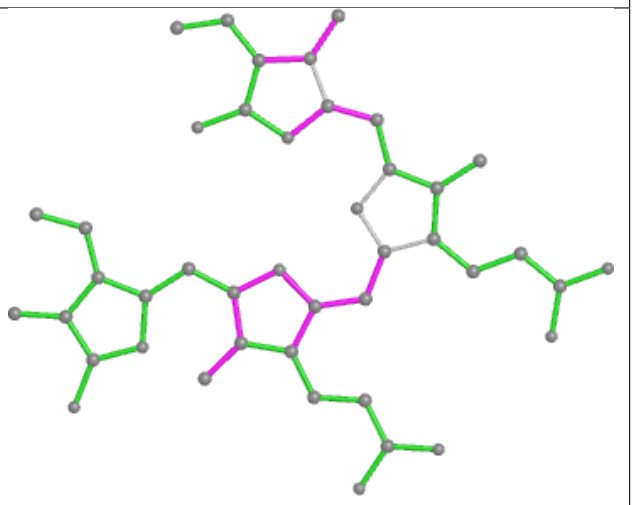

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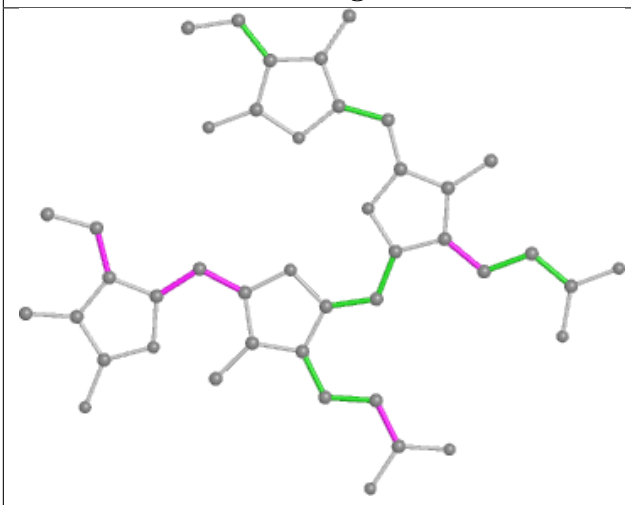

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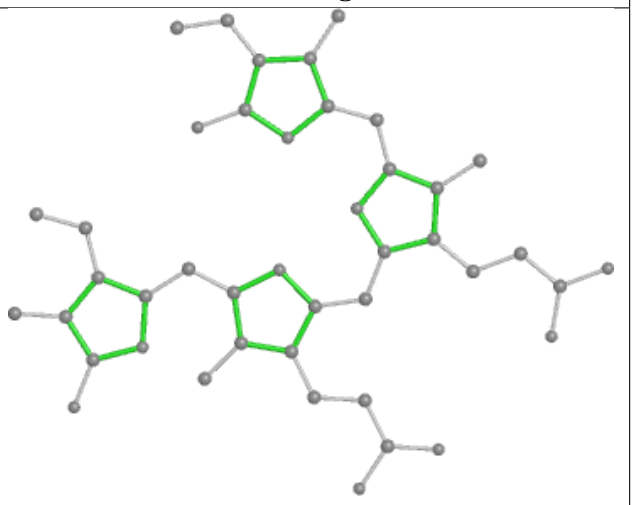
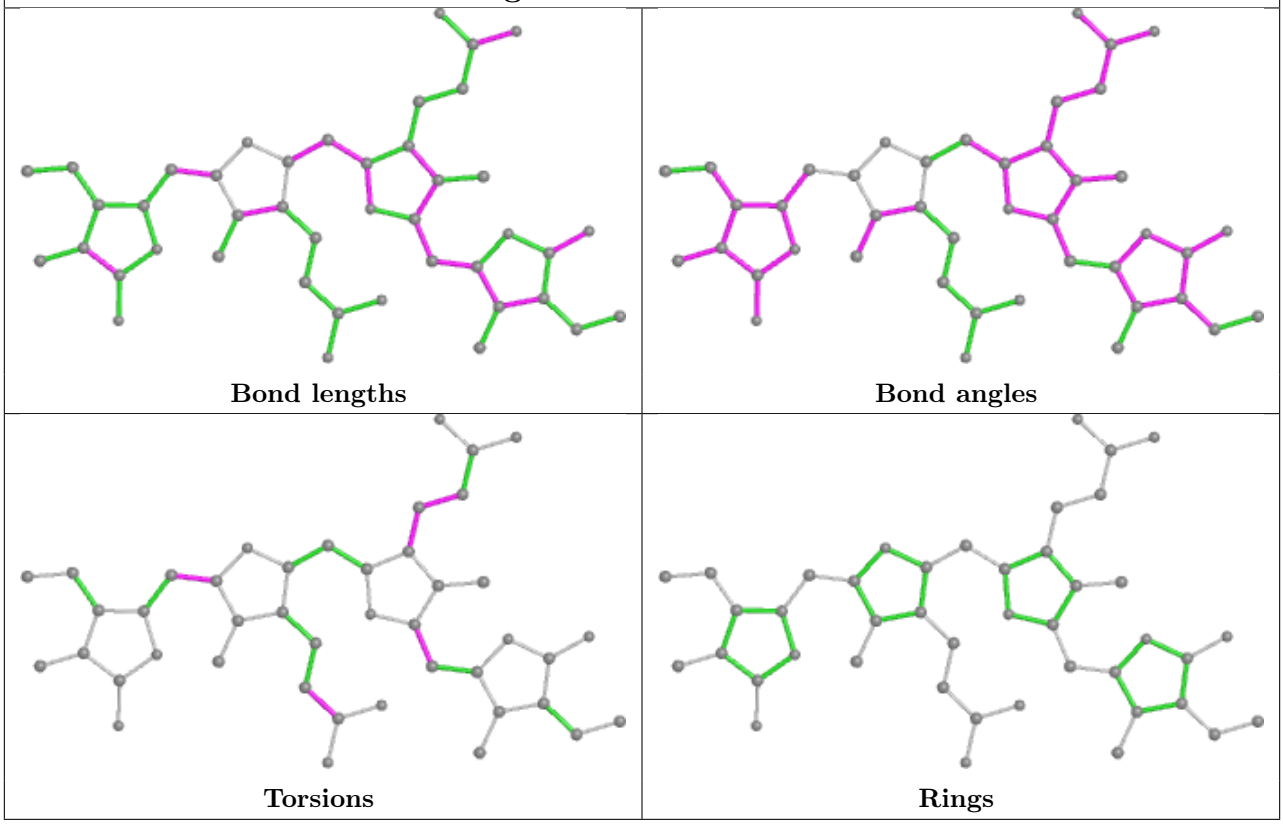


Rings

Ligand CYC G1 1001



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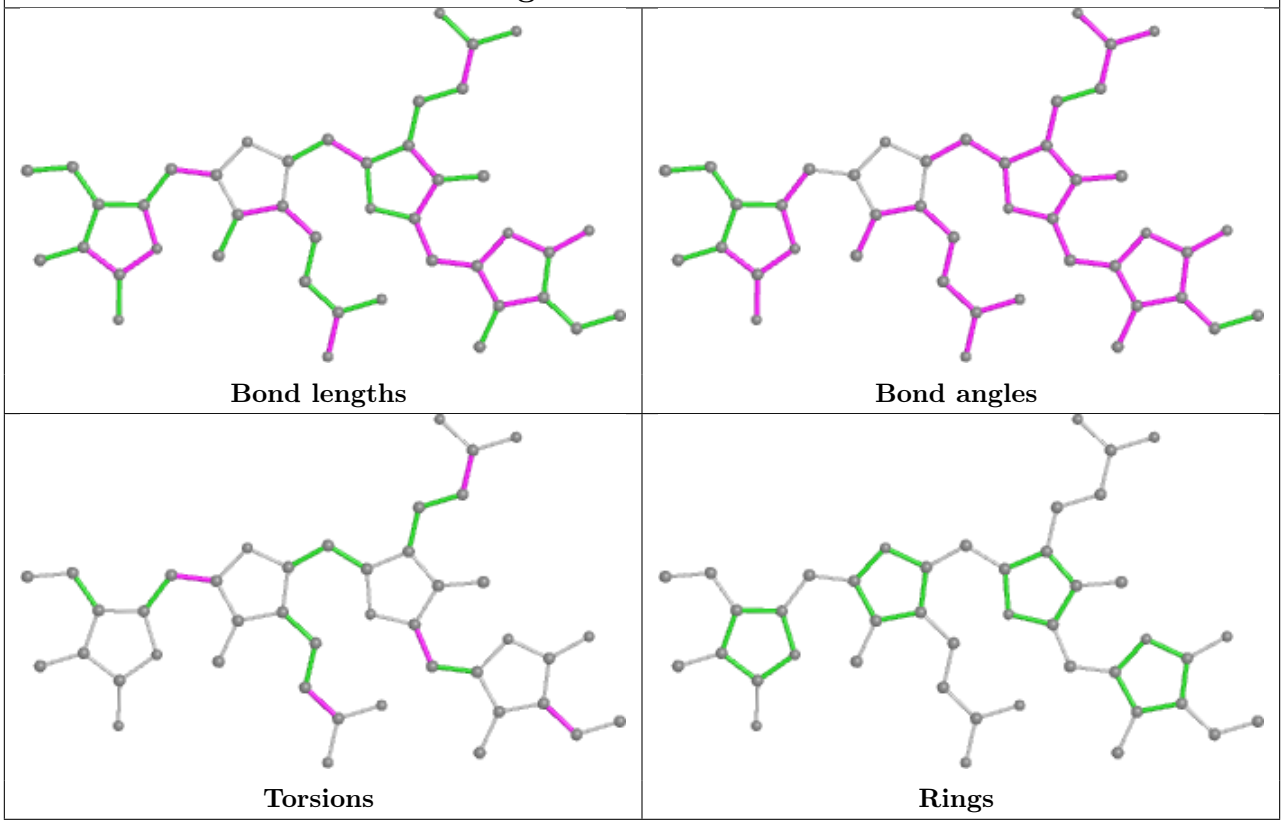

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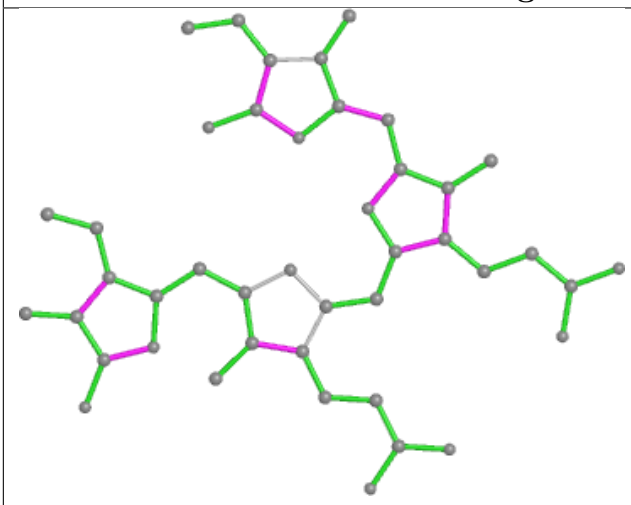

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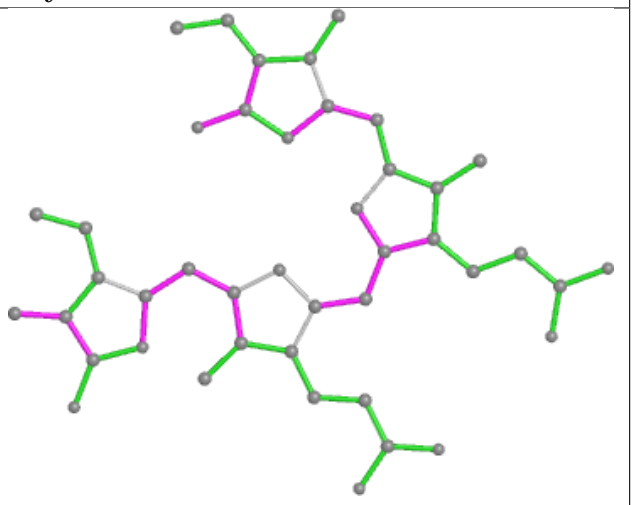
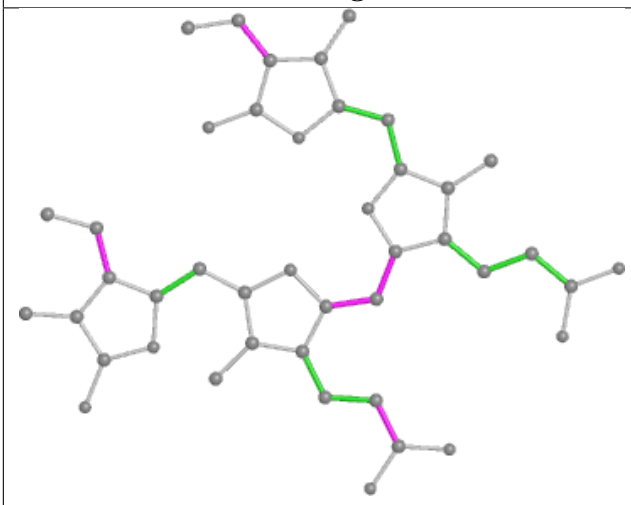
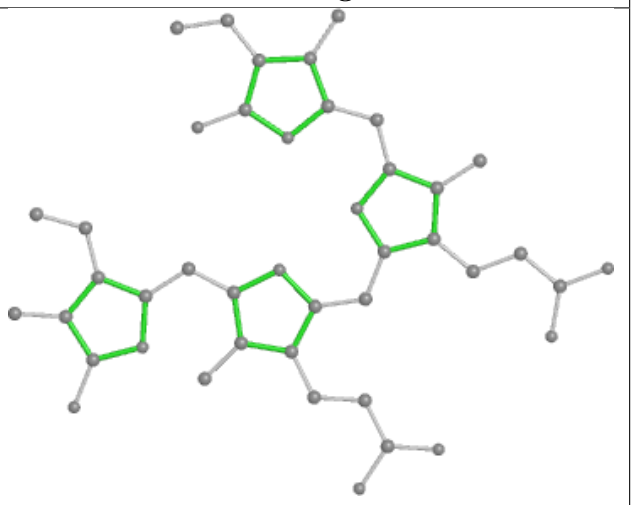


Bond angles

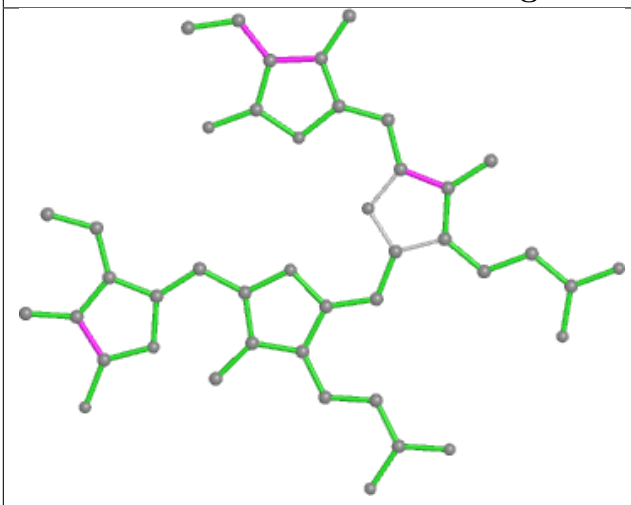


Torsions



Rings

Ligand PEB cx 202



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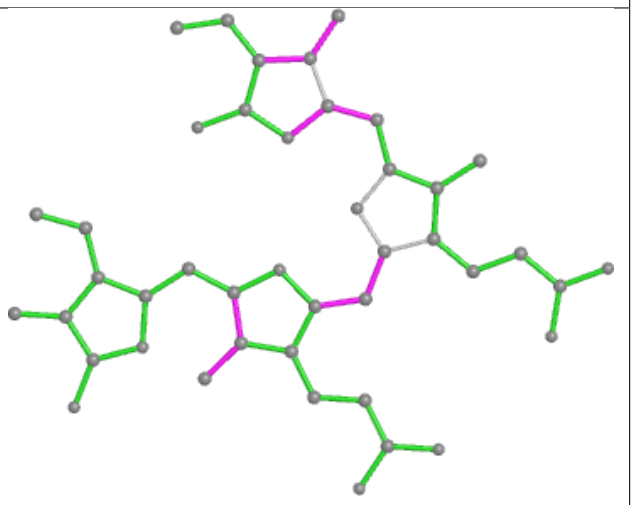

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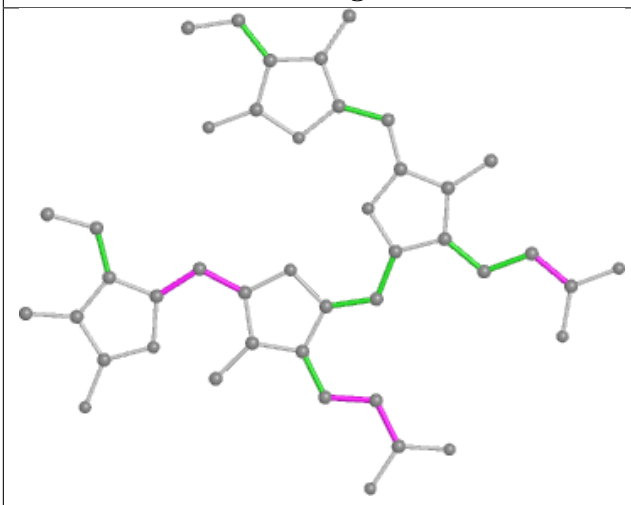

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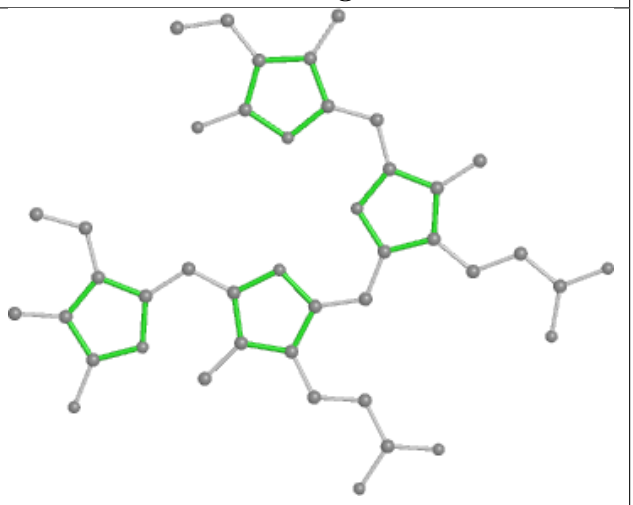

Rings

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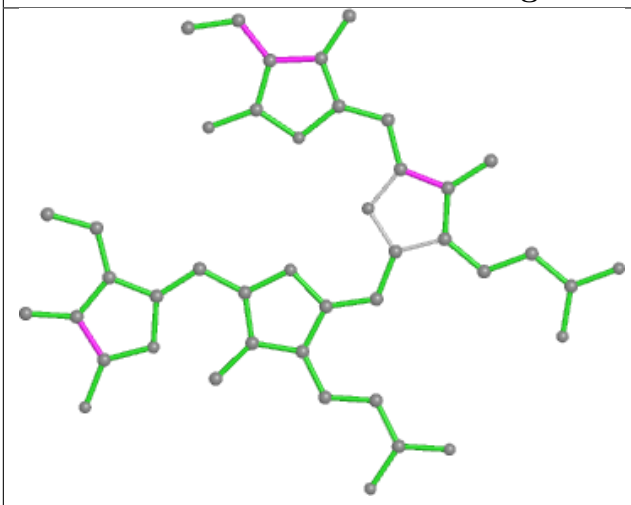

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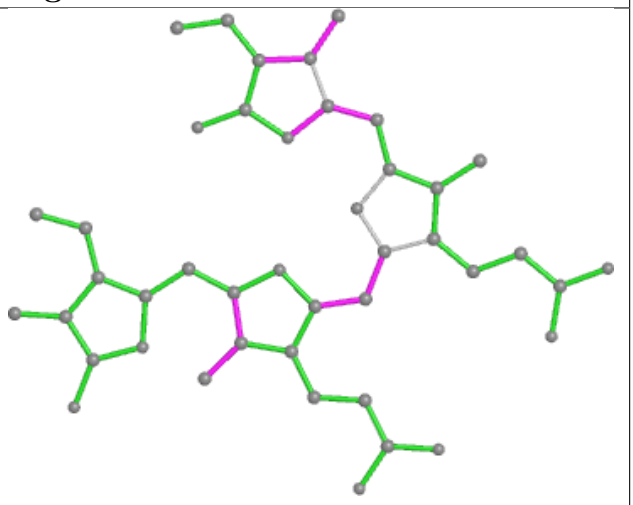
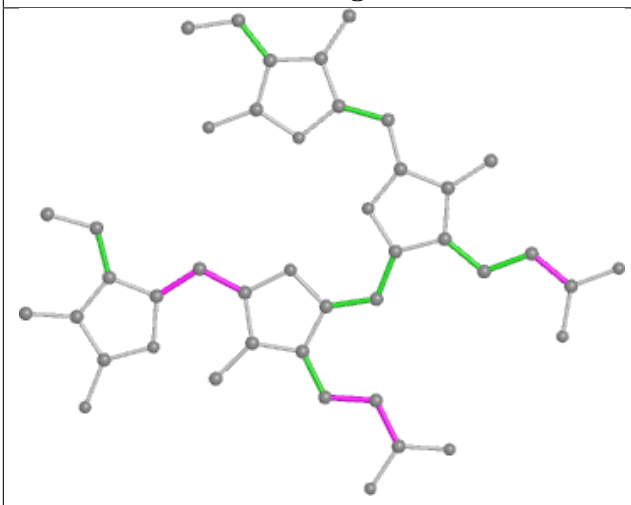


Bond angles



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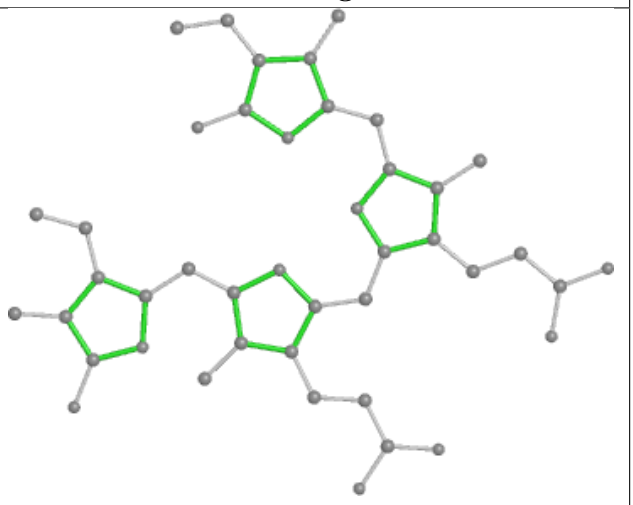
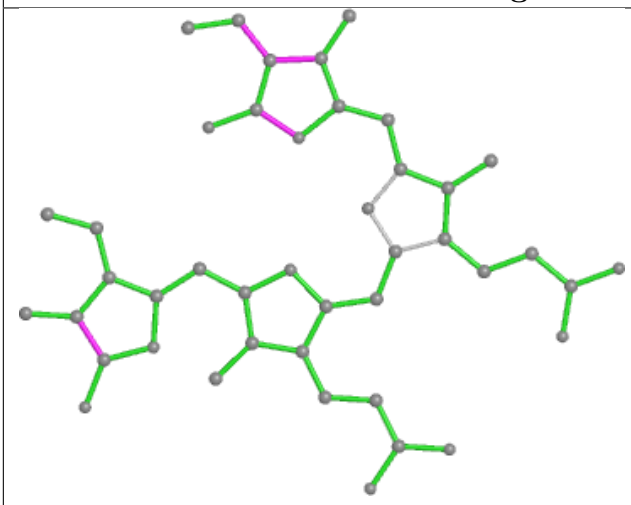
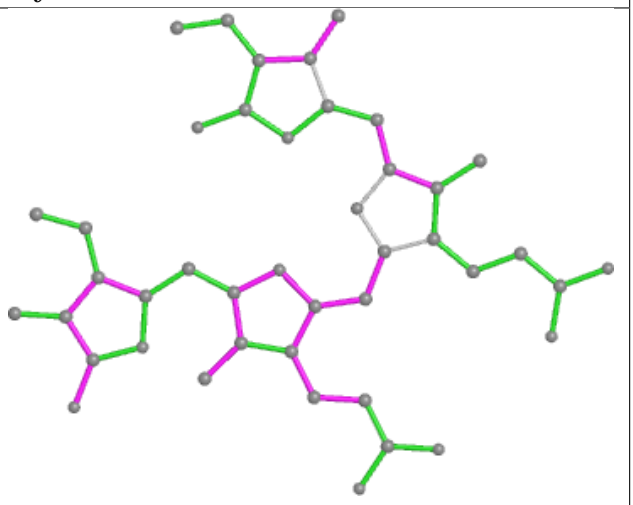


Rings

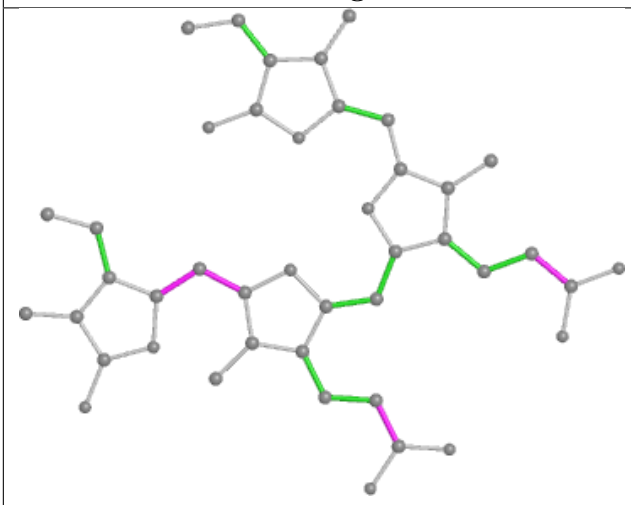
Ligand PEB y9 1001



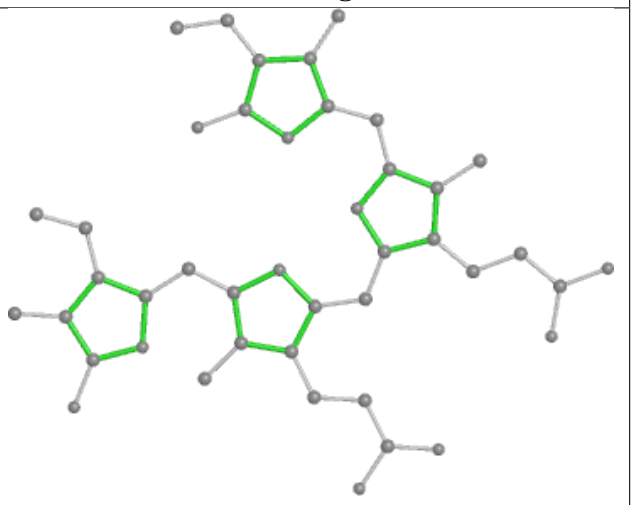
Bond lengths



Bond angles

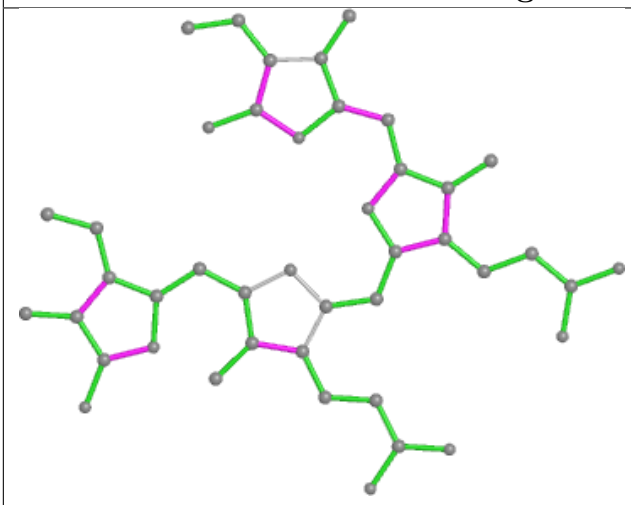


Torsions



Rings

Ligand PUB p6 203



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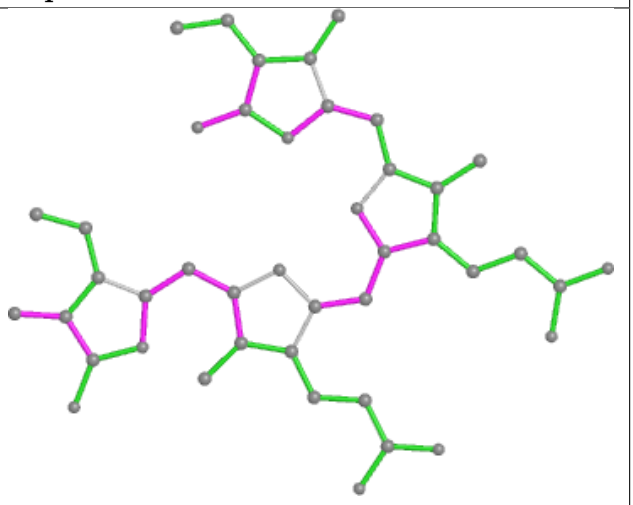

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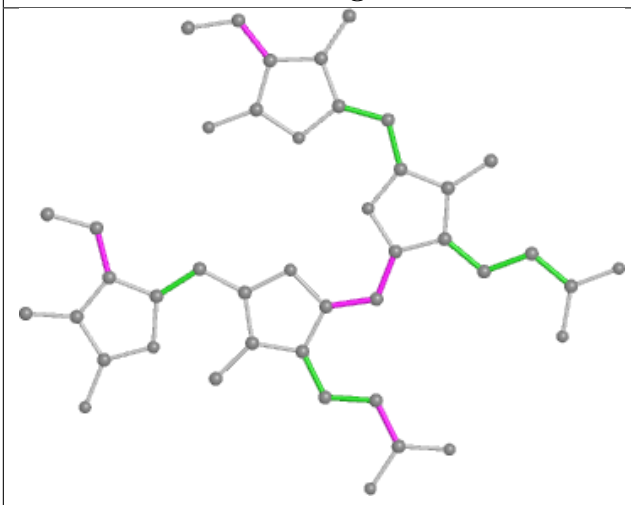

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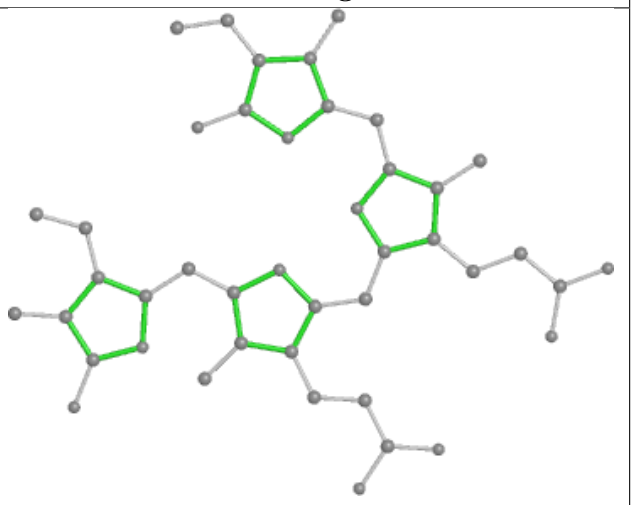
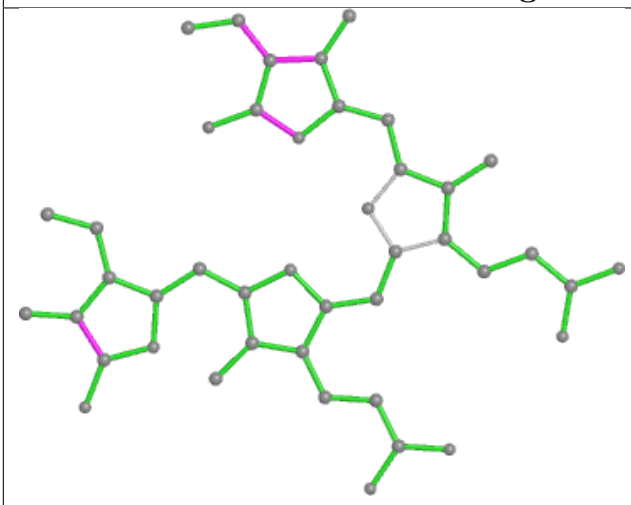


Rings

Ligand PEB v6 202



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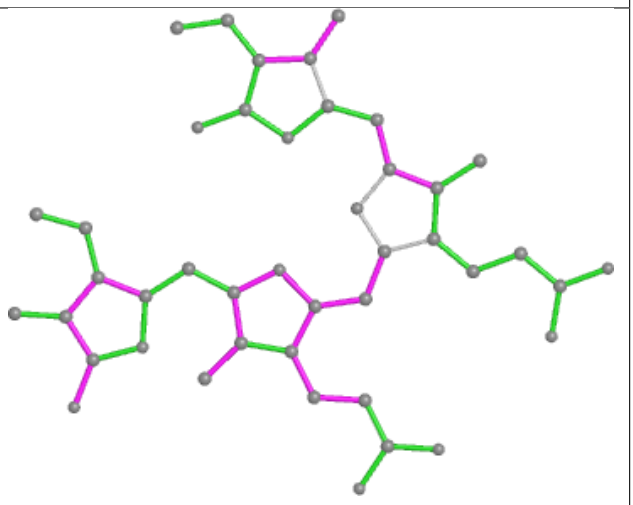

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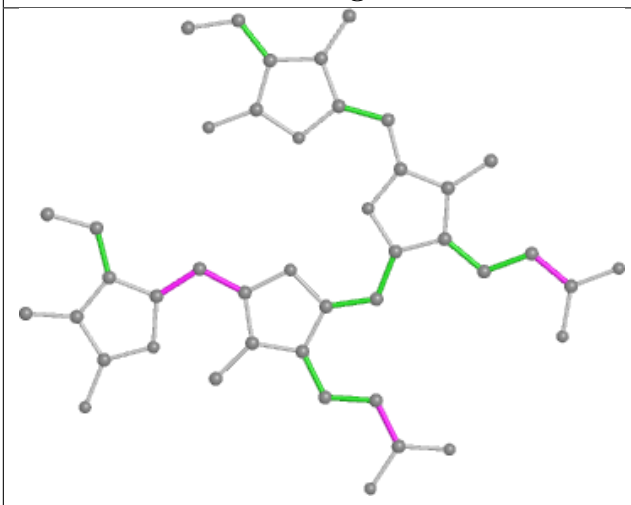

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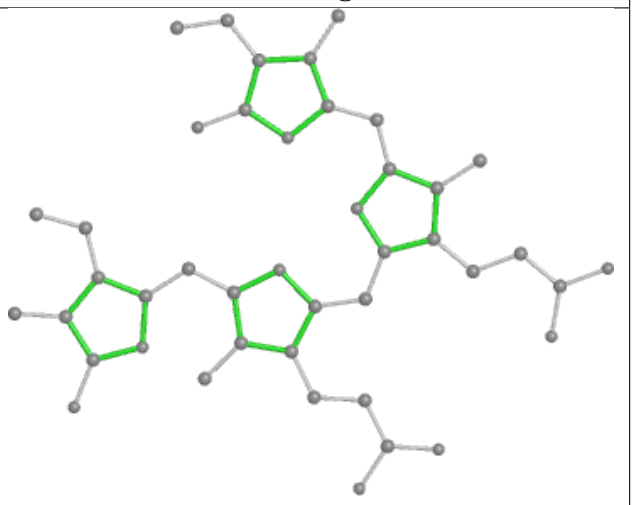
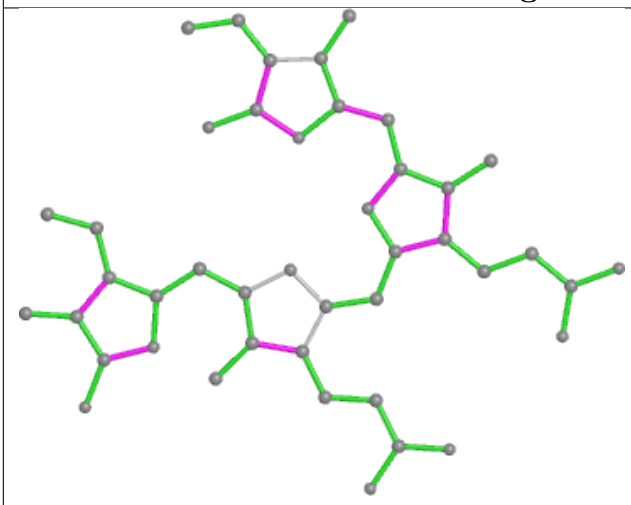


Rings

Ligand PUB I8 203



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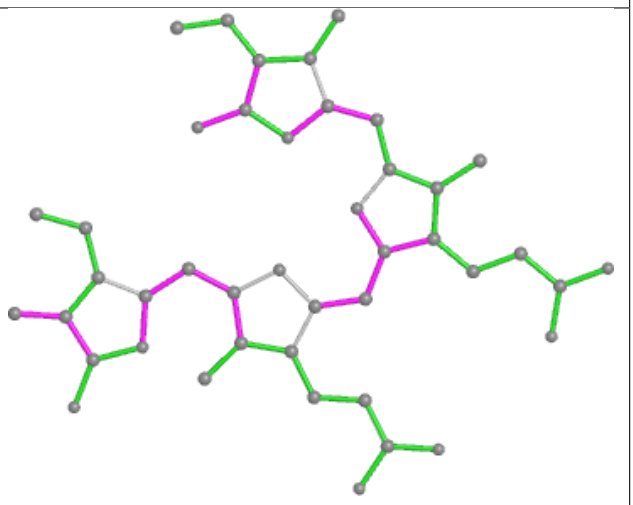

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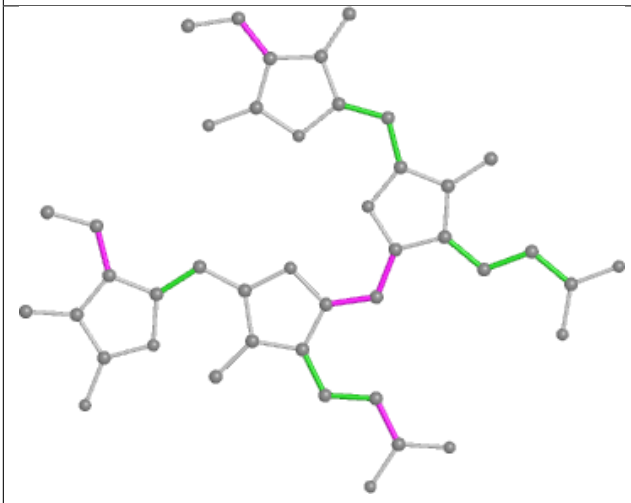

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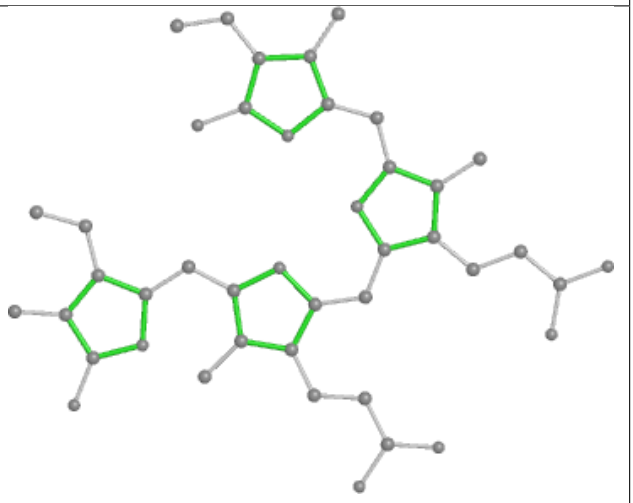
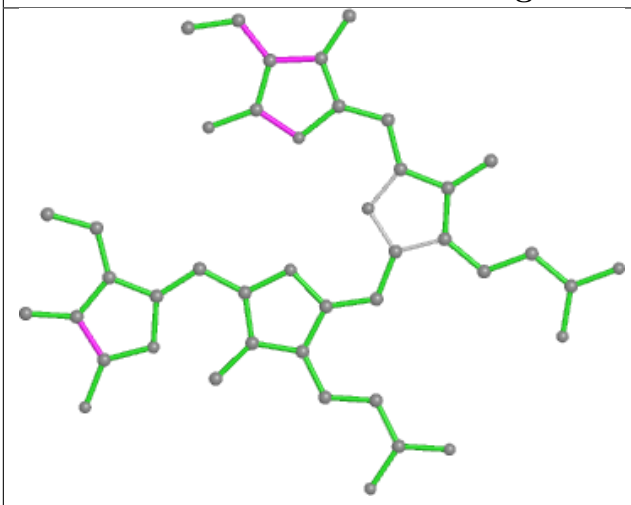


Rings

Ligand PEB X4 201



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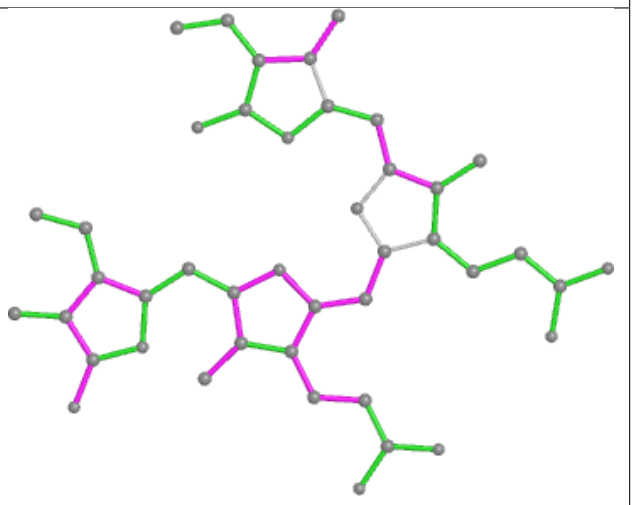

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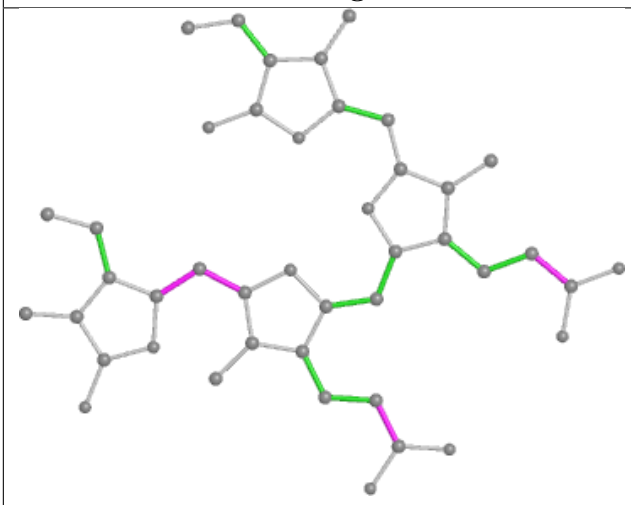

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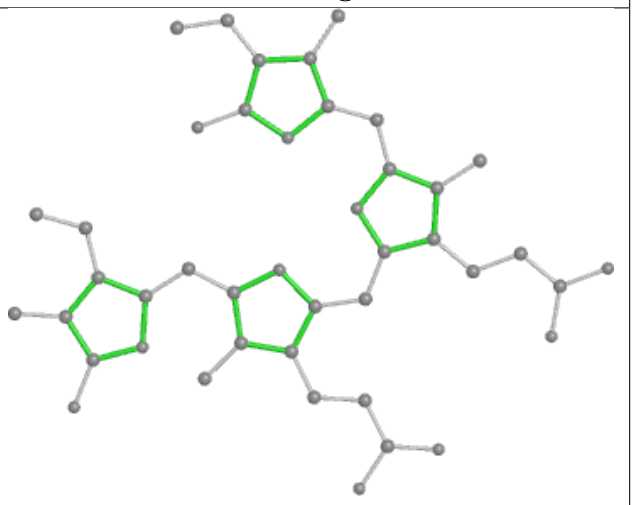
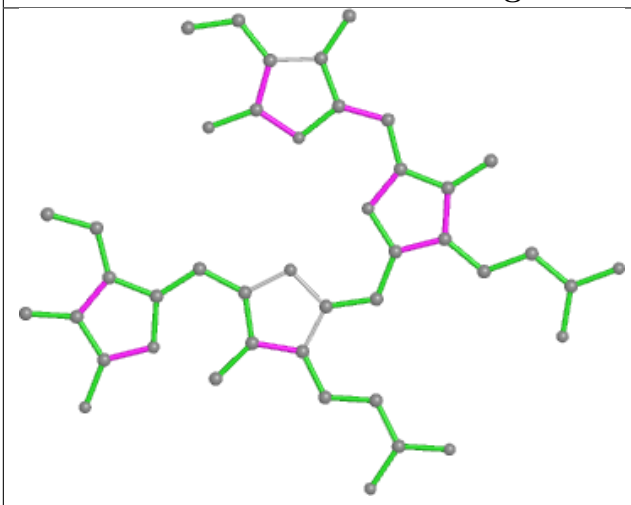


Rings

Ligand PUB U8 1005



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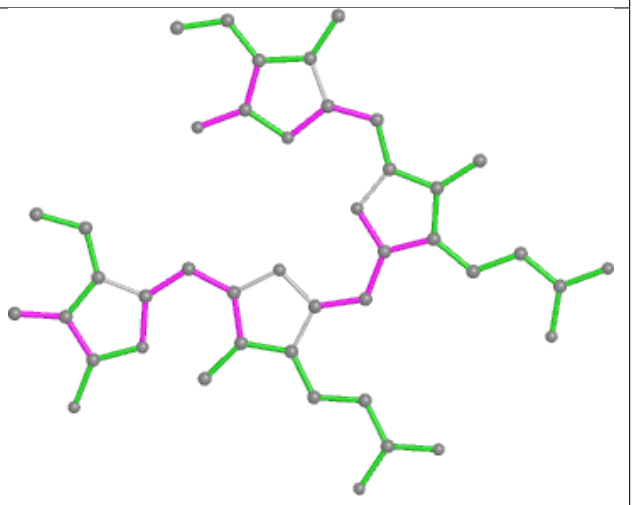
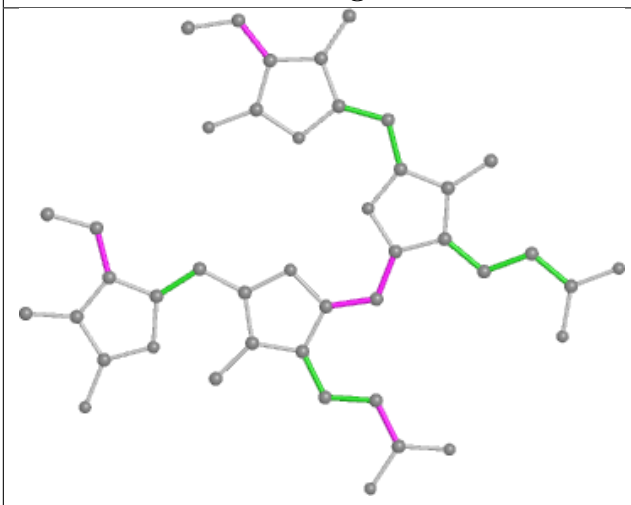


Bond angles



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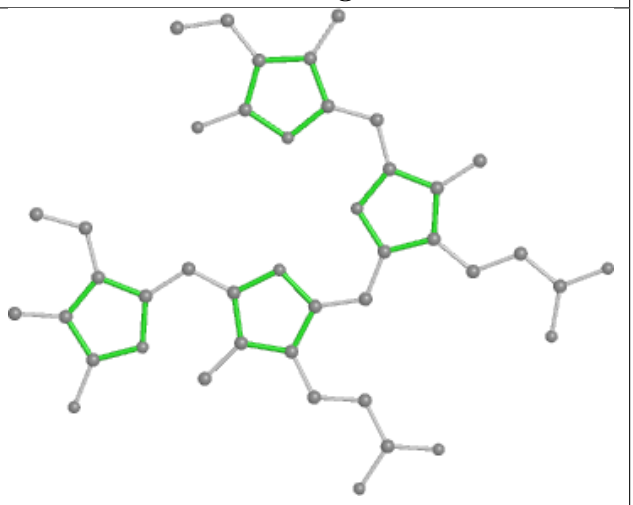
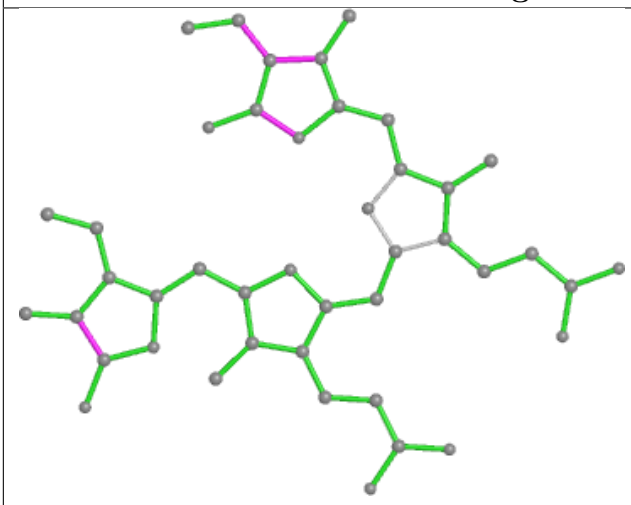


Rings

Ligand PEB M8 201



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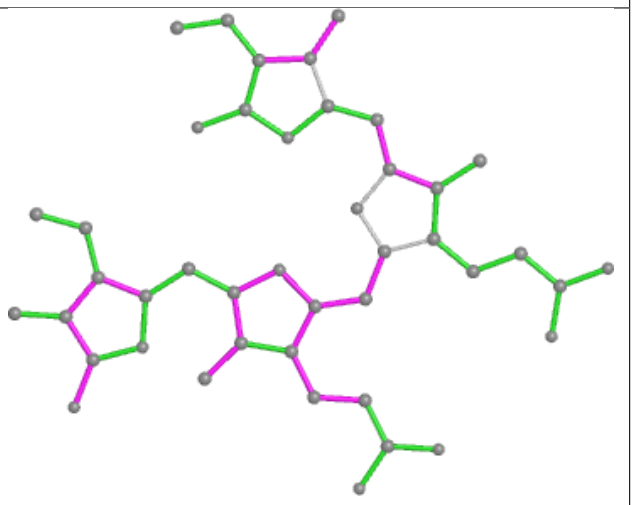

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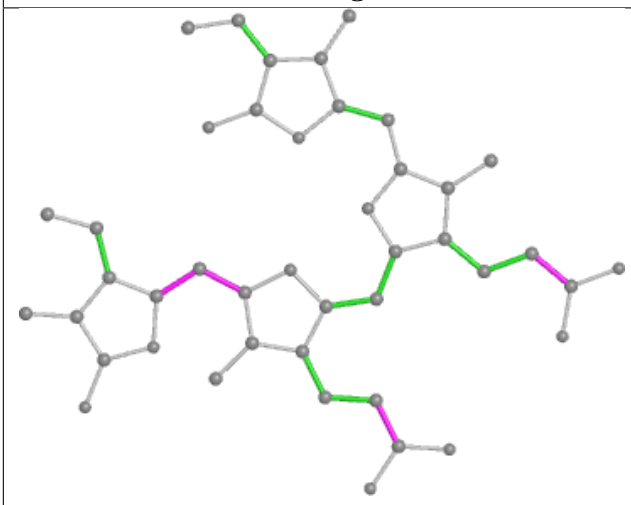

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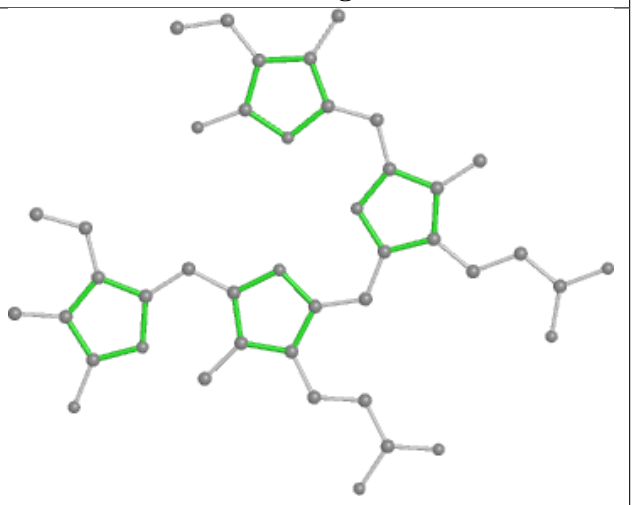
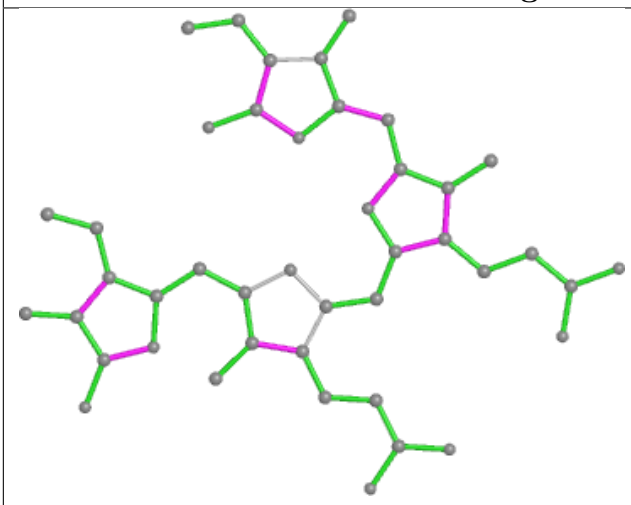


Rings

Ligand PUB fq 203



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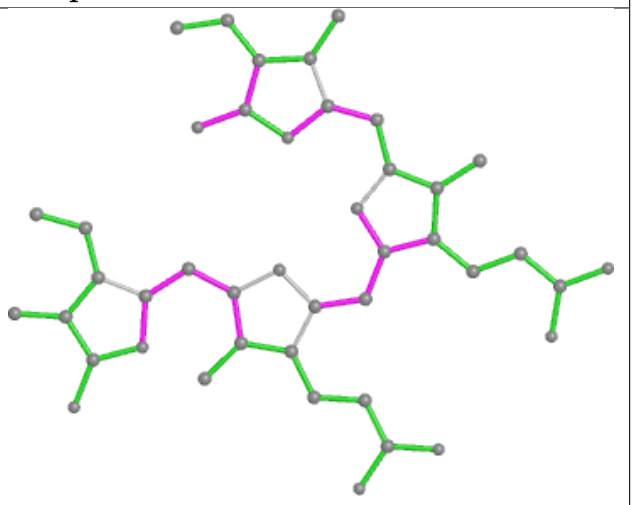

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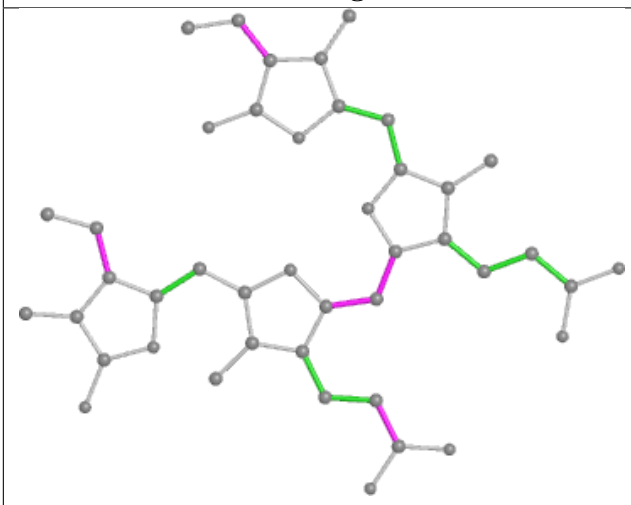

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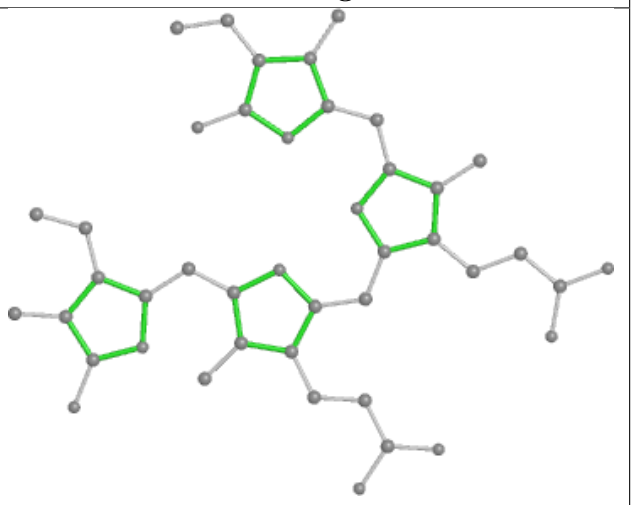
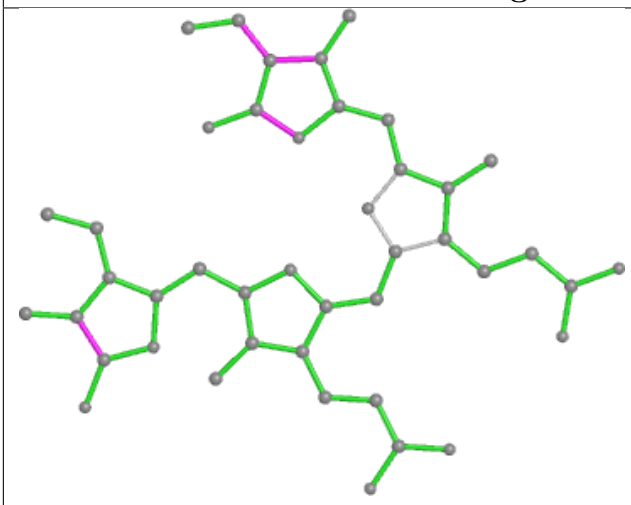


Rings

Ligand PEB k7 1001



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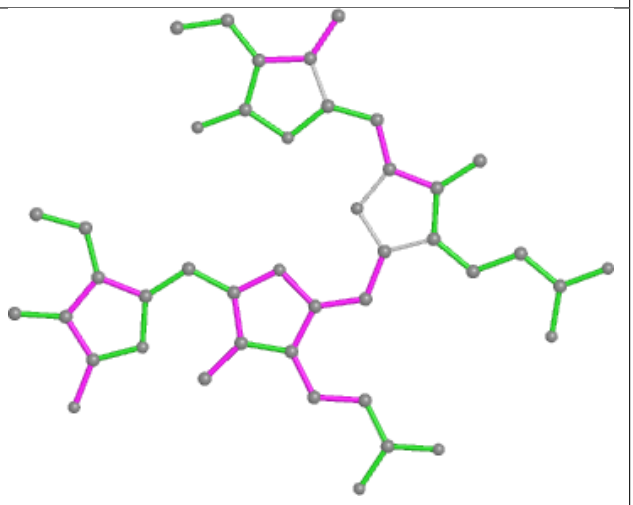

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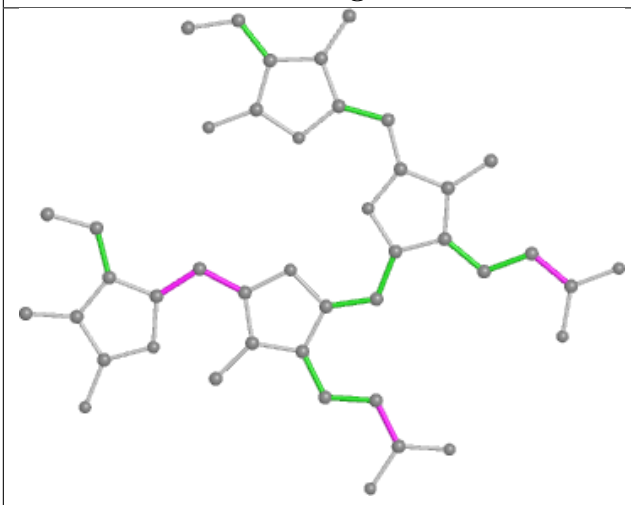

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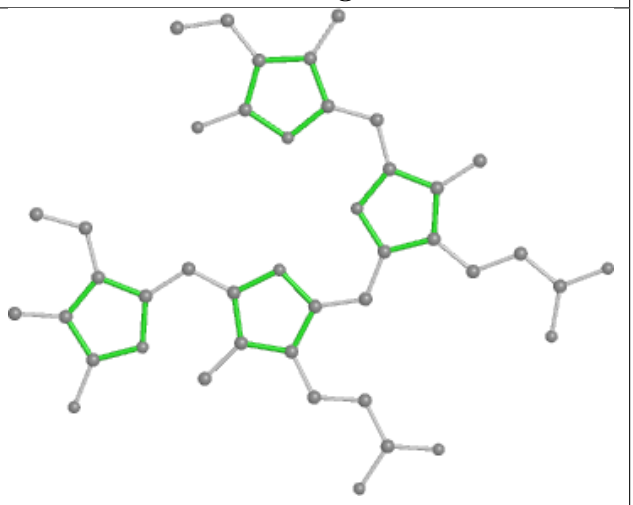
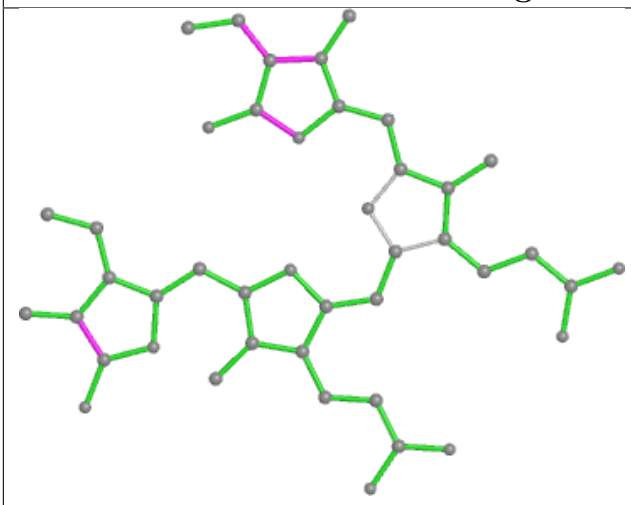


Rings

Ligand PEB H8 201



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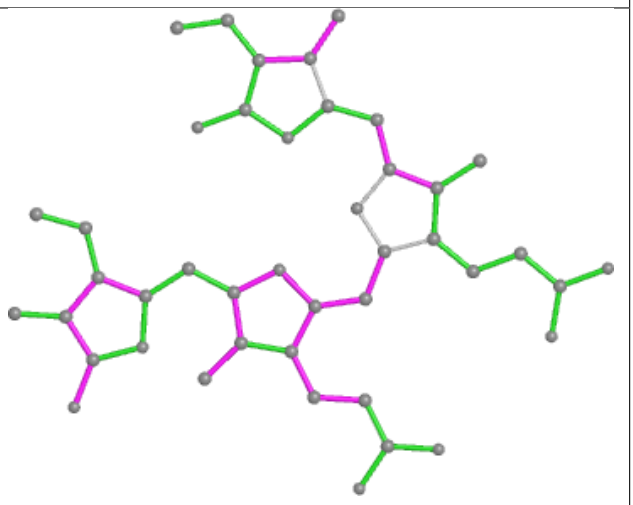

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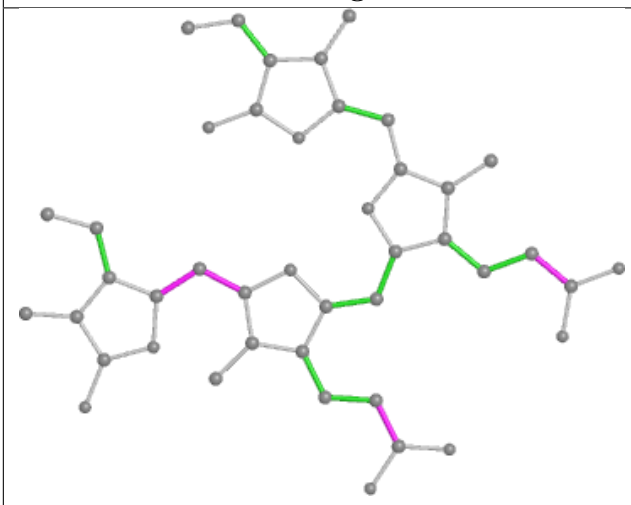

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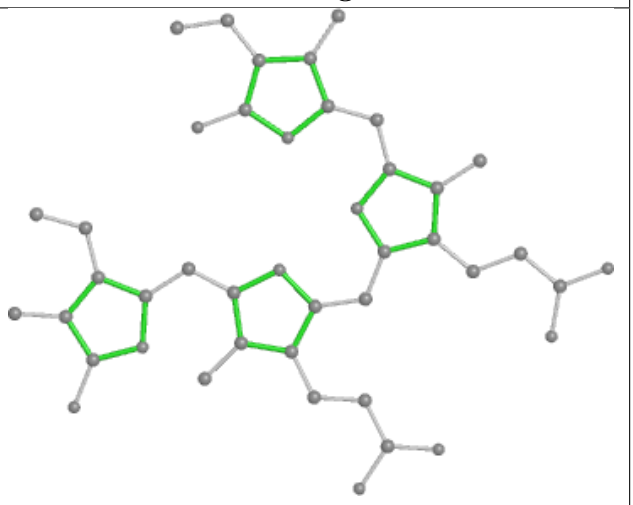
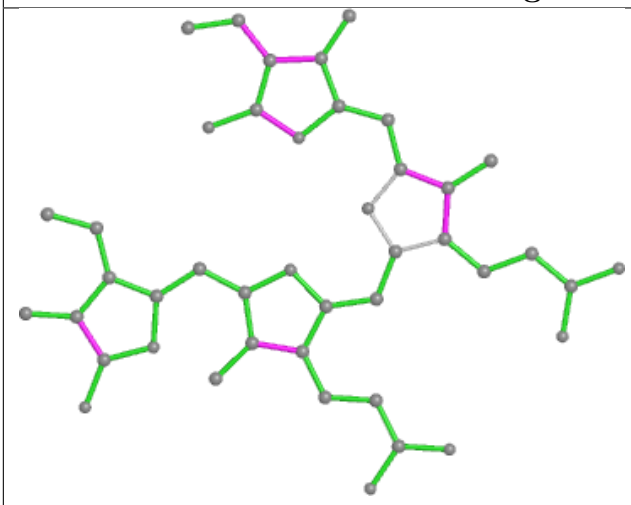


Rings

Ligand PEB l2 202



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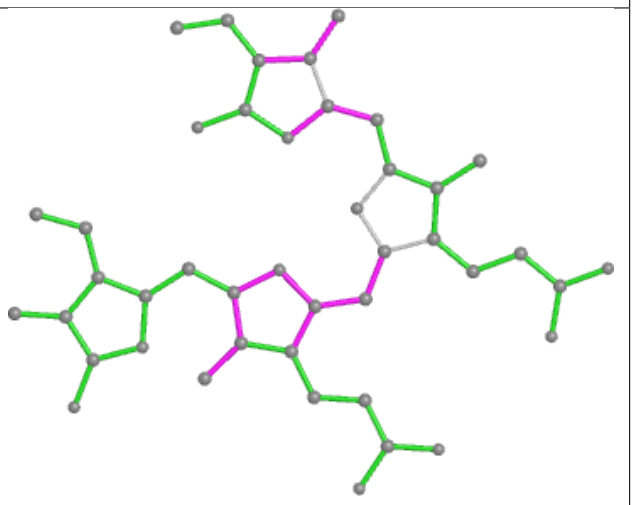

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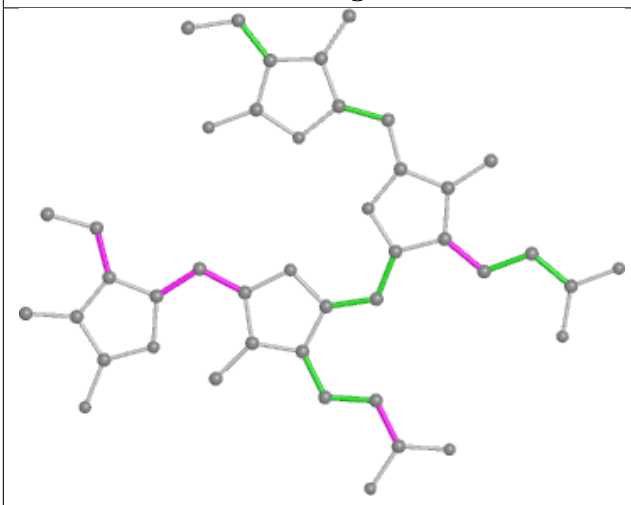

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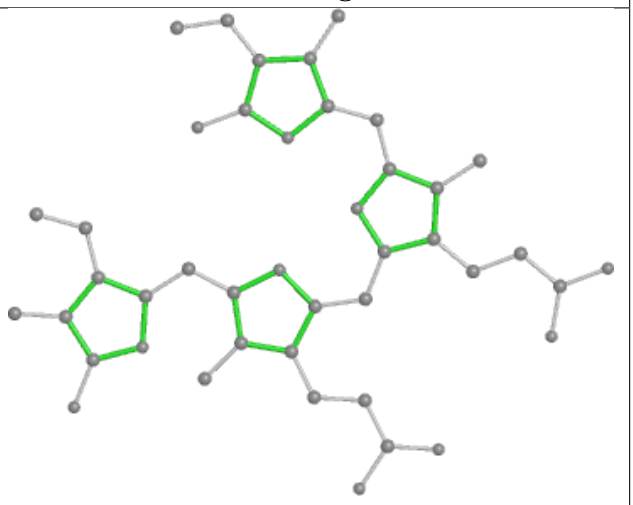
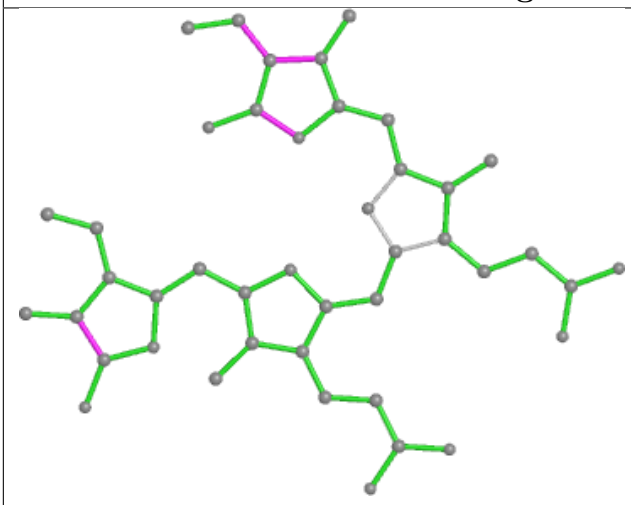


Rings

Ligand PEB dF 202



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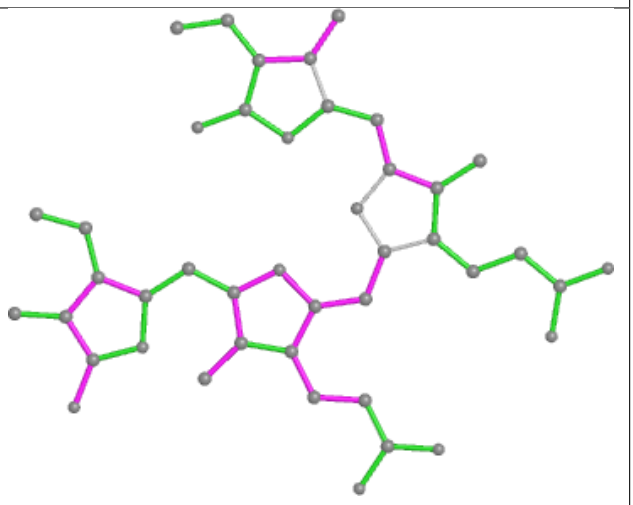

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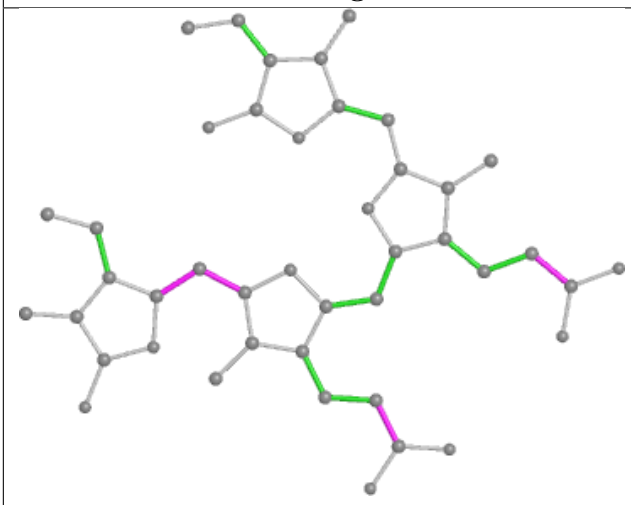

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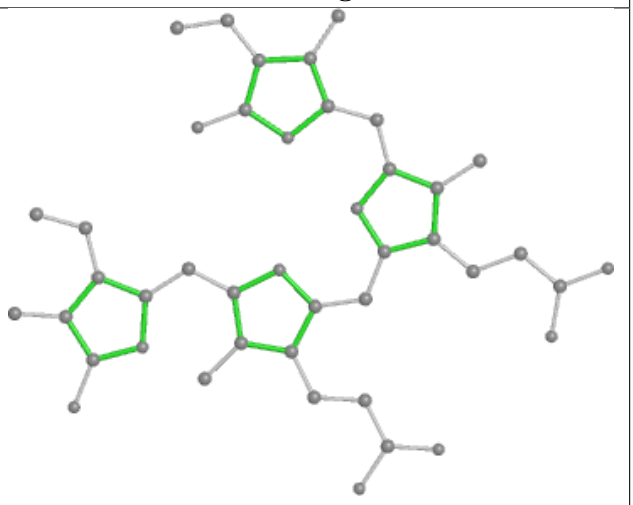
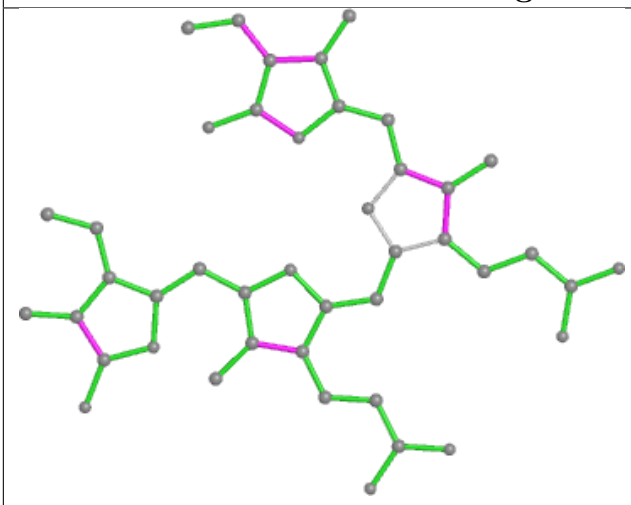


Rings

Ligand PEB X6 202



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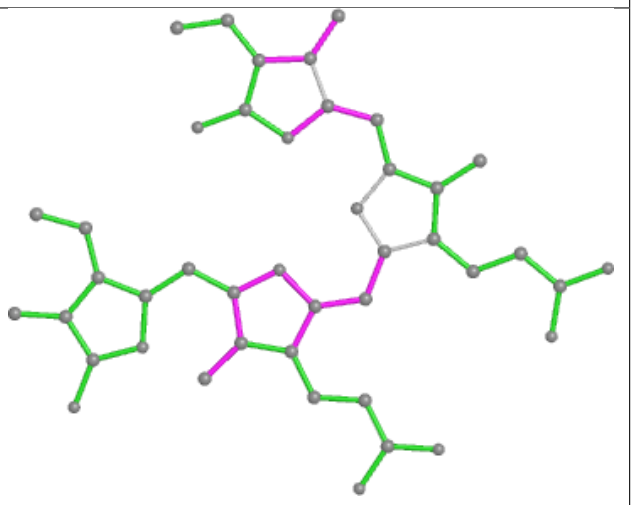
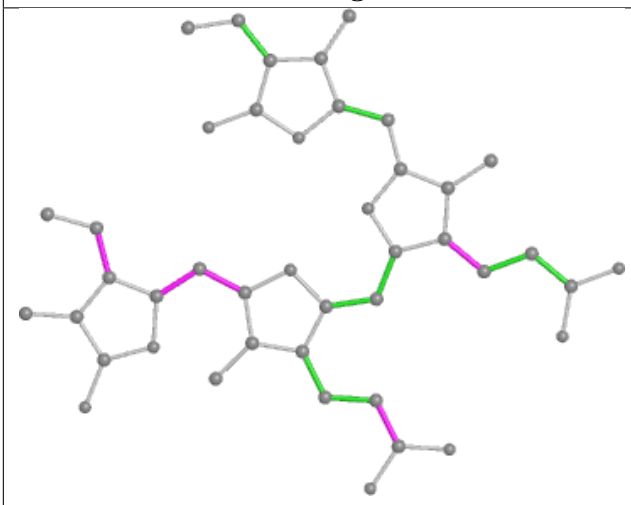


Bond angles



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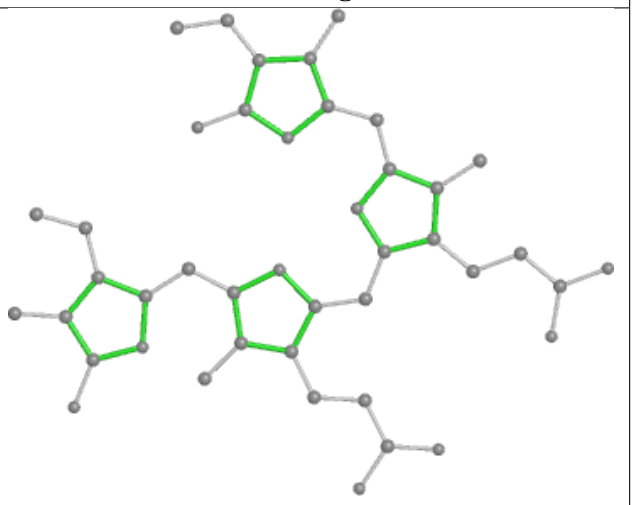
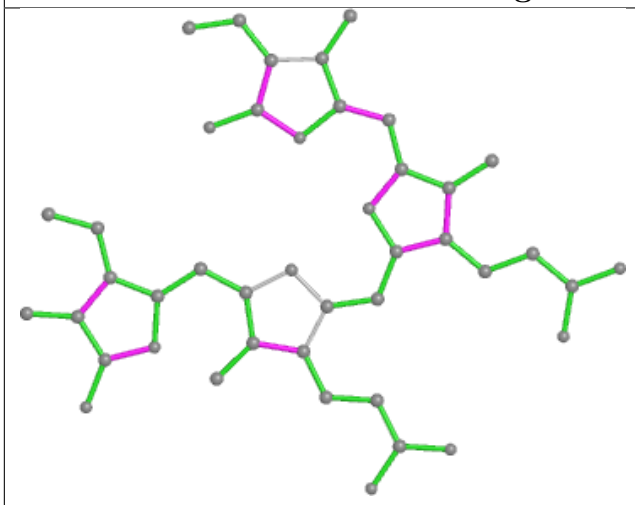


Rings

Ligand PUB V6 203



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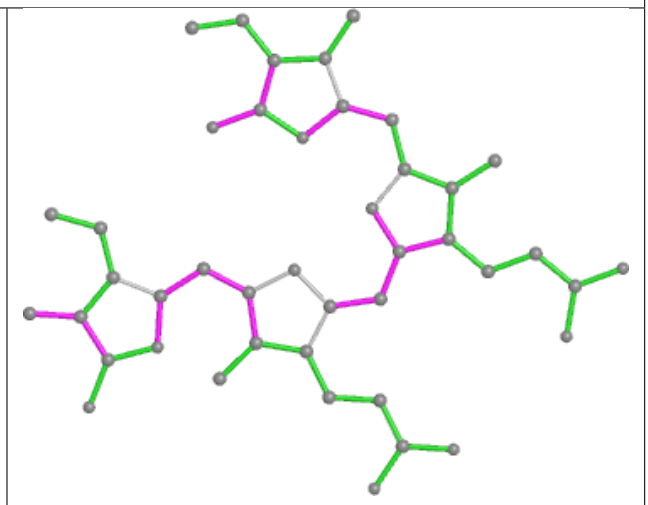
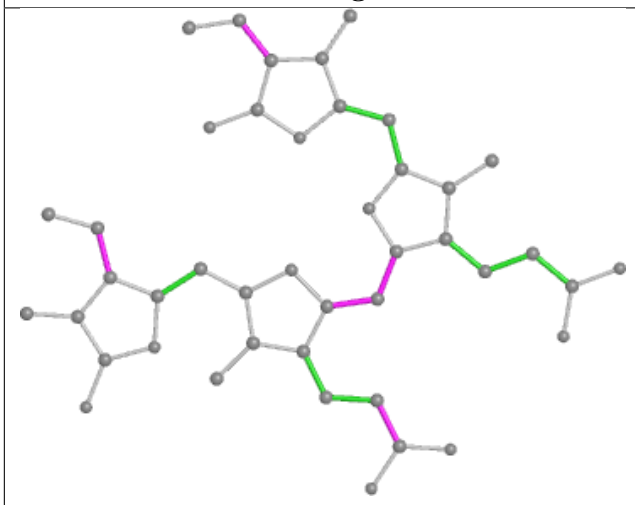
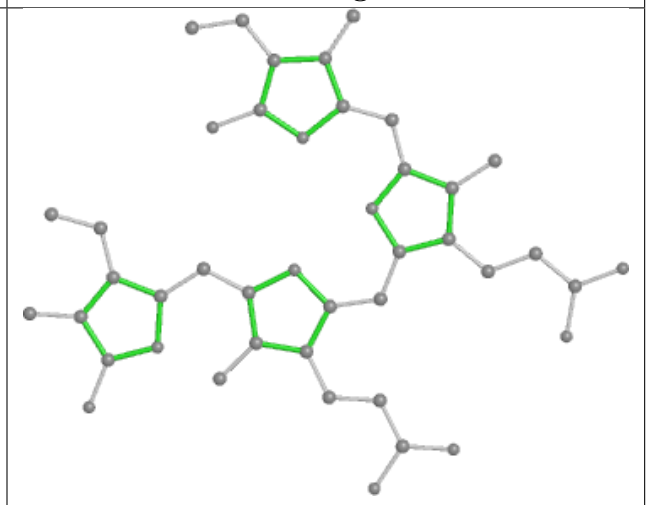


Bond angles

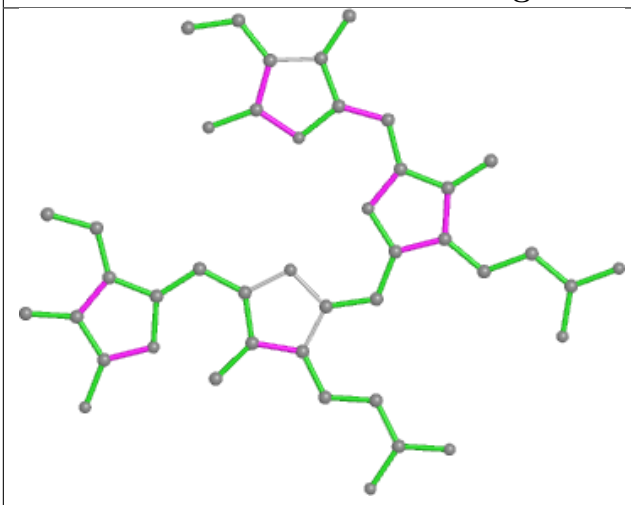


Torsions



Rings

Ligand PUB aH 203



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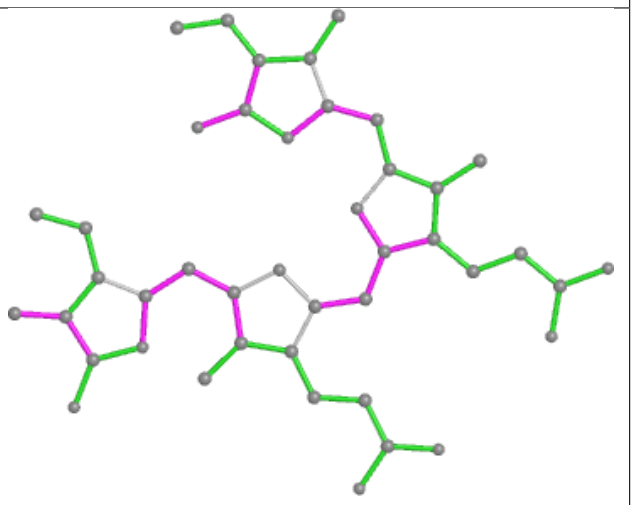

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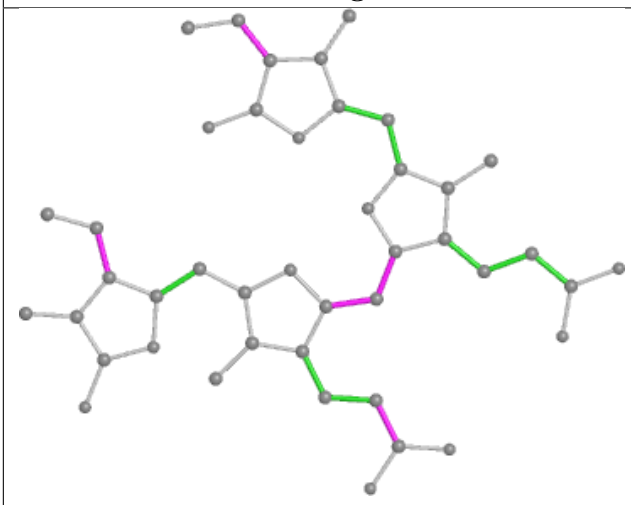

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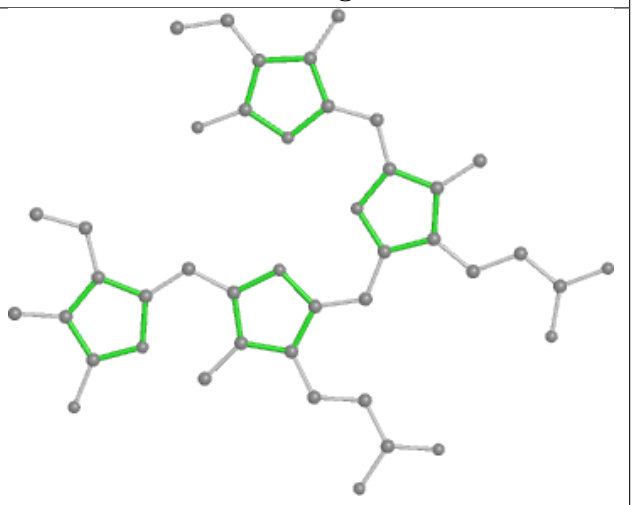
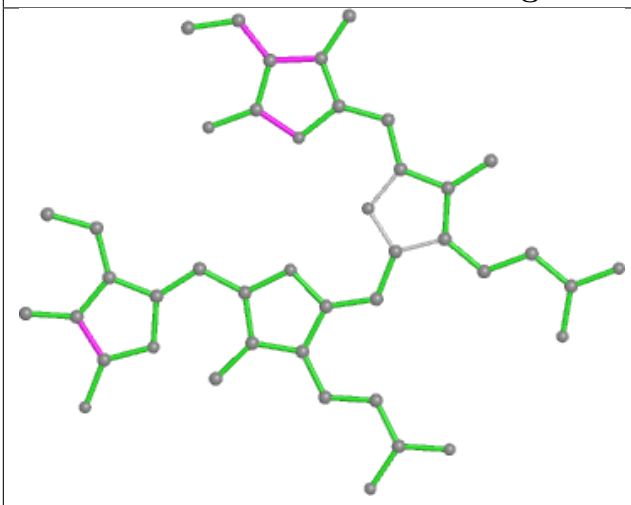


Rings

Ligand PEB r6 202



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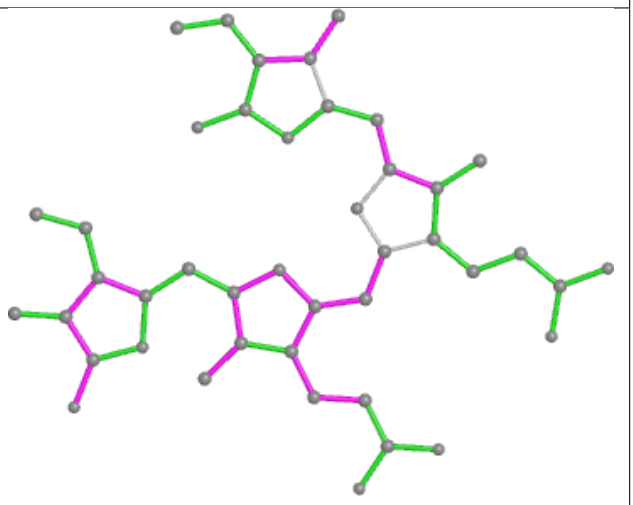

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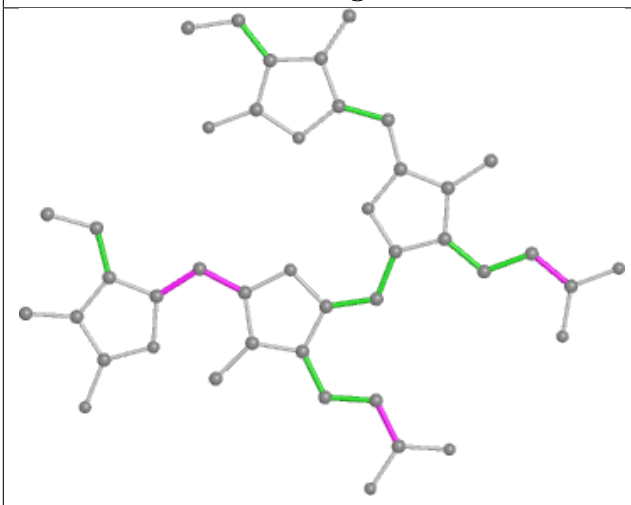

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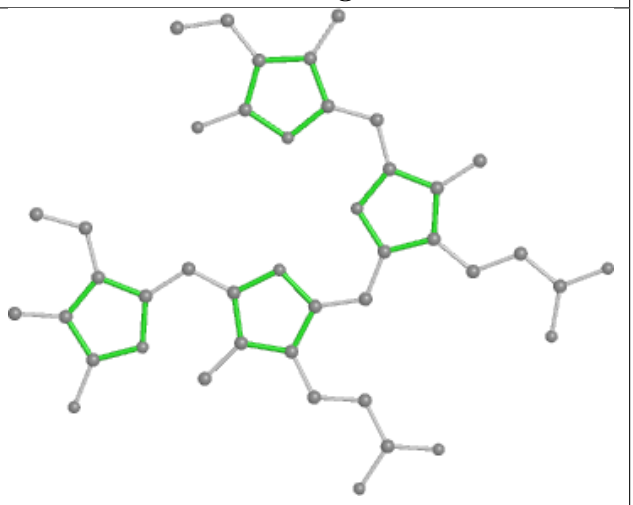

Rings

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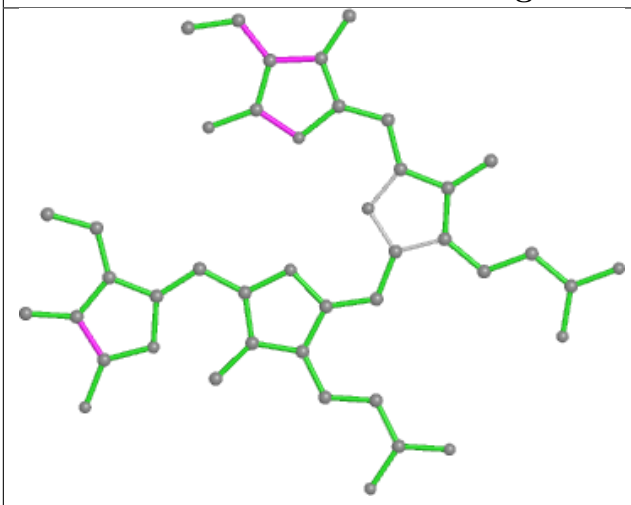

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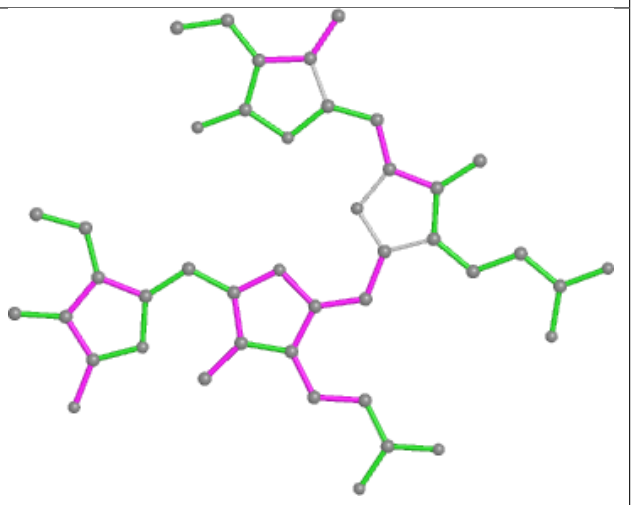

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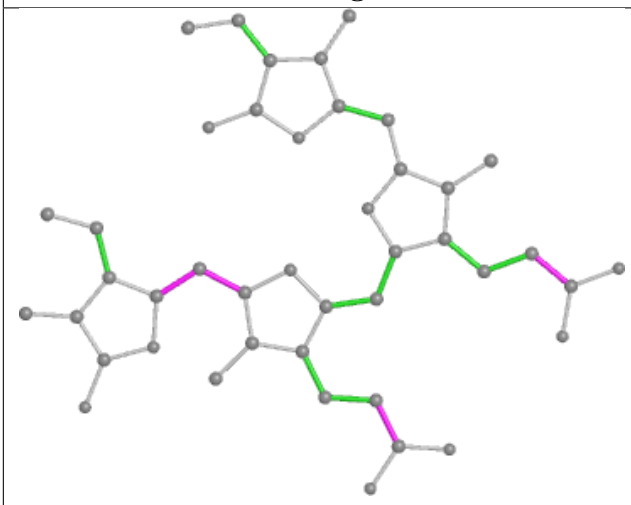

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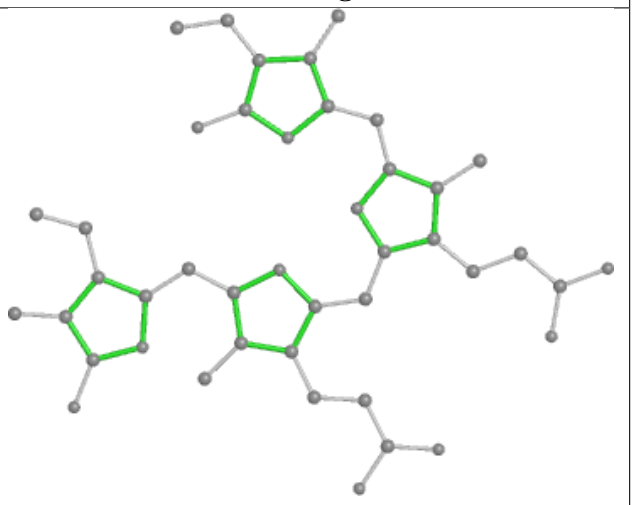

Rings

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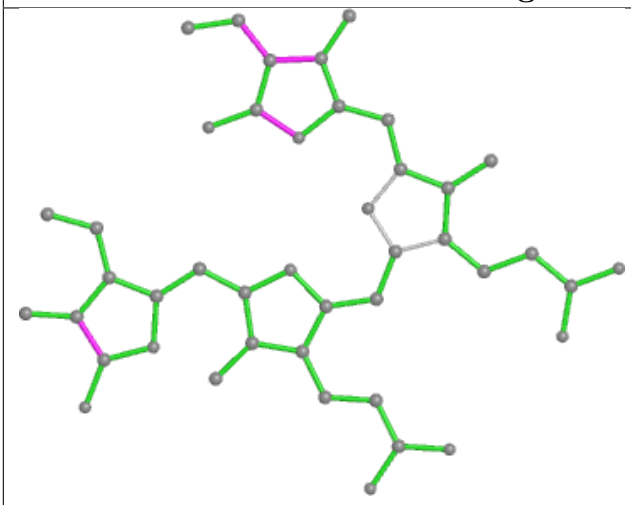

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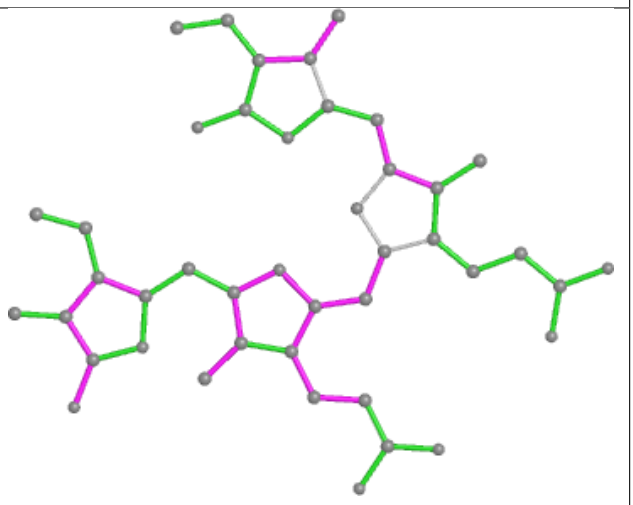

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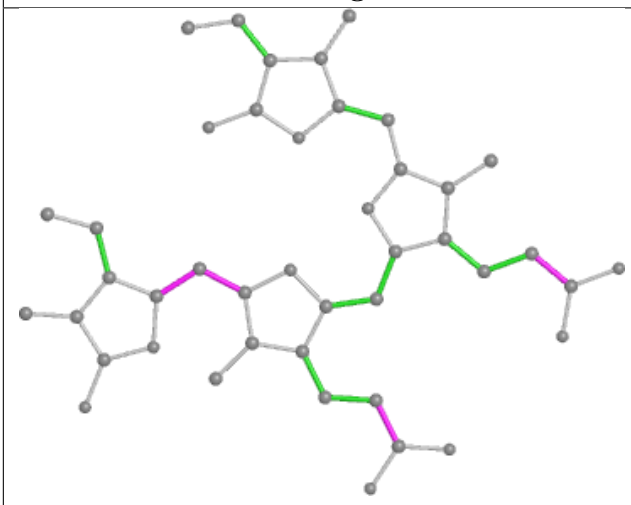

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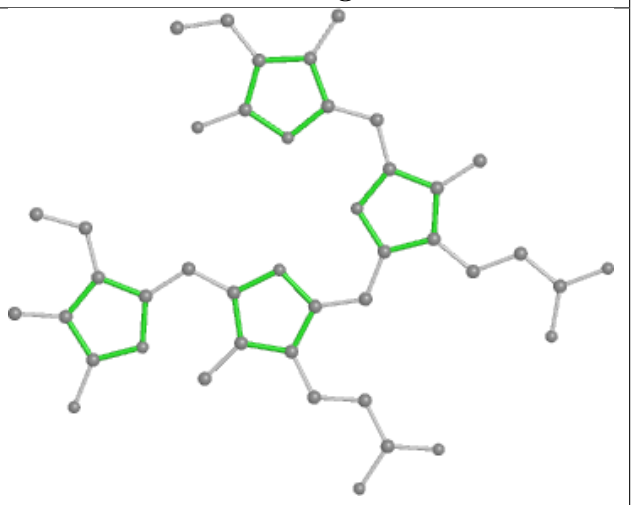

Rings

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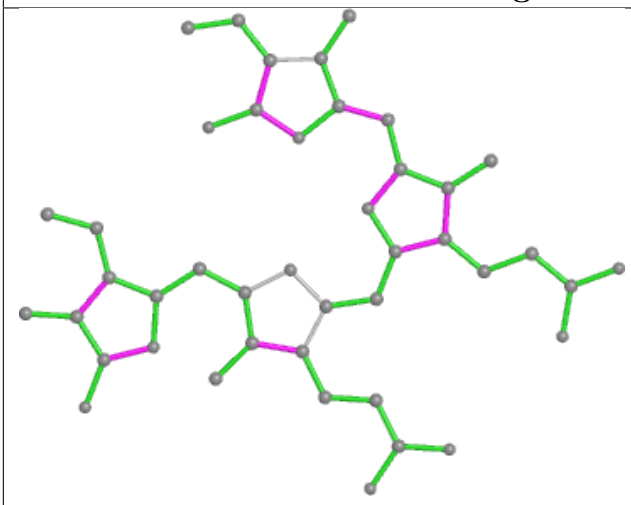

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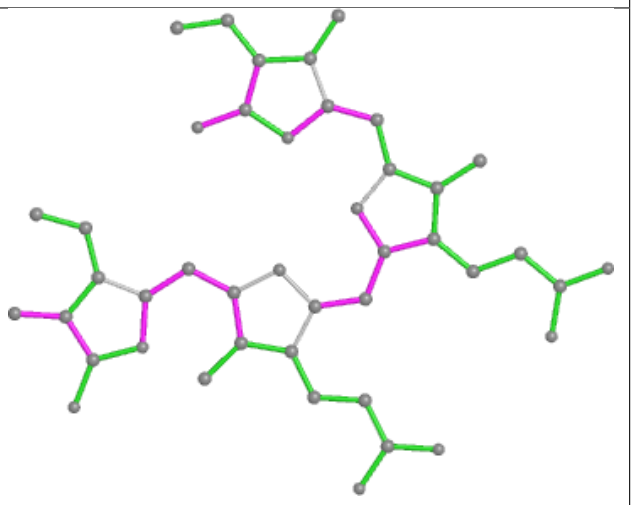

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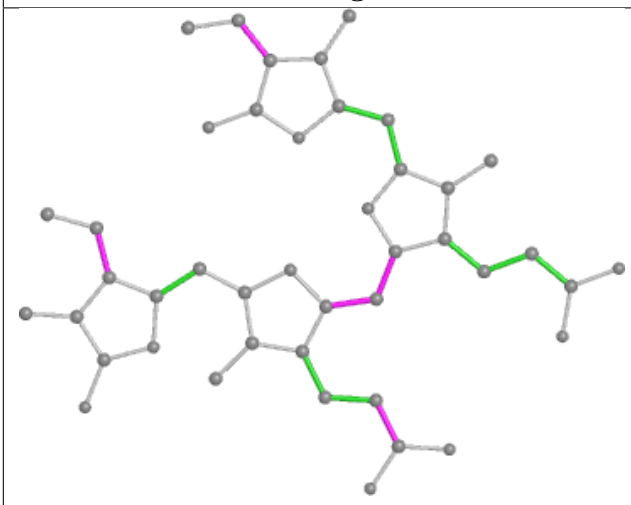

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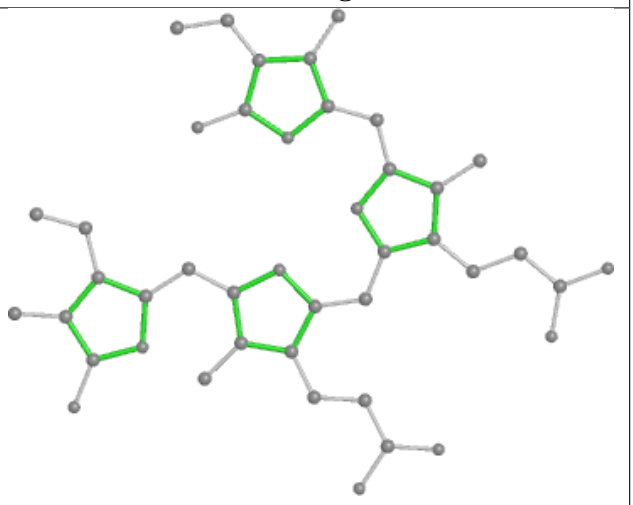

Rings

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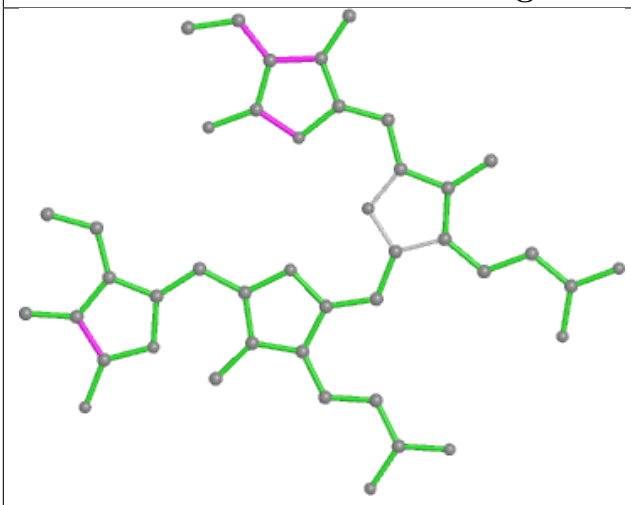

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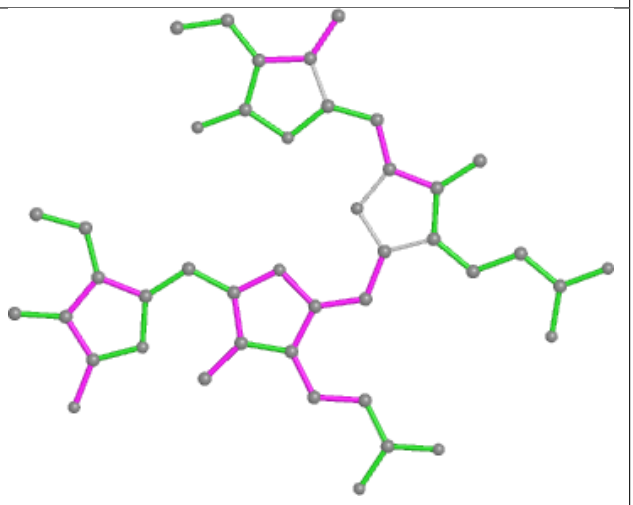

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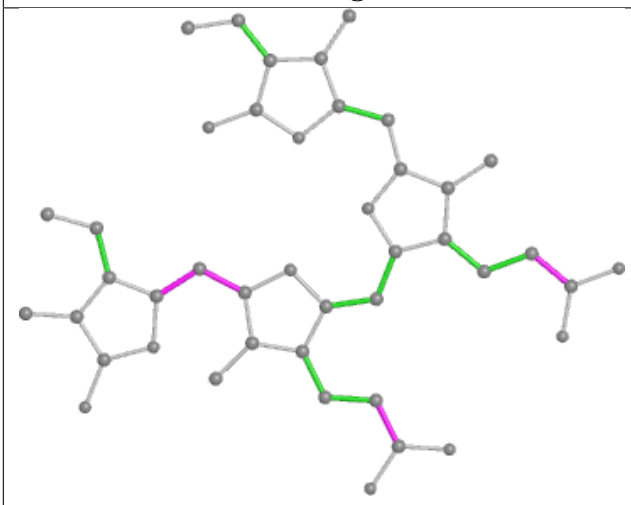

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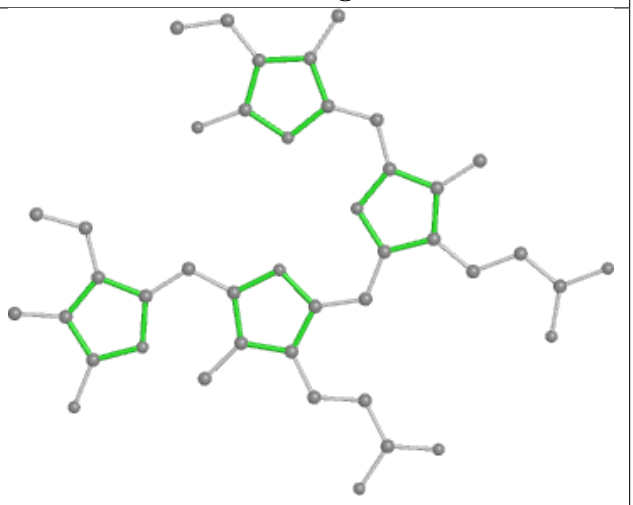

Rings

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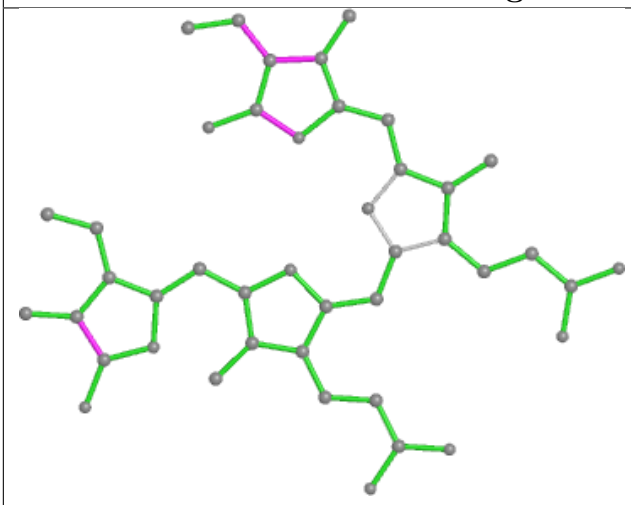

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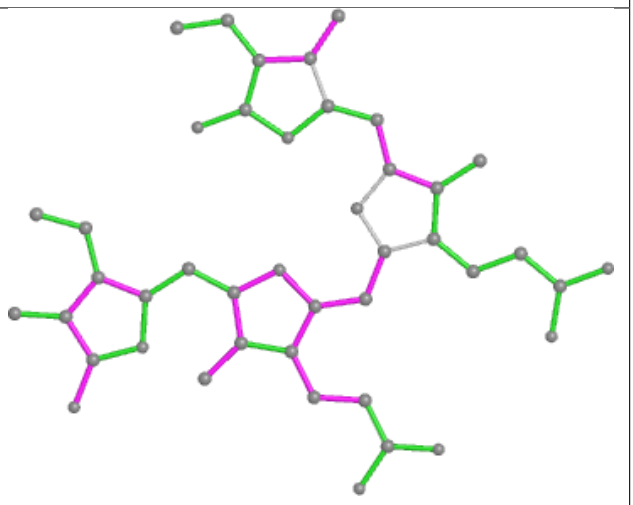

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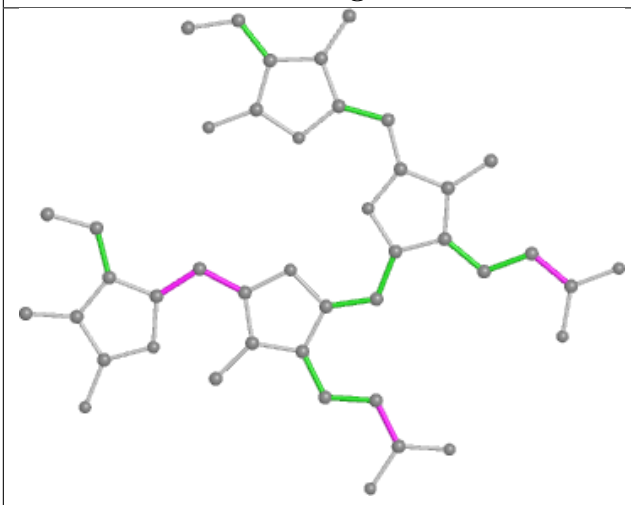

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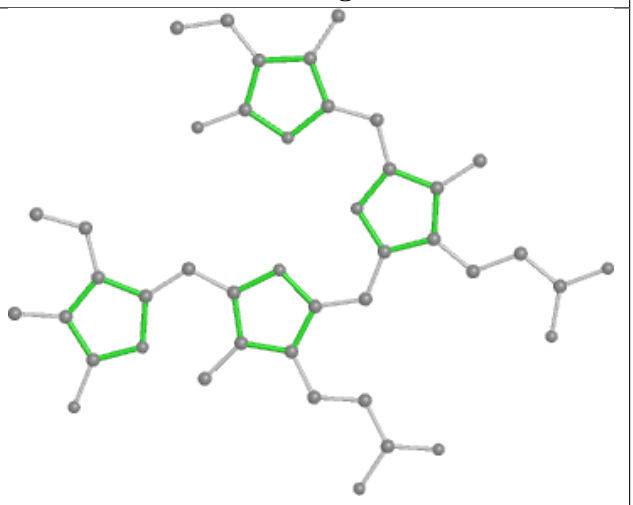
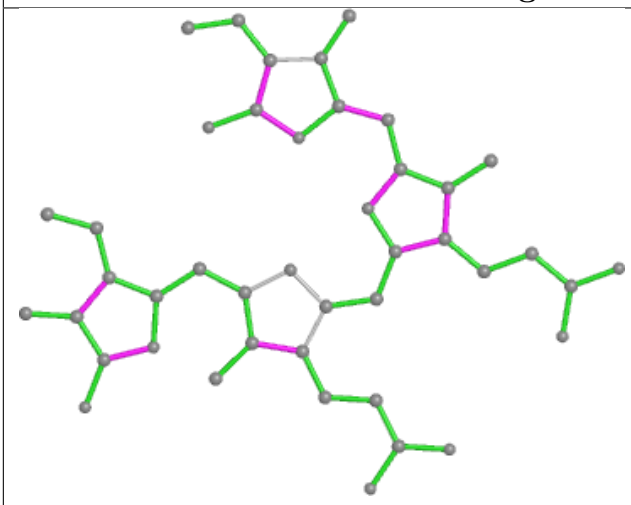


Rings

Ligand PUB ge 203



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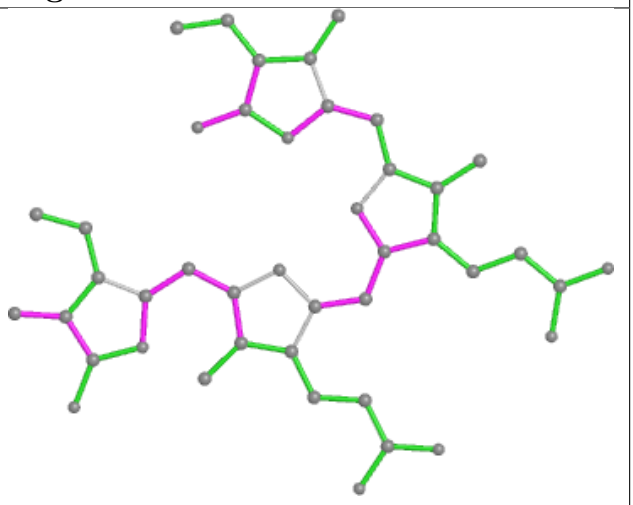

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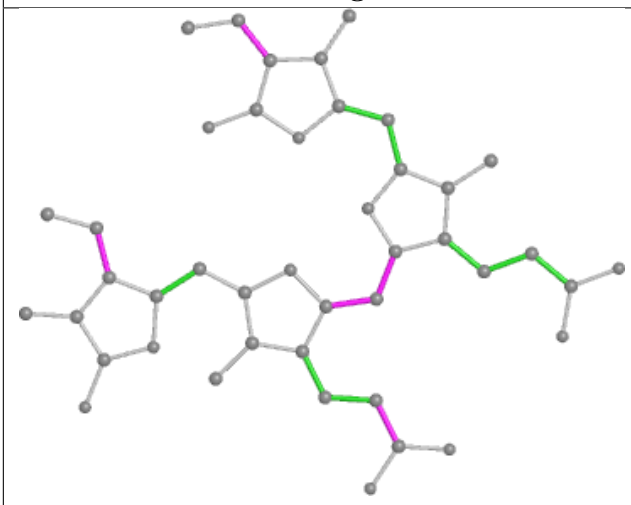

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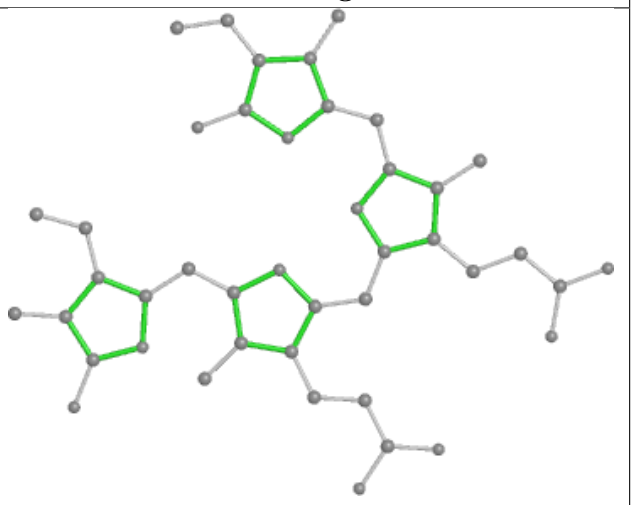
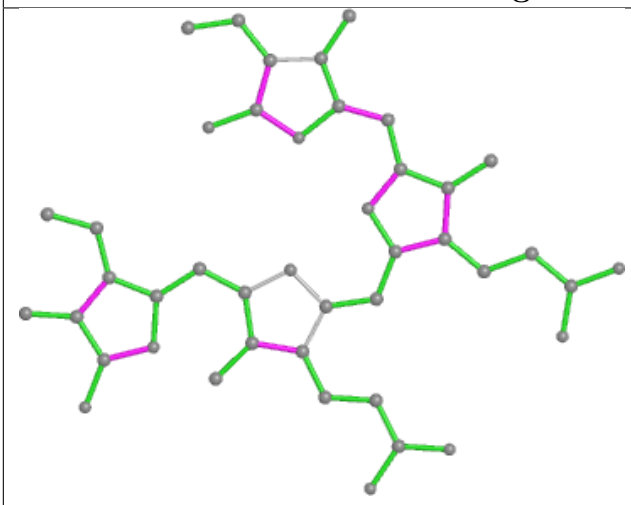


Rings

Ligand PUB dw 405



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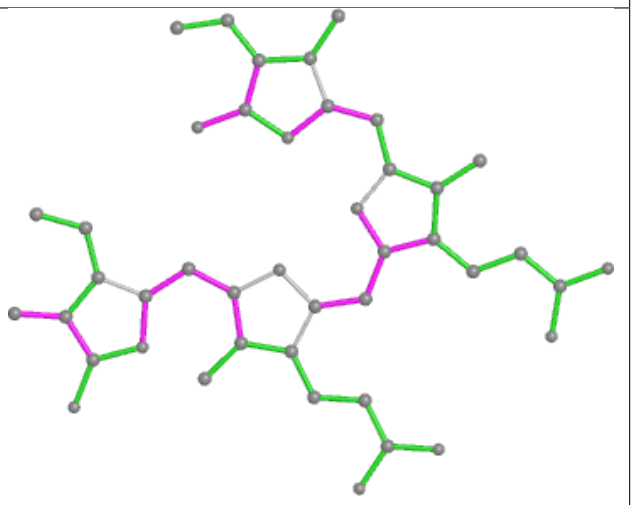

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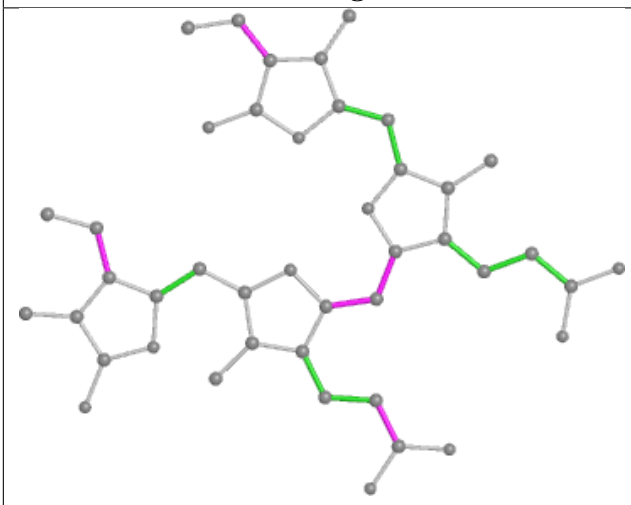

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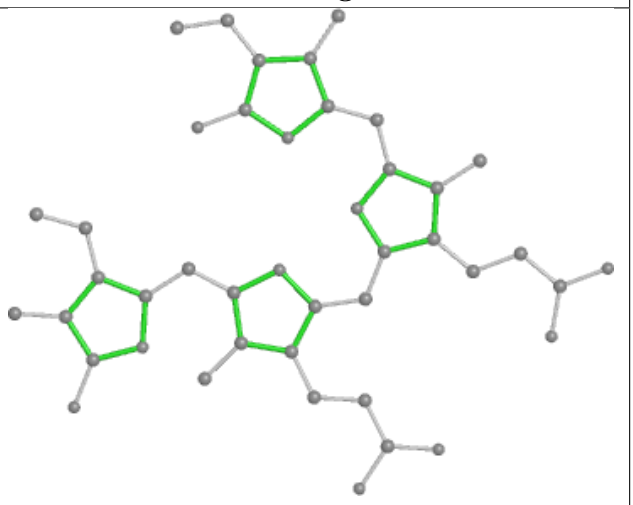

Rings

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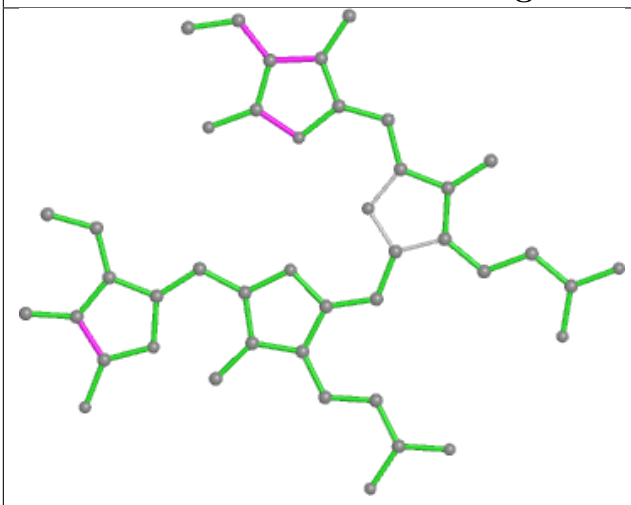

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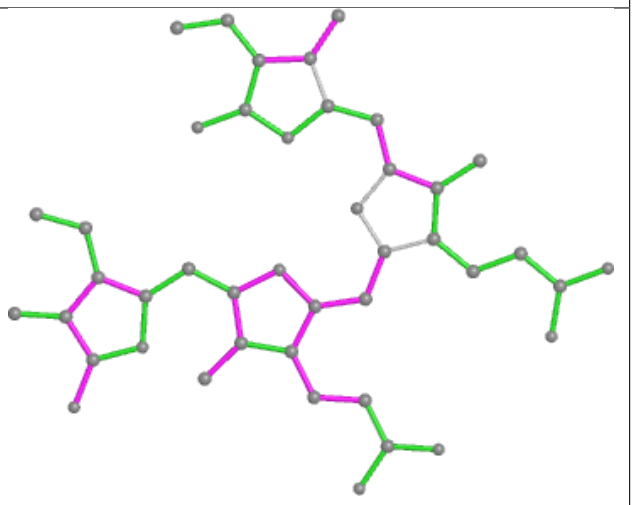

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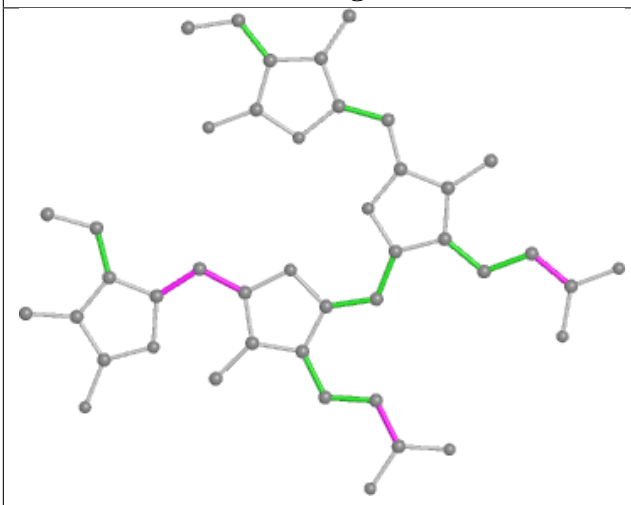

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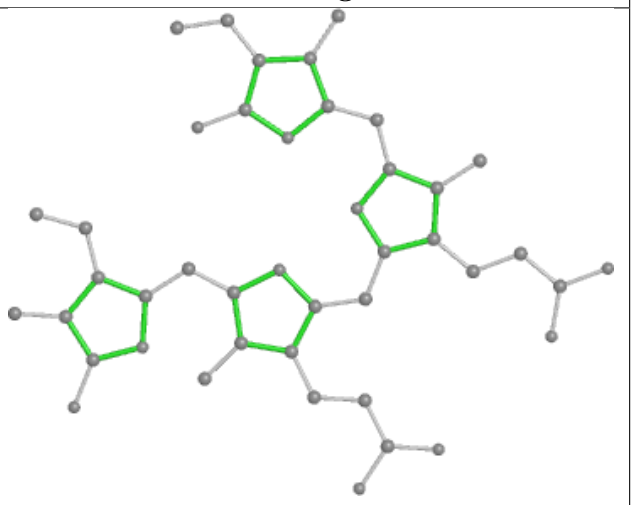
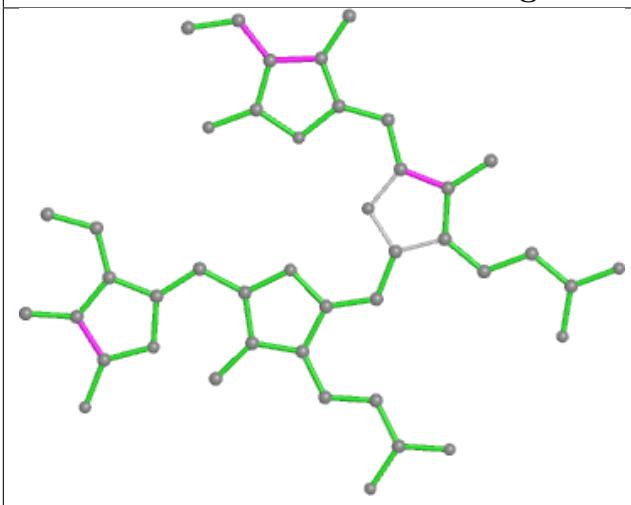


Rings

Ligand PEB go 202



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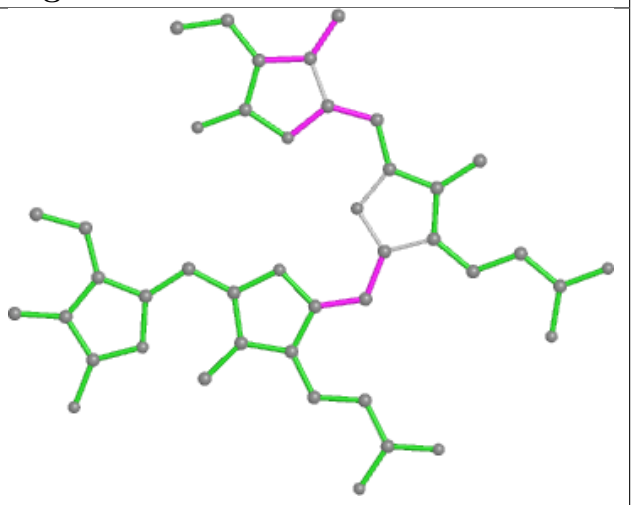

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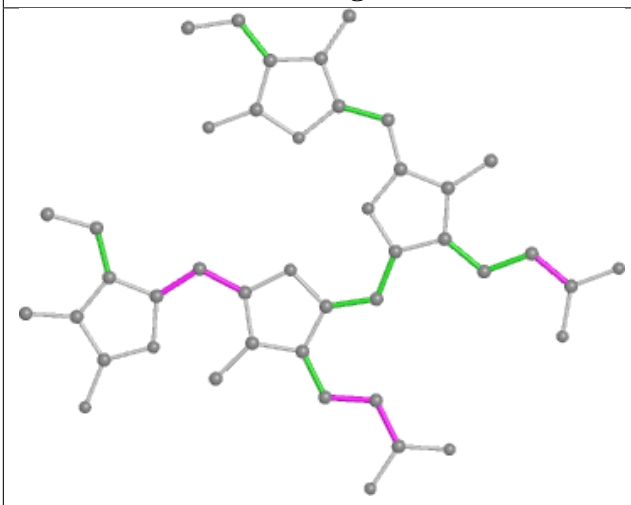

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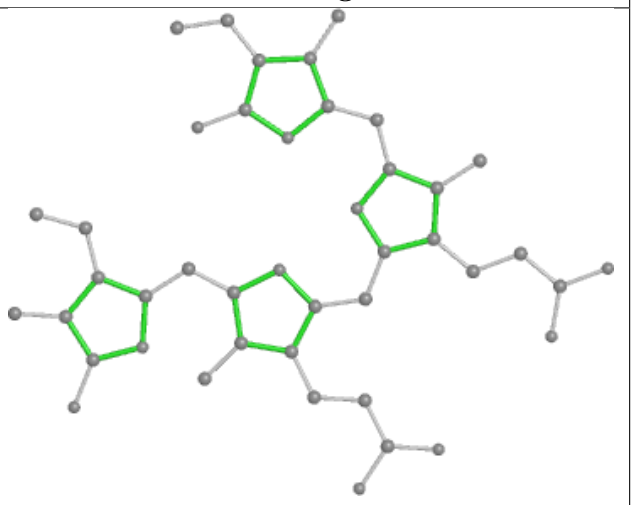

Rings

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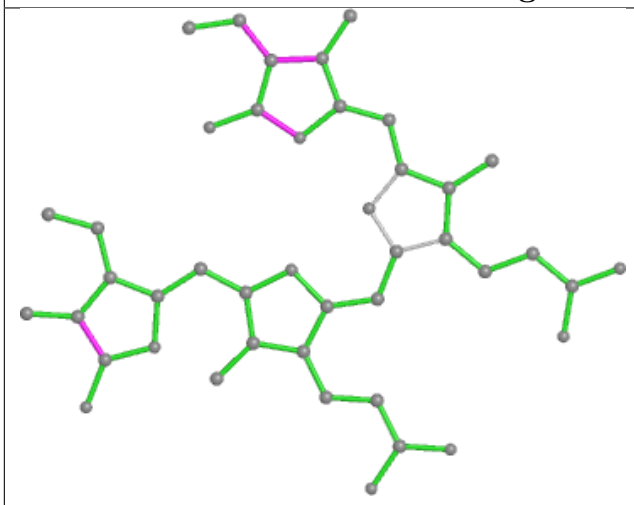

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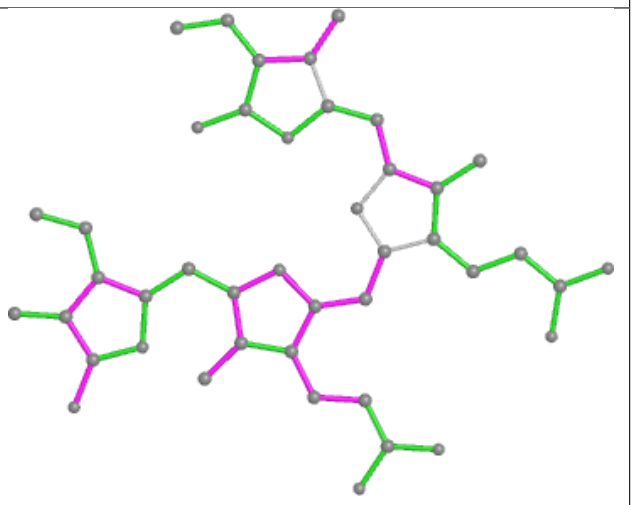

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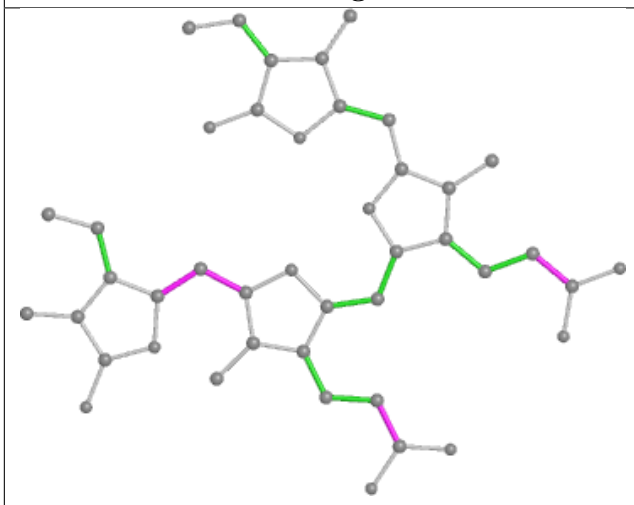

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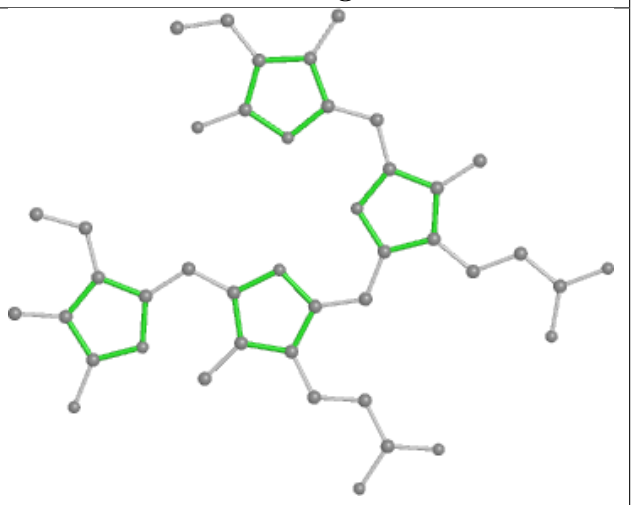
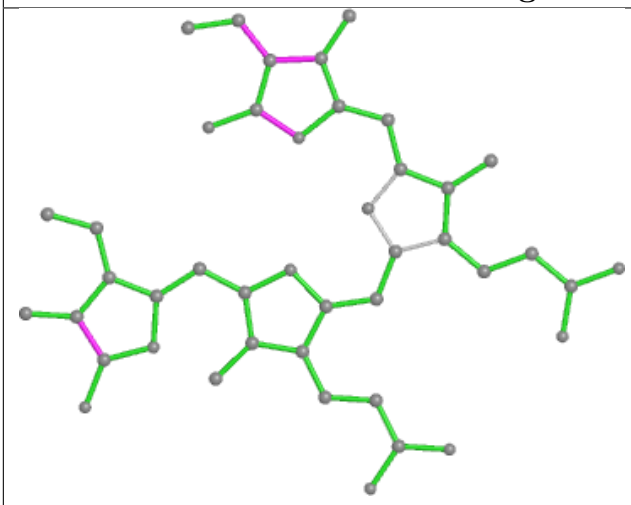


Rings

Ligand PEB S2 201



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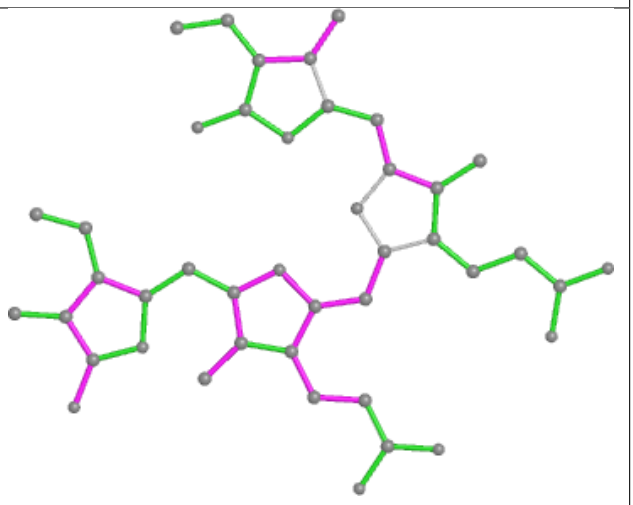
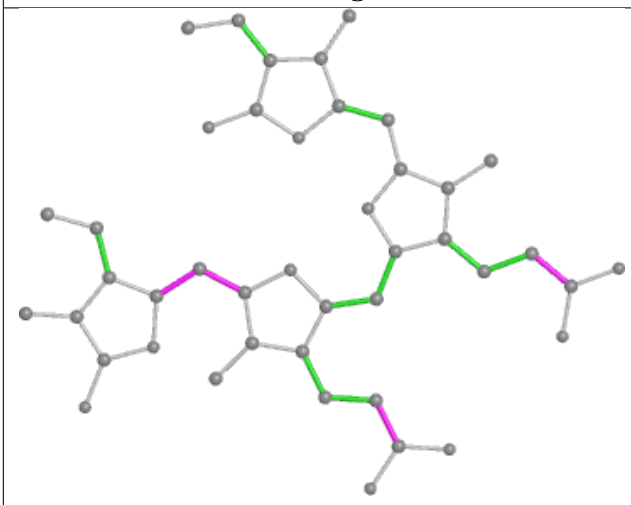
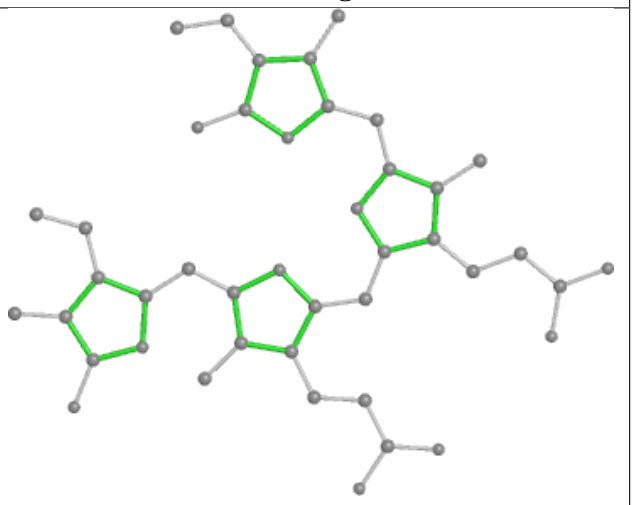


Bond angles

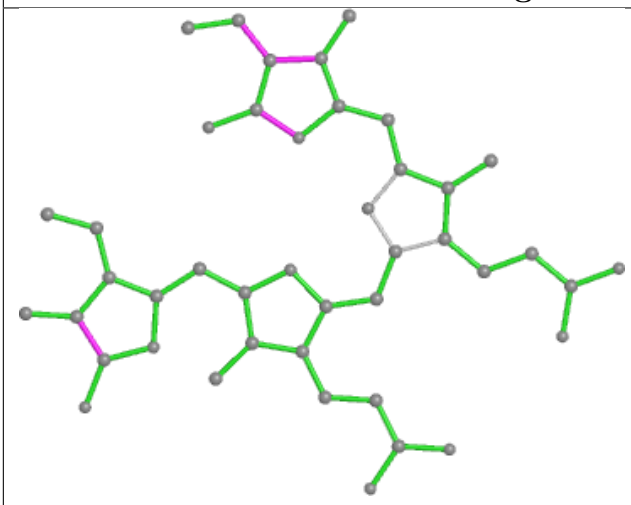


Torsions



Rings

Ligand PEB K7 201



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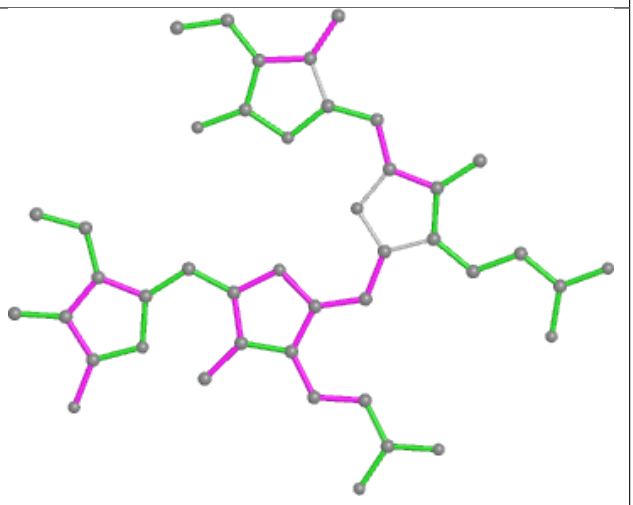
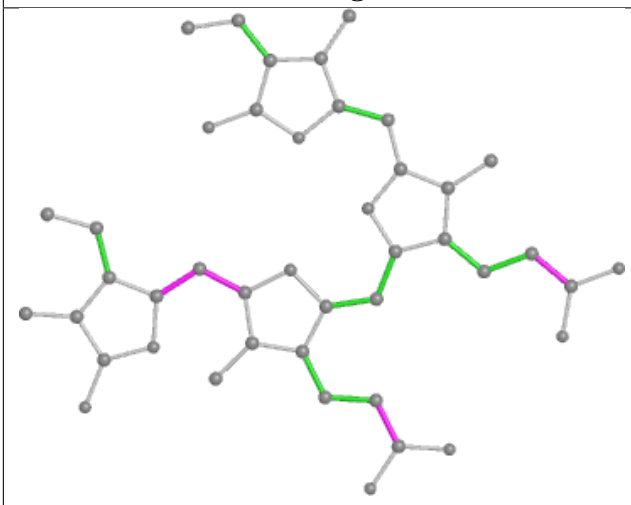


Bond angles



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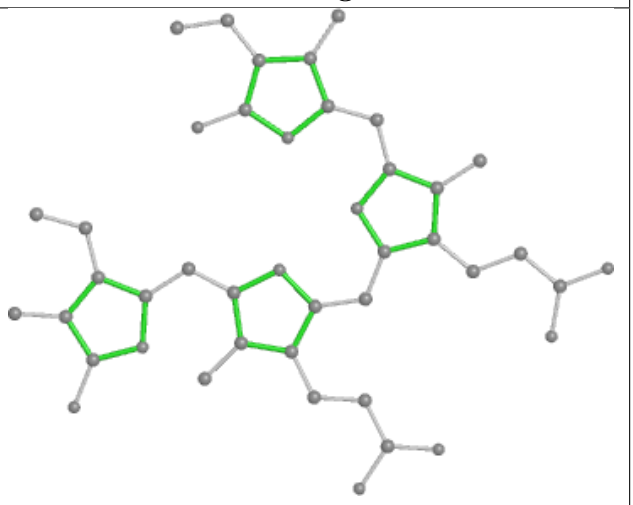
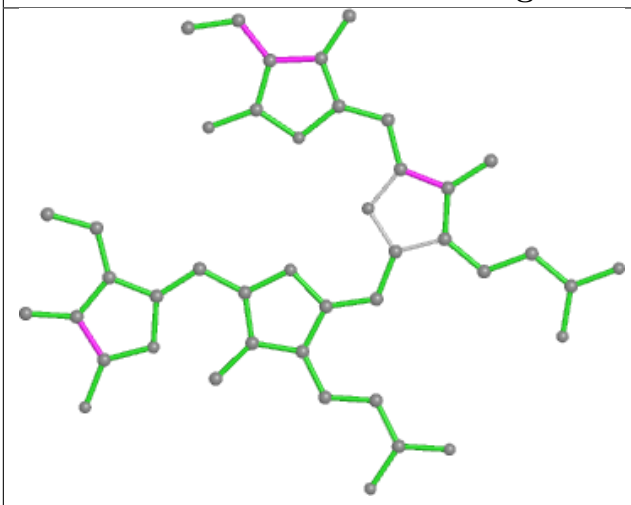


Rings

Ligand PEB P2 202



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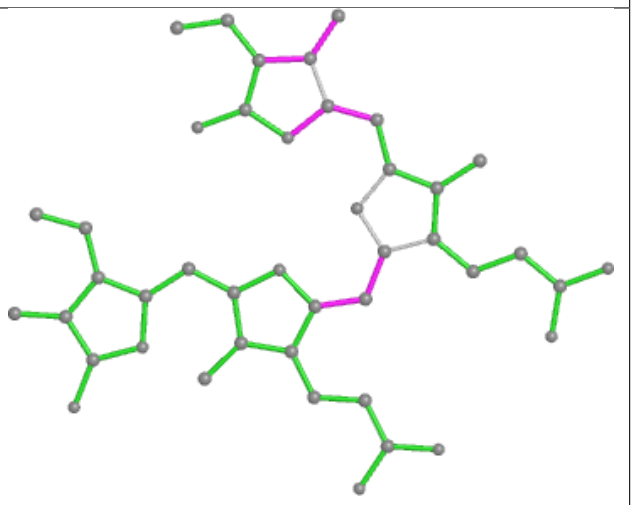

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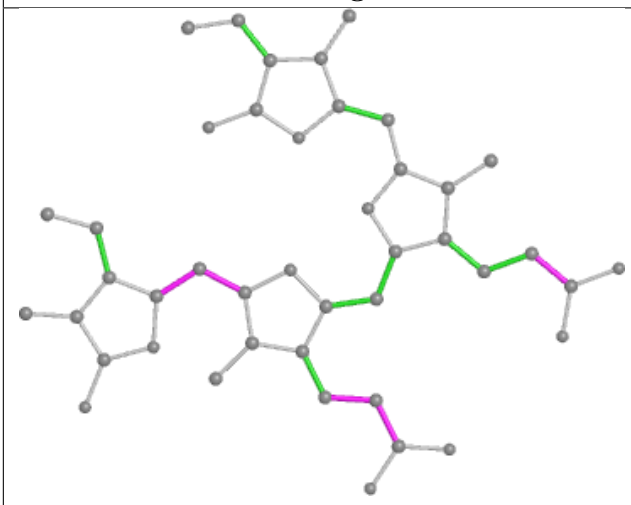

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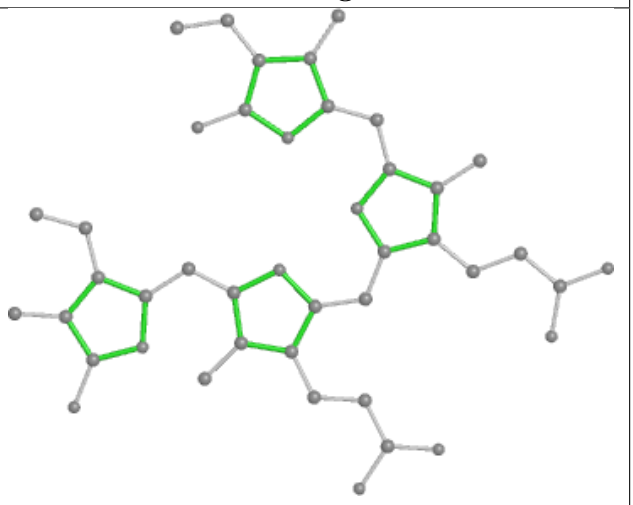
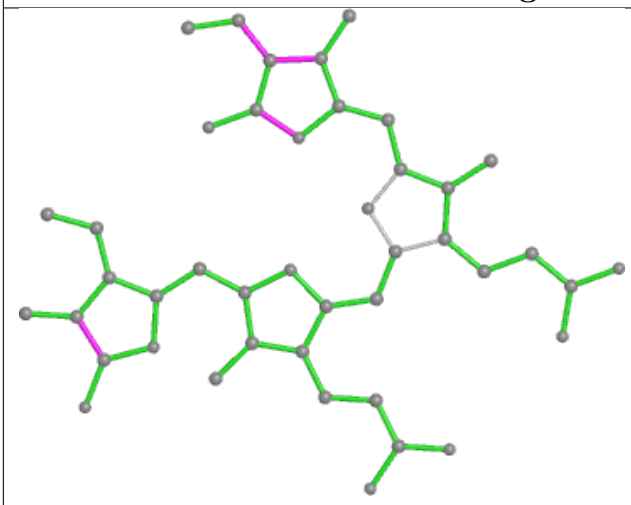


Rings

Ligand PEB y2 201



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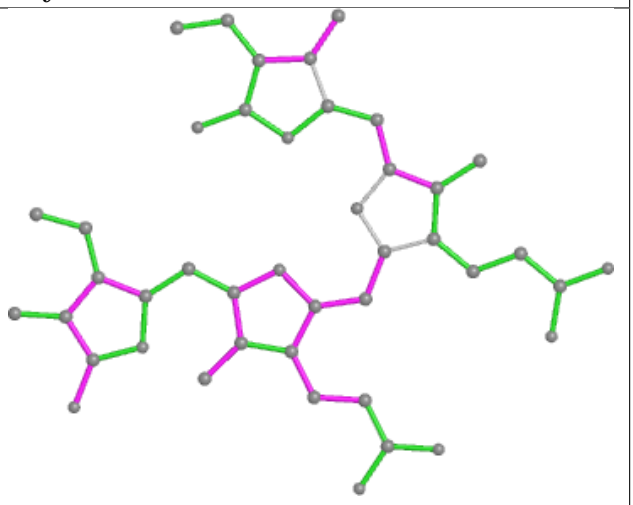

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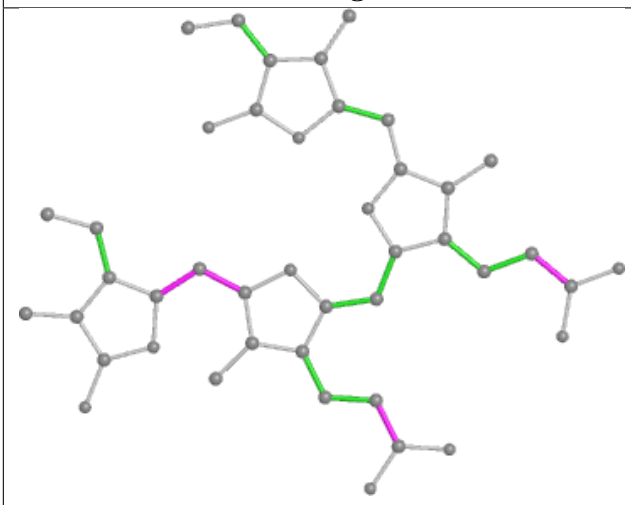

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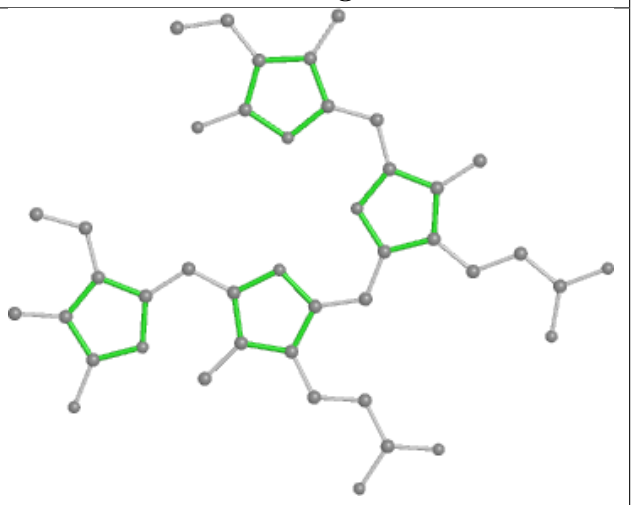
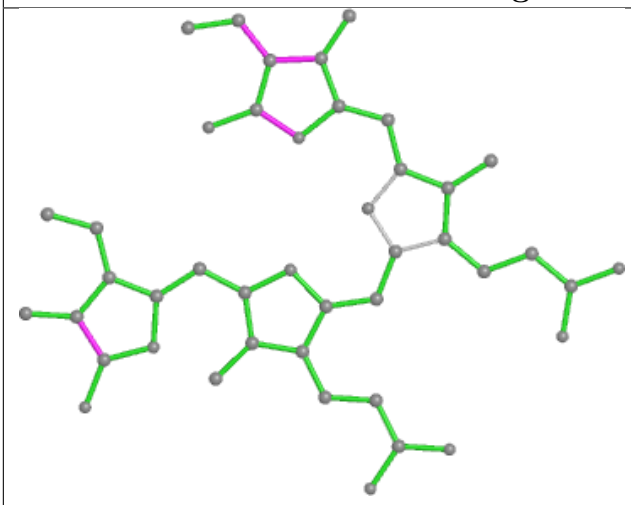


Rings

Ligand PEB dI 1001



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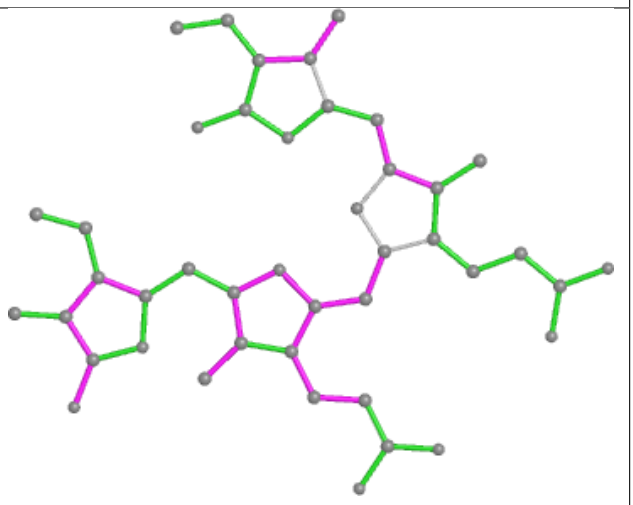

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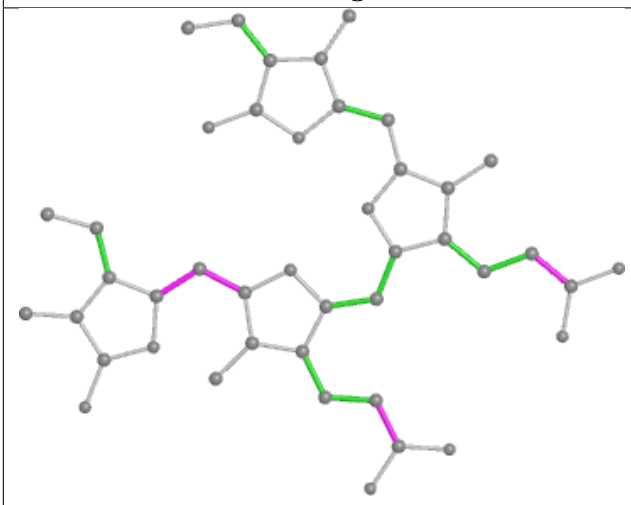

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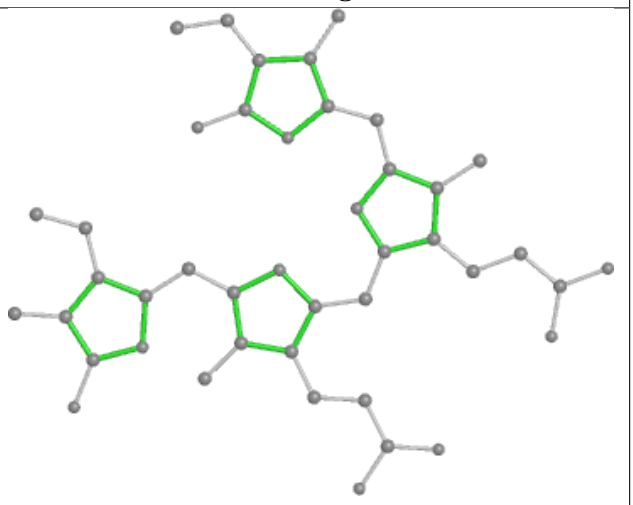
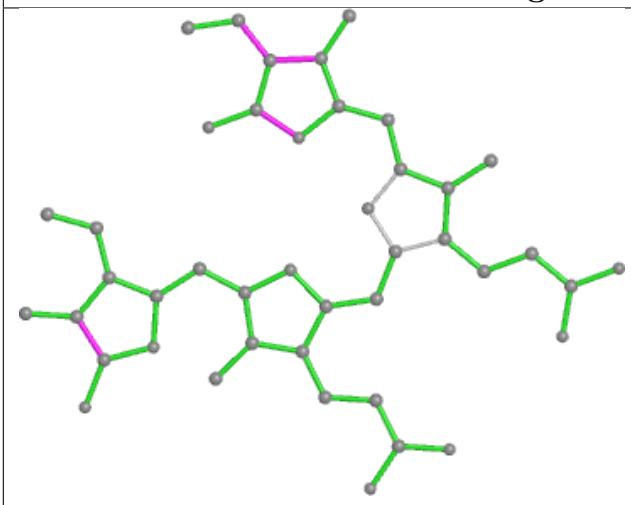


Rings

Ligand PEB fl 201



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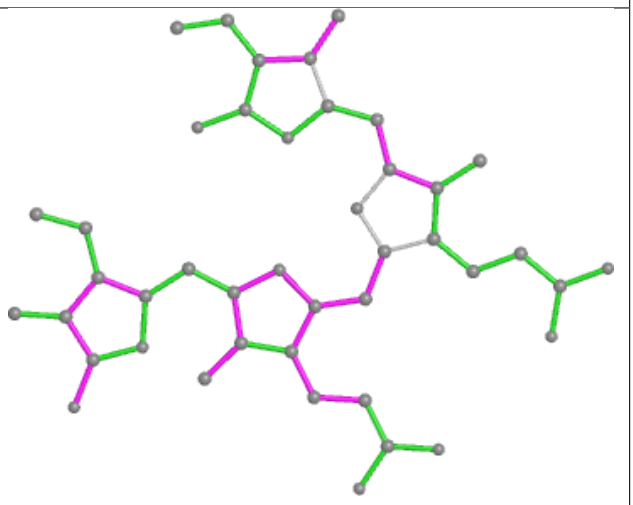

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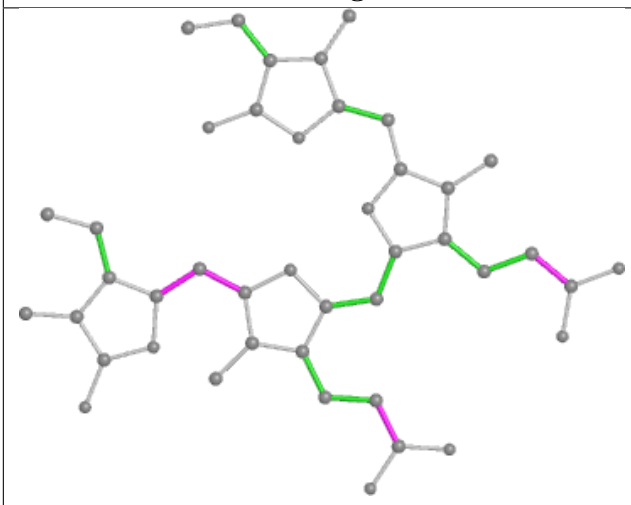

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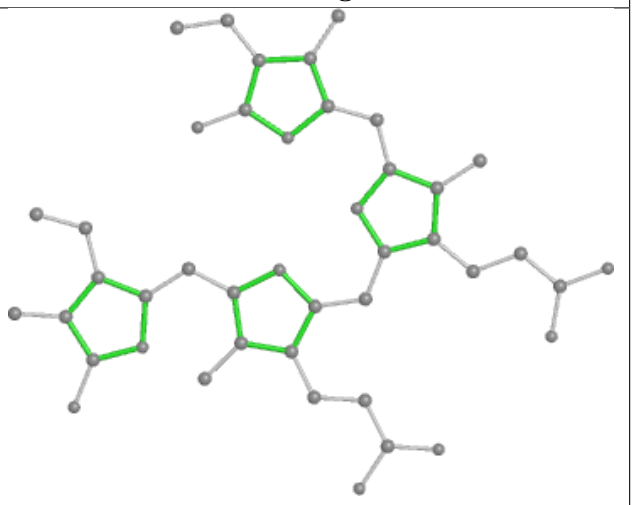
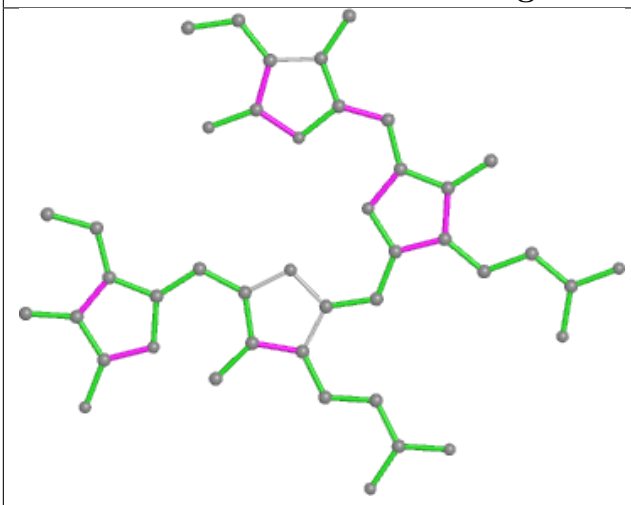


Rings

Ligand PUB x5 202



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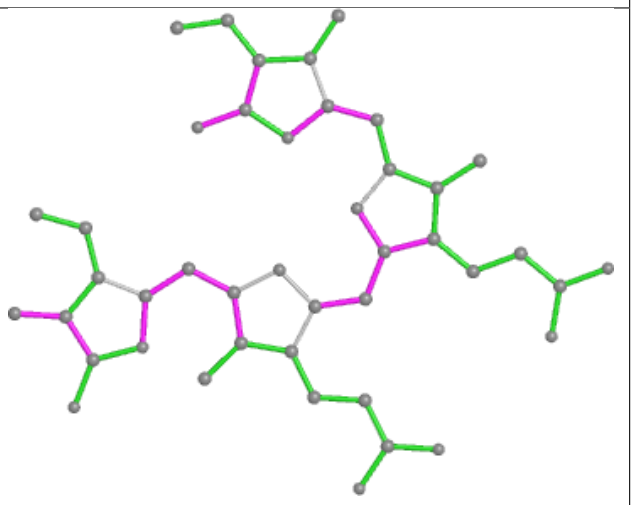

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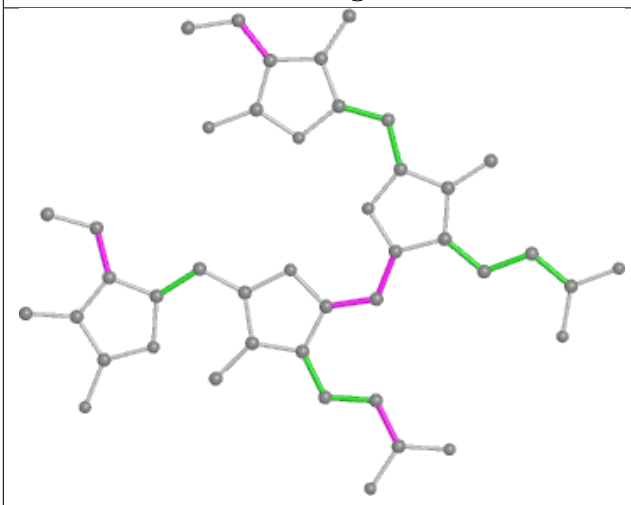

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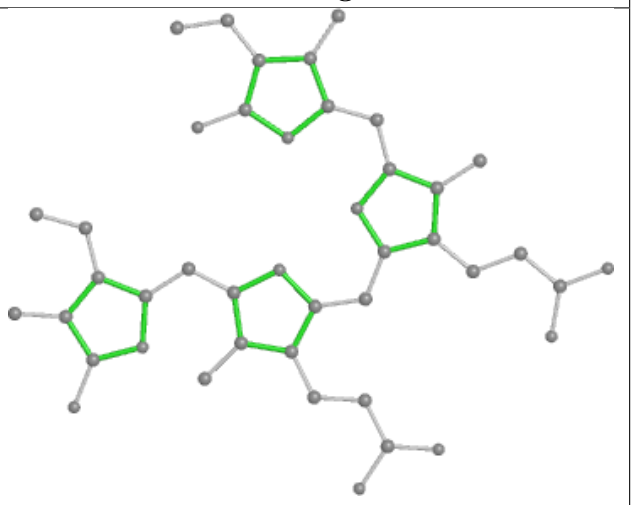

Rings

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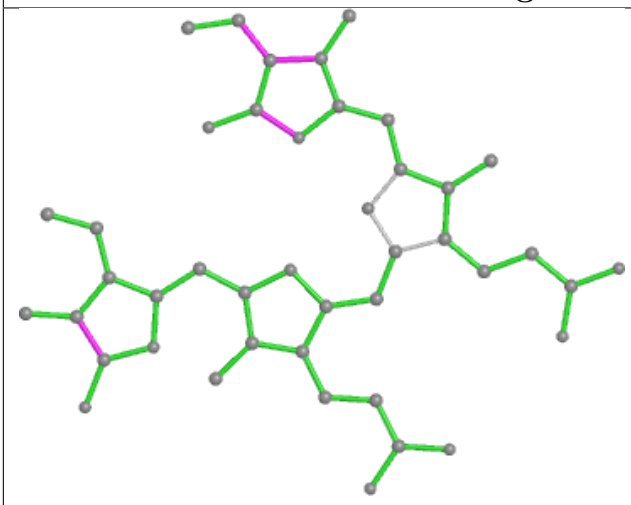

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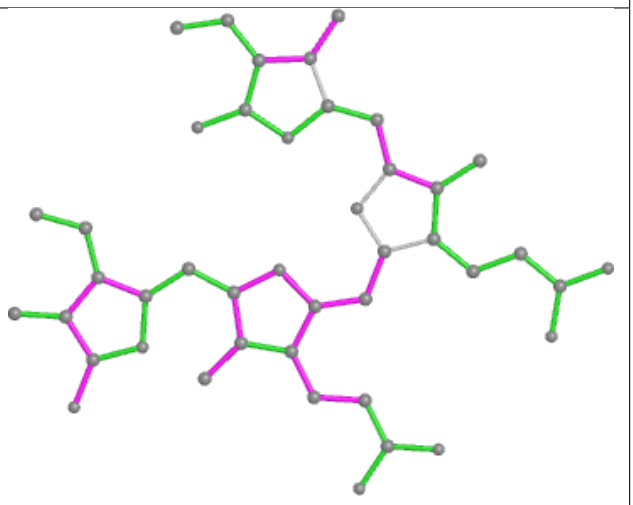

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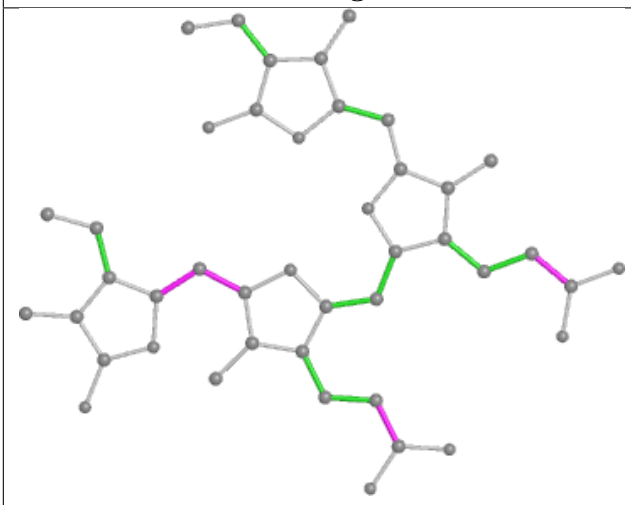

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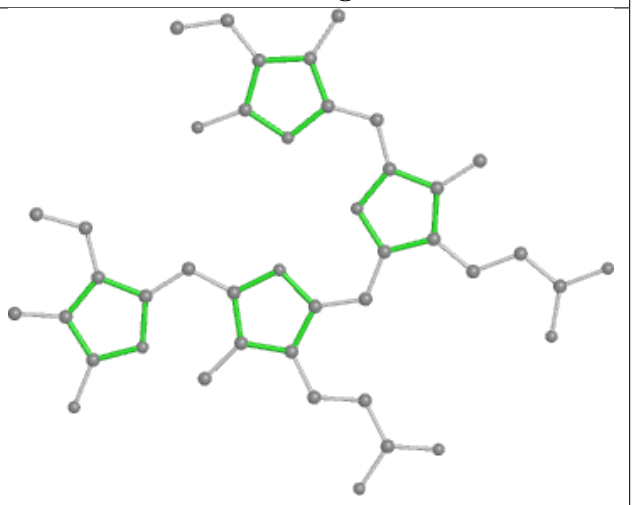

Rings

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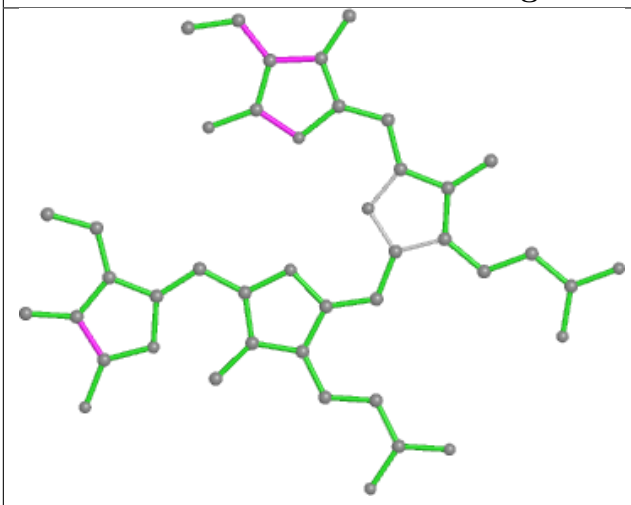

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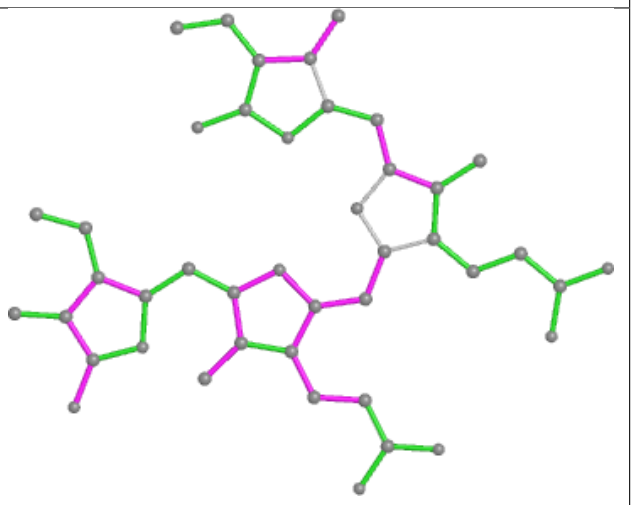

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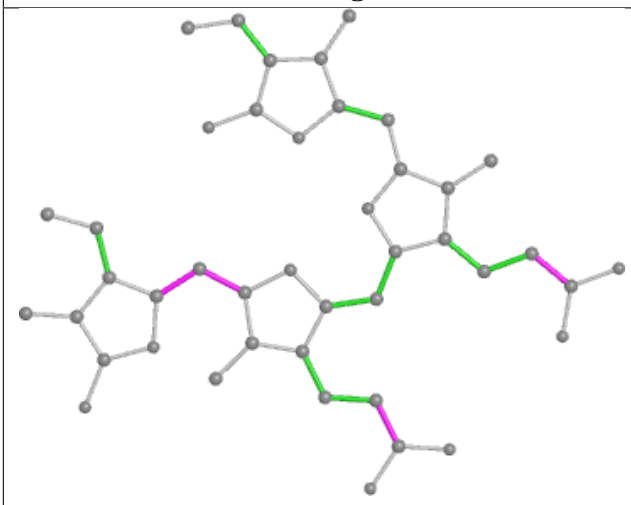

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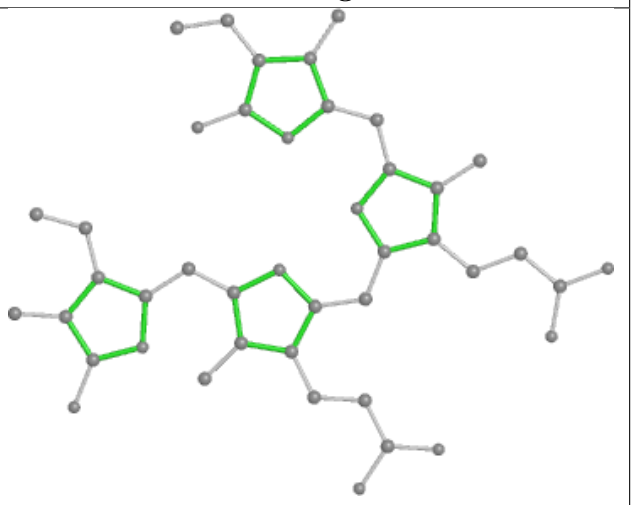

Rings

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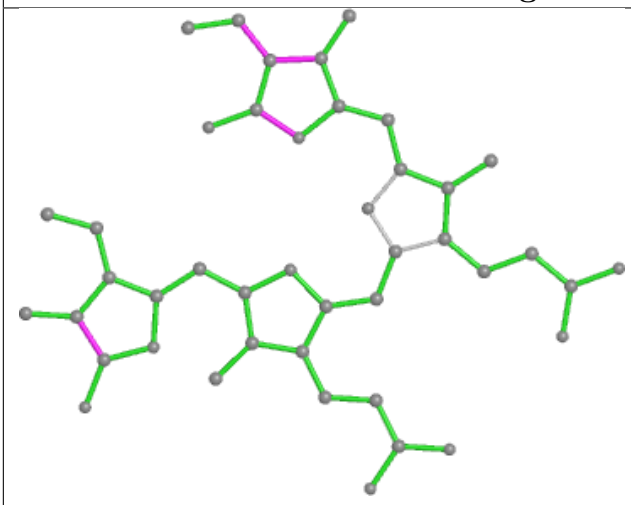

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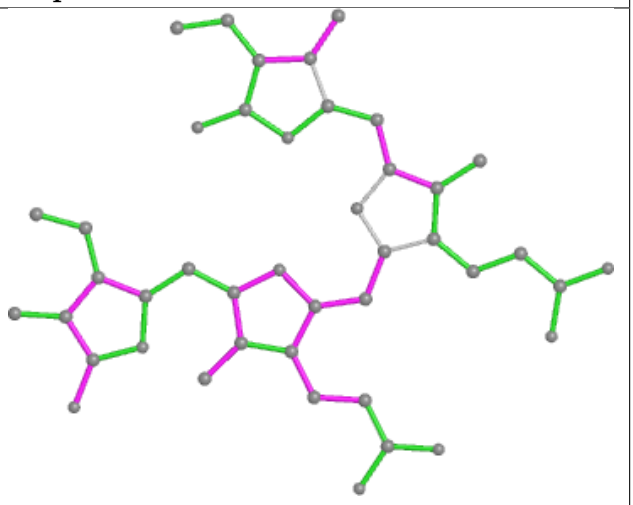

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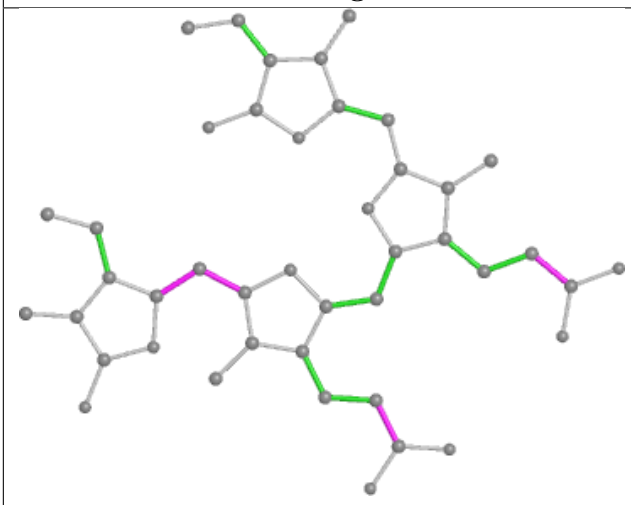

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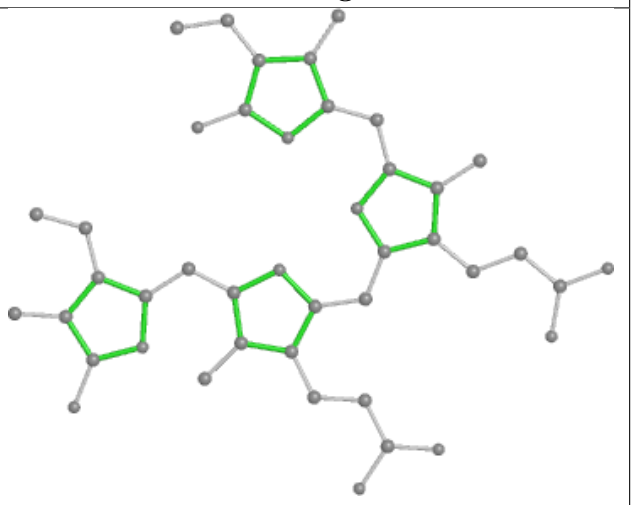
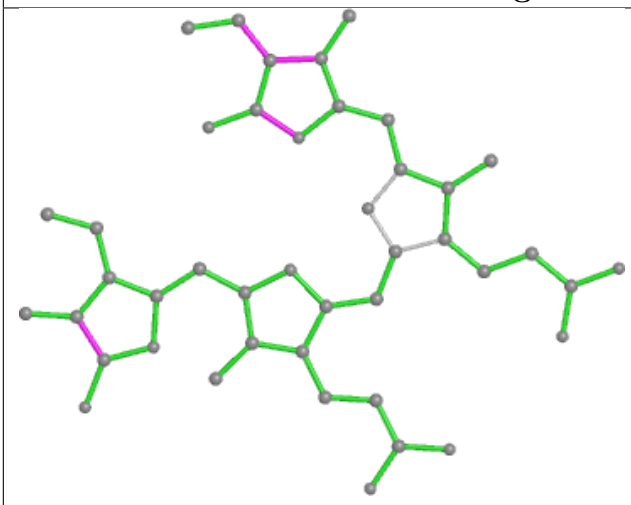


Rings

Ligand PEB dH 201



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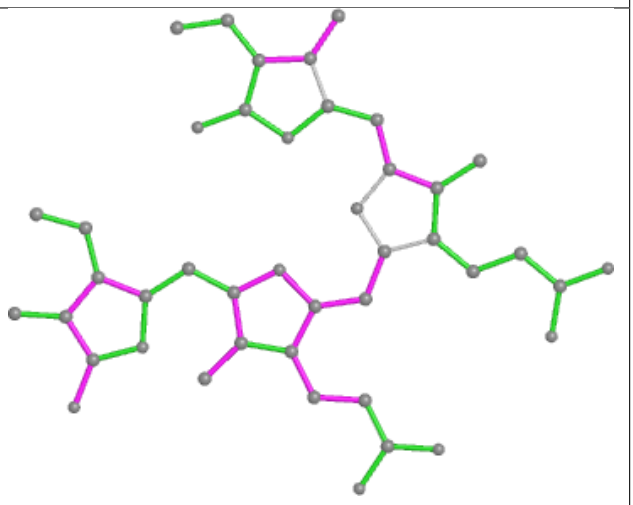

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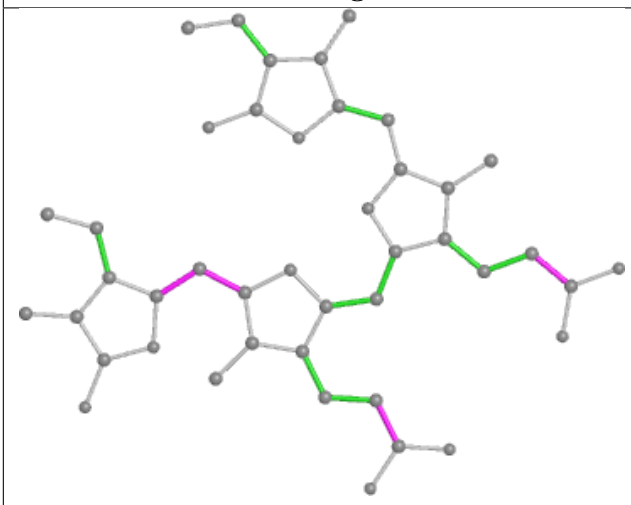

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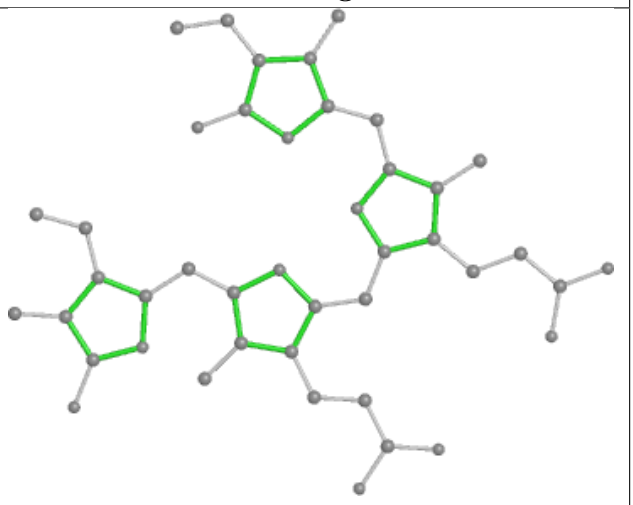
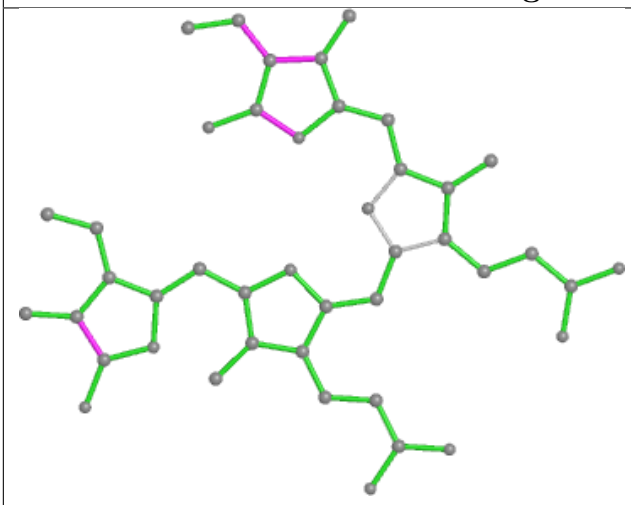


Rings

Ligand PEB lp 201



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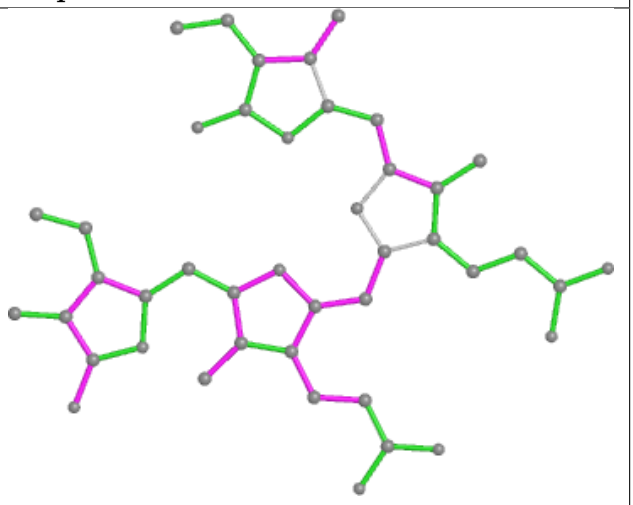

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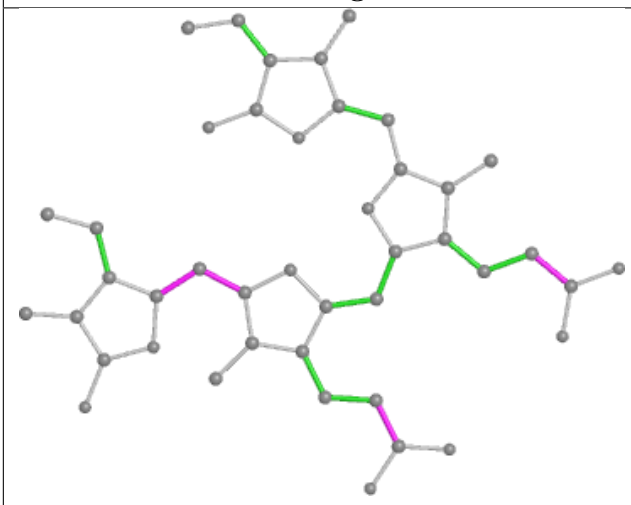

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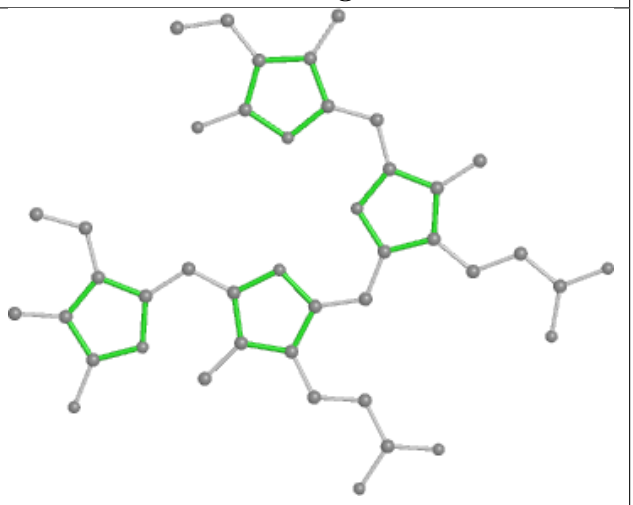
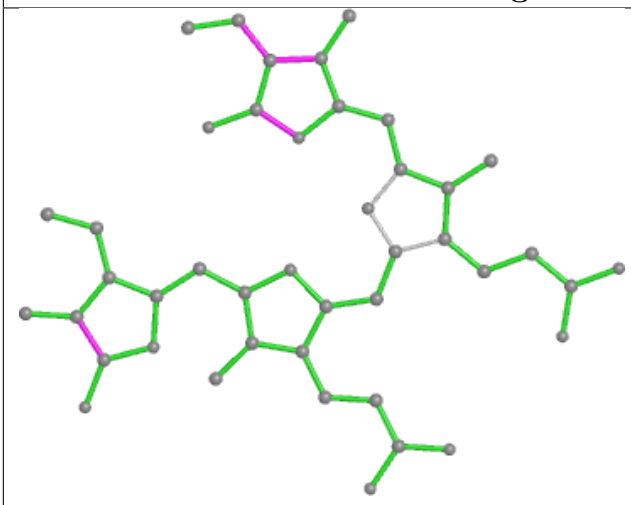


Rings

Ligand PEB a3 1003



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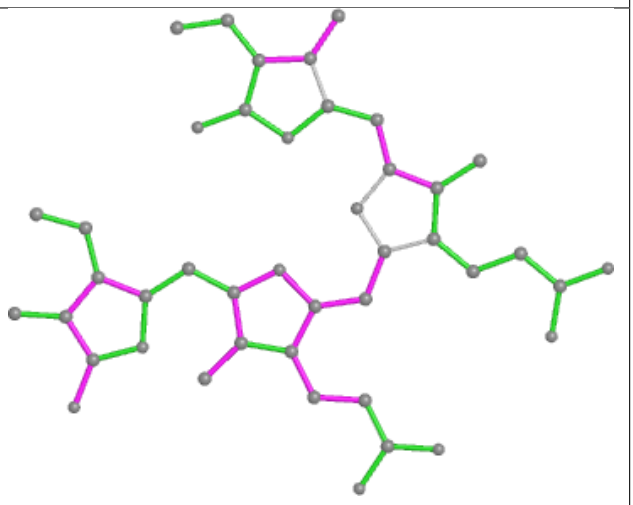

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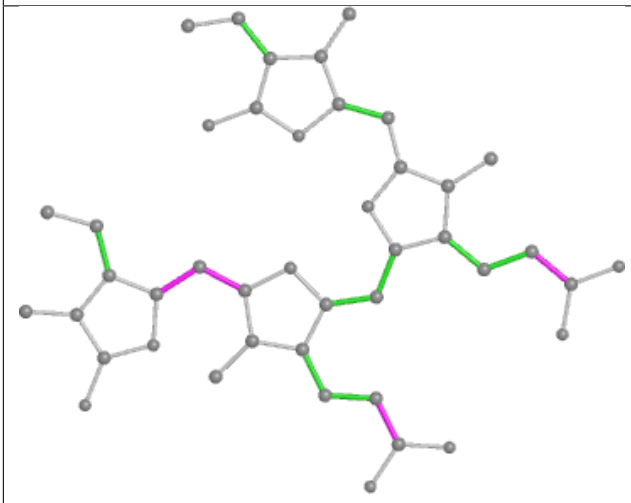

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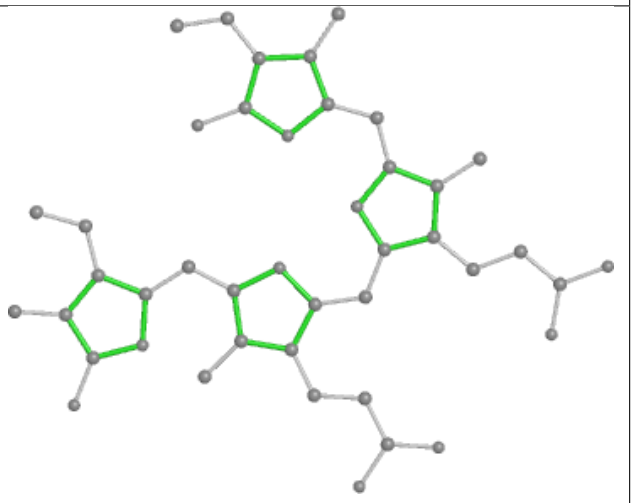

Rings

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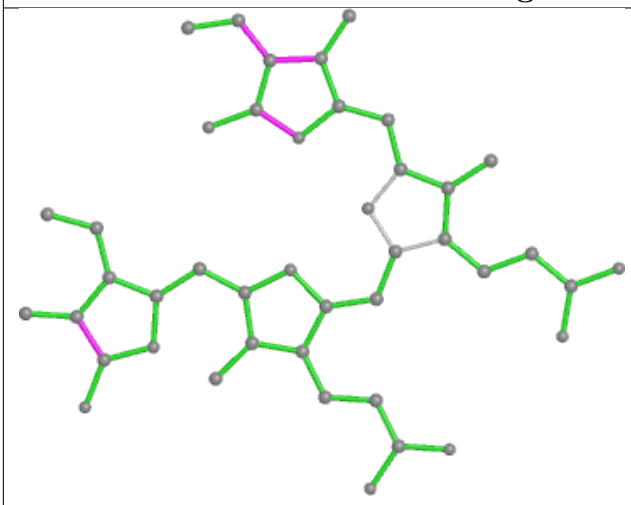

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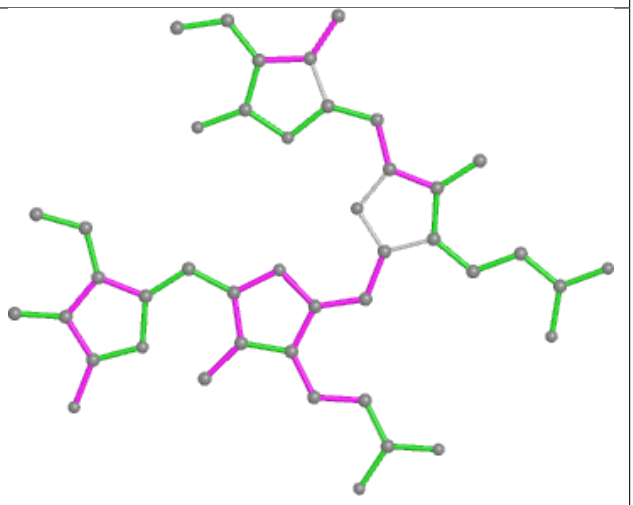

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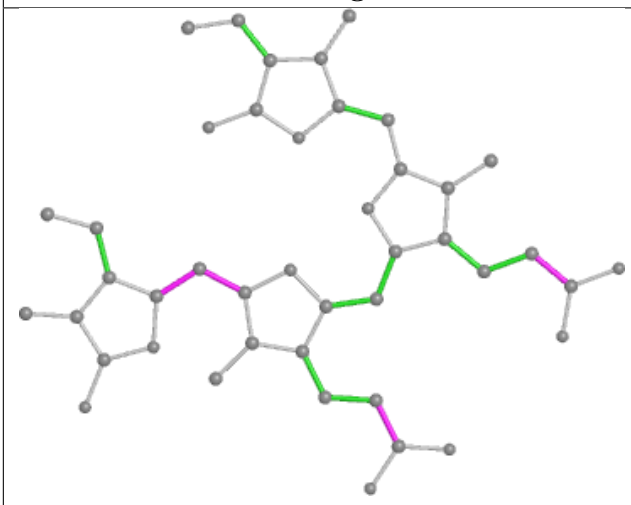

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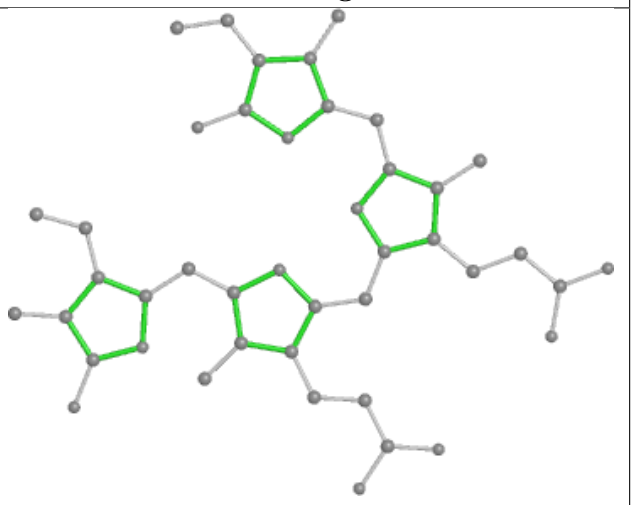
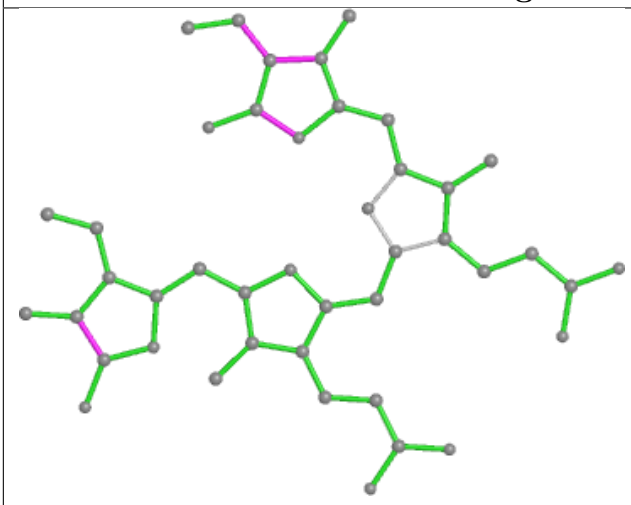
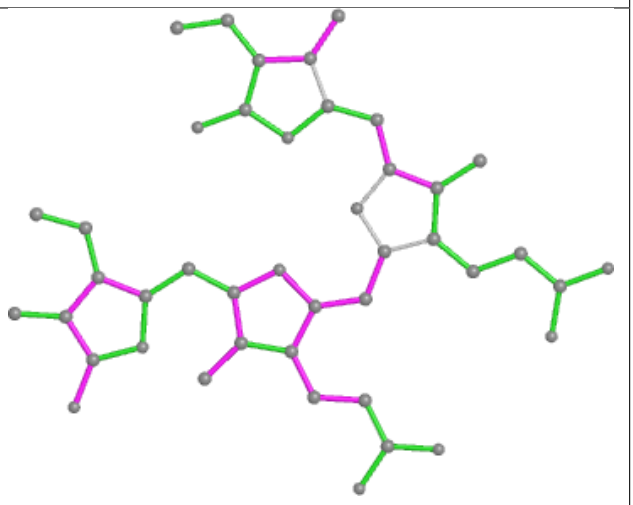


Rings

Ligand PEB V7 201



Bond lengths



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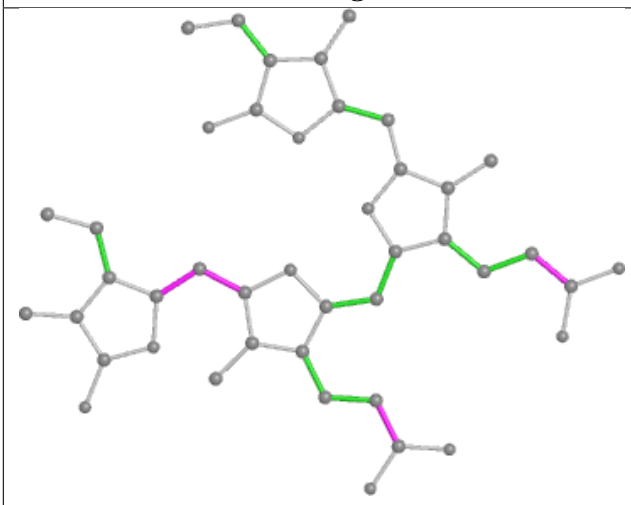
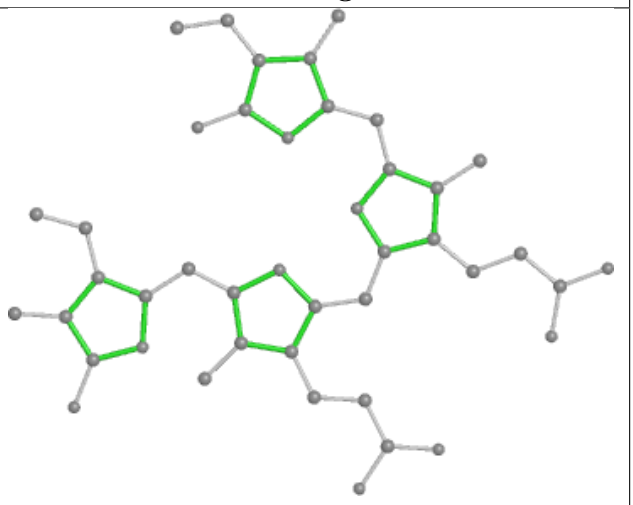
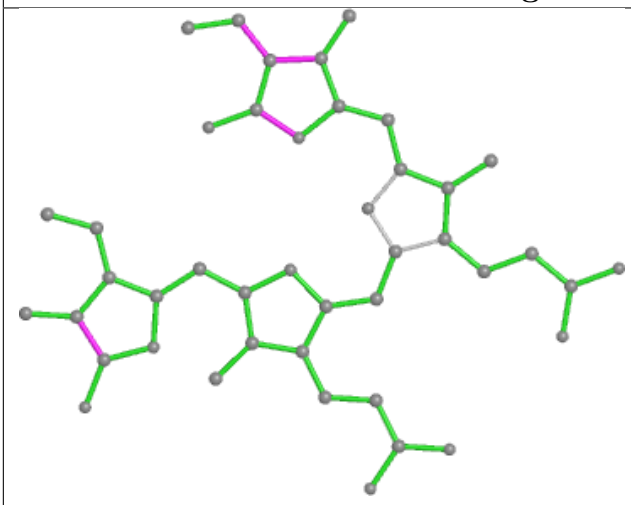


Torsions



Rings

Ligand PEB s6 202



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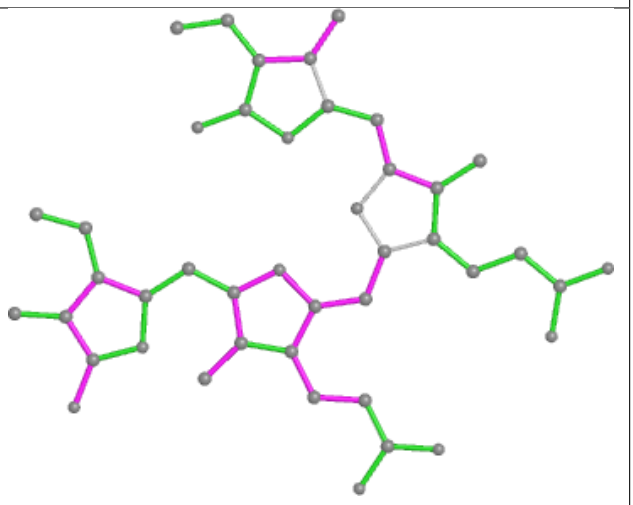

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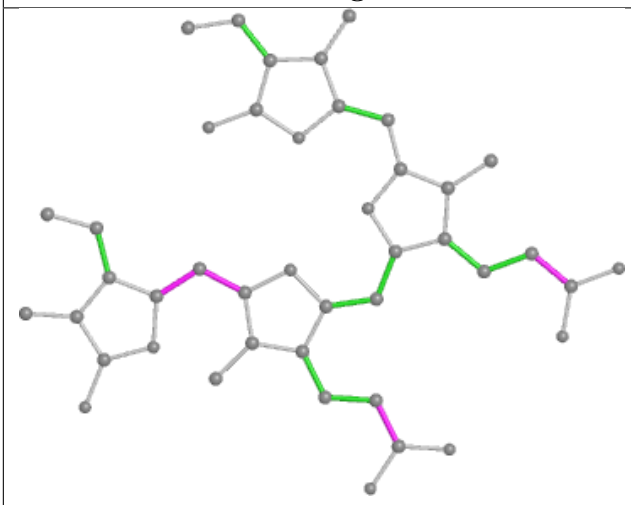

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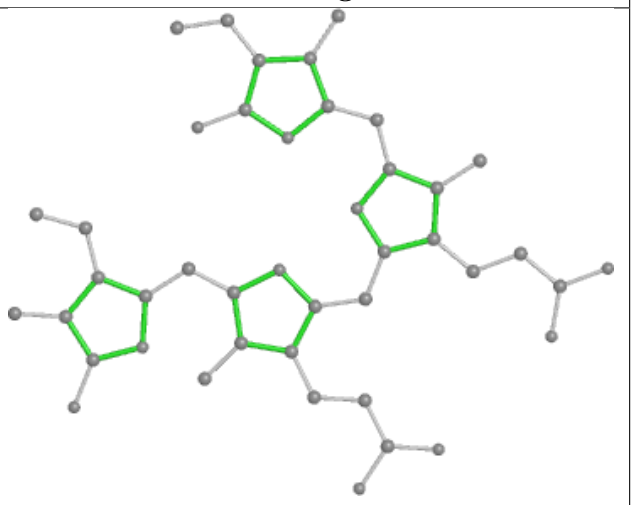

Rings

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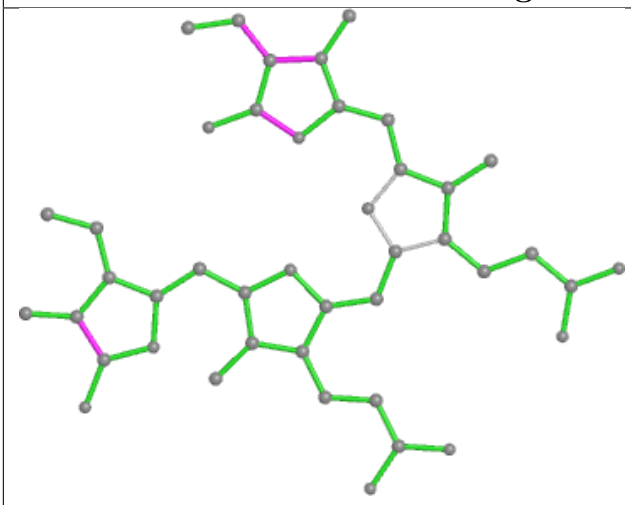

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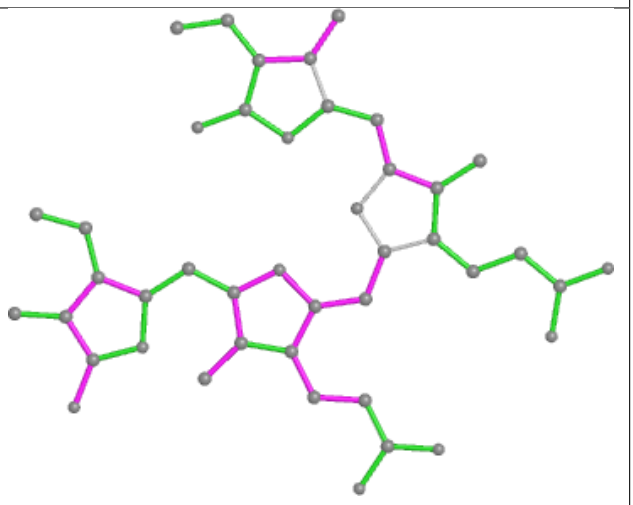

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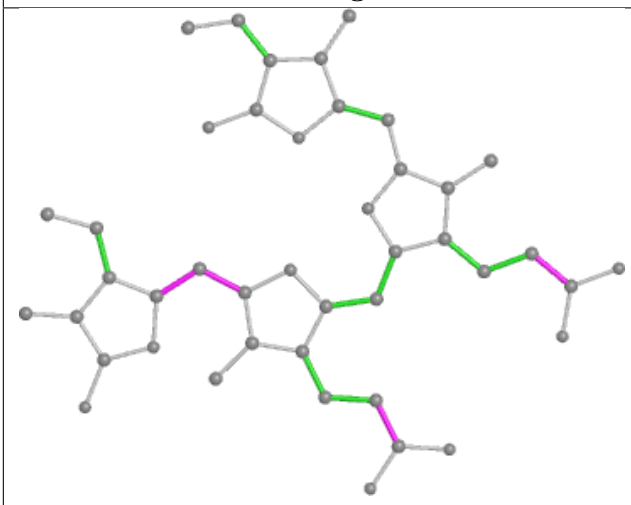

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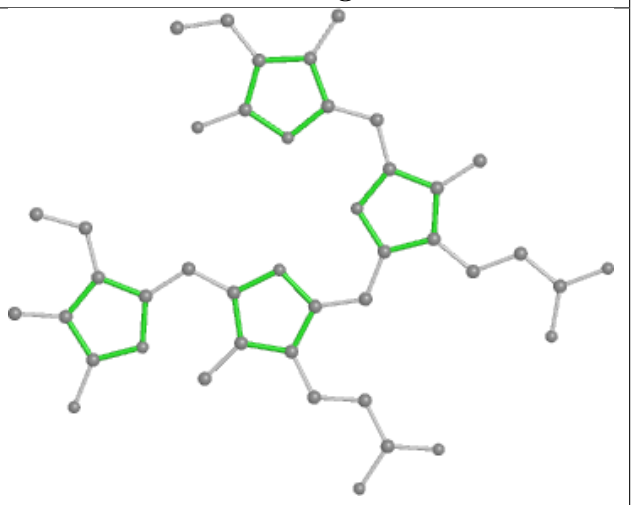
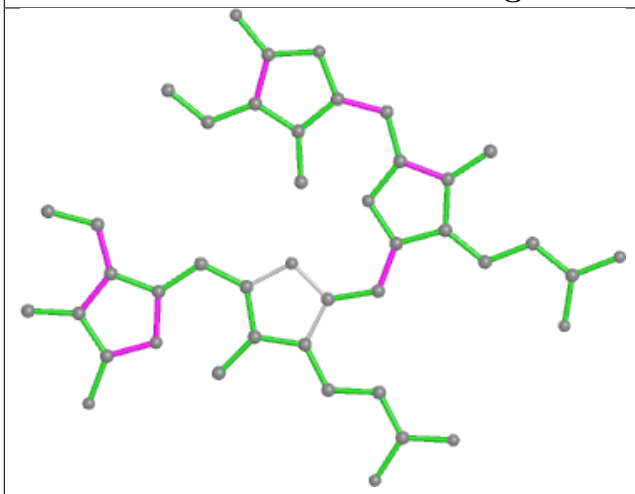


Rings

Ligand PVN A2 1004



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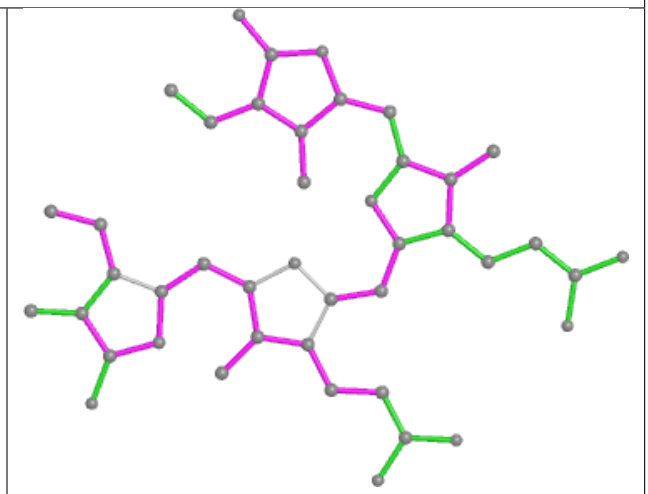

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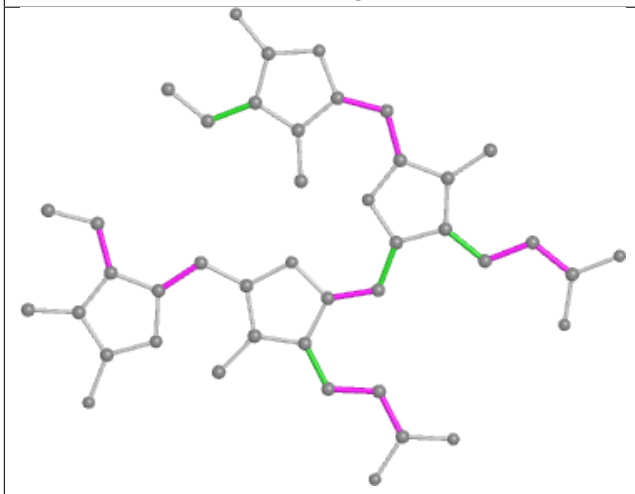

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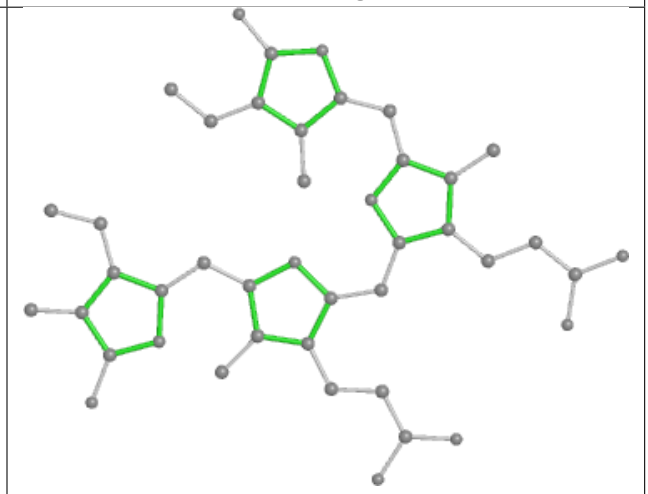

Rings

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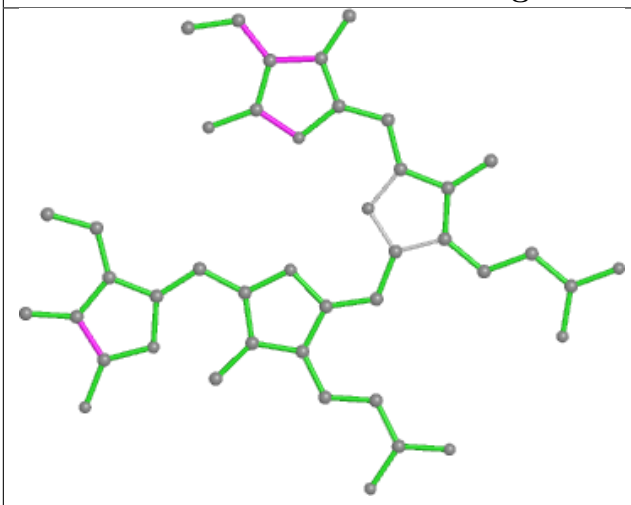

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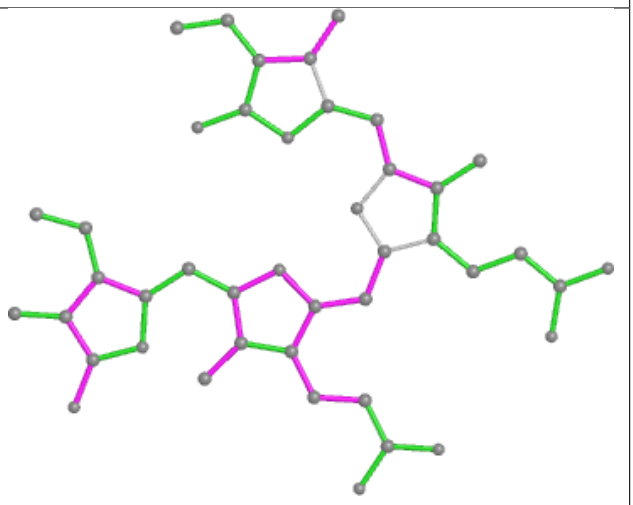

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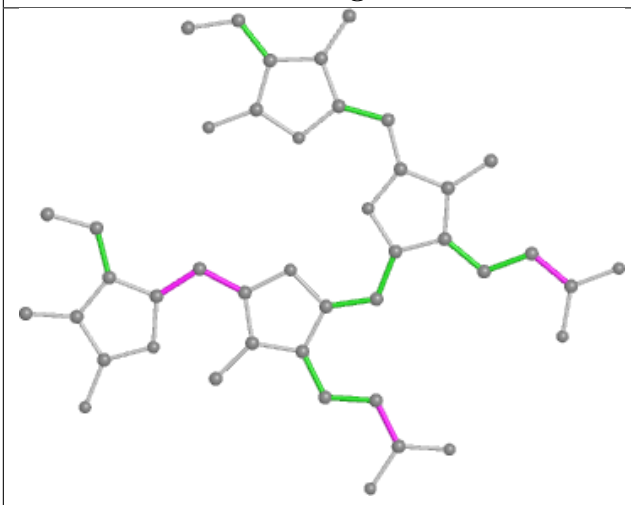

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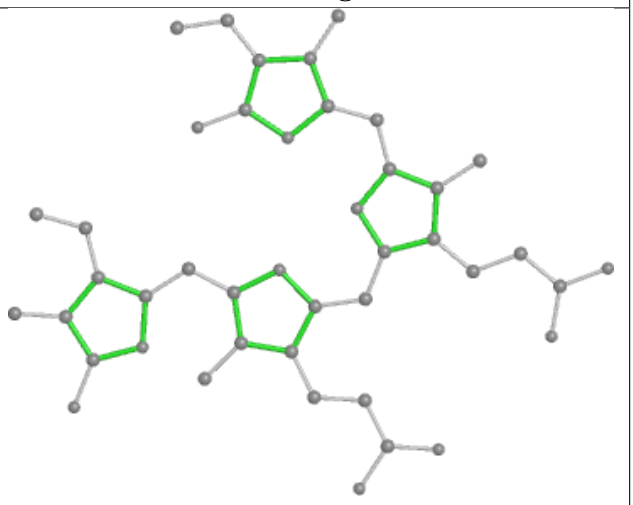

Rings

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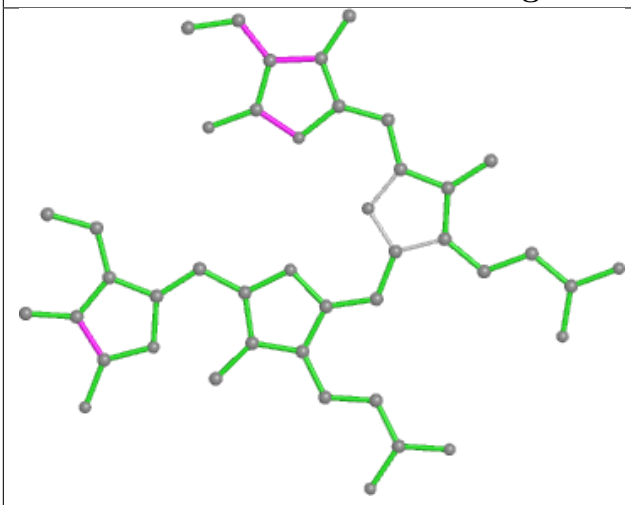

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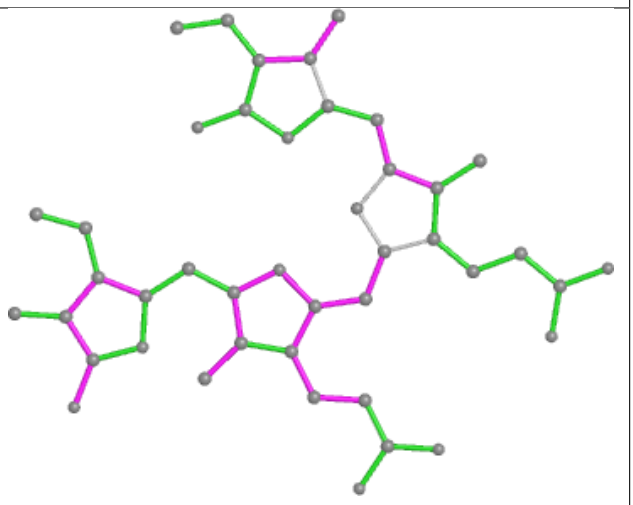

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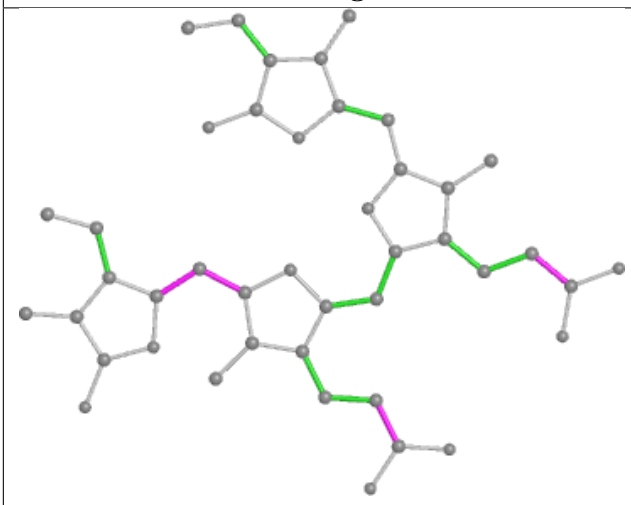

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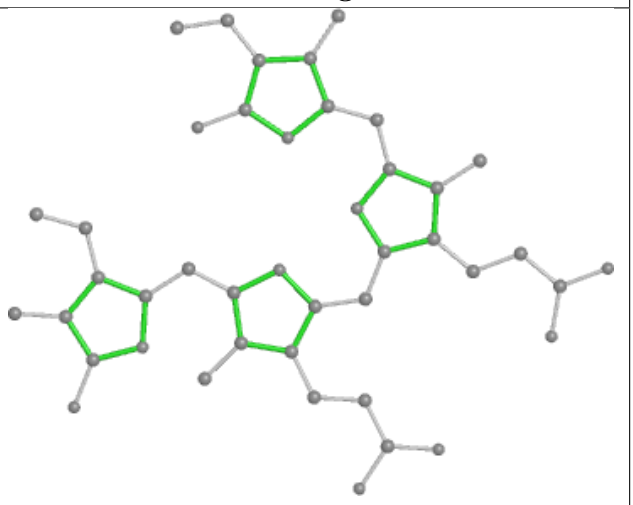

Rings

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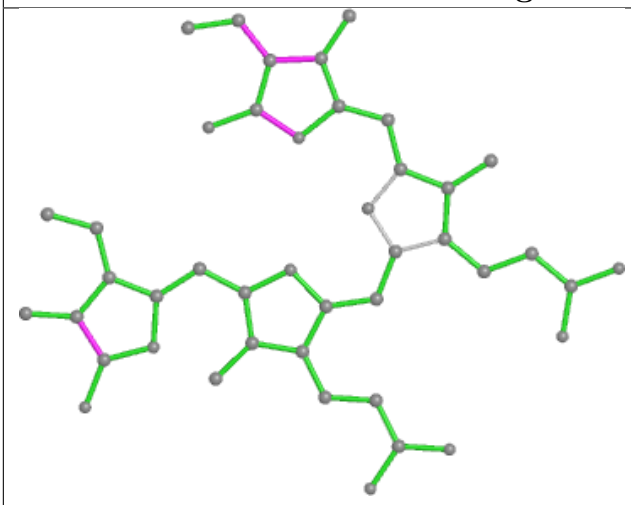

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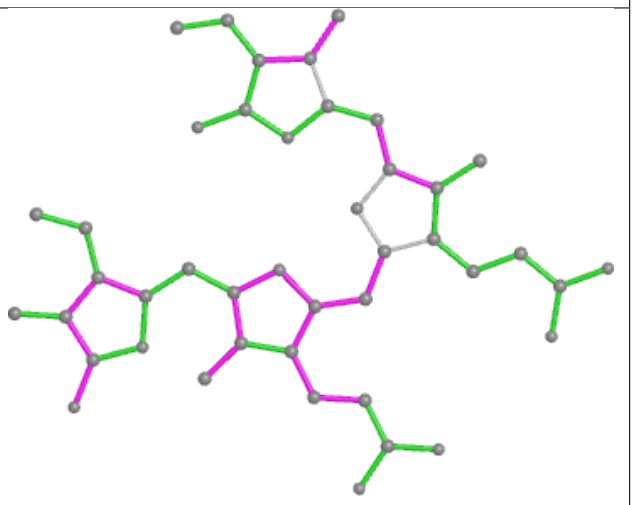

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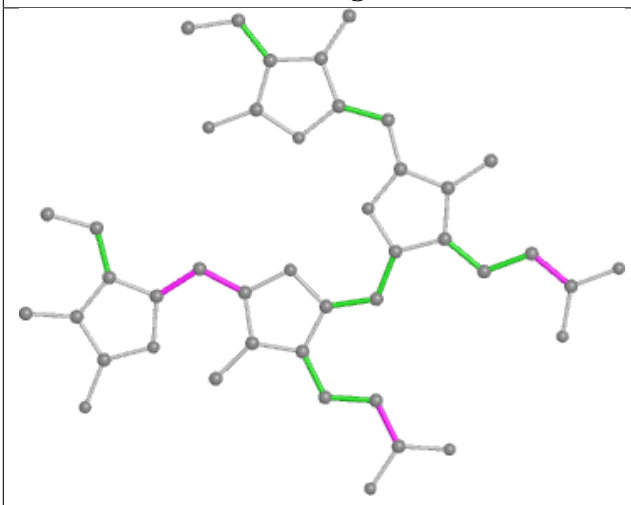

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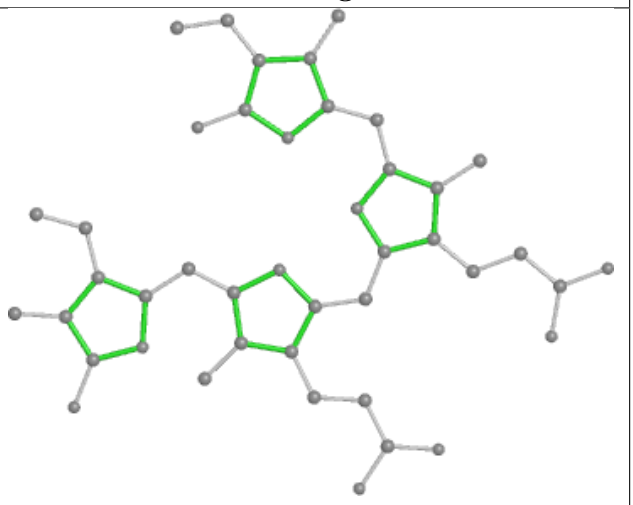
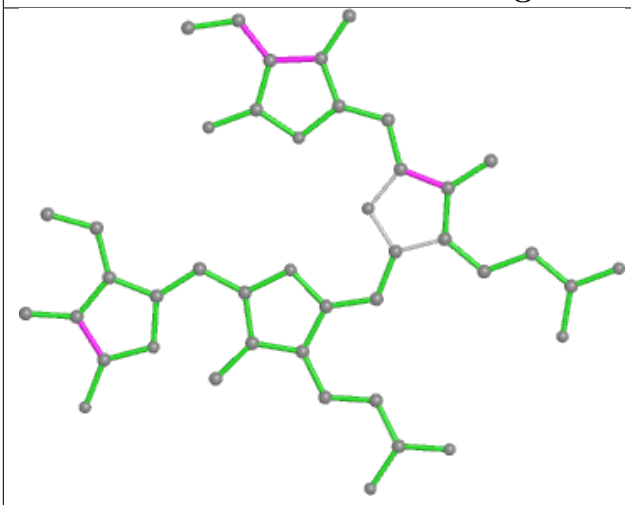


Rings

Ligand PEB hY 402



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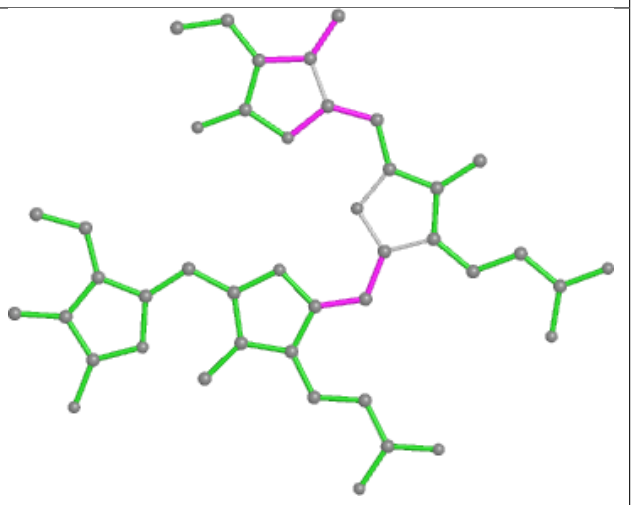

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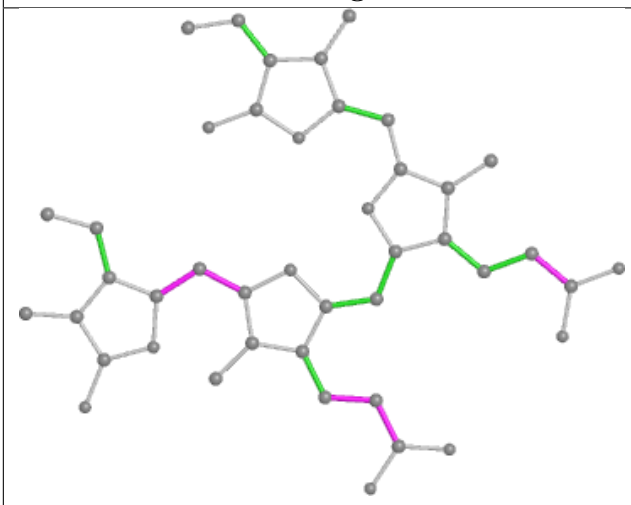

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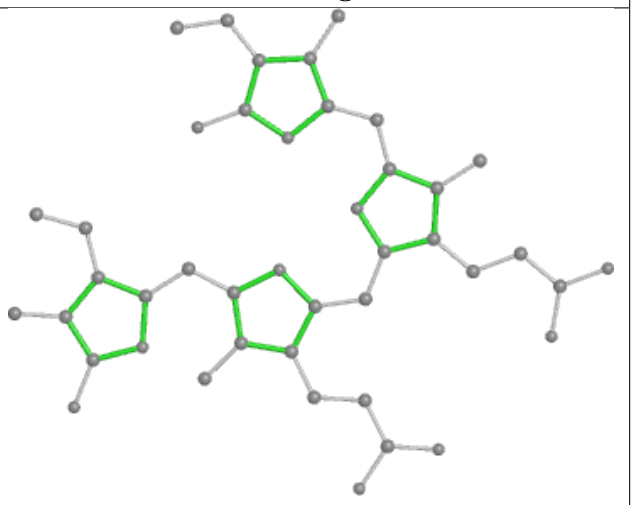

Rings

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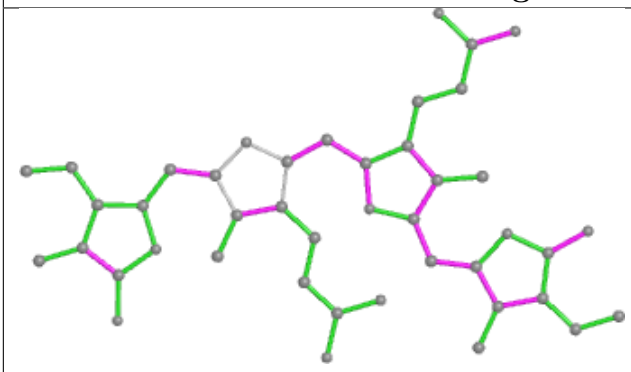

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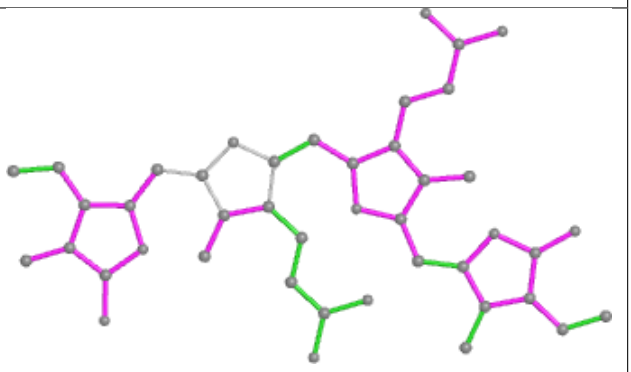

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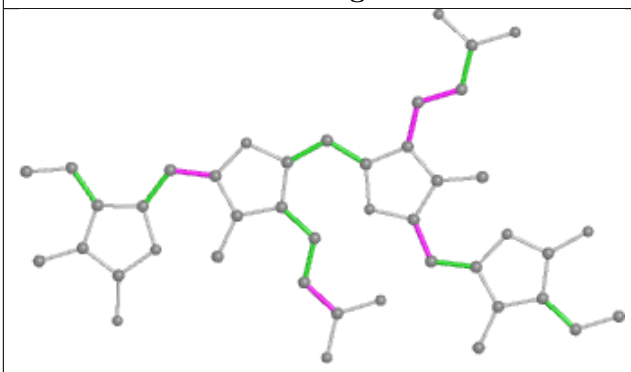

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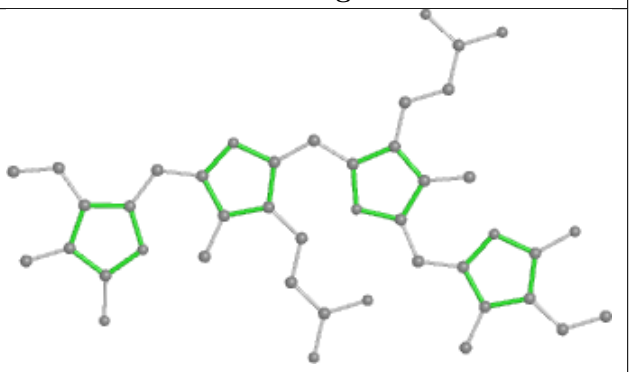
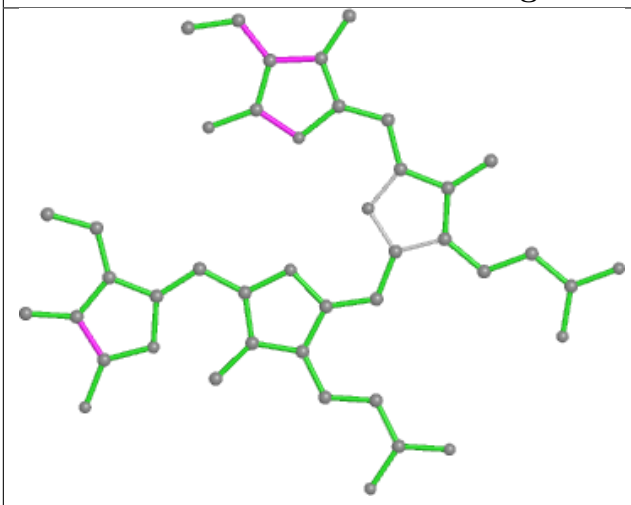


Rings

Ligand PEB a8 601



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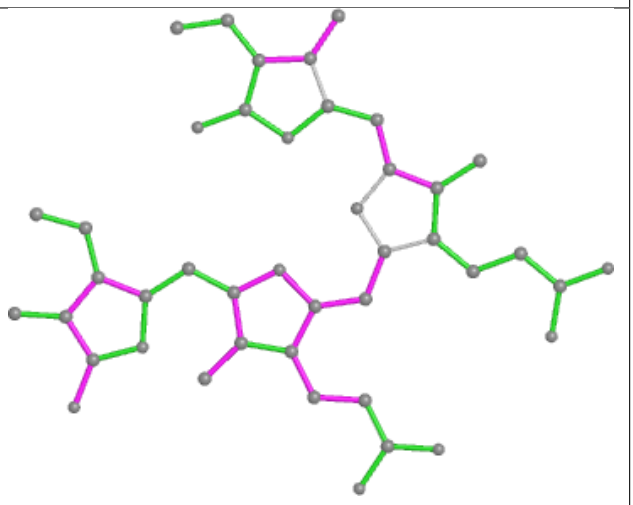

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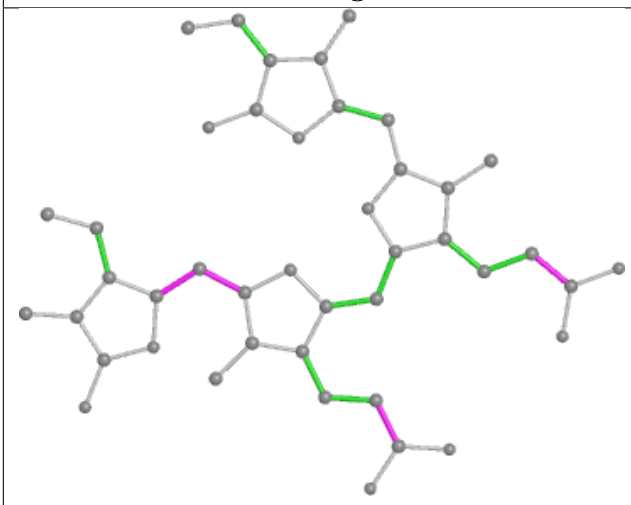

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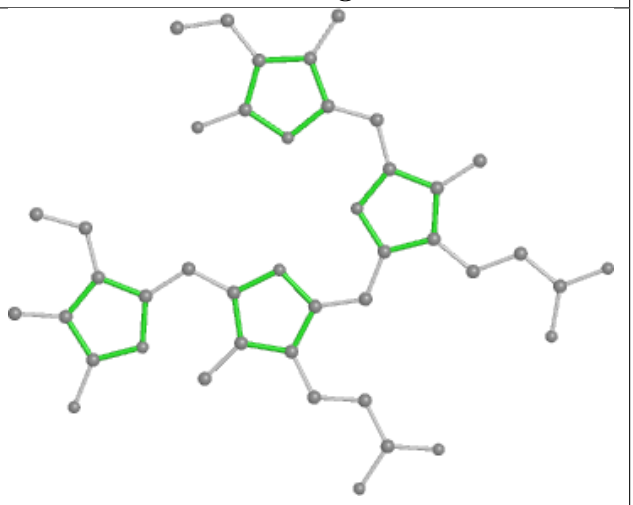
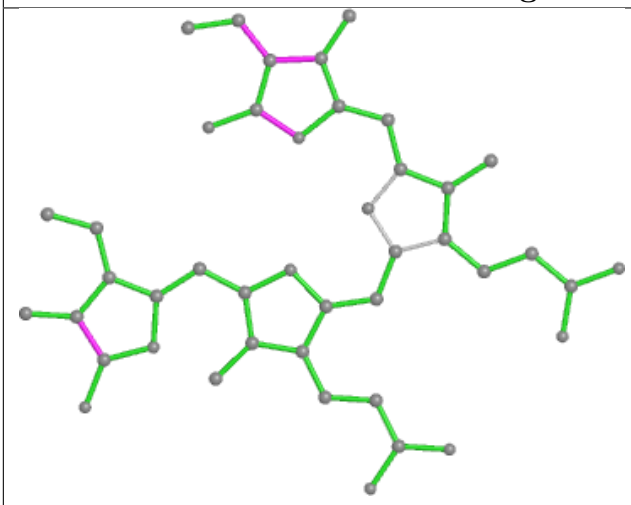


Rings

Ligand PEB g6 202



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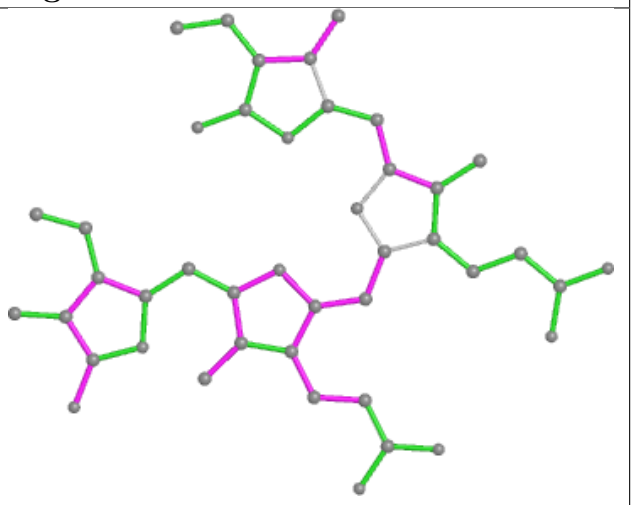

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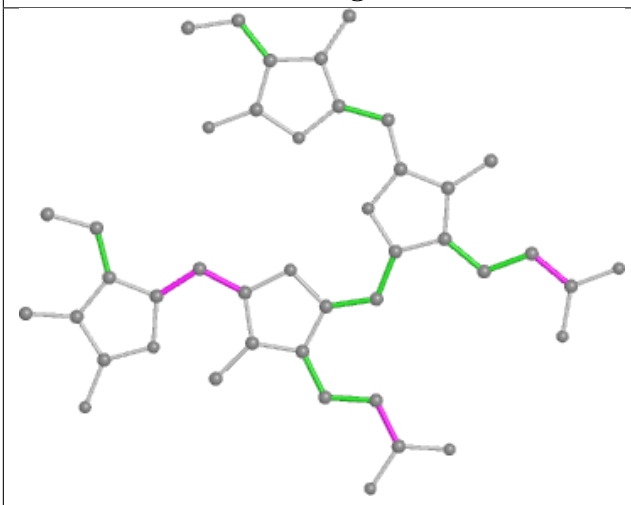

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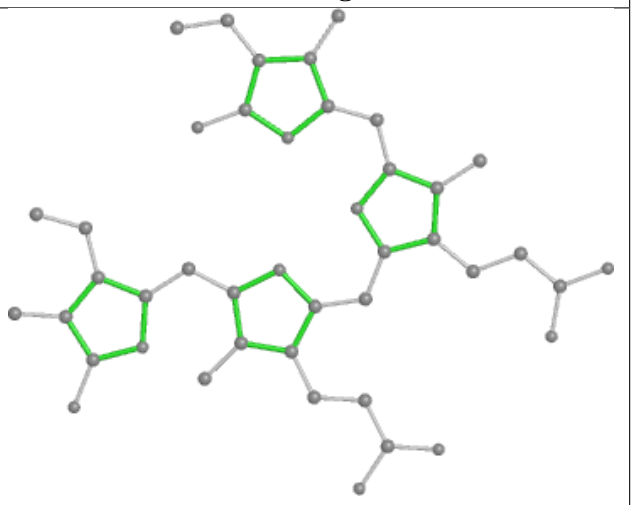

Rings

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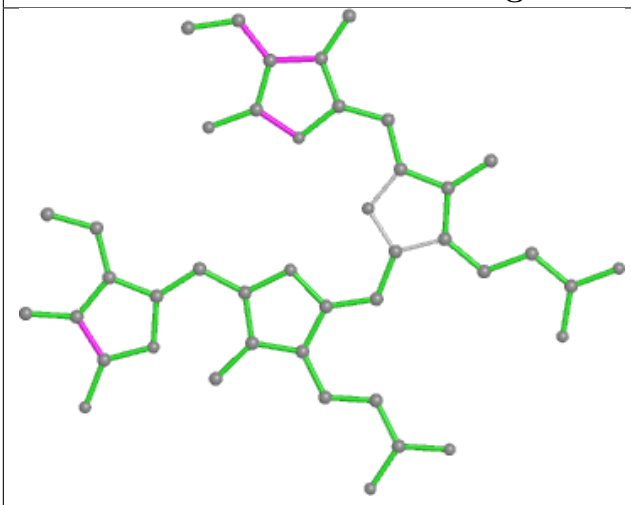

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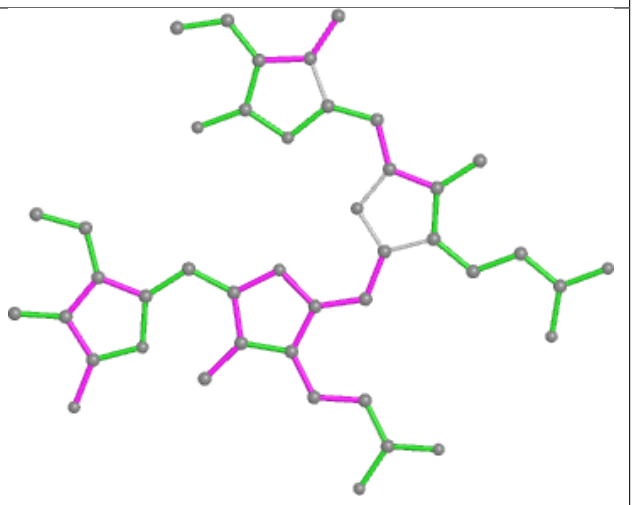

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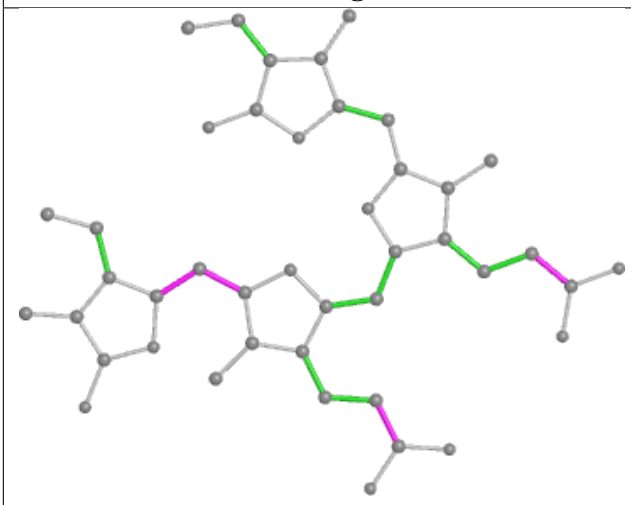

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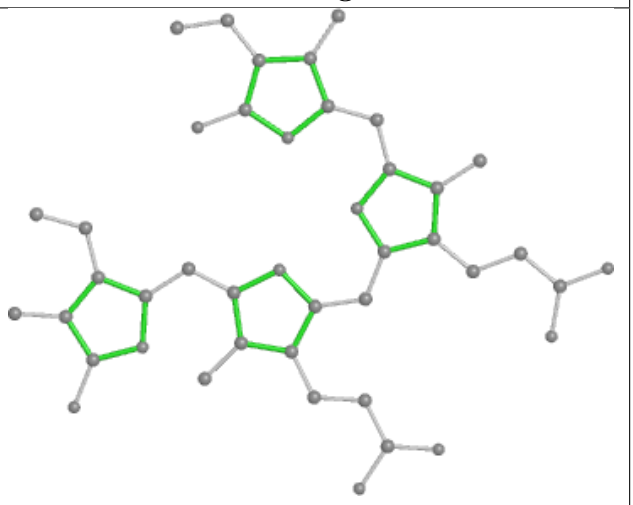

Rings

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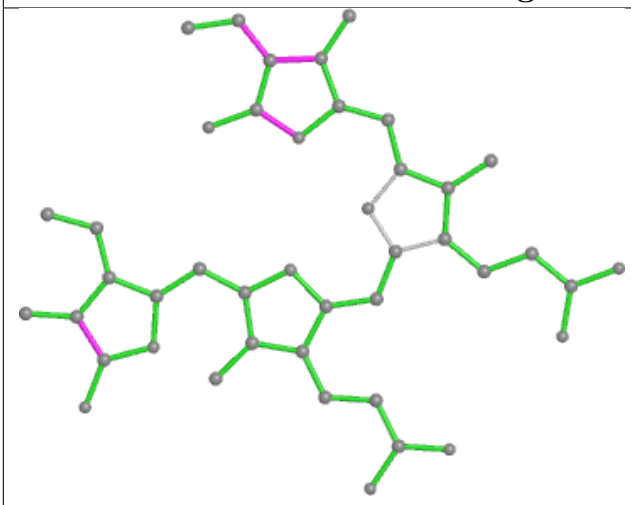

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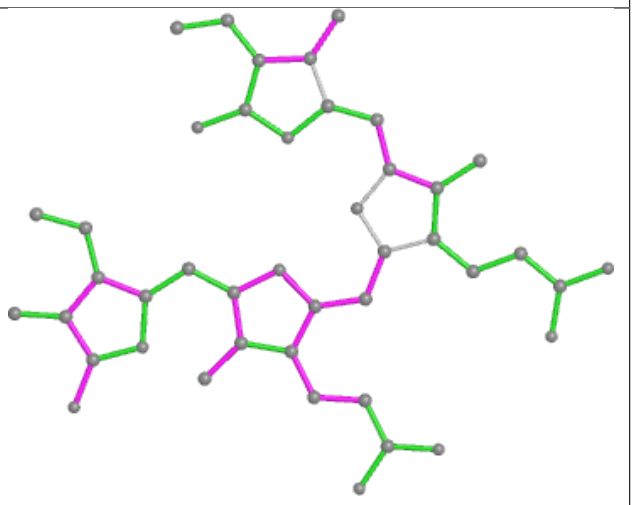
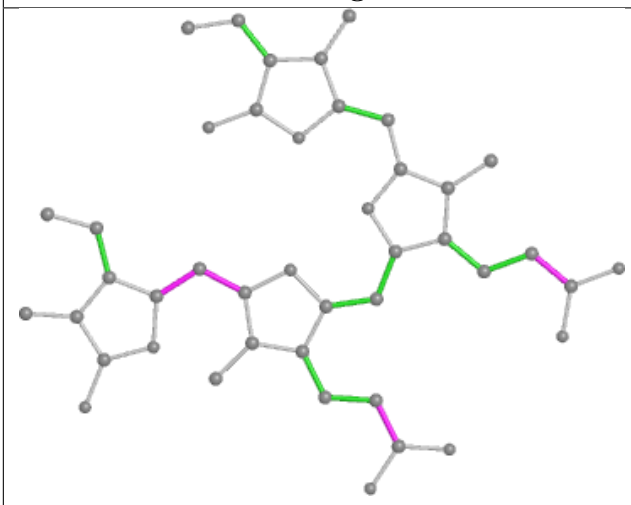


Bond angles



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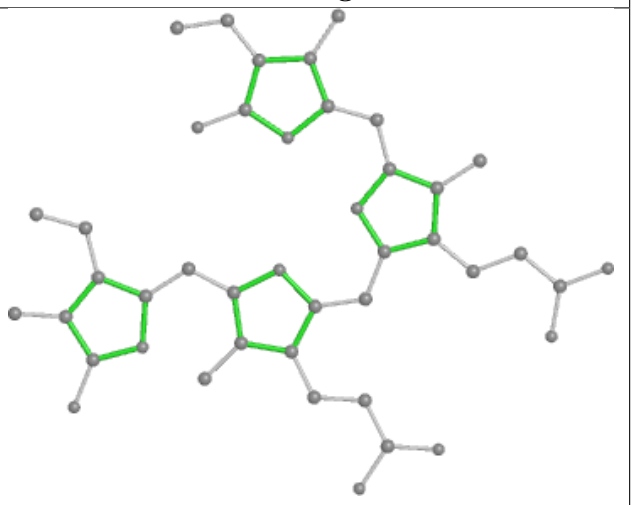

Rings

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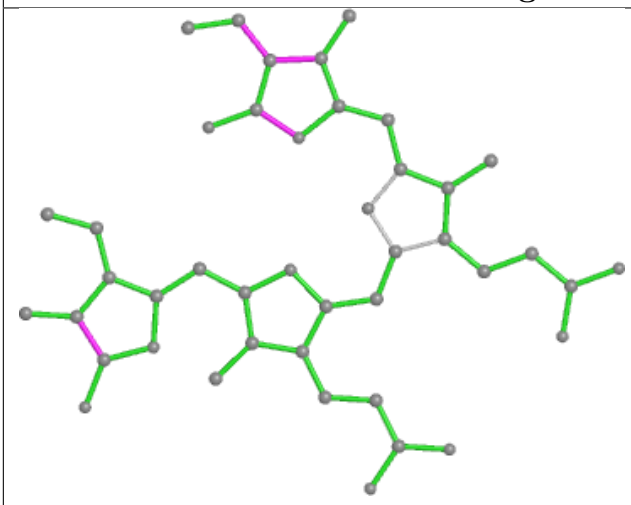

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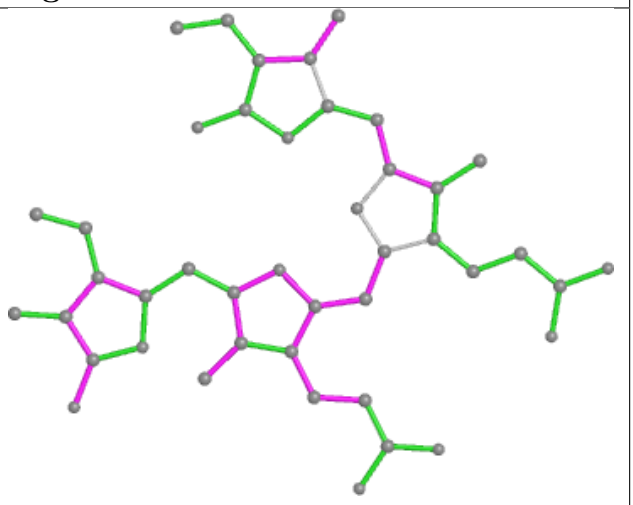
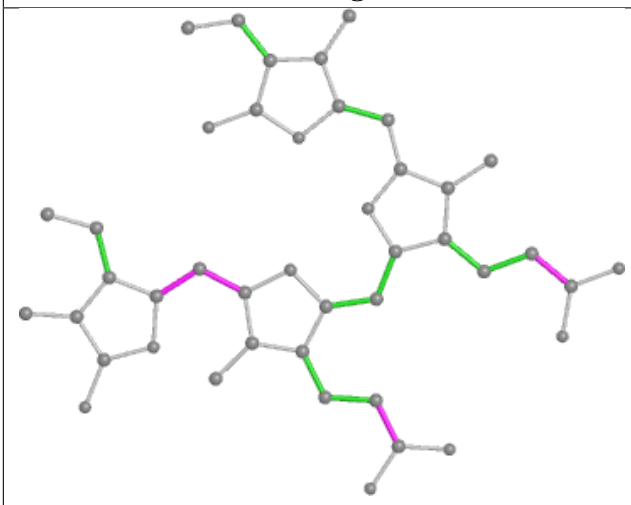
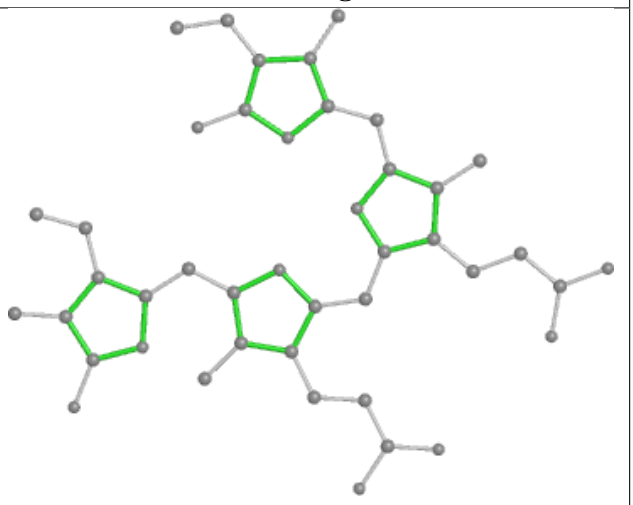


Bond angles

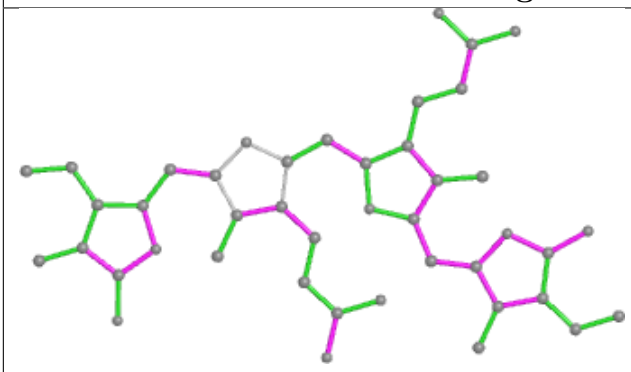


Torsions



Rings

Ligand CYC p1 201



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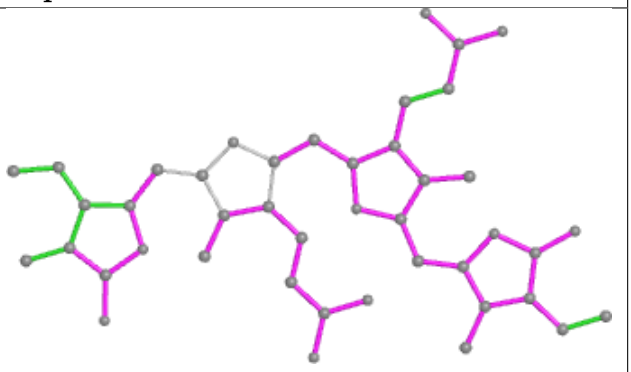

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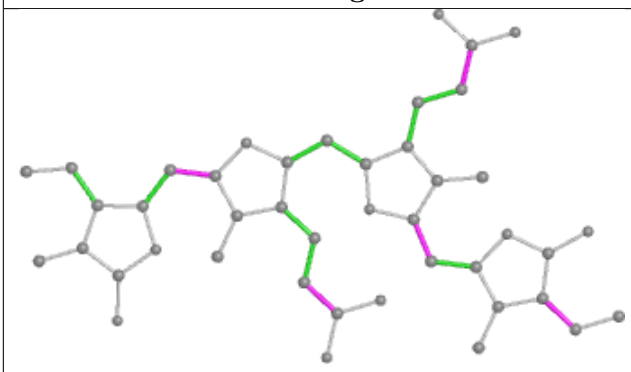

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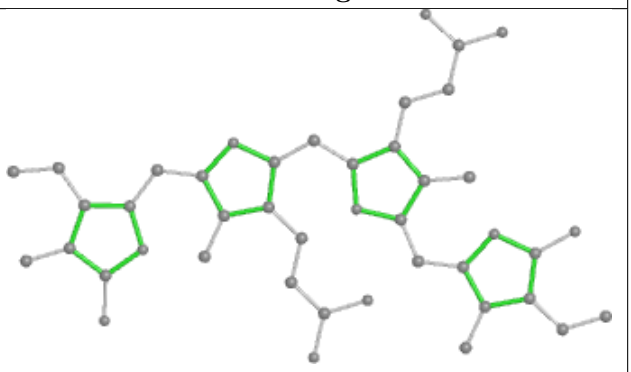
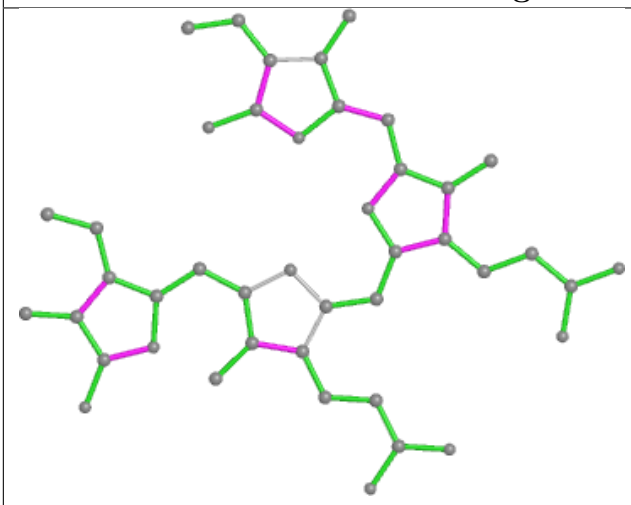


Rings

Ligand PUB D5 203



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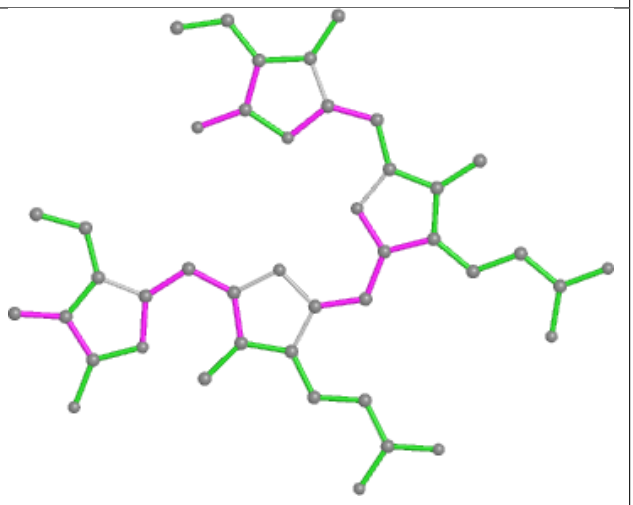

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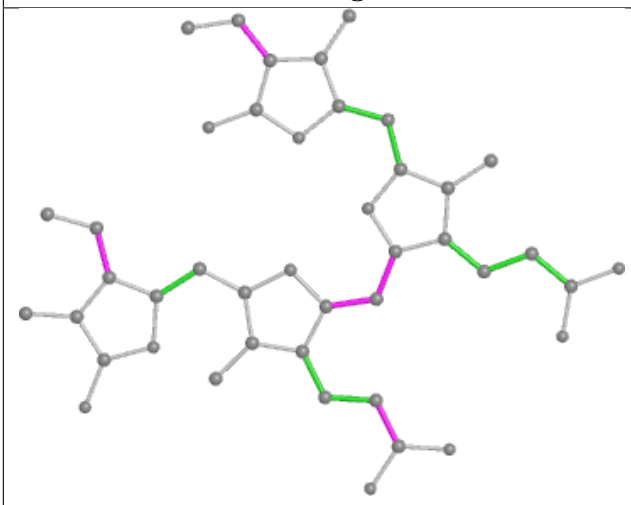

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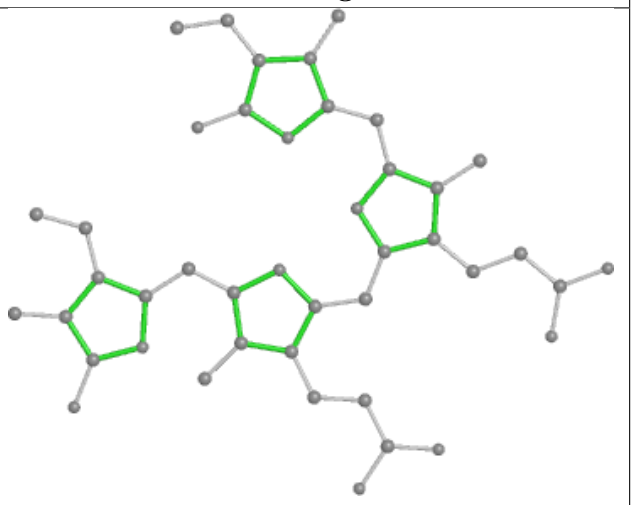
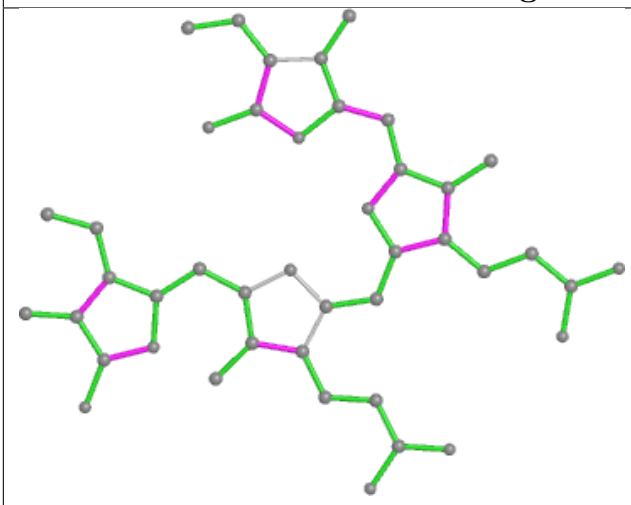


Rings

Ligand PUB ec 203



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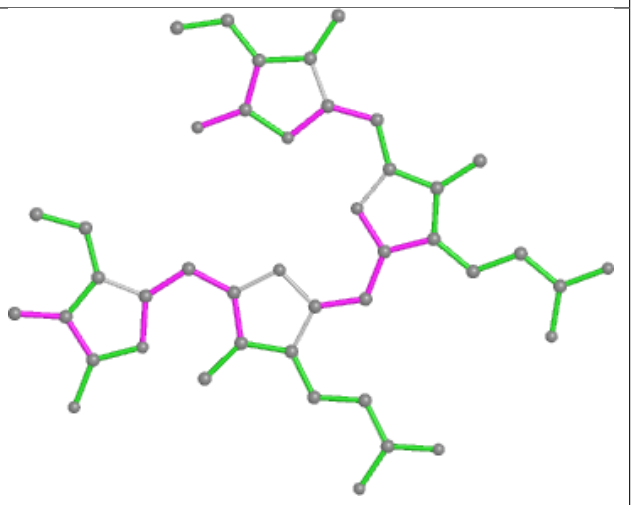

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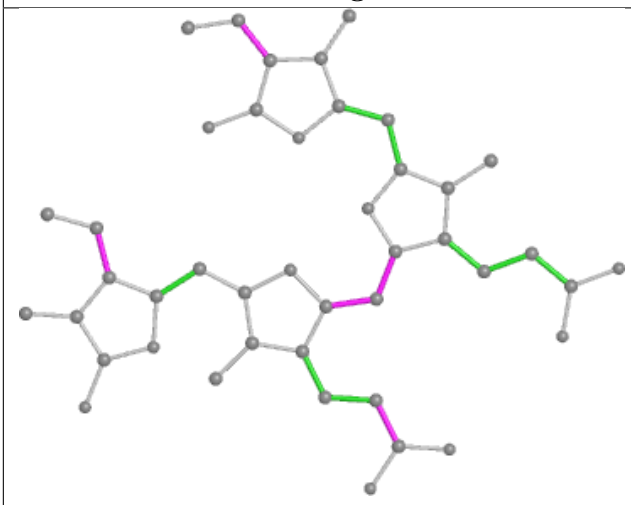

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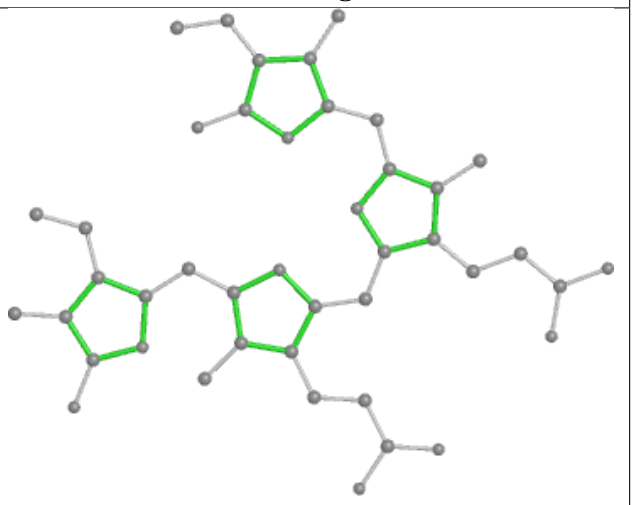
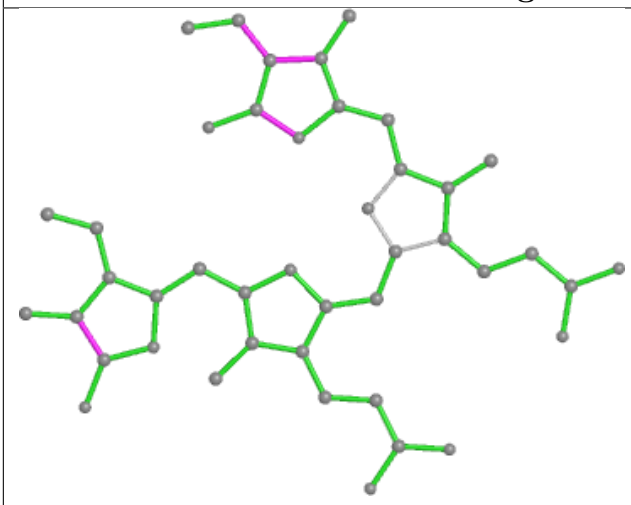


Rings

Ligand PEB cP 202



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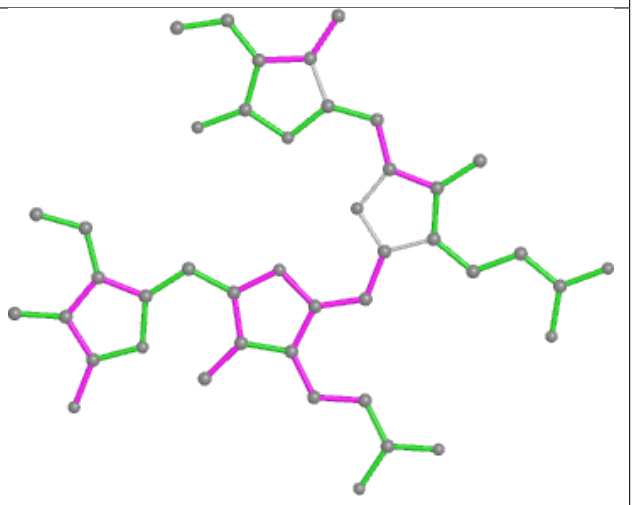

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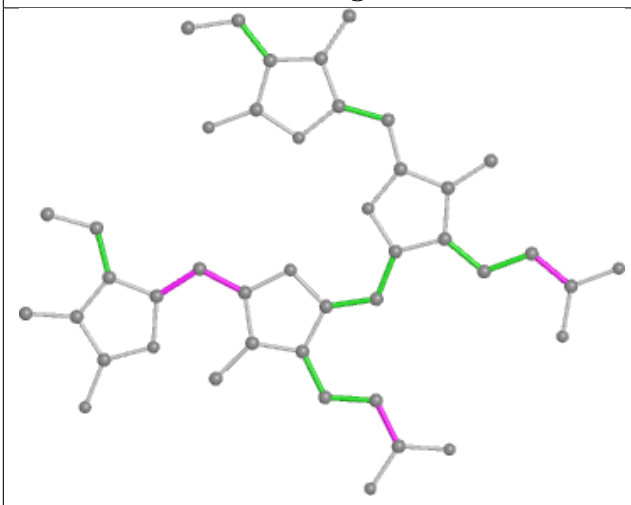

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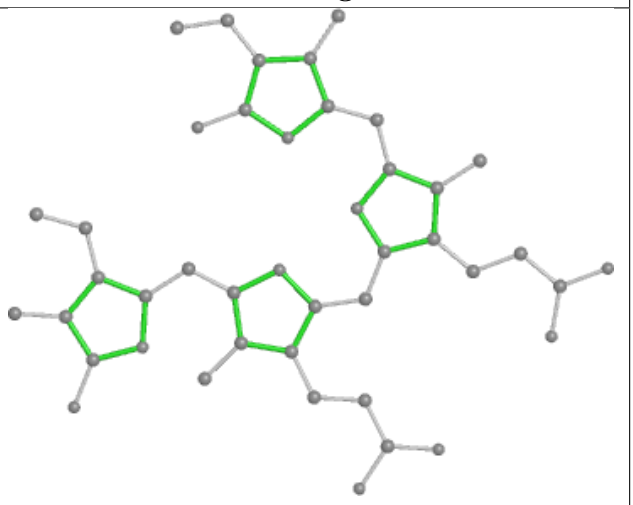
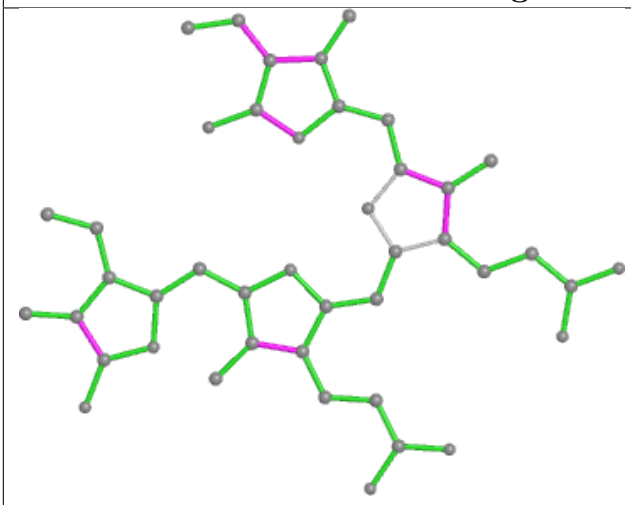


Rings

Ligand PEB jP 1002



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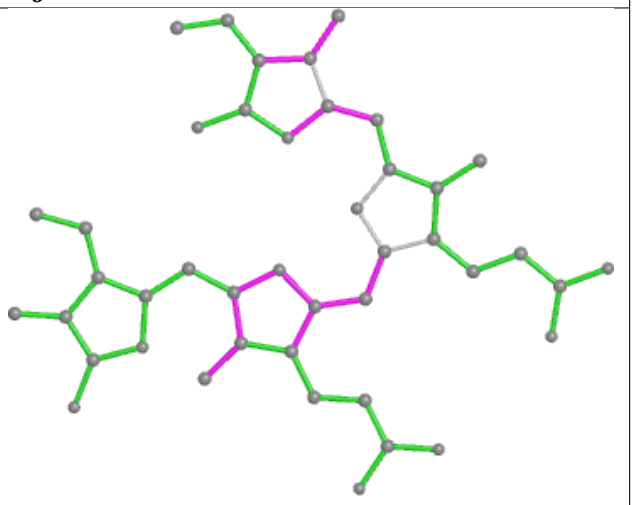

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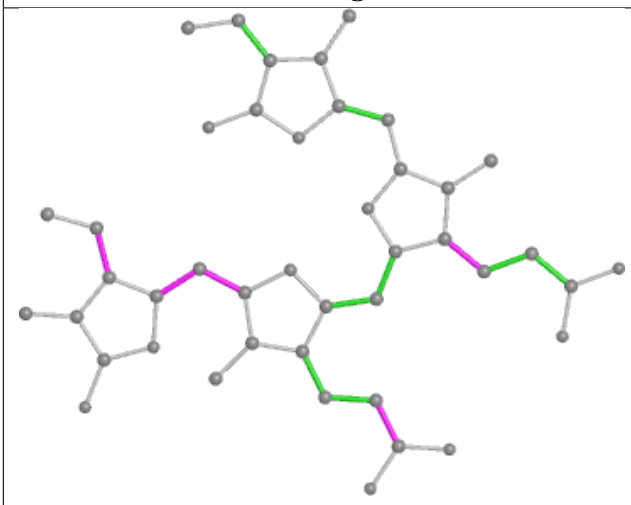

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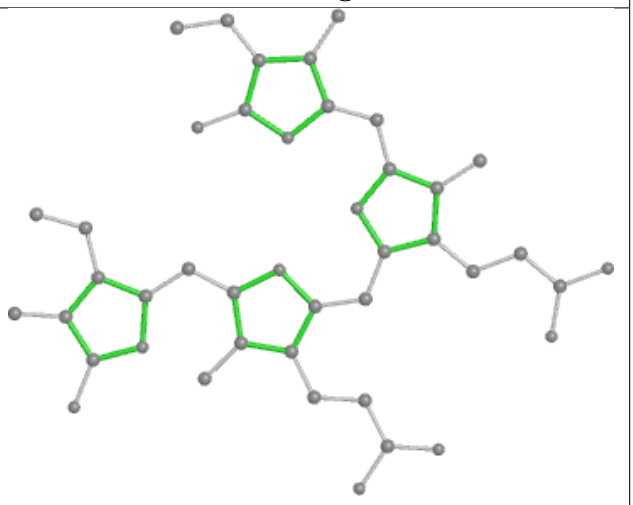

Rings

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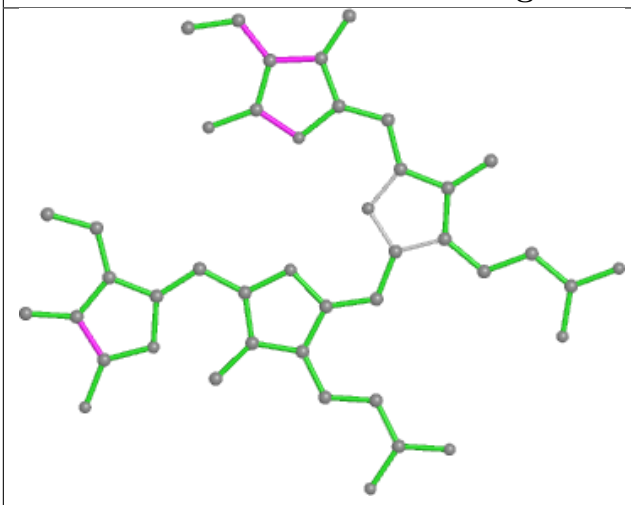

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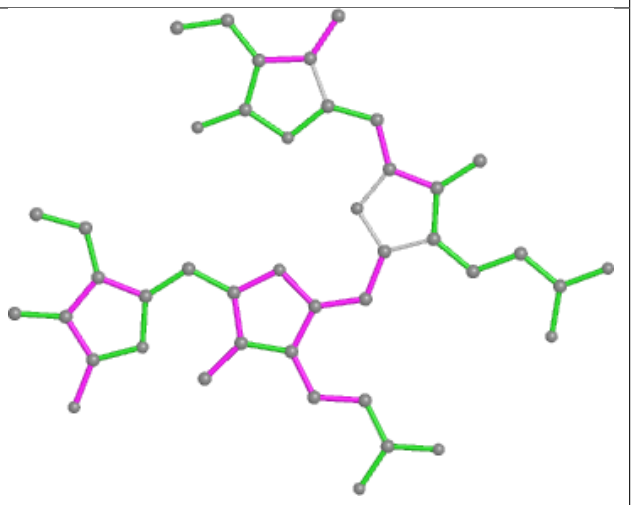

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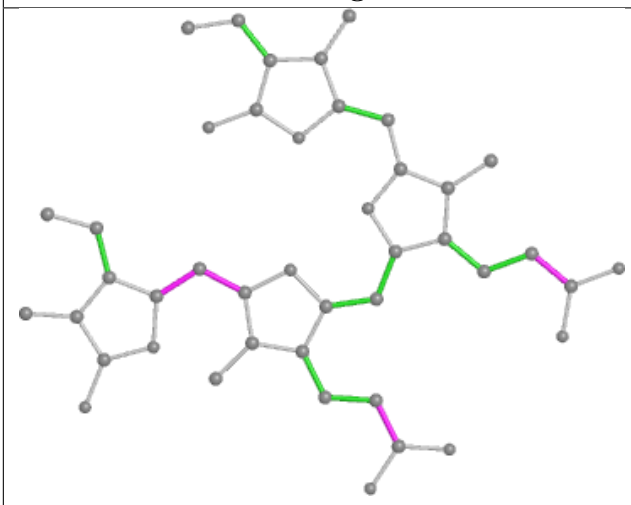

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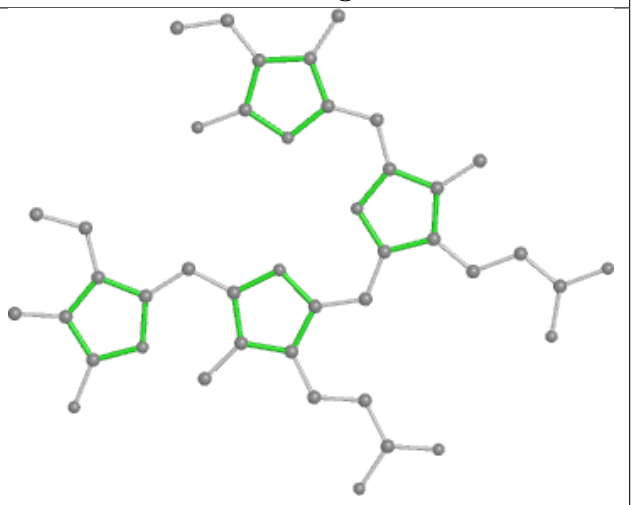

Rings

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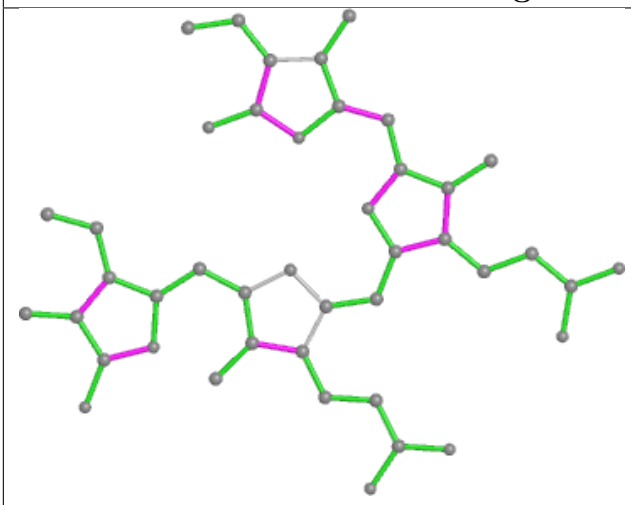

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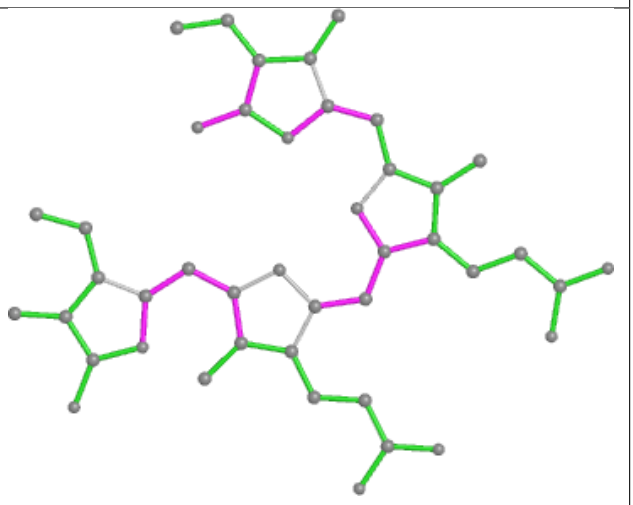

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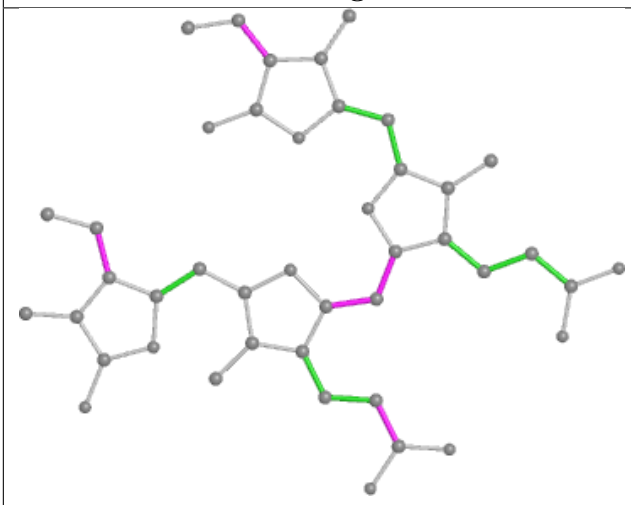

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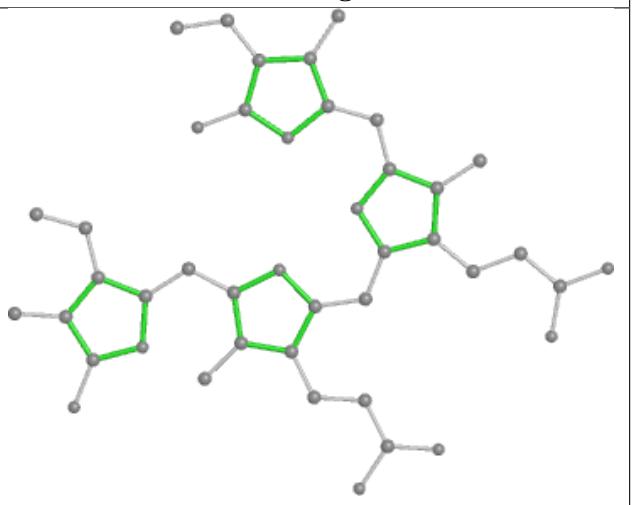
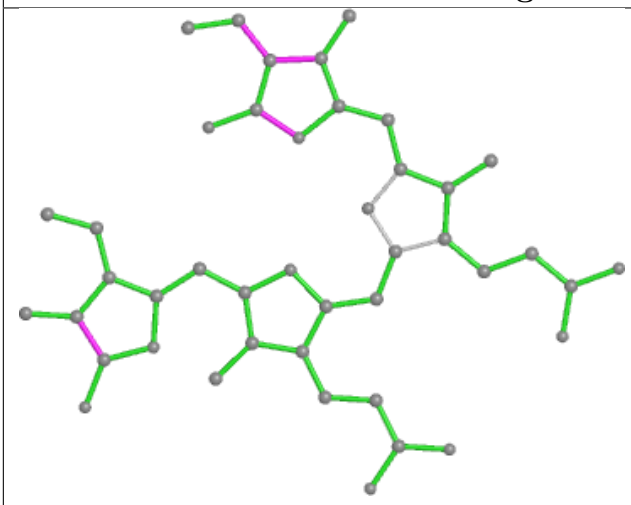


Rings

Ligand PEB cR 201



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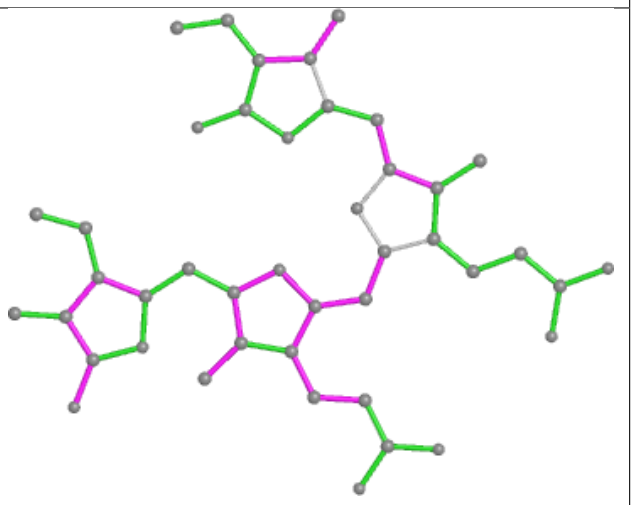

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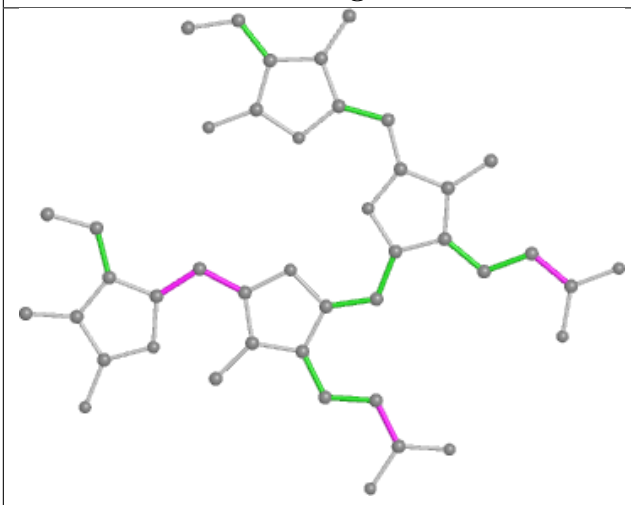

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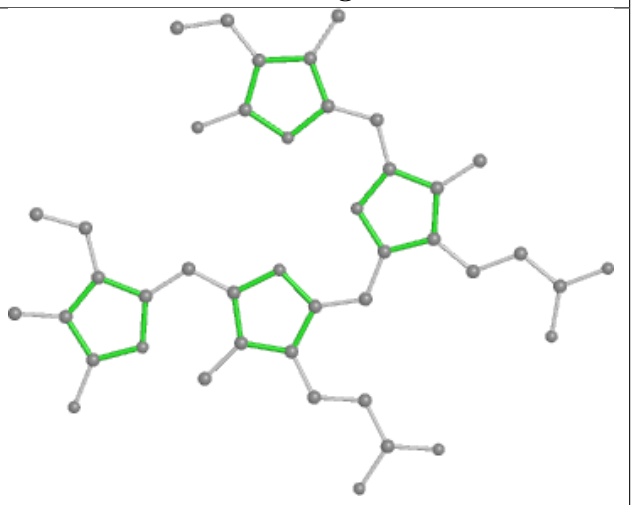
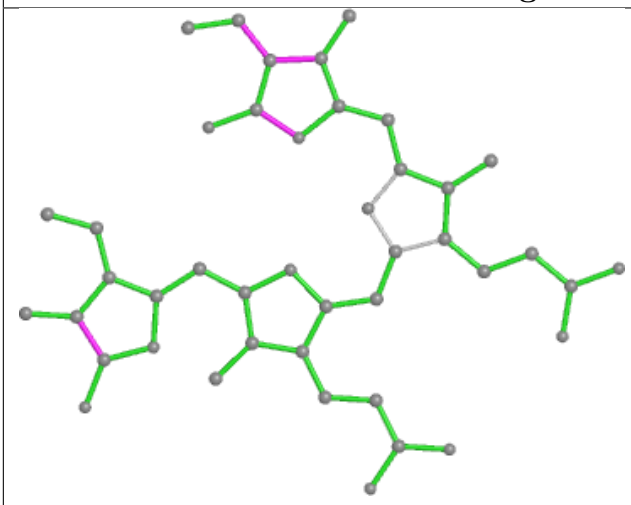


Rings

Ligand PEB v9 201



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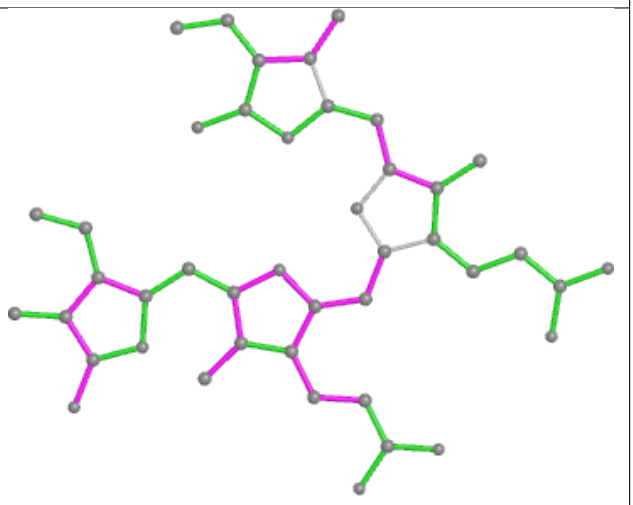

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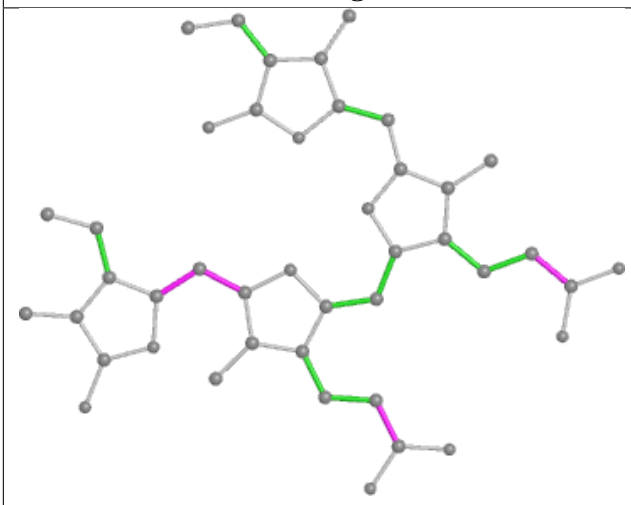

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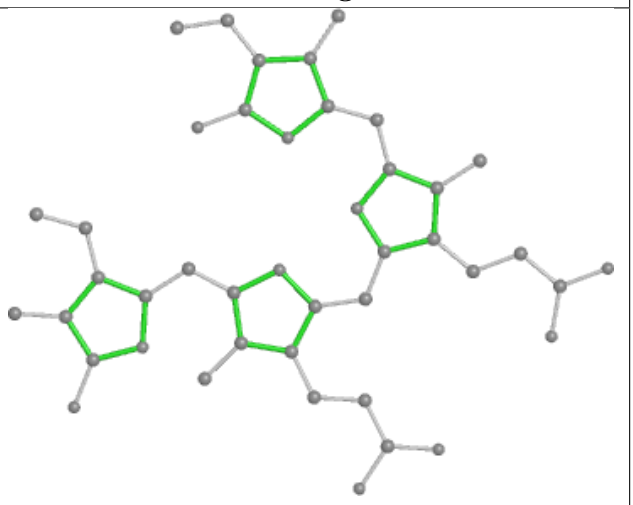
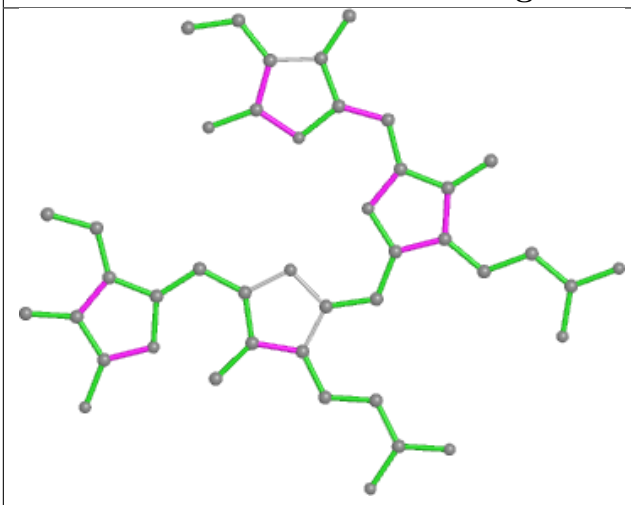


Rings

Ligand PUB Z5 306



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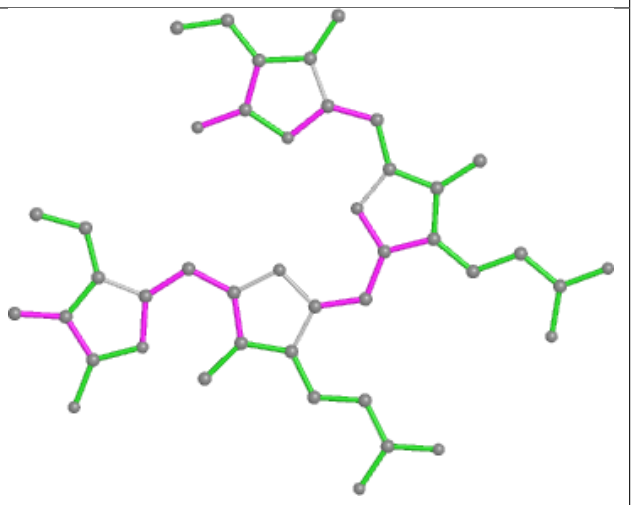

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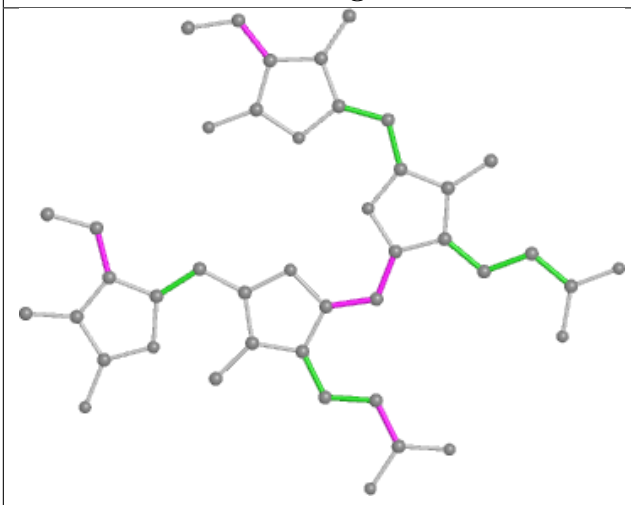

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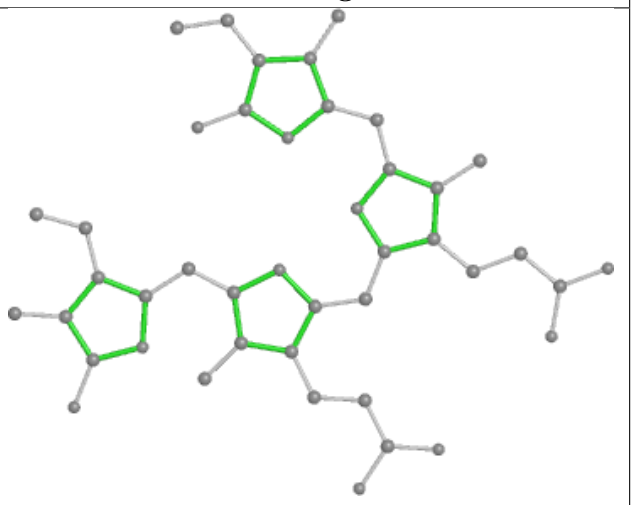
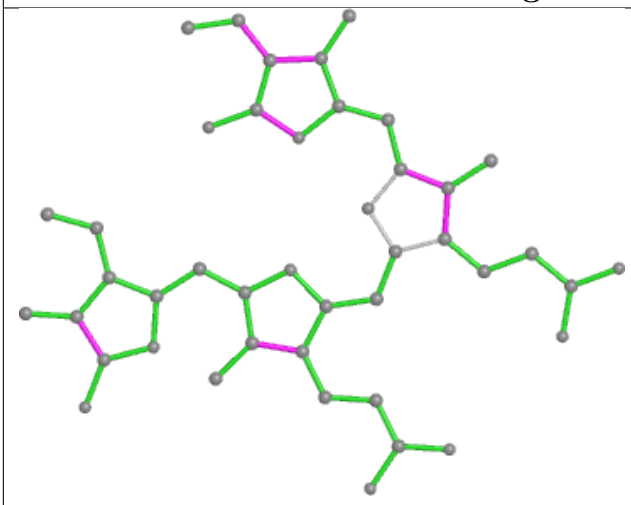


Rings

Ligand PEB lp 202



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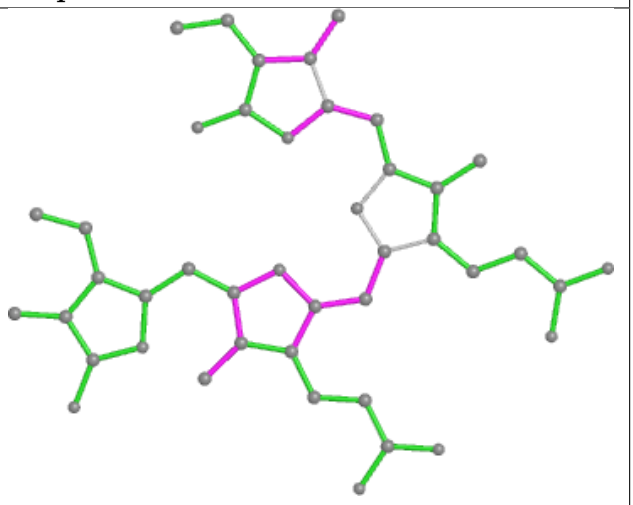

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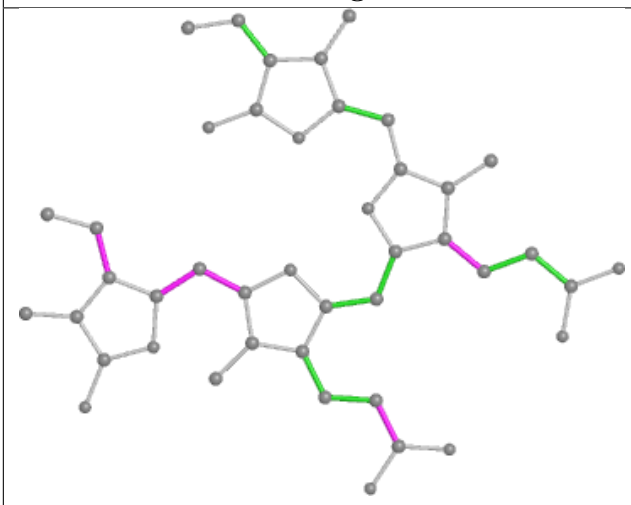

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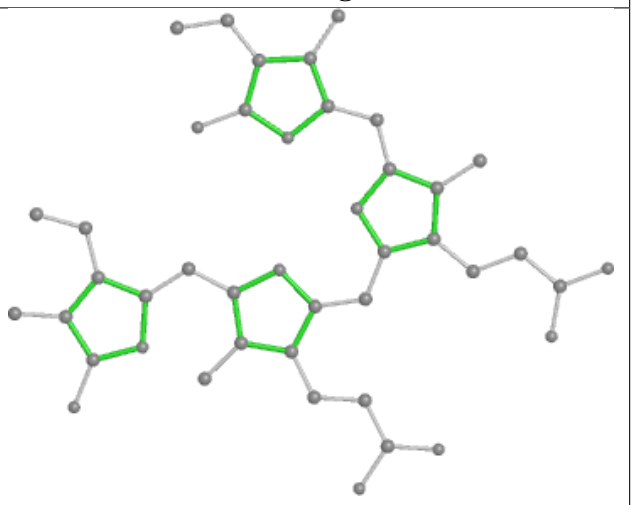
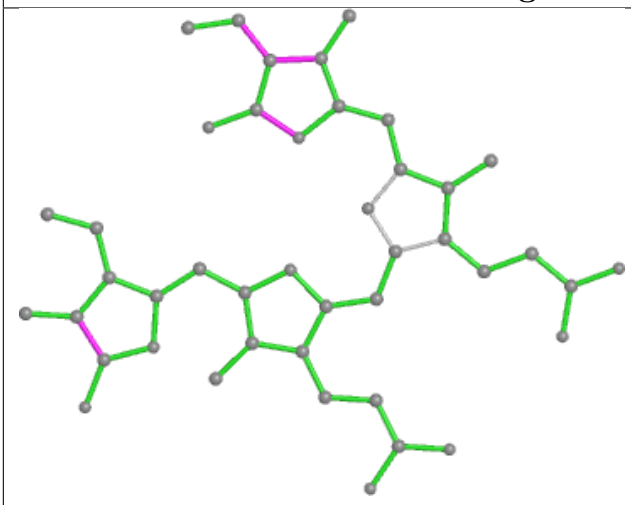


Rings

Ligand PEB b9 402



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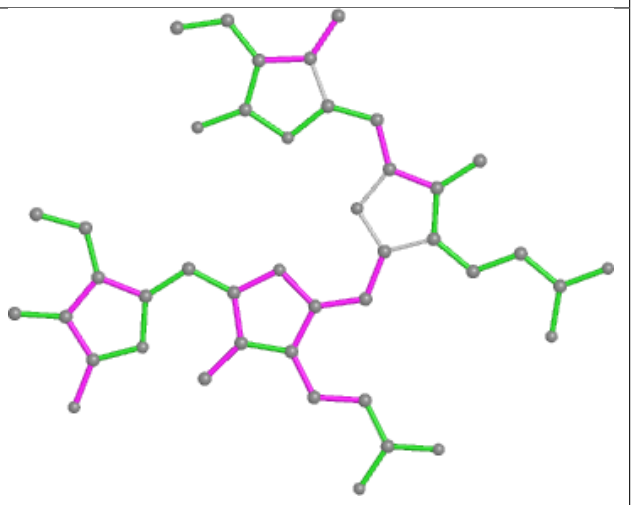

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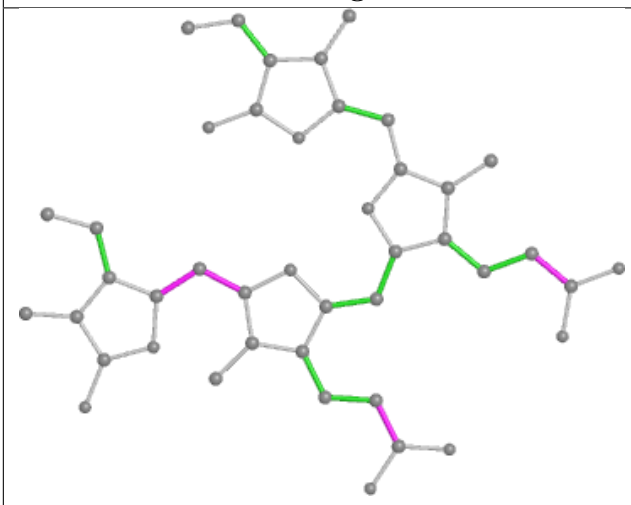

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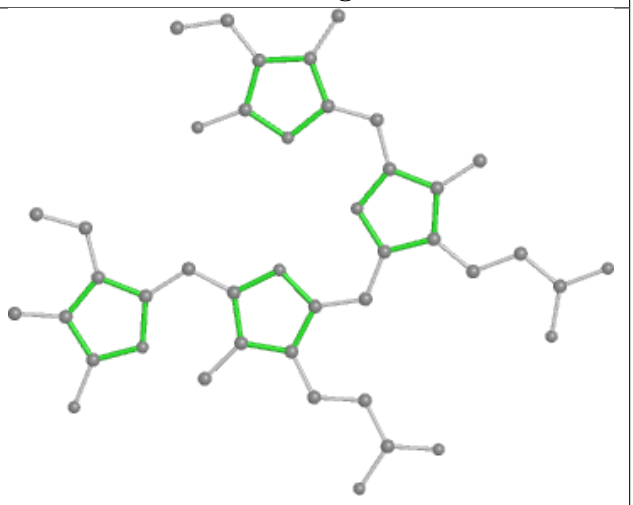
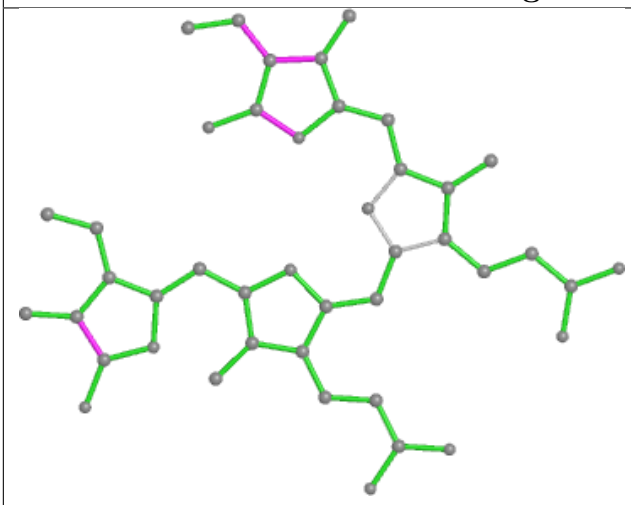


Rings

Ligand PEB lb 201



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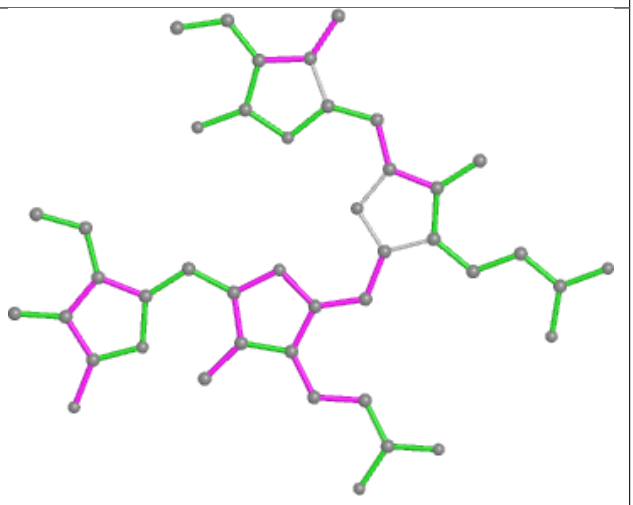
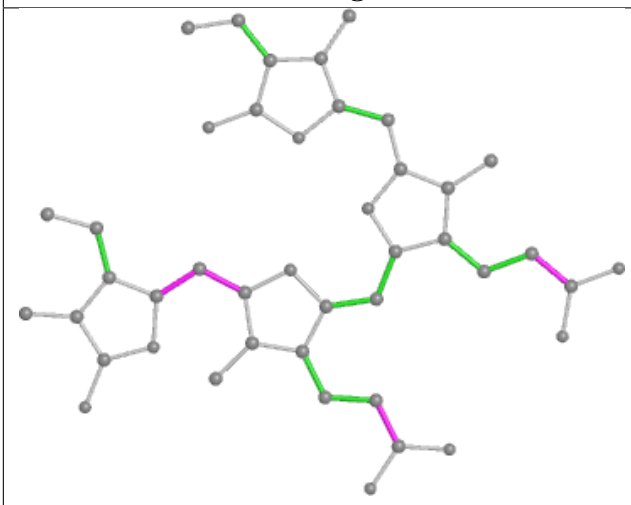
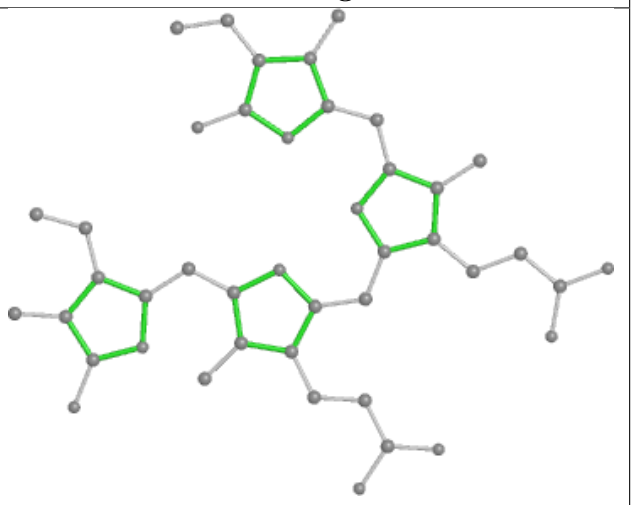


Bond angles

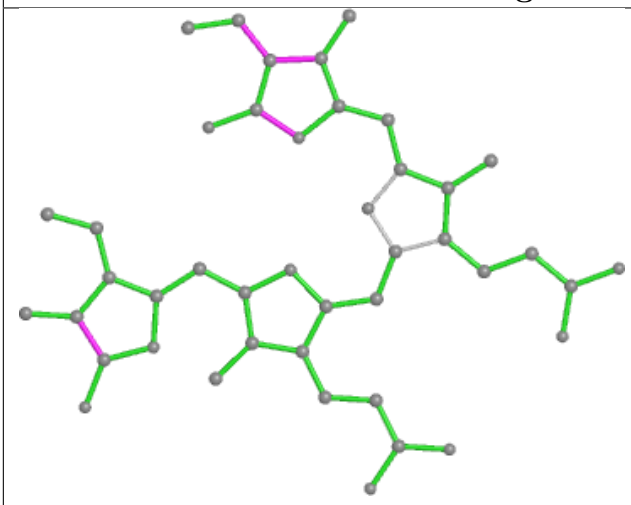


Torsions



Rings

Ligand PEB C6 202



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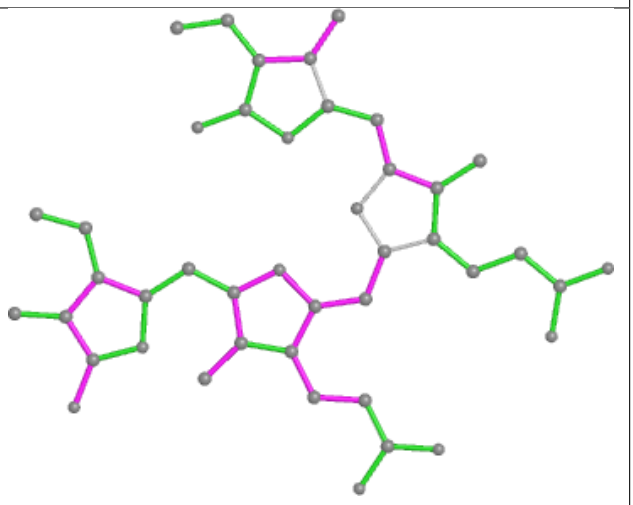

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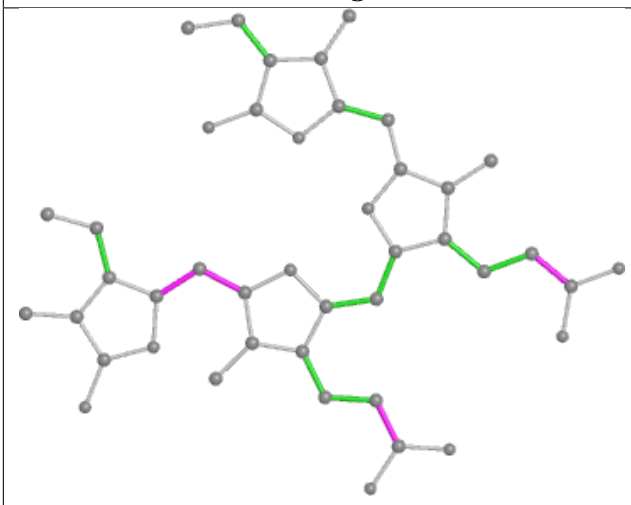

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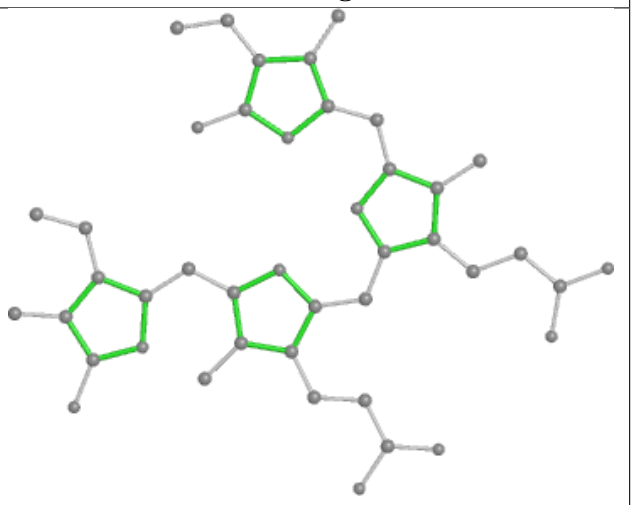
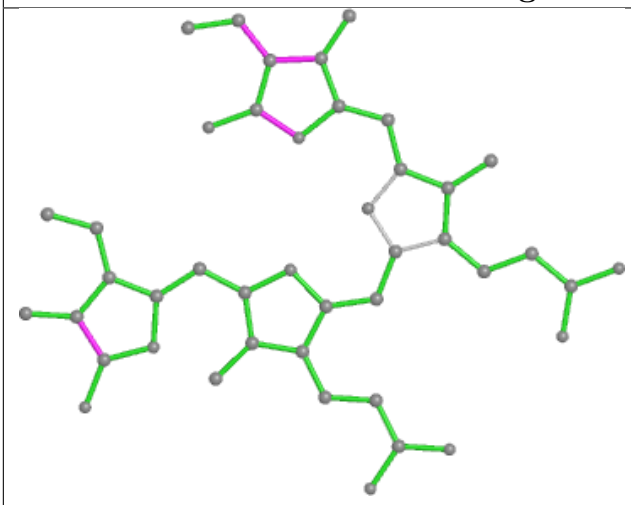


Rings

Ligand PEB h6 201



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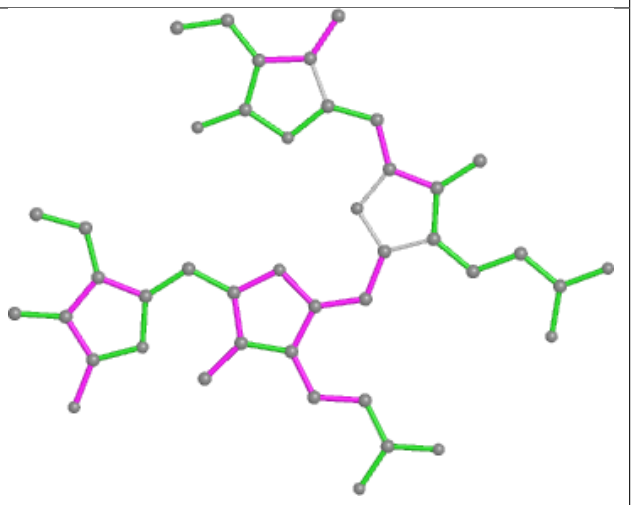

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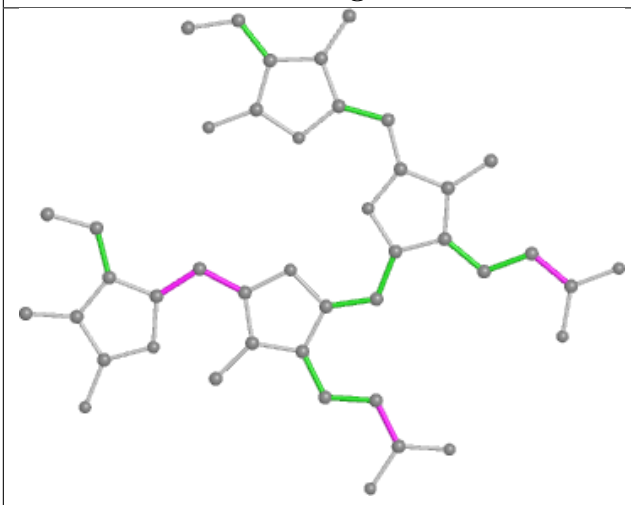

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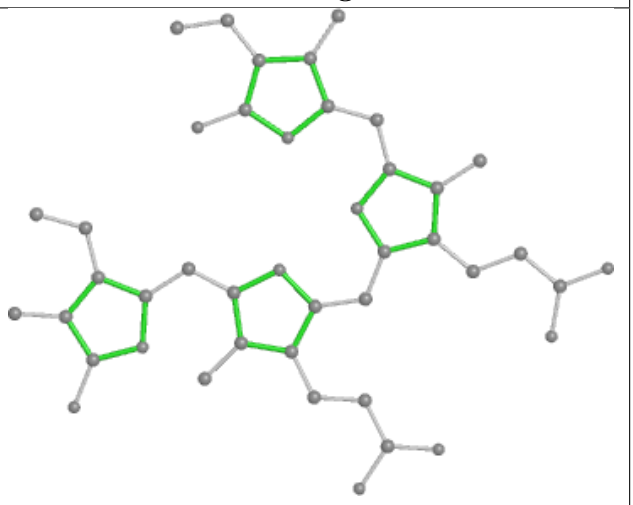
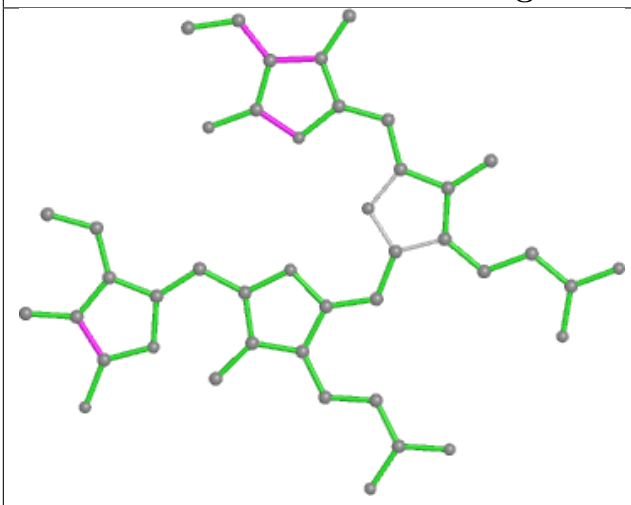


Rings

Ligand PEB cD 201



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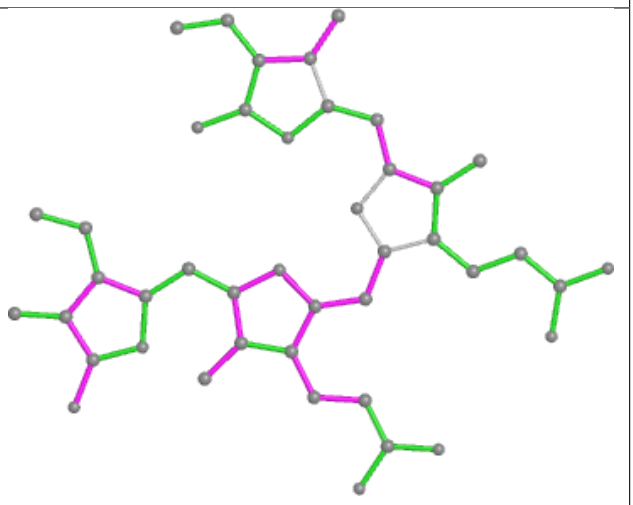

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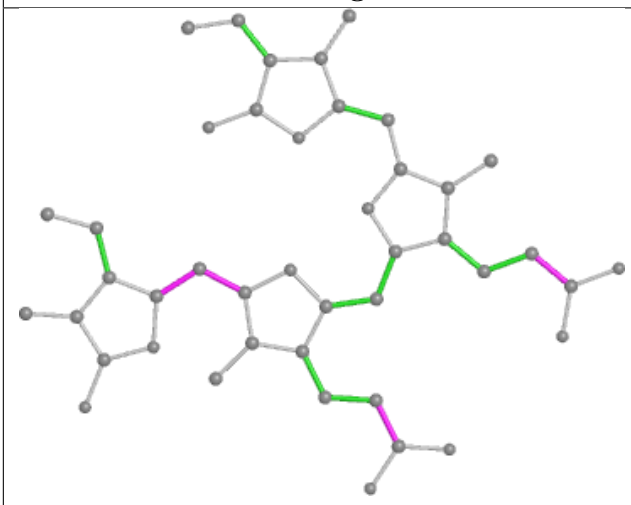

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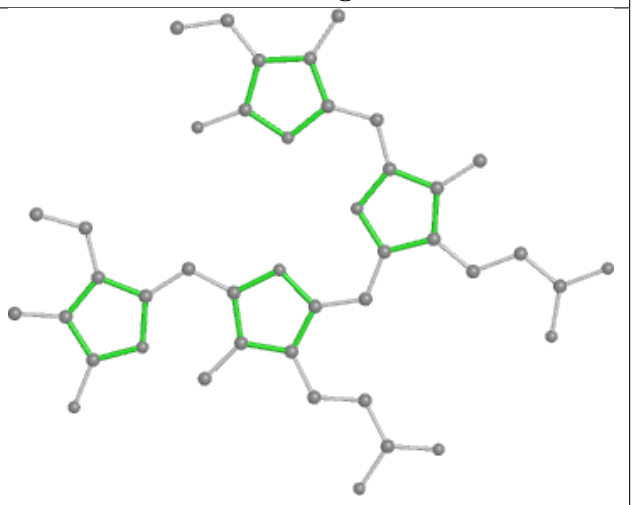
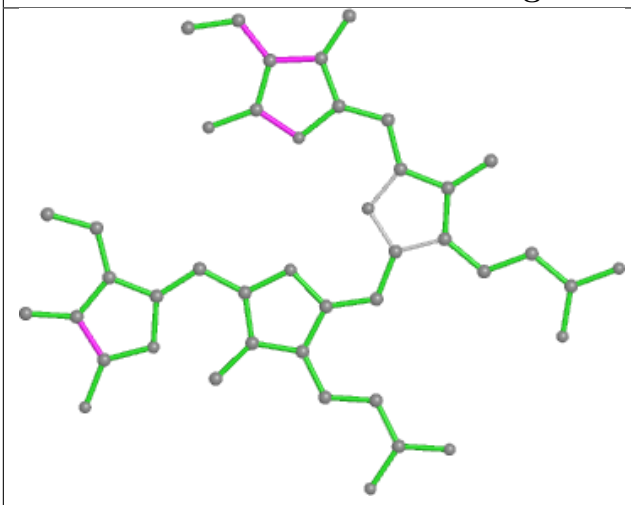


Rings

Ligand PEB j2 201



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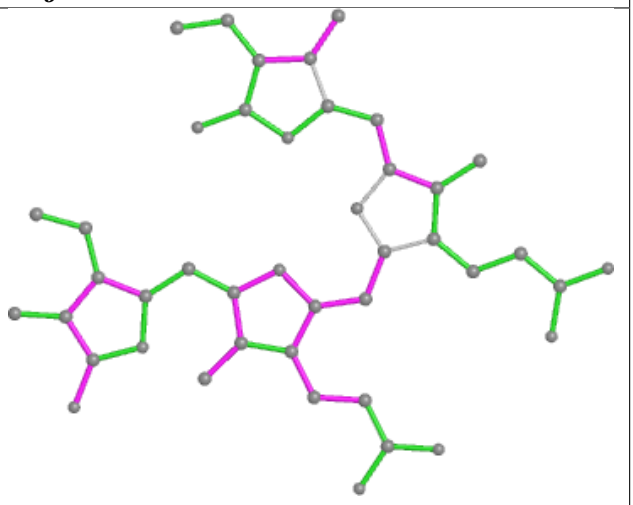

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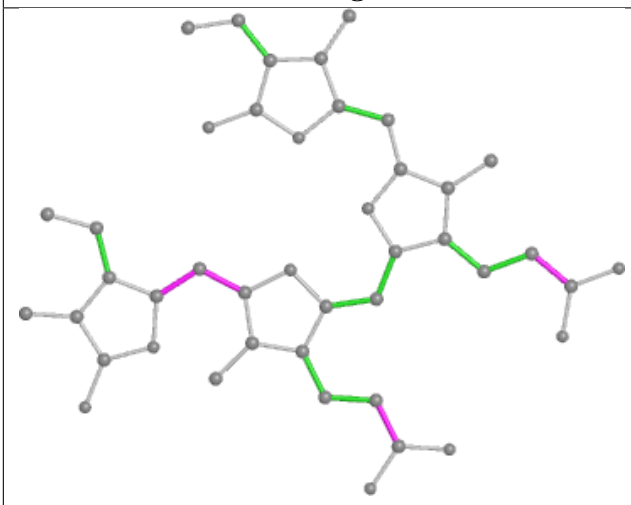

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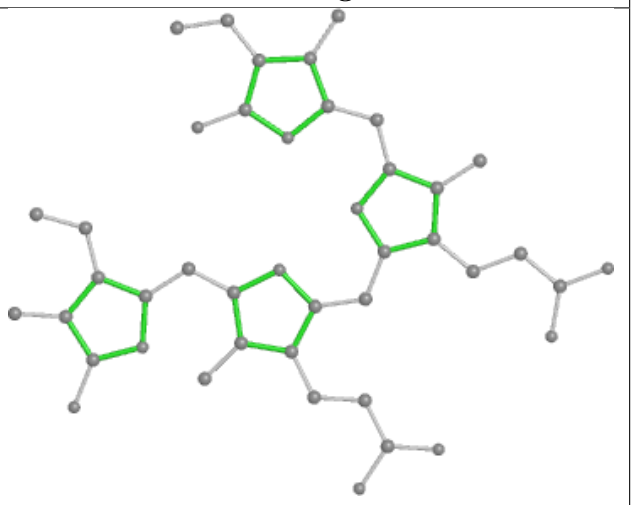

Rings

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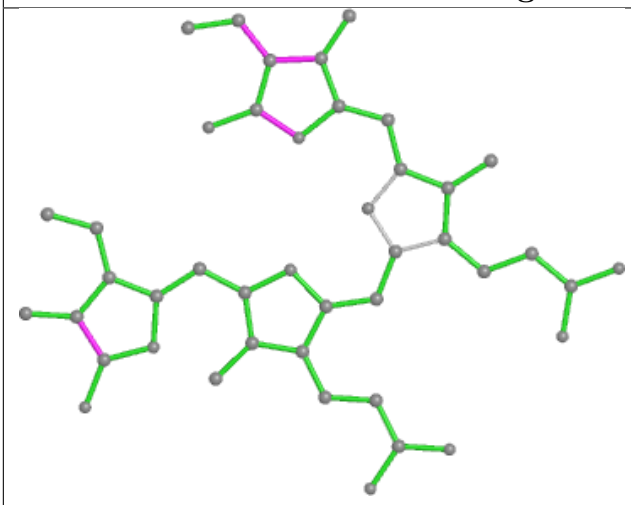

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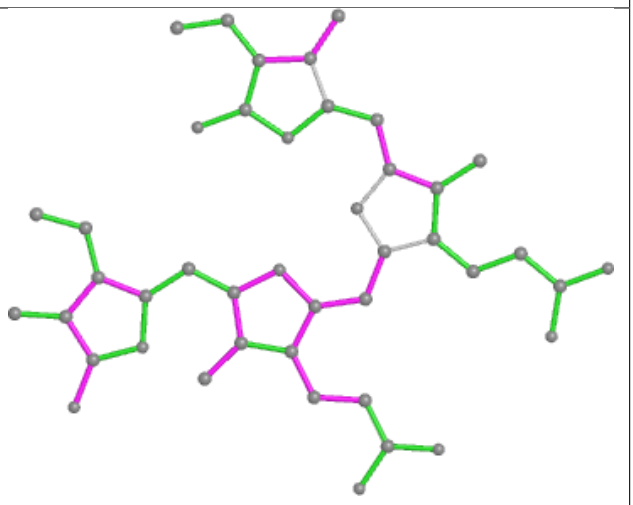

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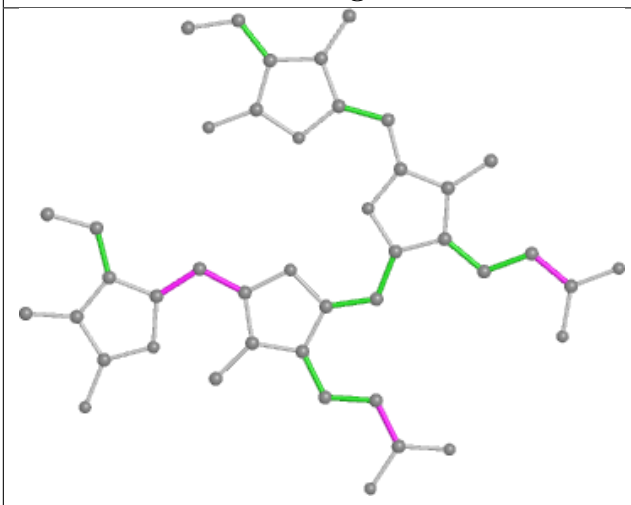

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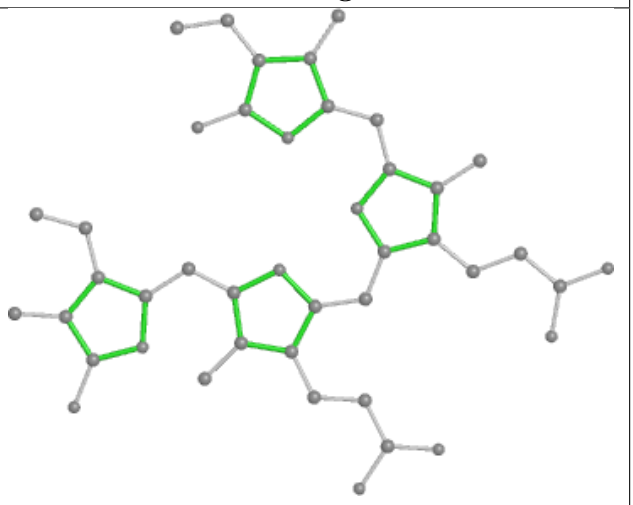
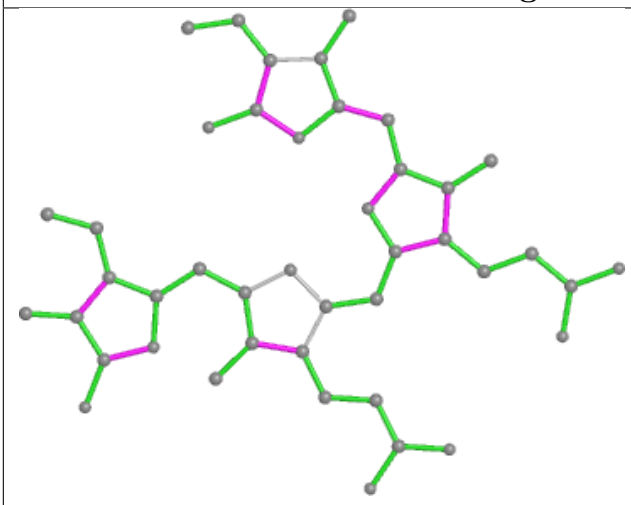


Rings

Ligand PUB cz 203



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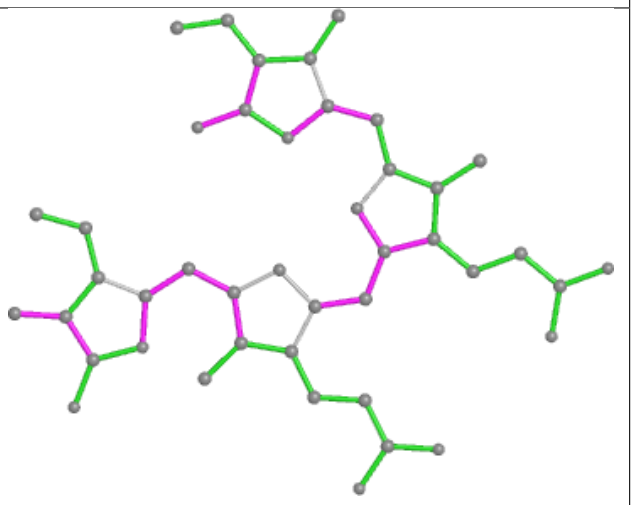

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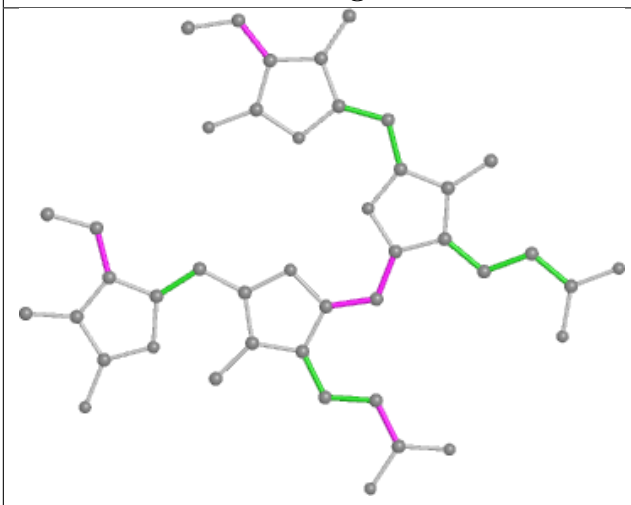

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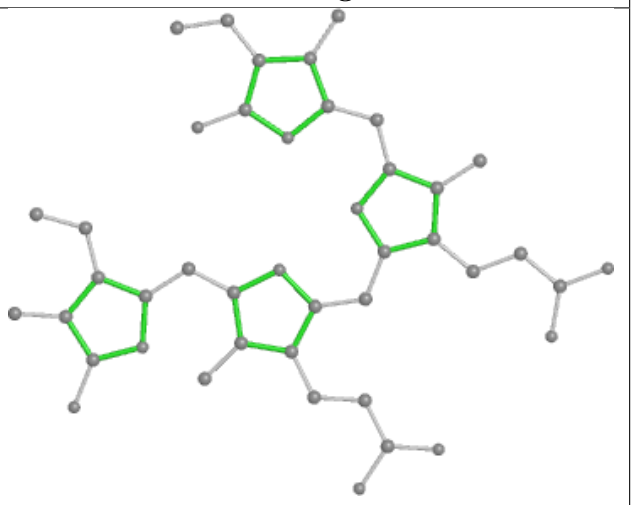
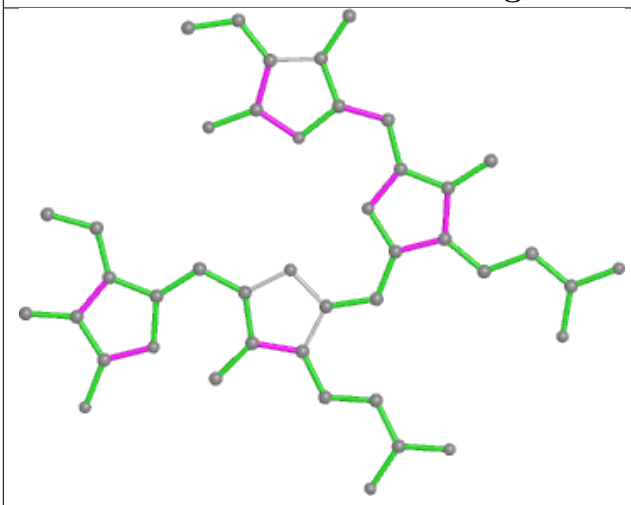


Rings

Ligand PUB U8 1006



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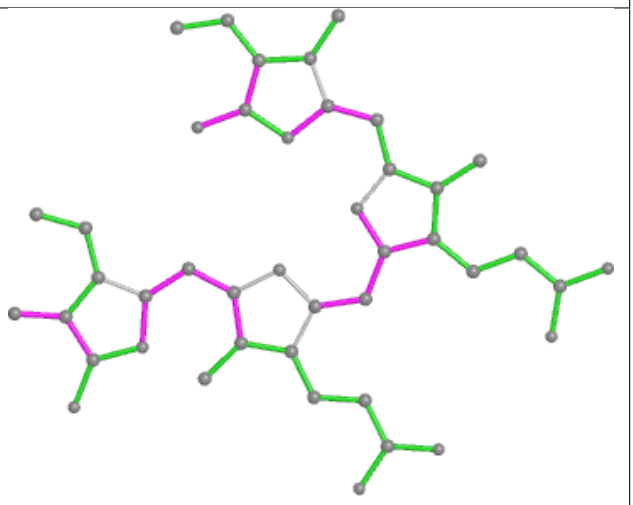

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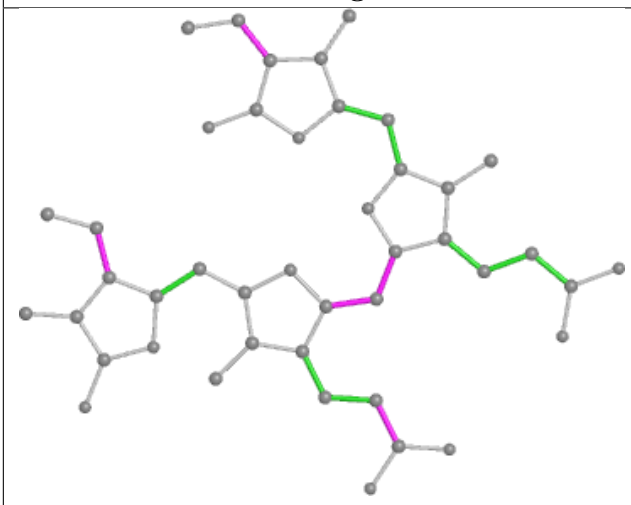

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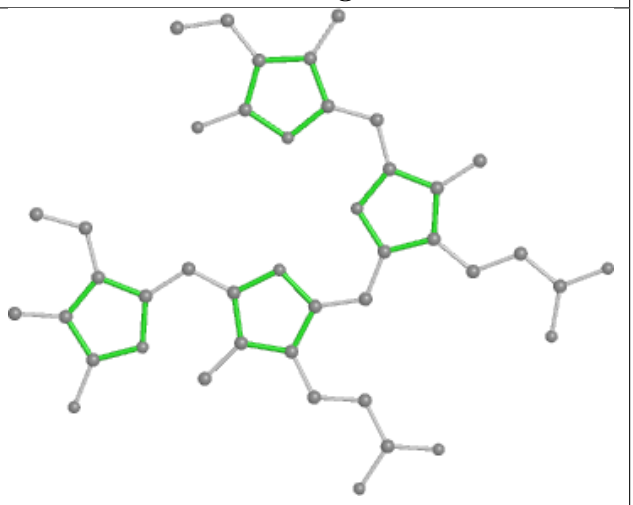
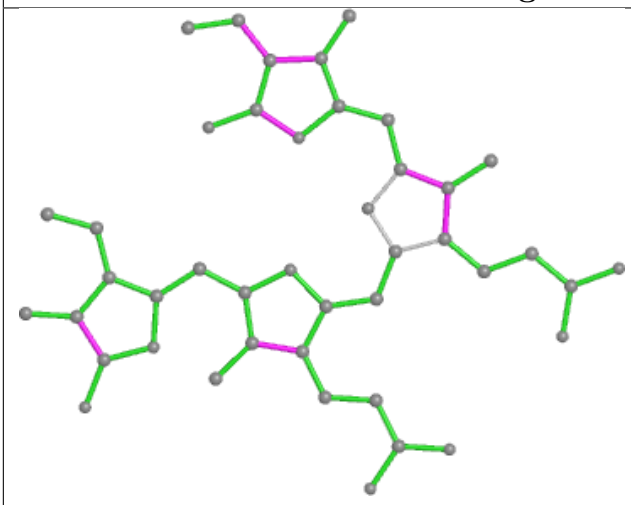


Rings

Ligand PEB p8 202



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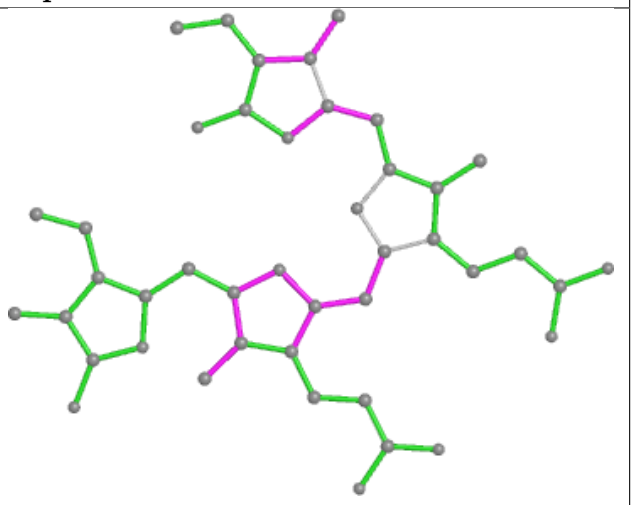

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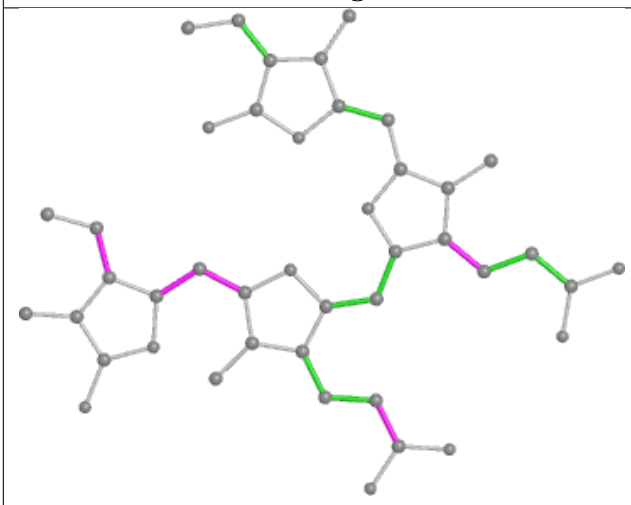

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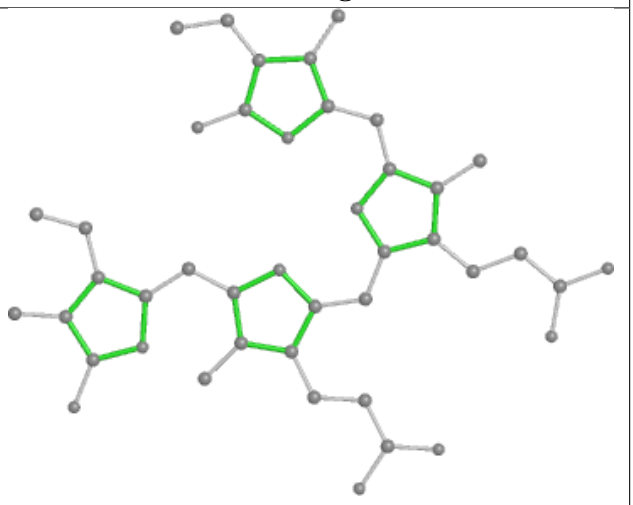
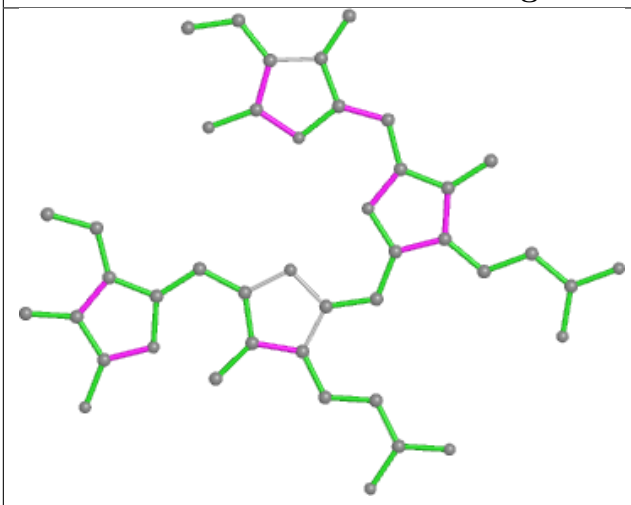


Rings

Ligand PUB cs 203



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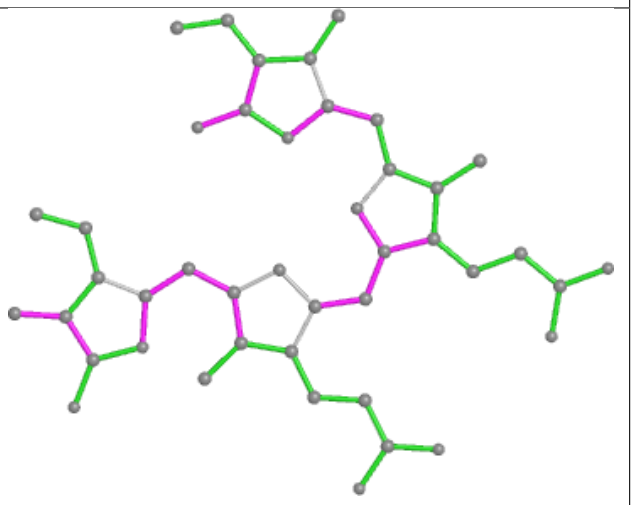

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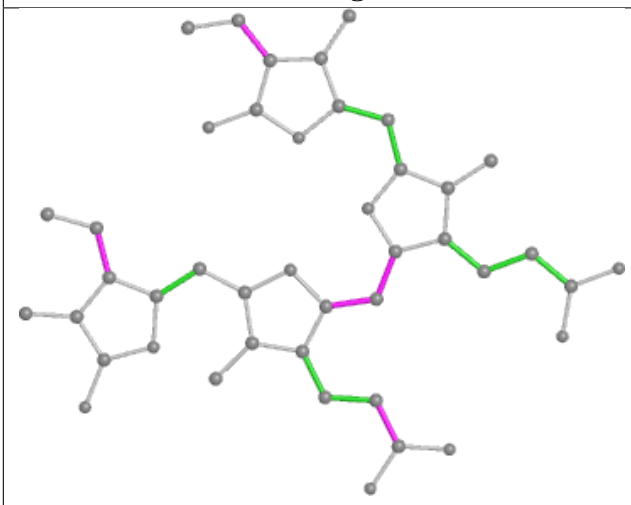

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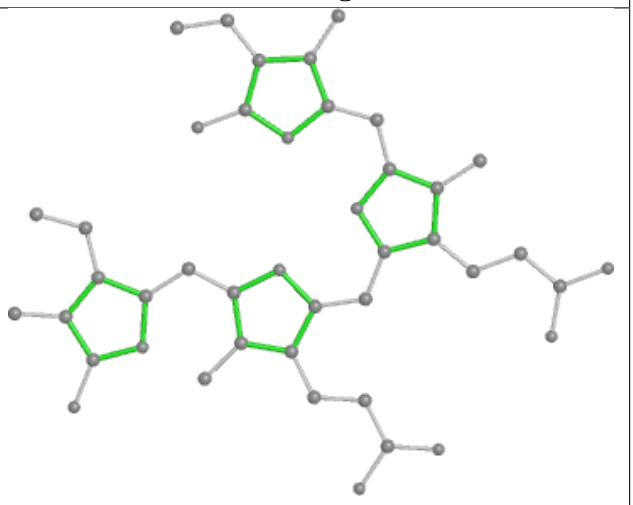
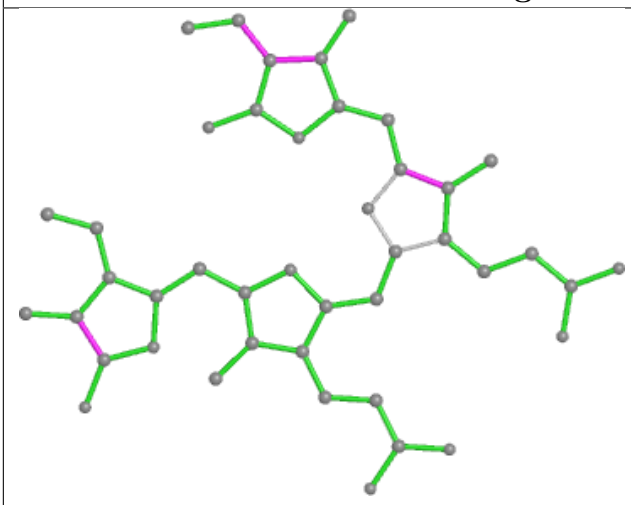


Rings

Ligand PEB hQ 202



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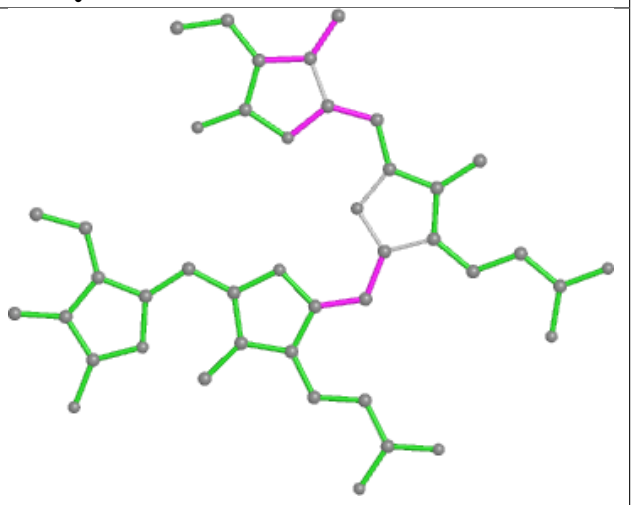

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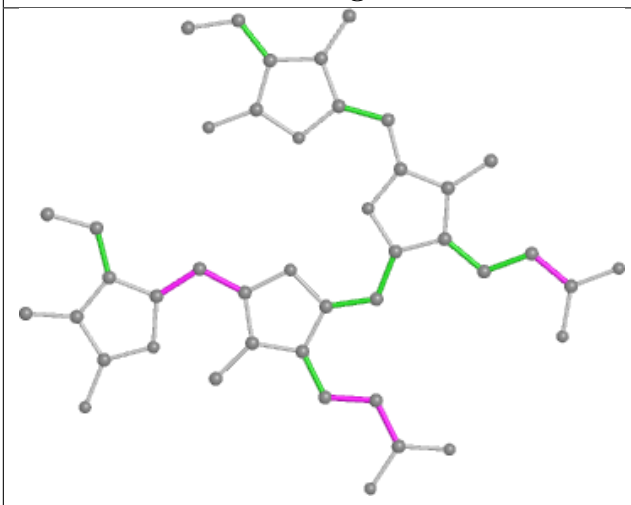

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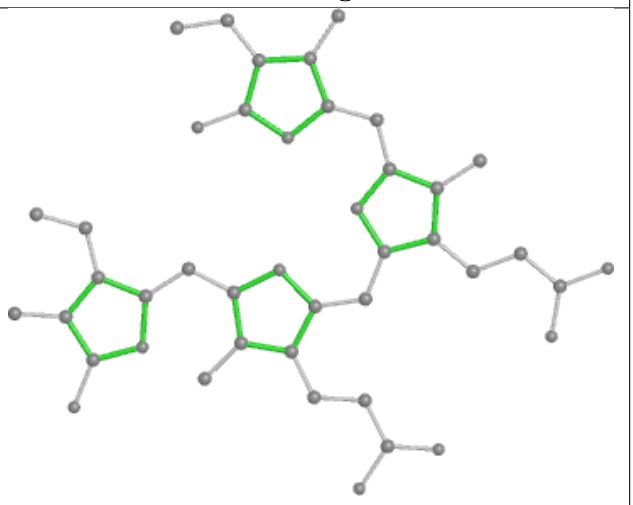
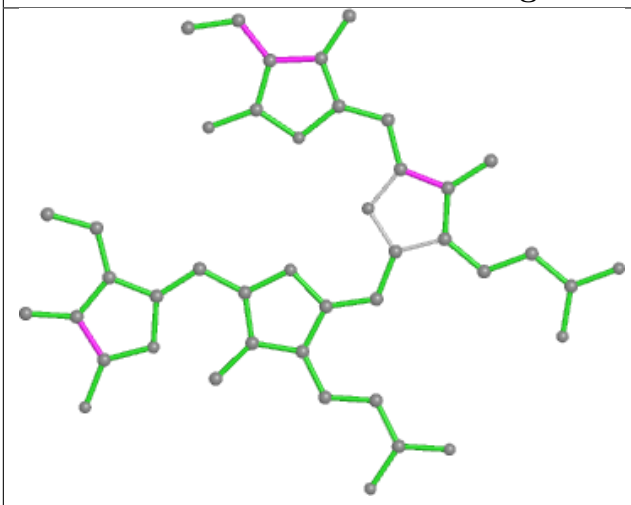


Rings

Ligand PEB lw 202



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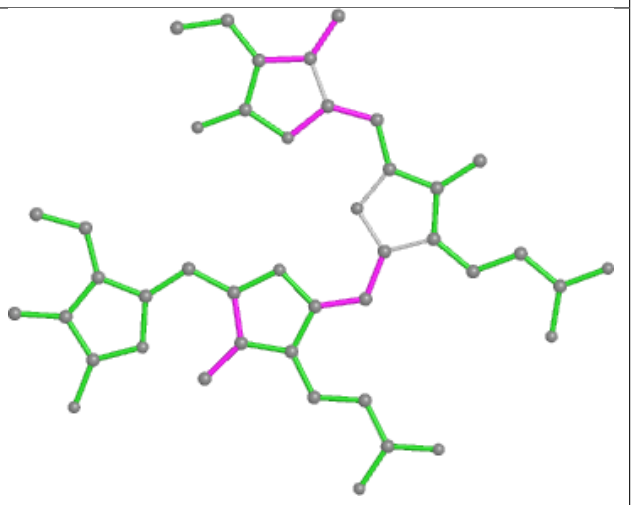

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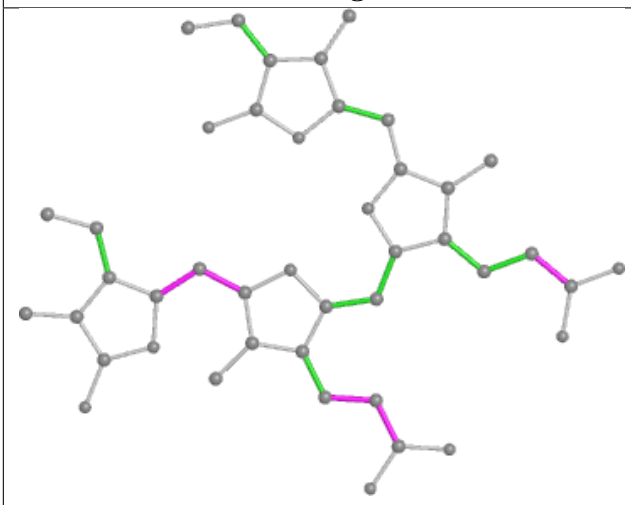

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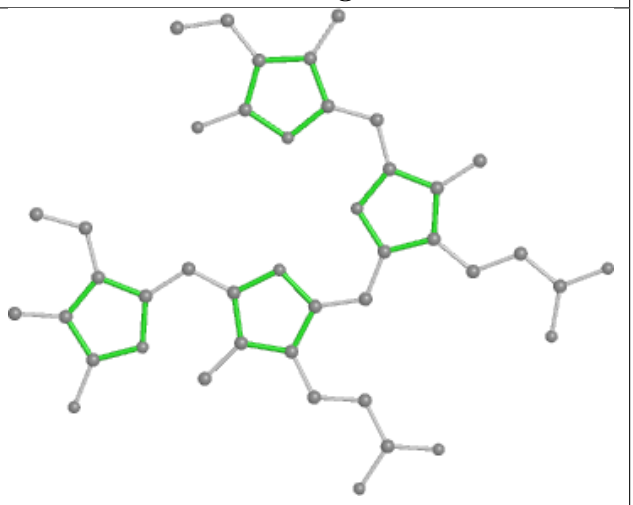
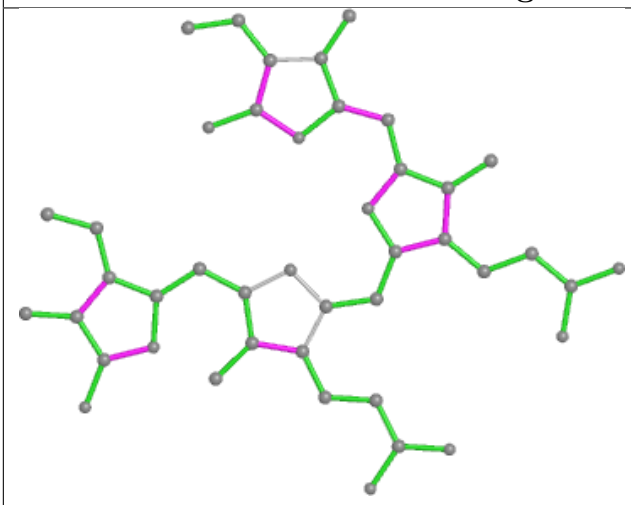


Rings

Ligand PUB d6 203



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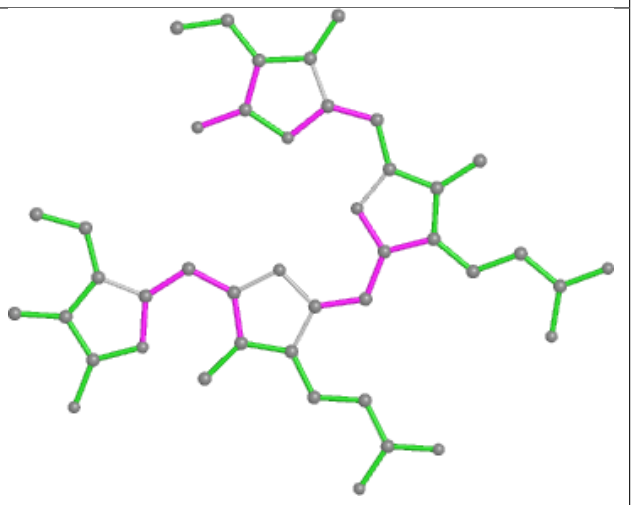

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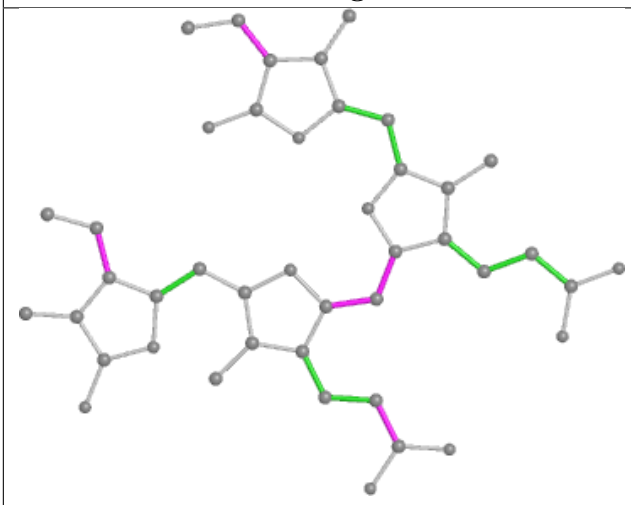

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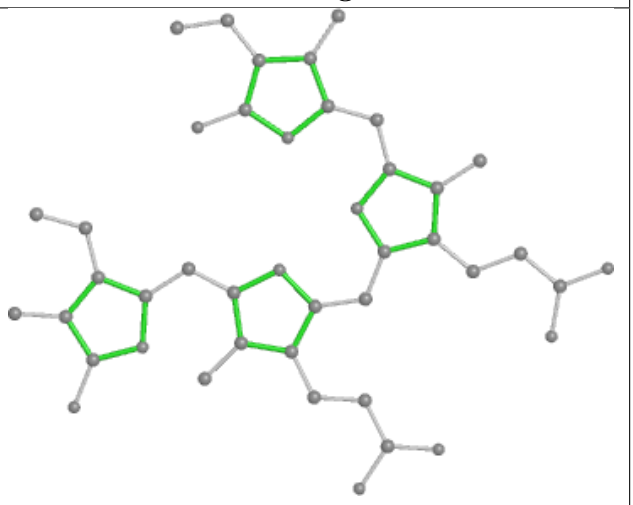
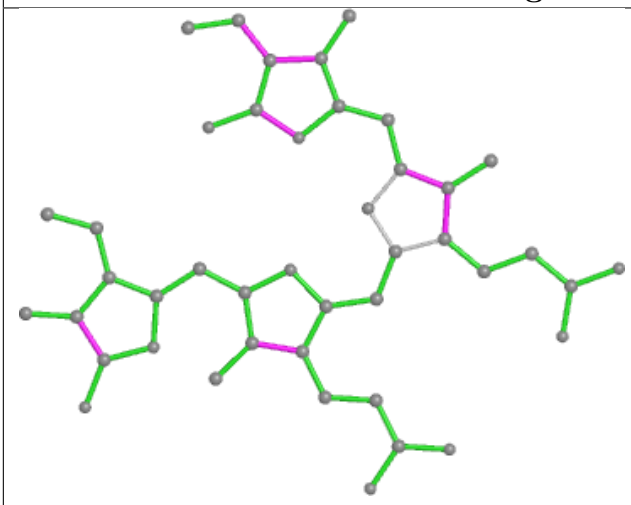


Rings

Ligand PEB lr 202



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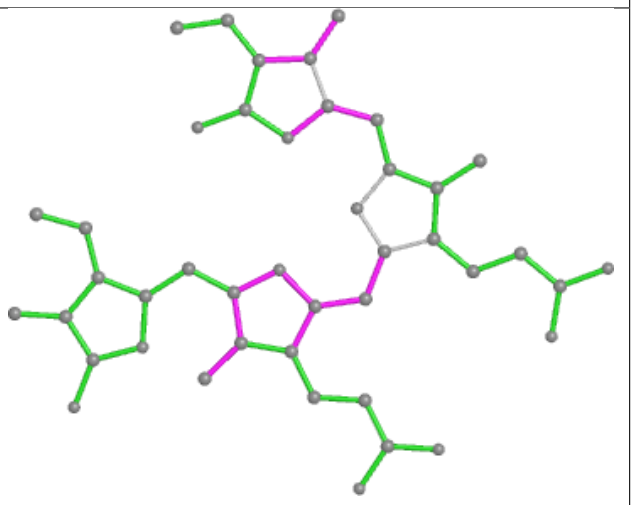

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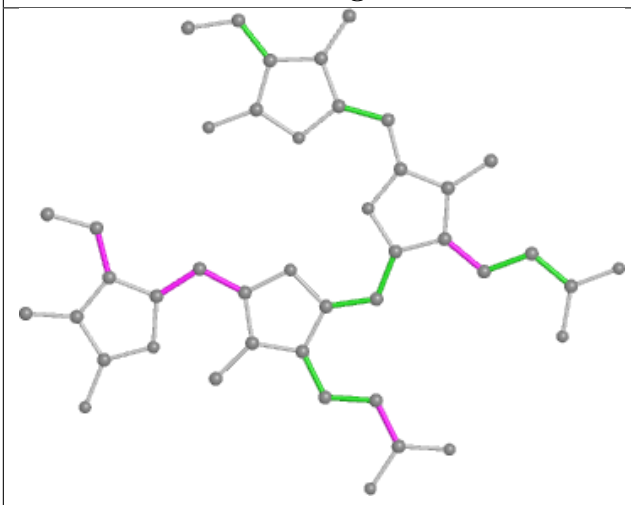

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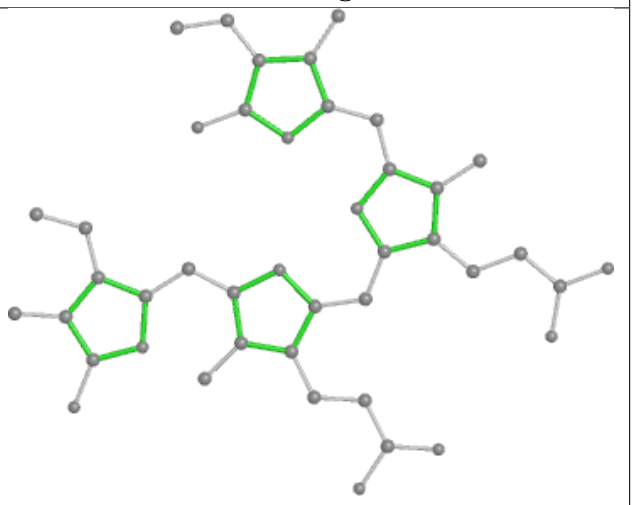
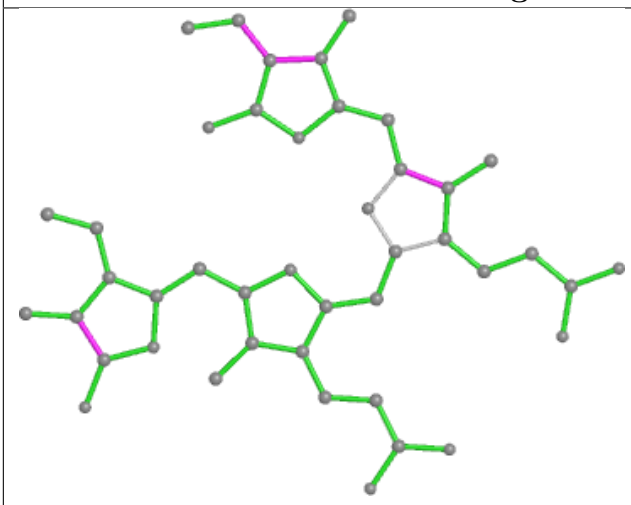


Rings

Ligand PEB bM 202



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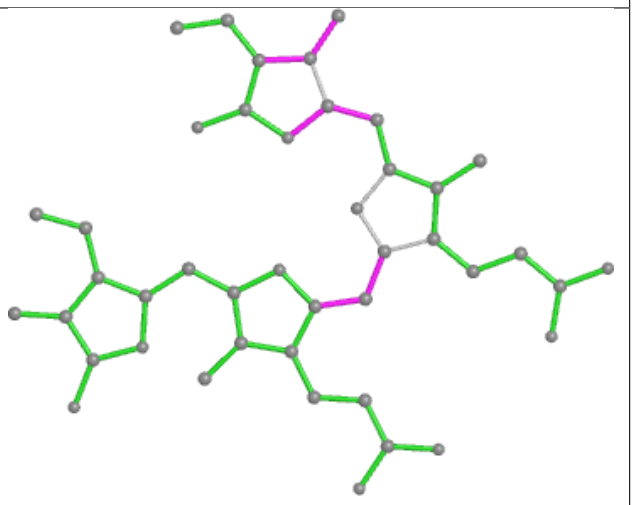

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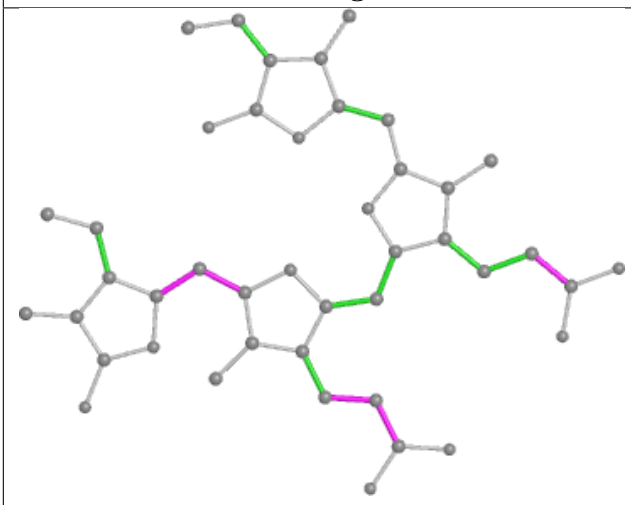
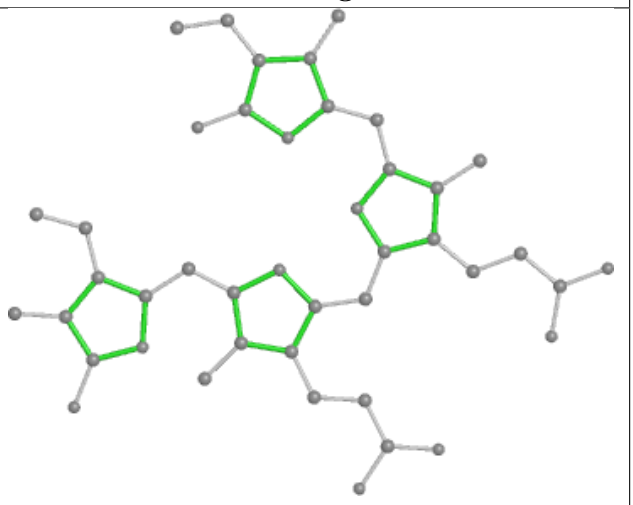
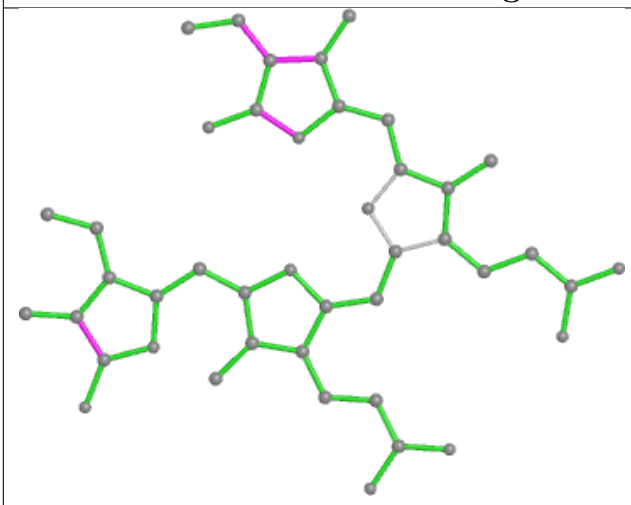


Torsions



Rings

Ligand PEB M6 1002



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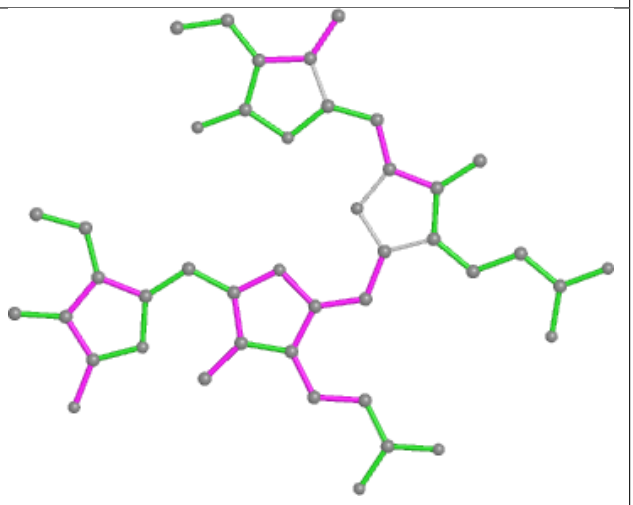

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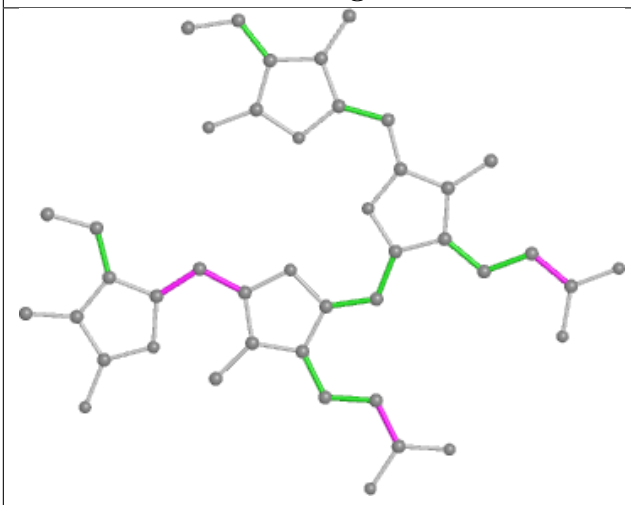

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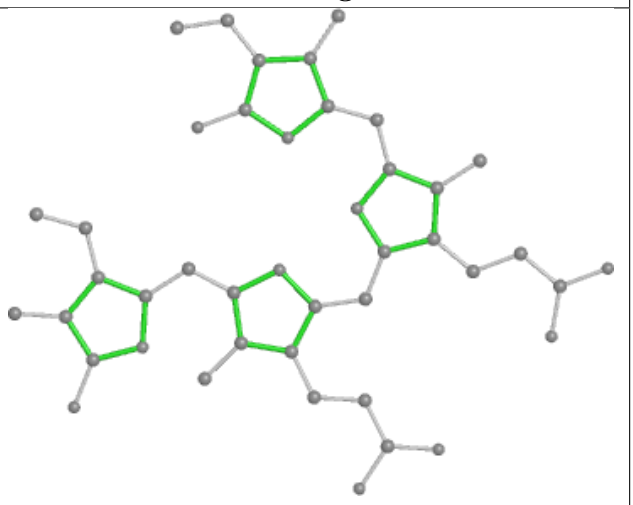

Rings

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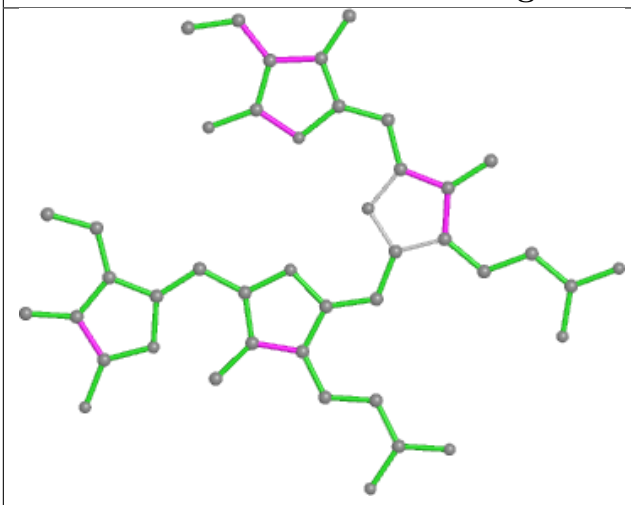

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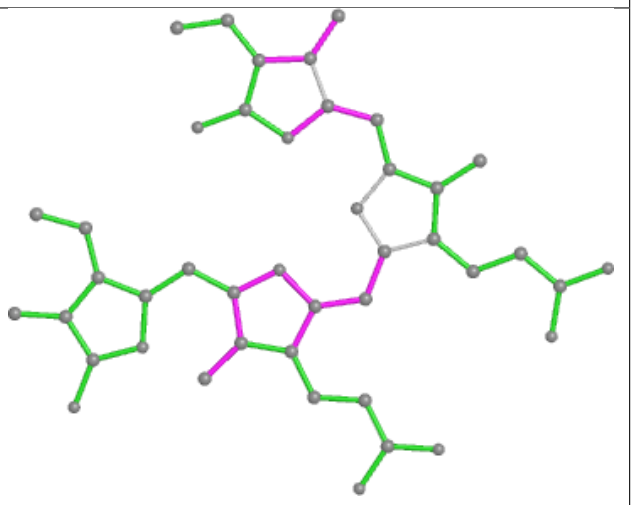

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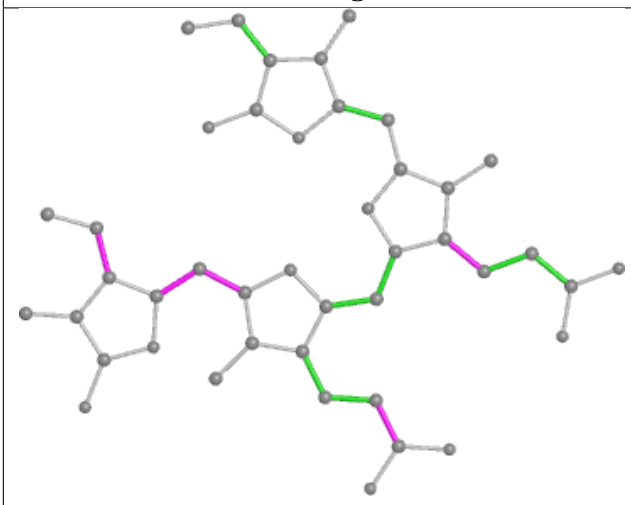

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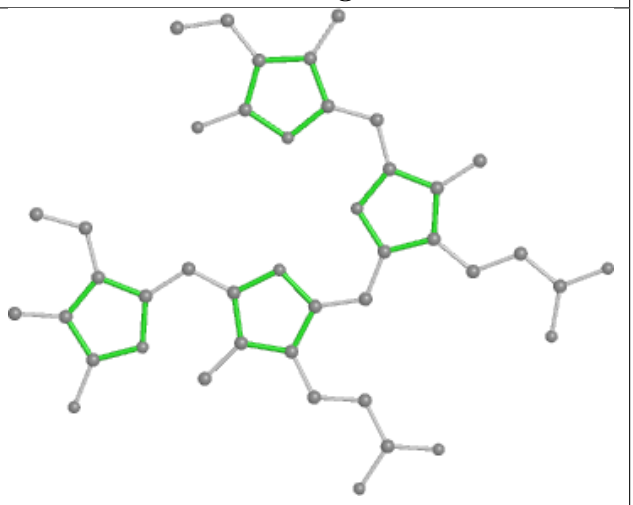

Rings

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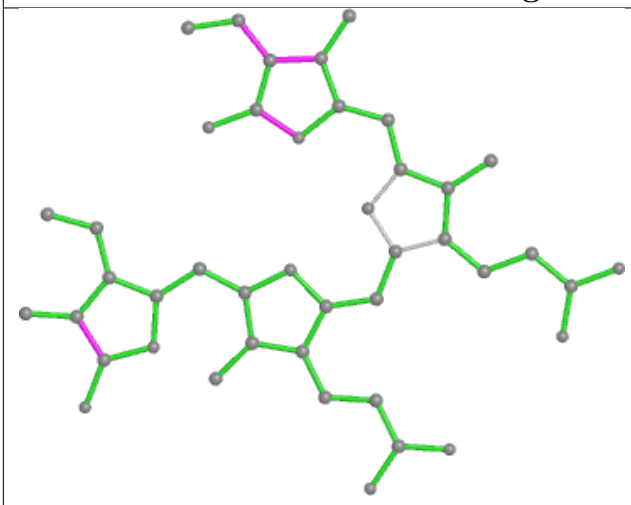

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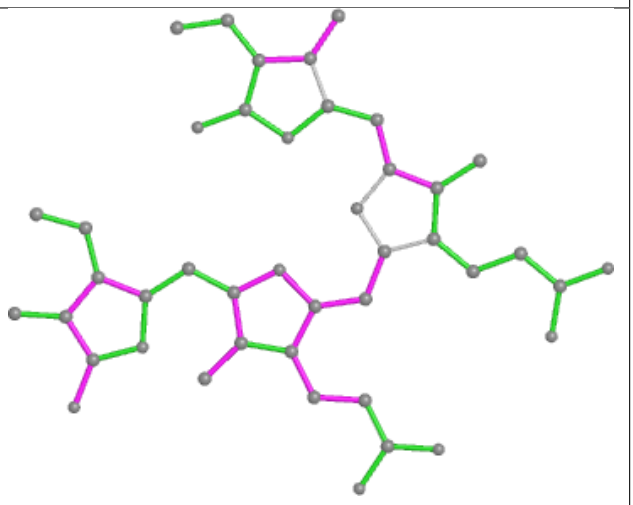

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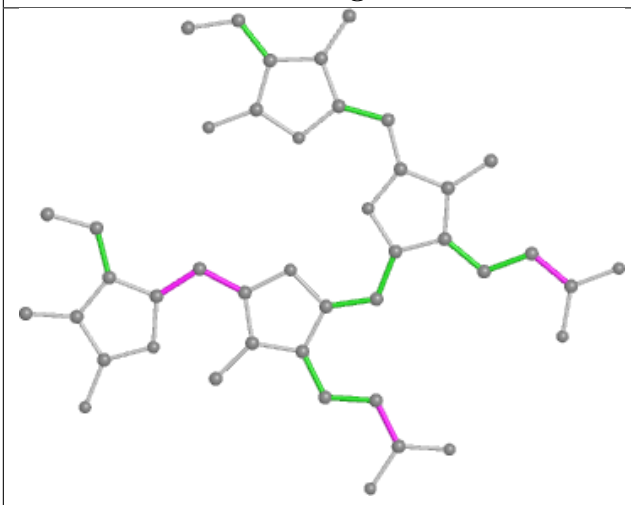

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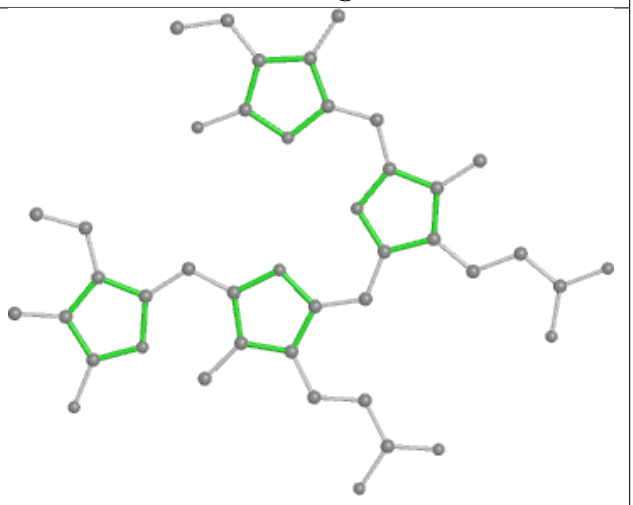

Rings

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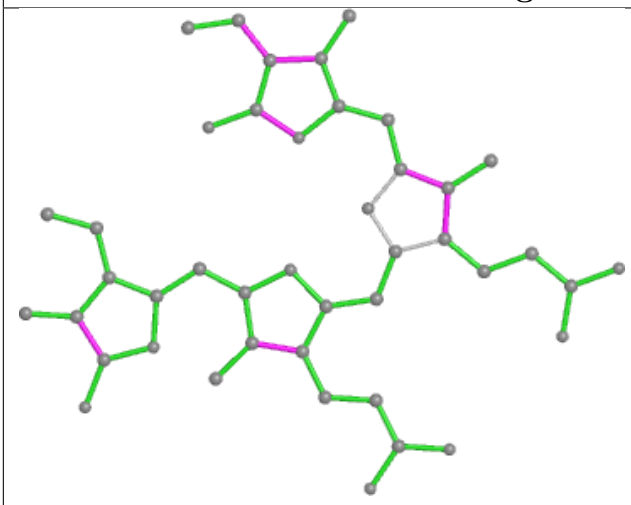

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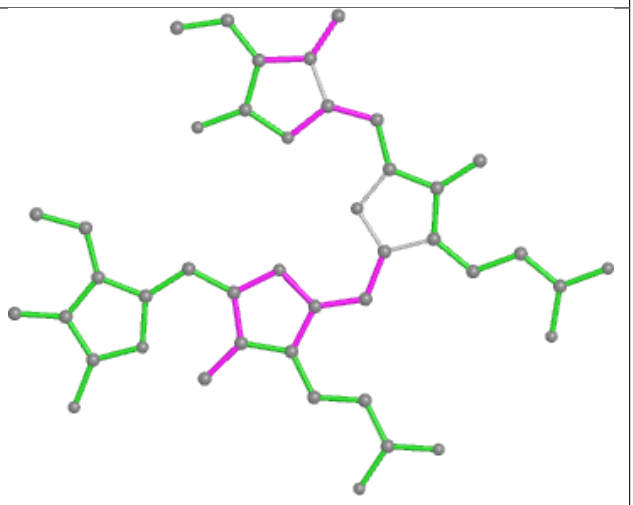

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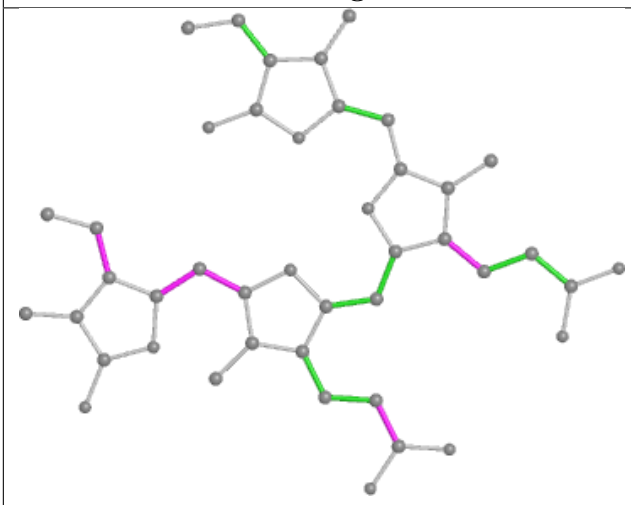

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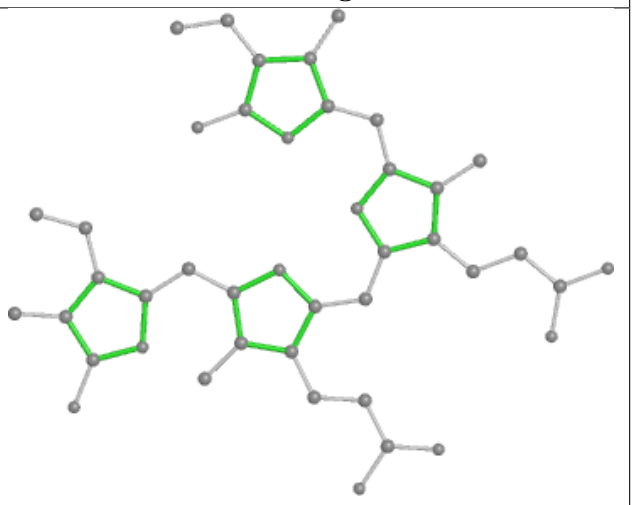

Rings

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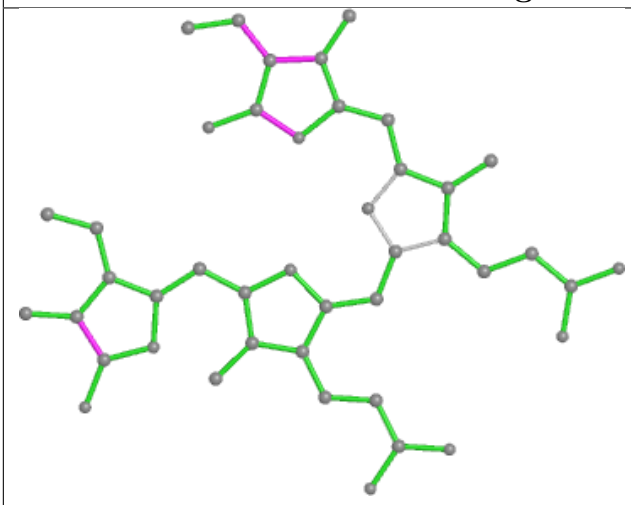

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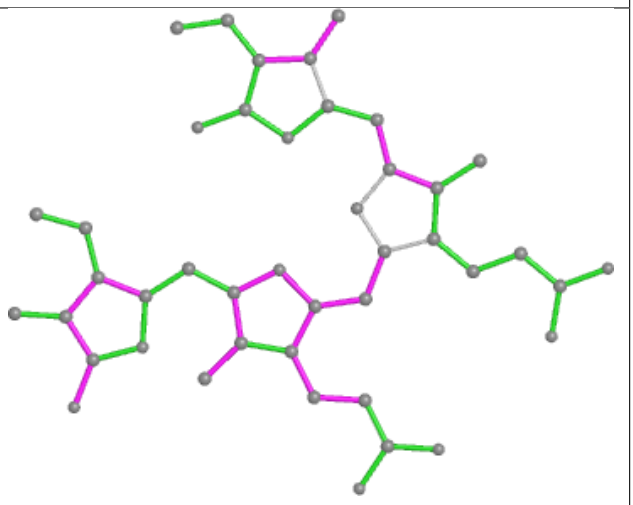

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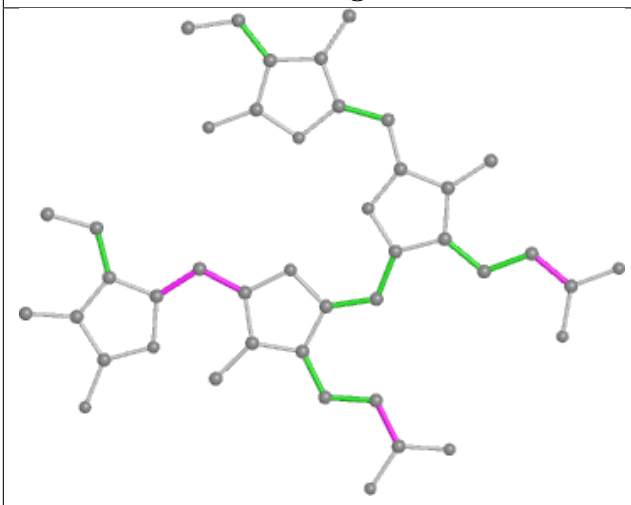

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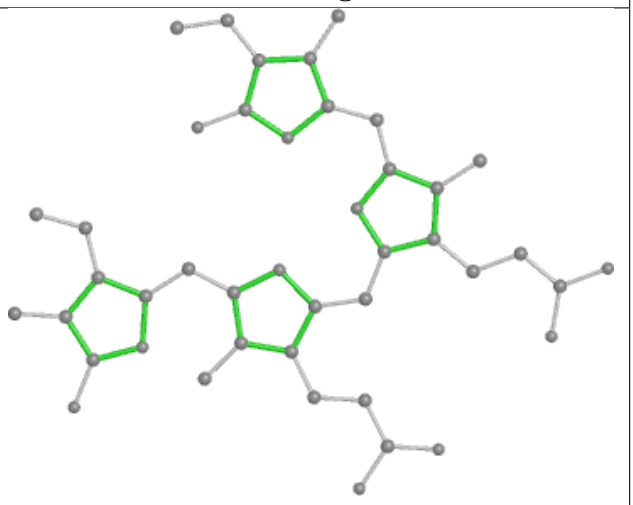

Rings

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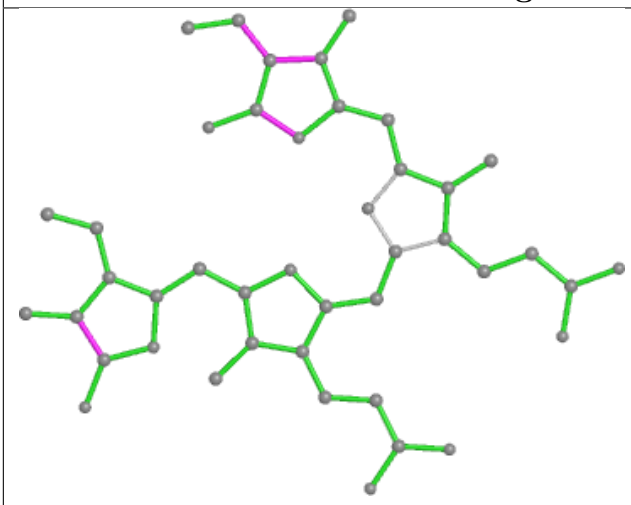

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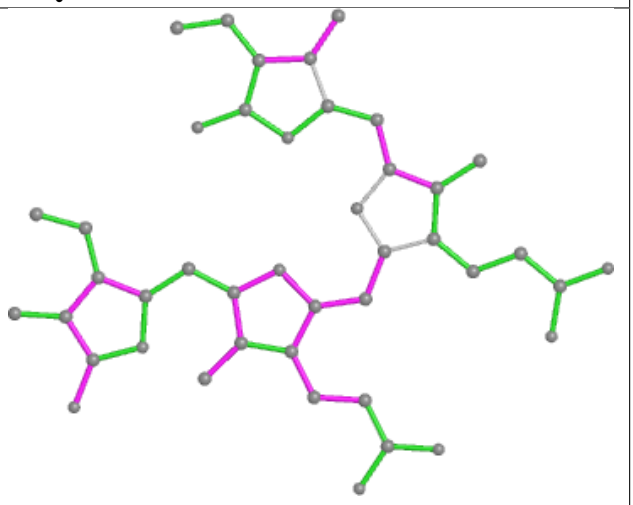

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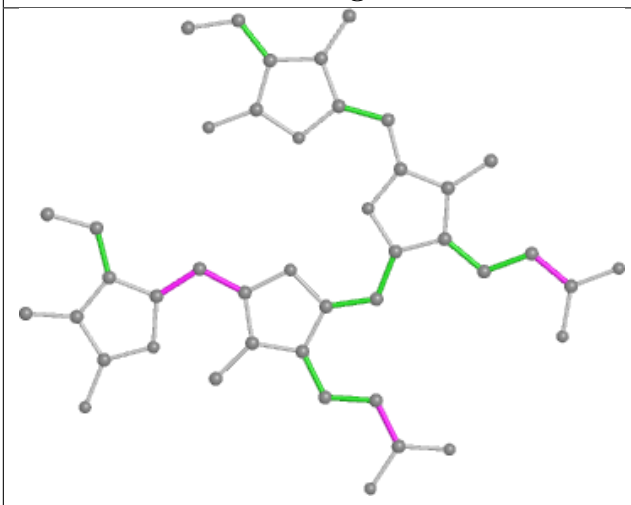

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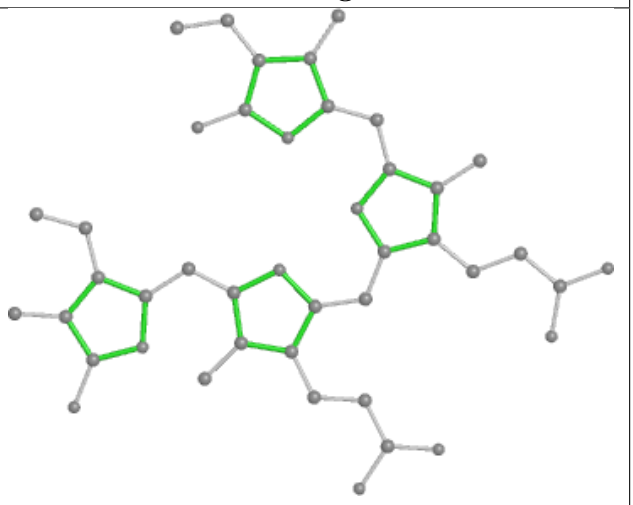

Rings

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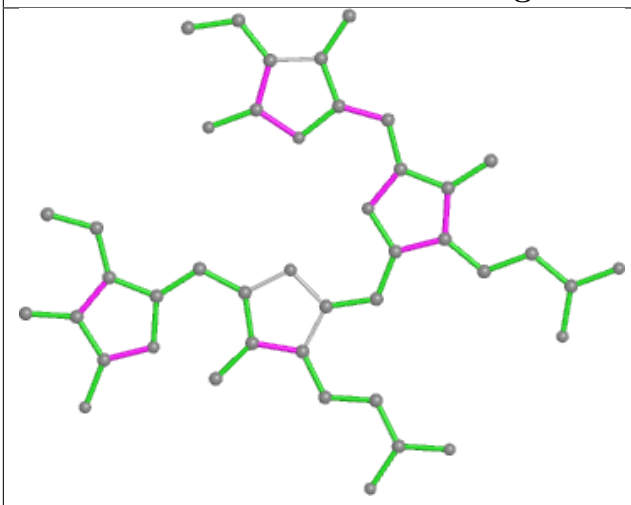

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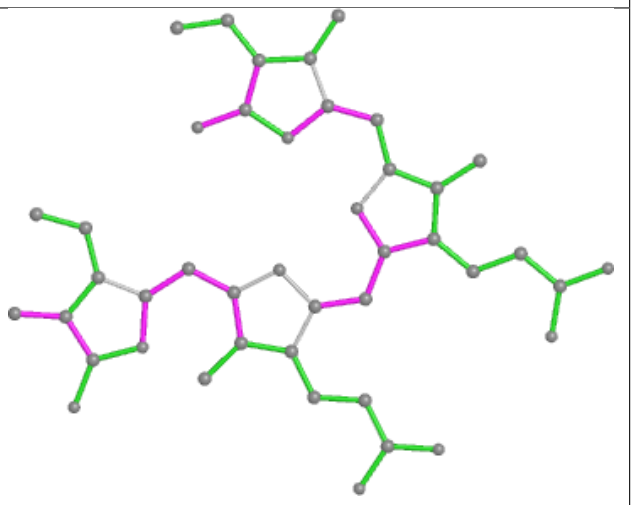

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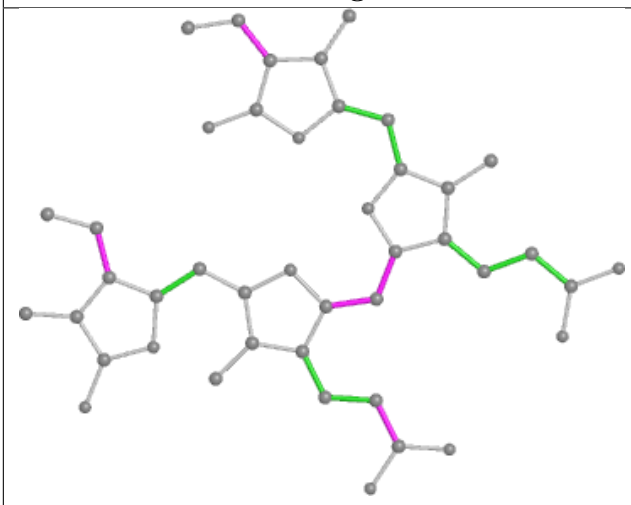

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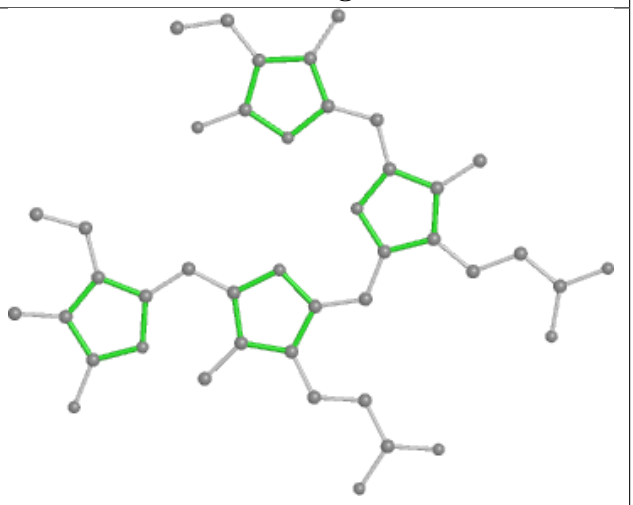

Rings

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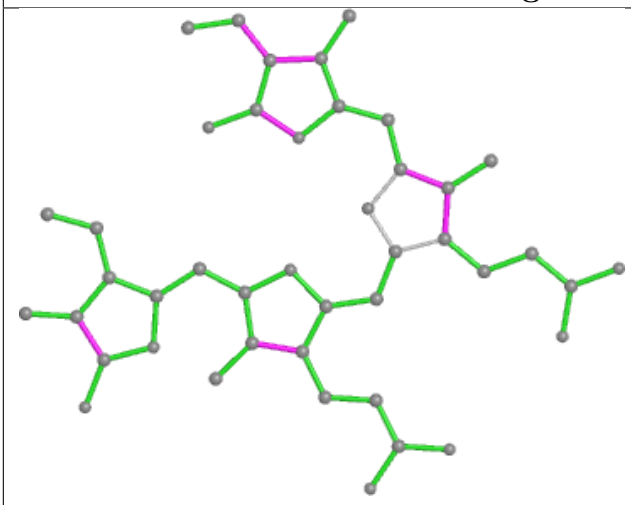

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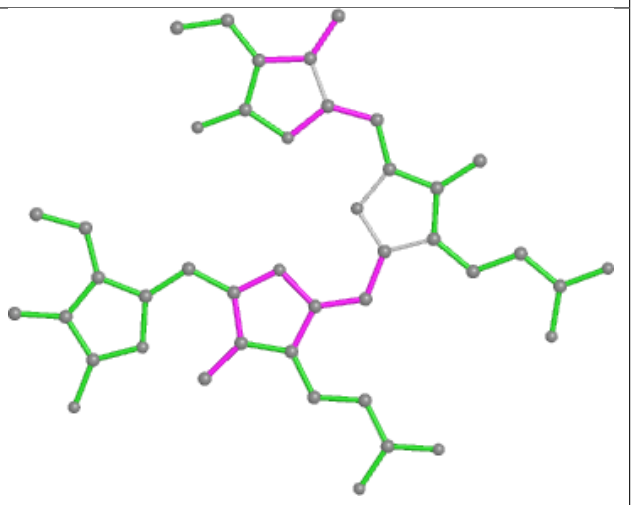

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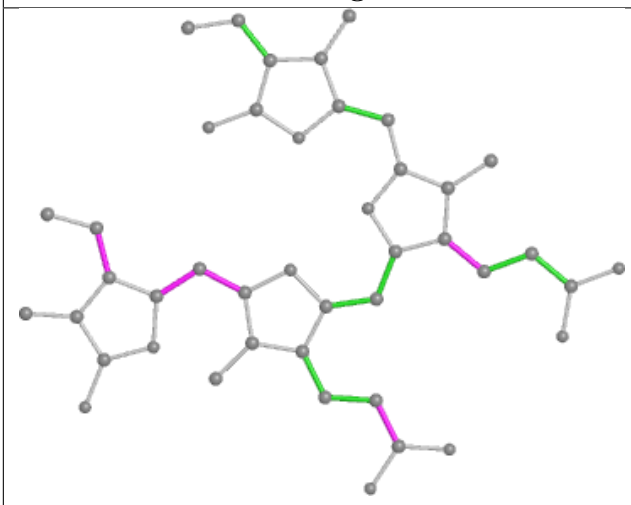

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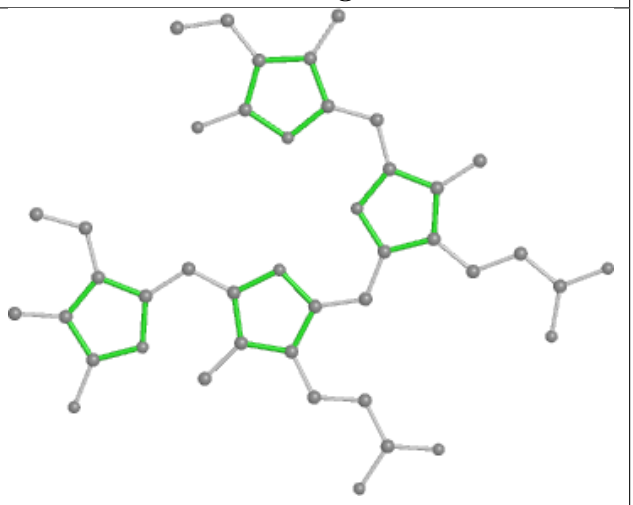

Rings

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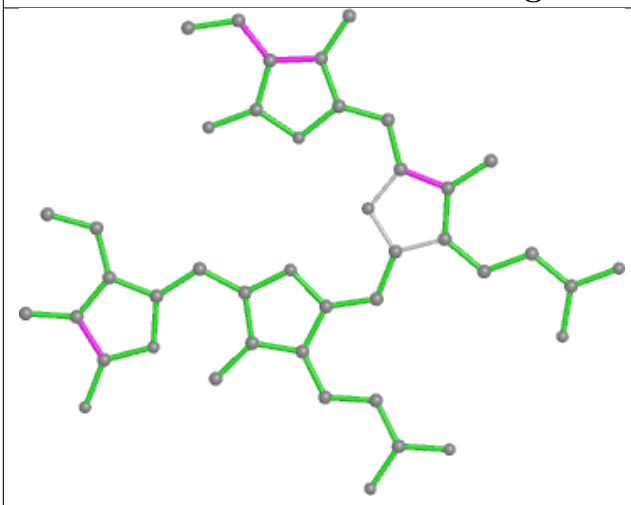

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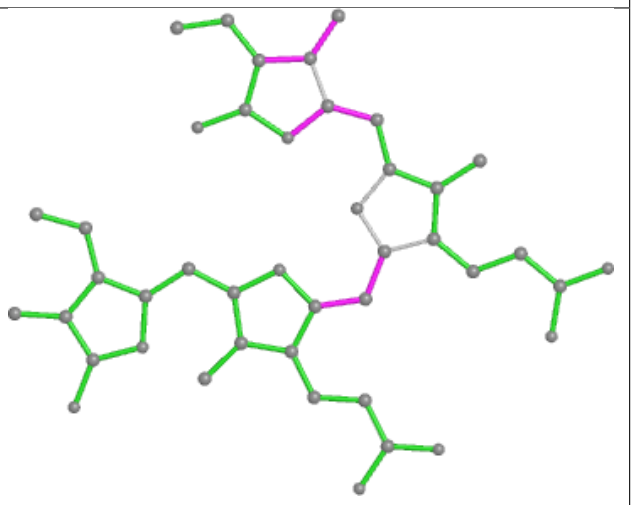

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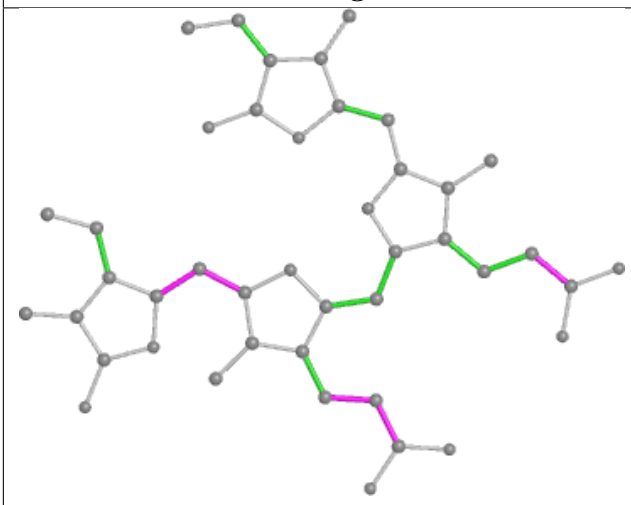

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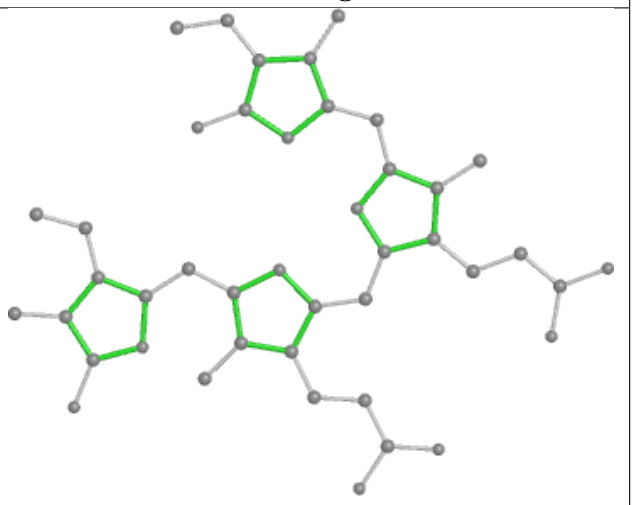

Rings

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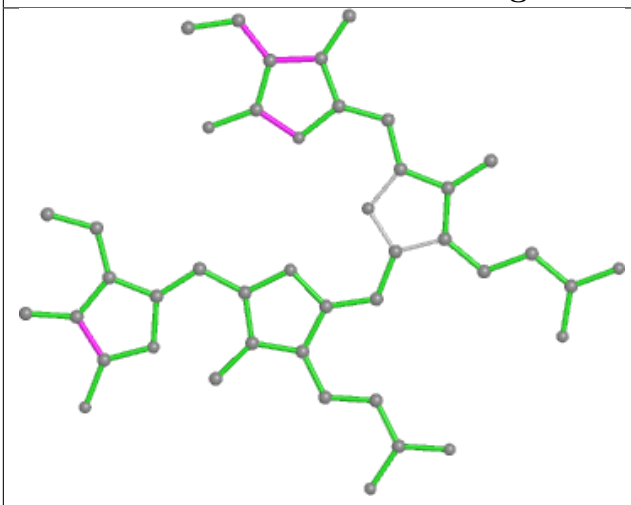

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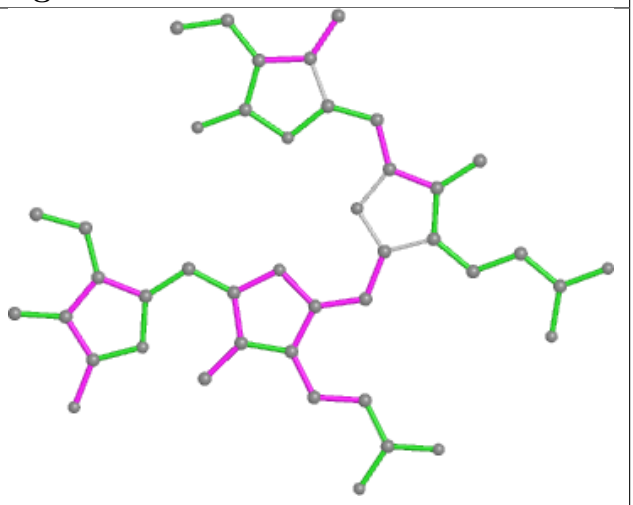

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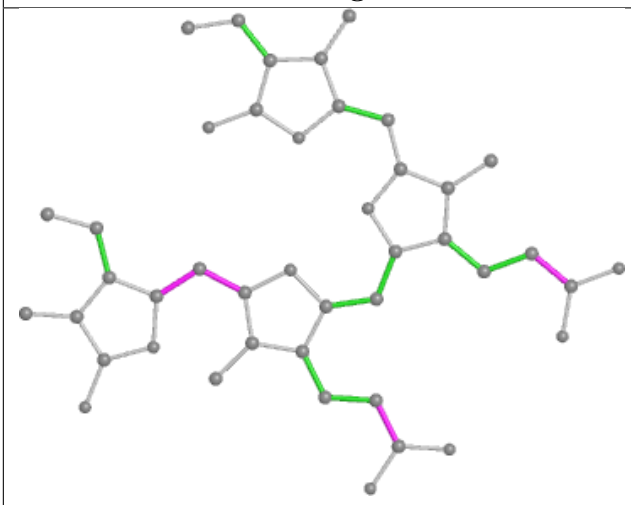

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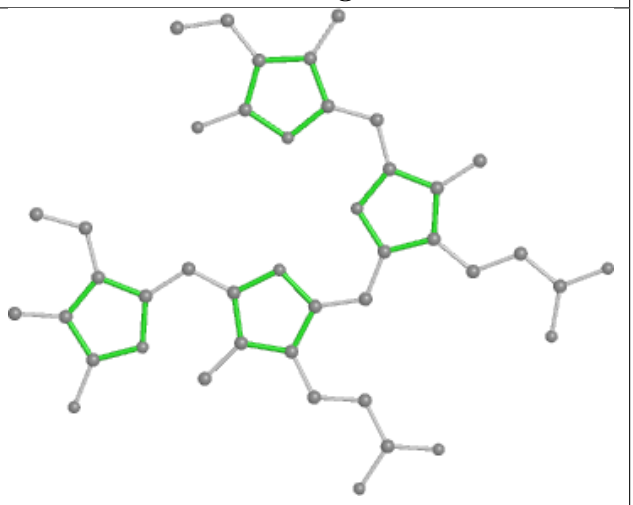

Rings

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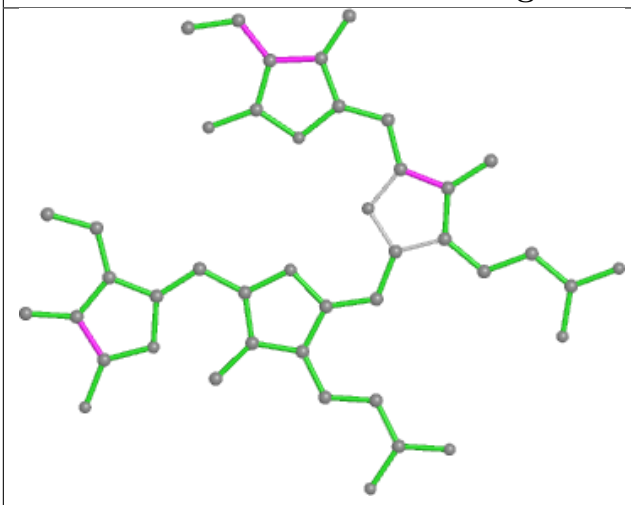

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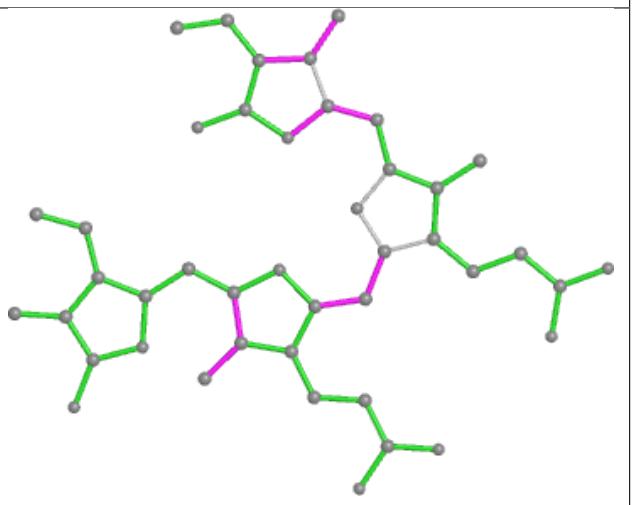

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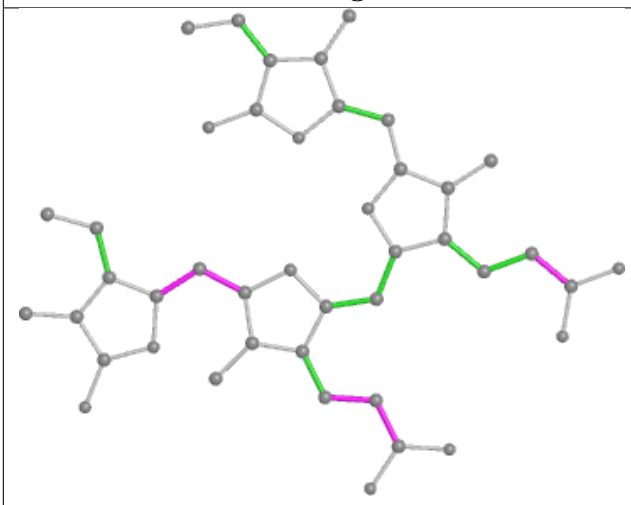

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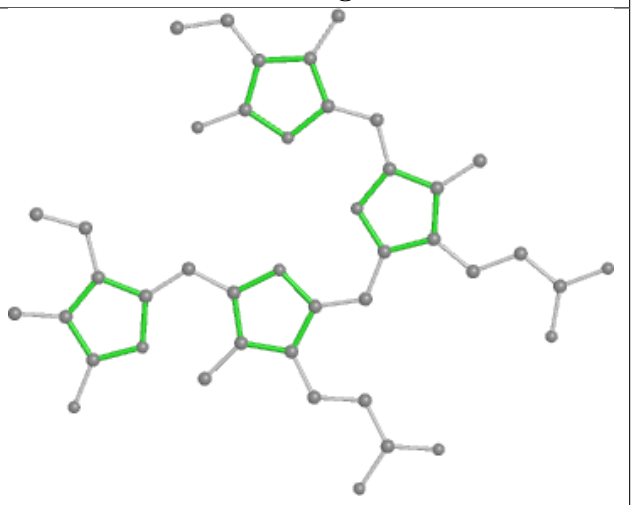

Rings

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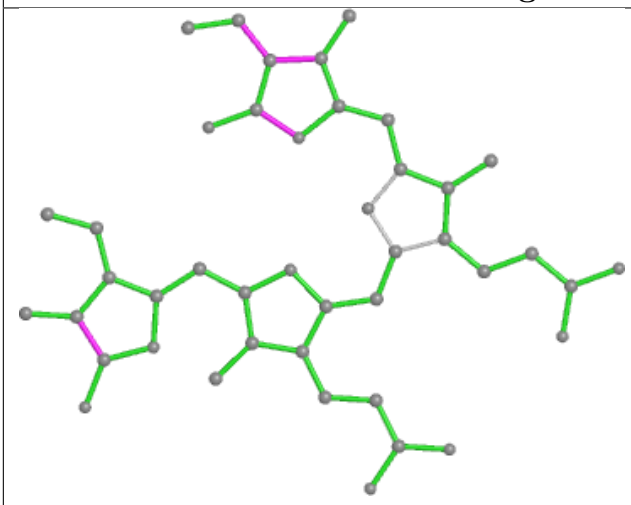

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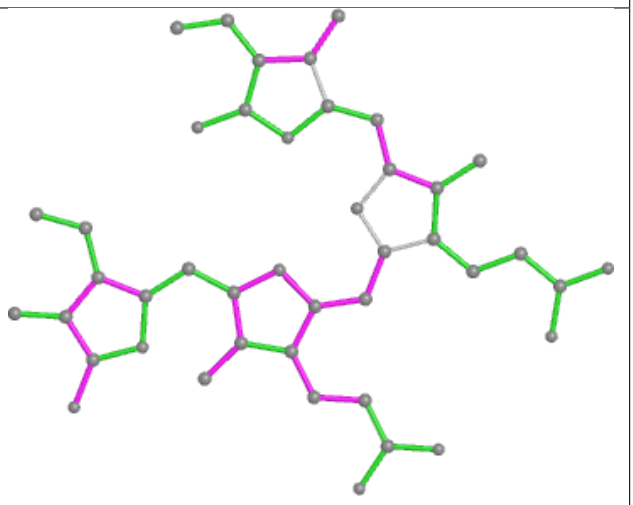

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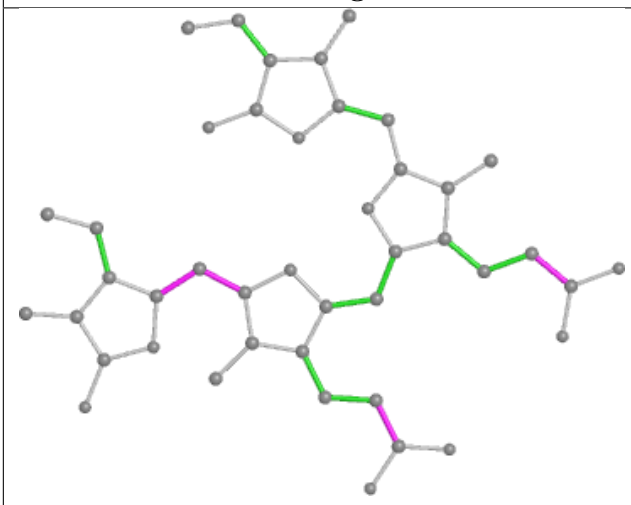

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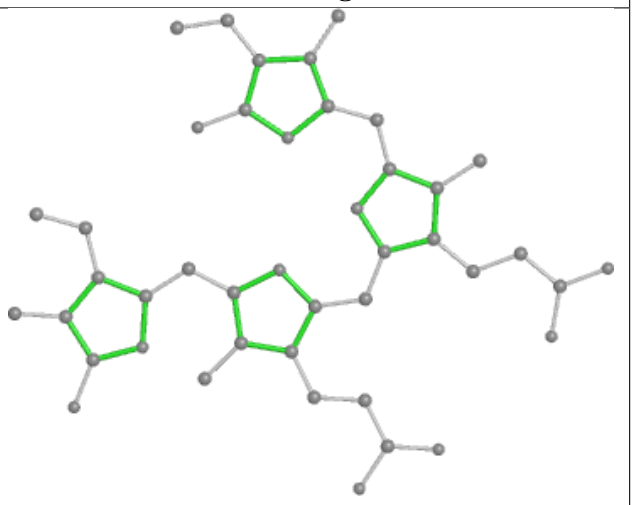

Rings

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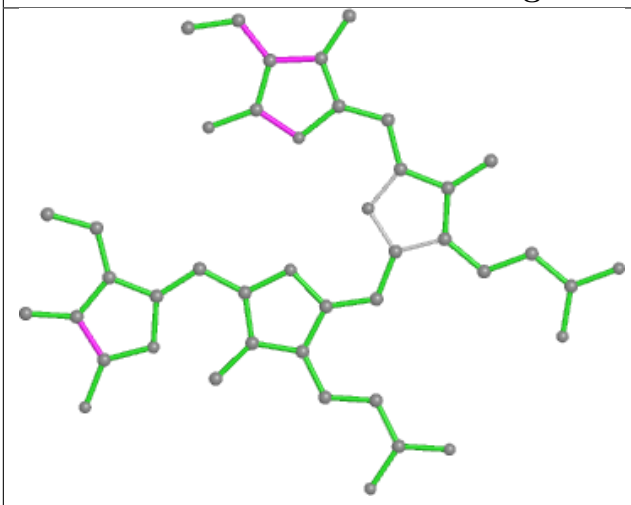

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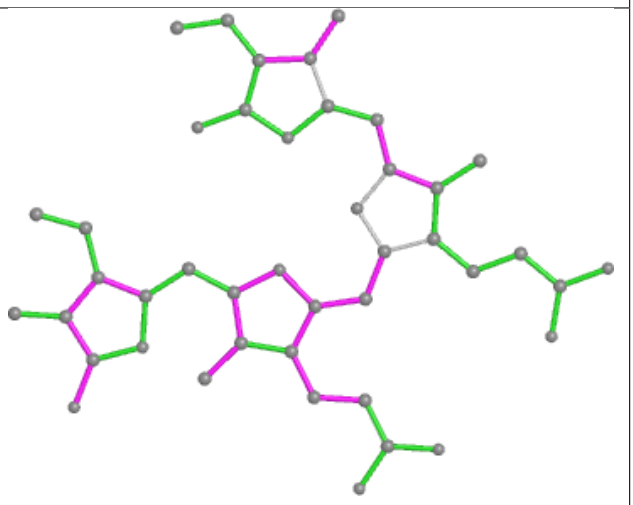
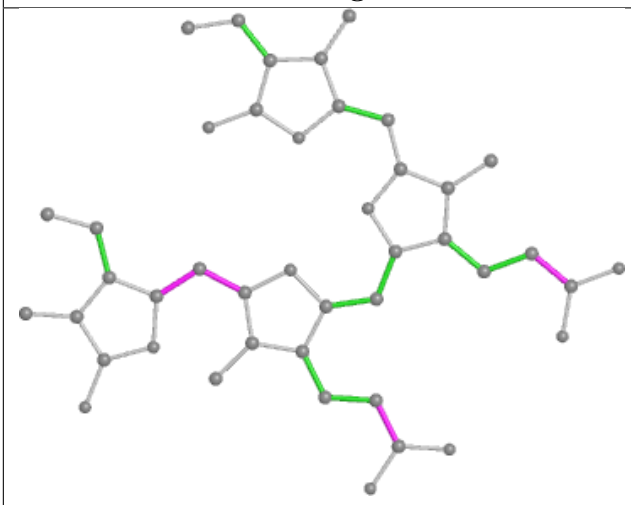
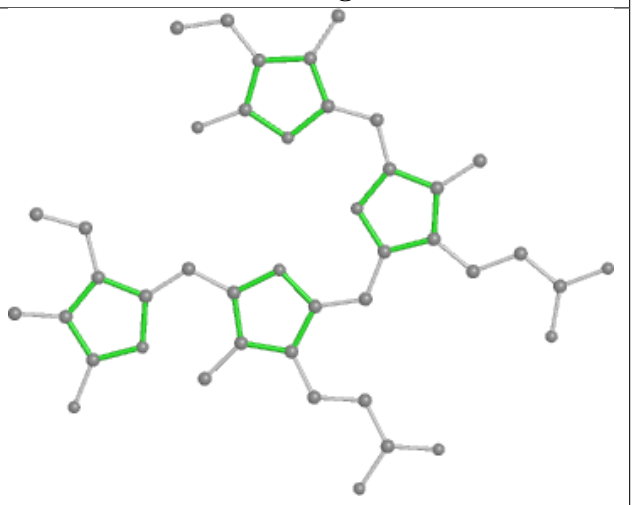


Bond angles

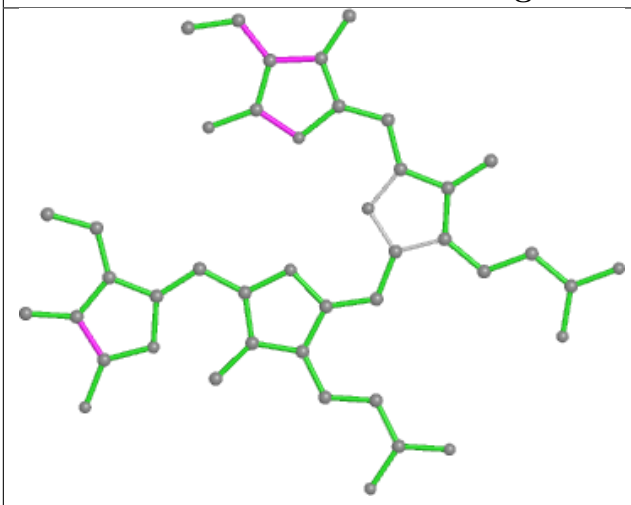


Torsions



Rings

Ligand PEB G5 201



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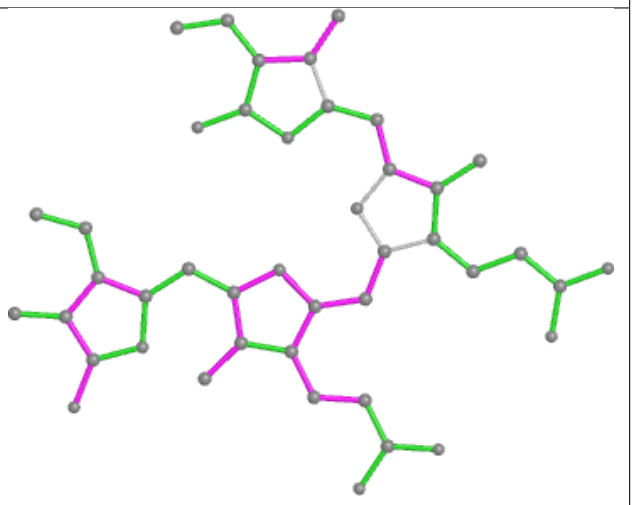

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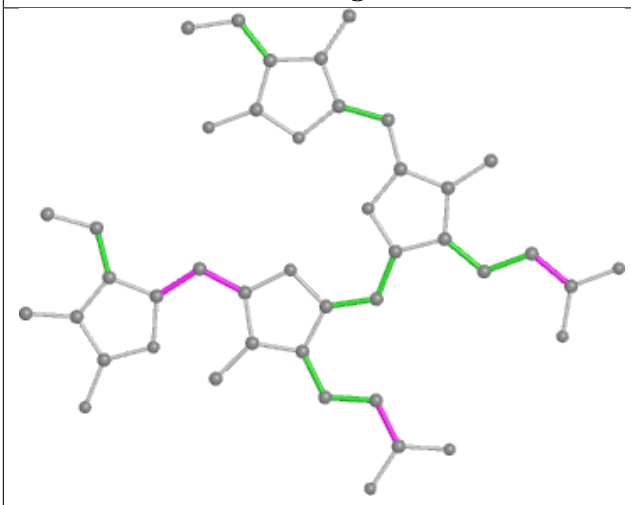

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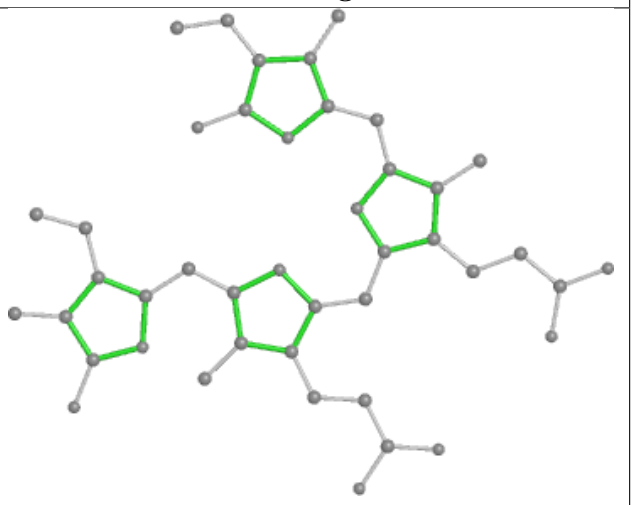
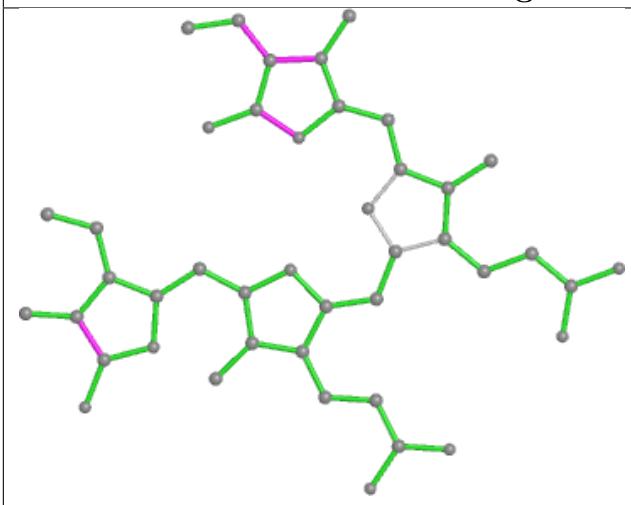


Rings

Ligand PEB w5 201



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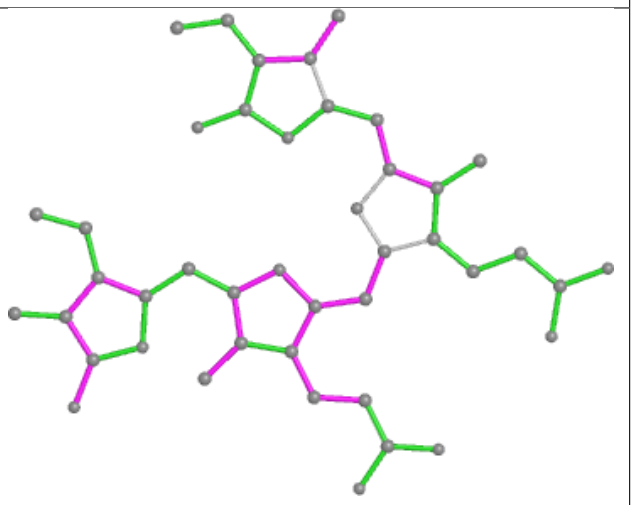

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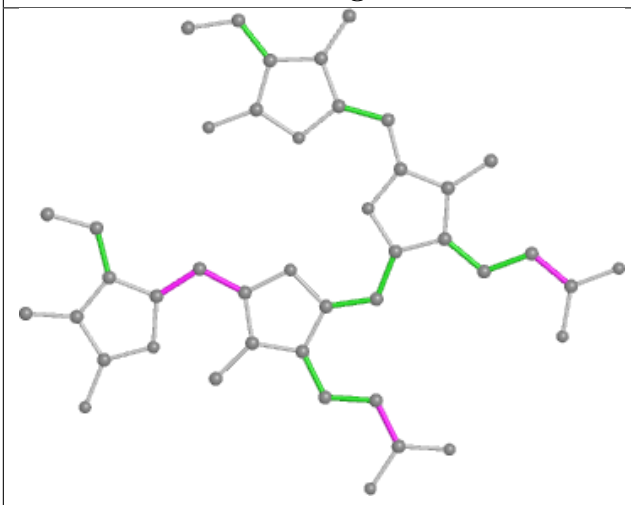

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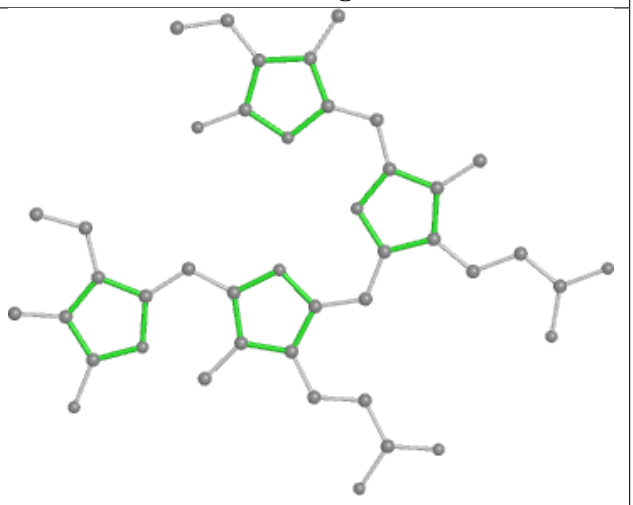
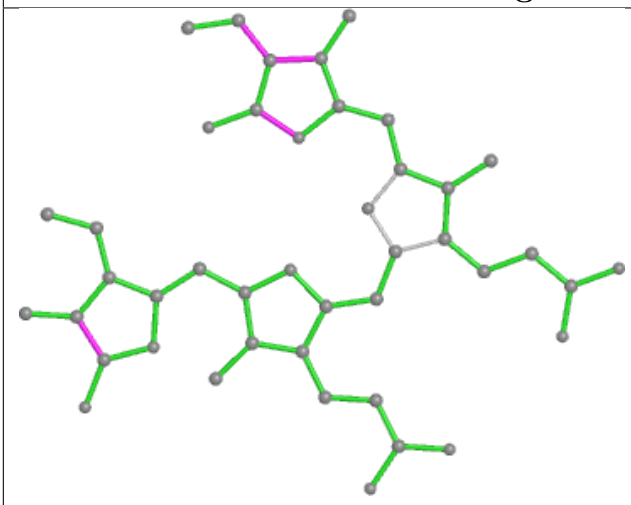


Rings

Ligand PEB C8 201



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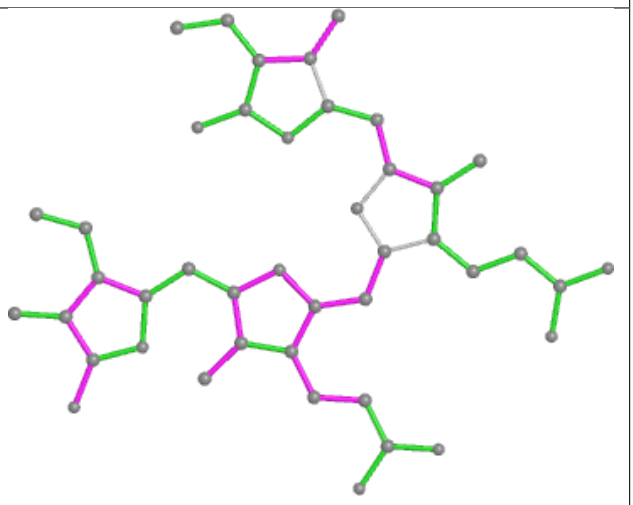

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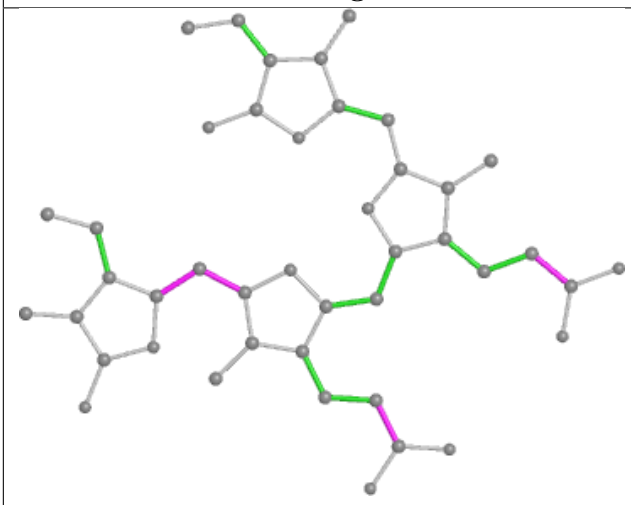

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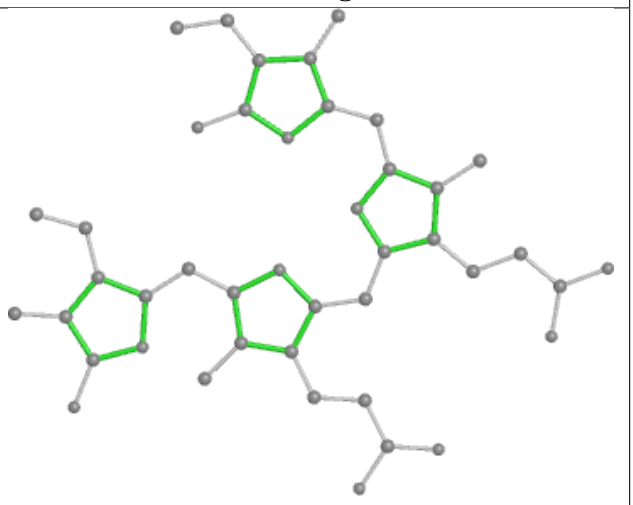
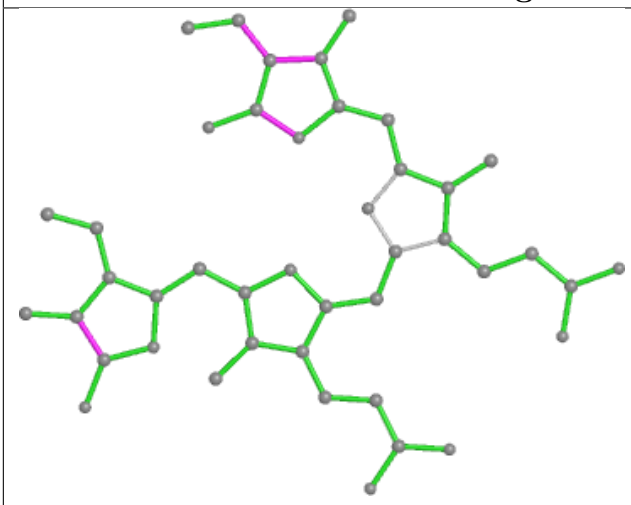


Rings

Ligand PEB hT 201



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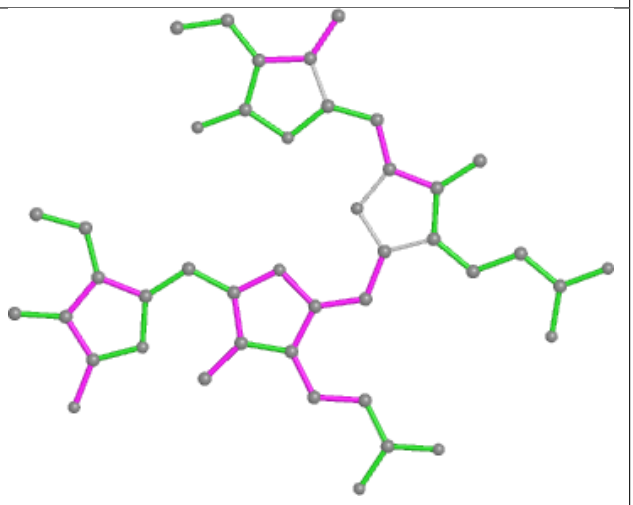
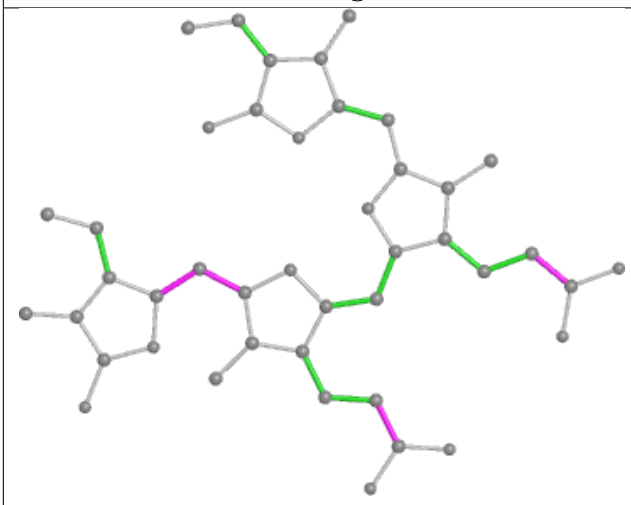


Bond angles



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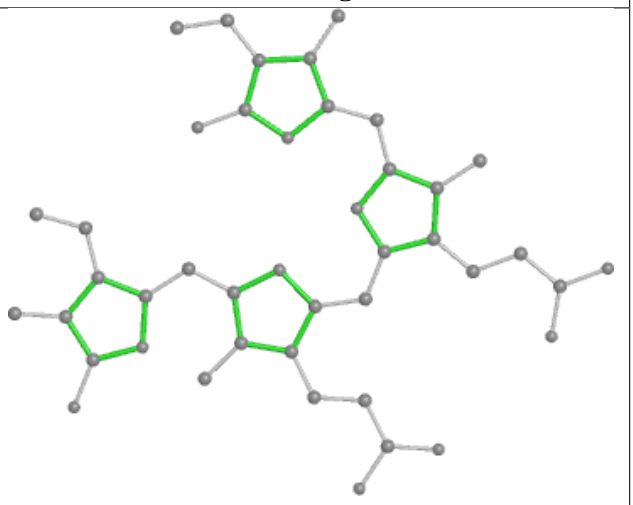

Rings

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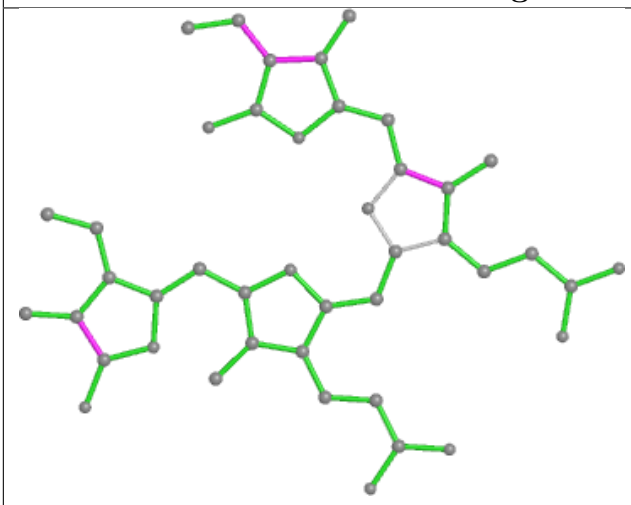

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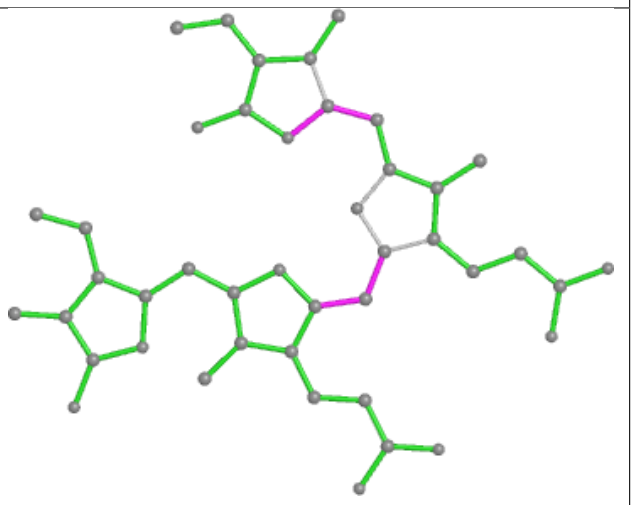

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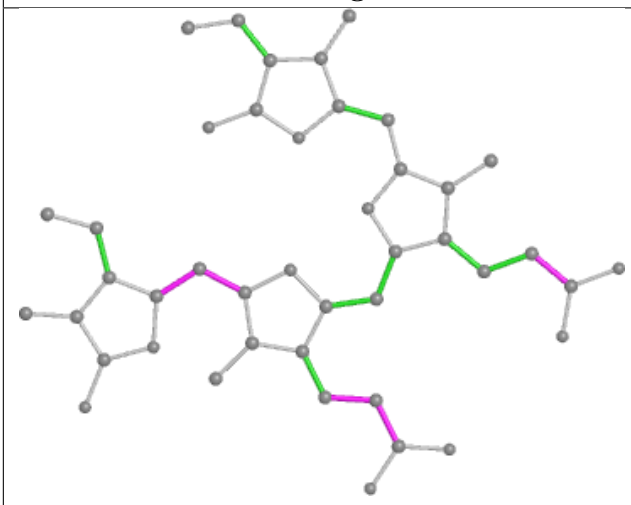

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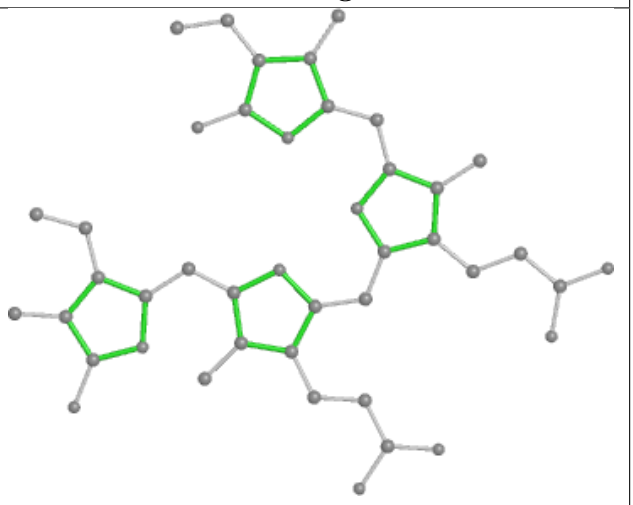
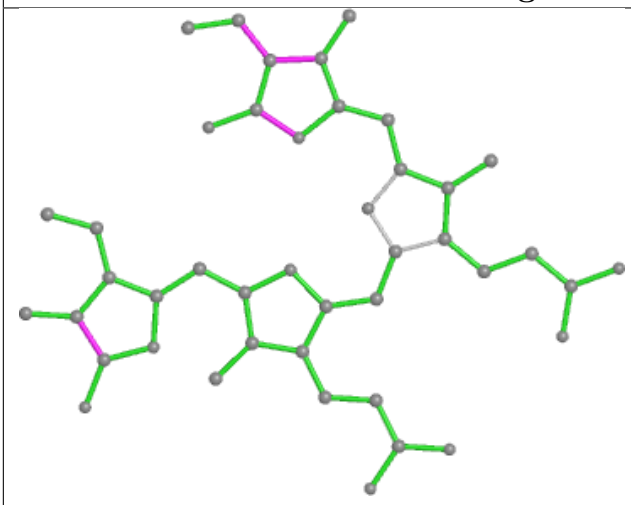


Rings

Ligand PEB L4 202



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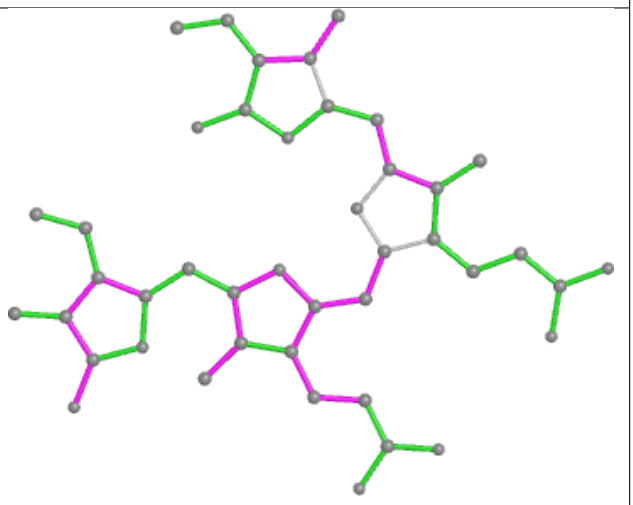

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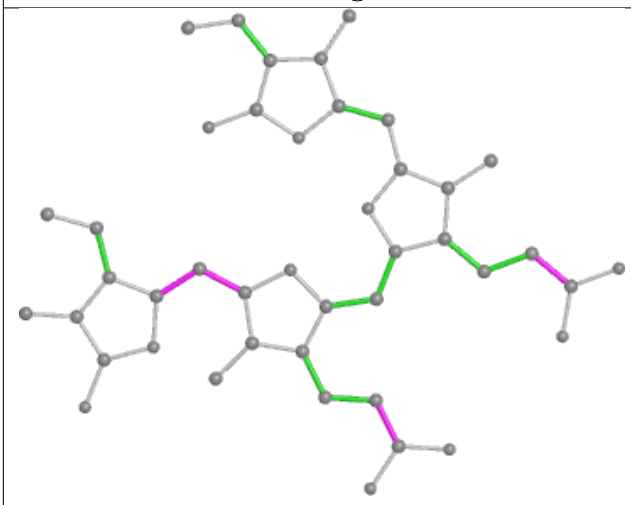

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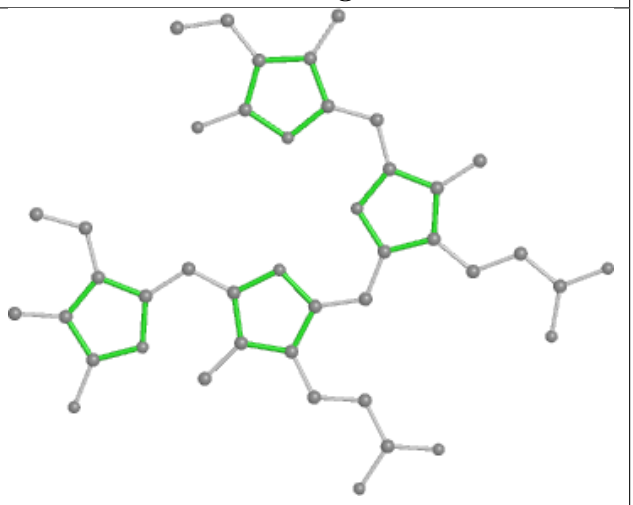

Rings

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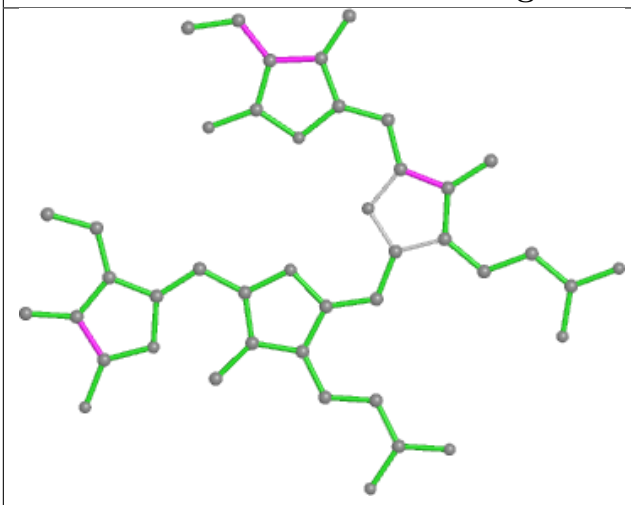

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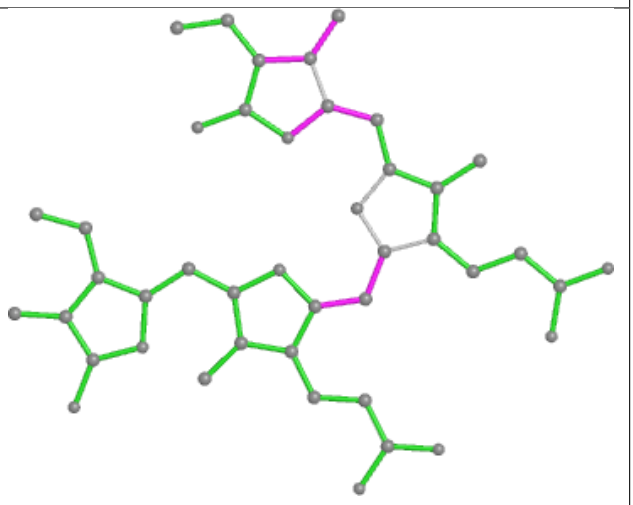

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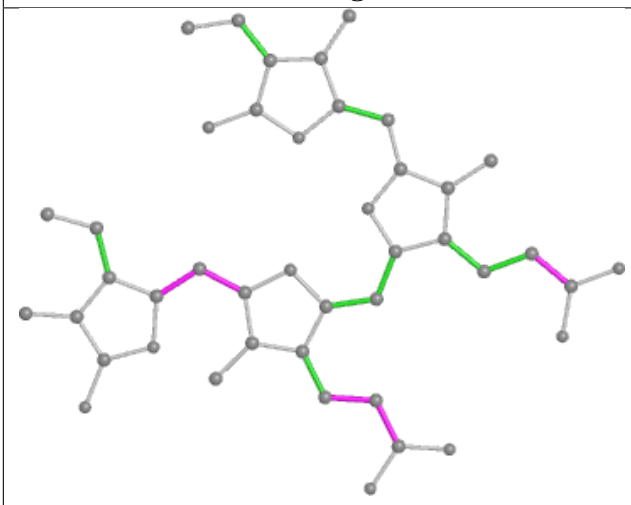

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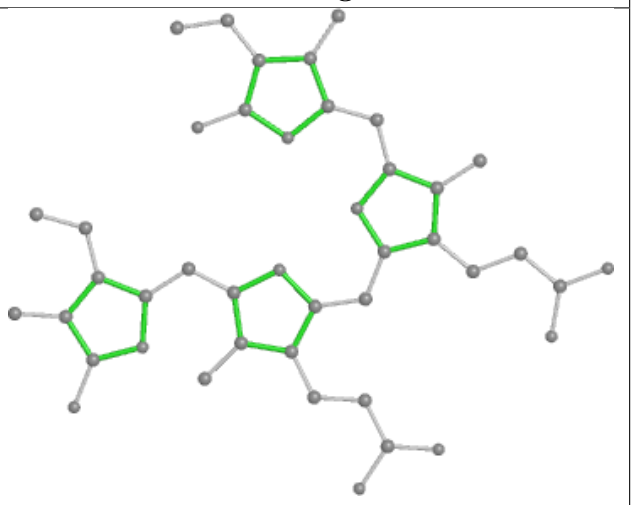
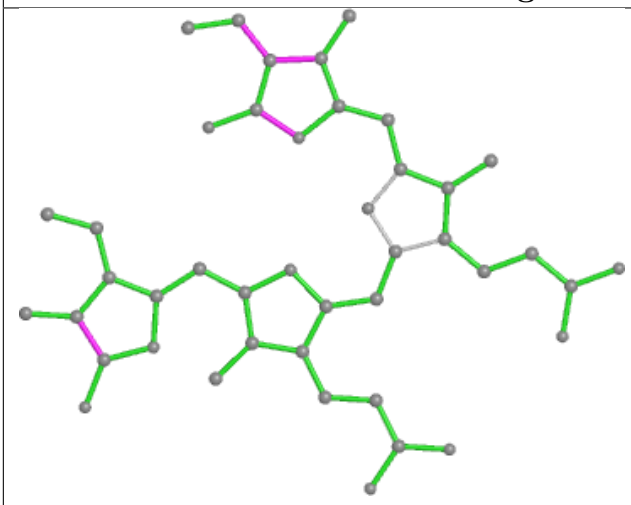


Rings

Ligand PEB bd 202



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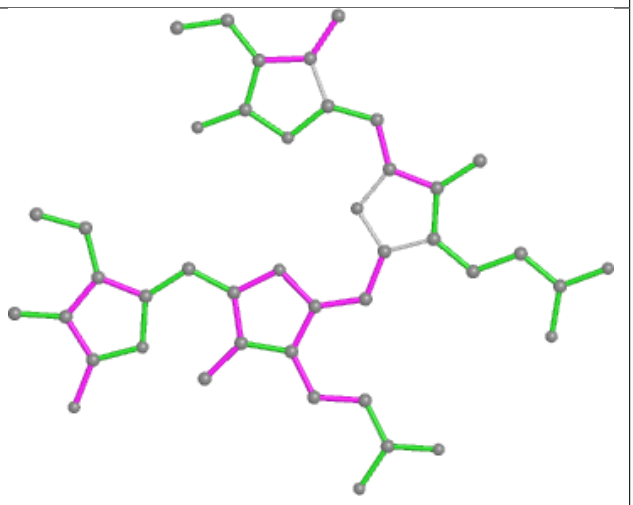

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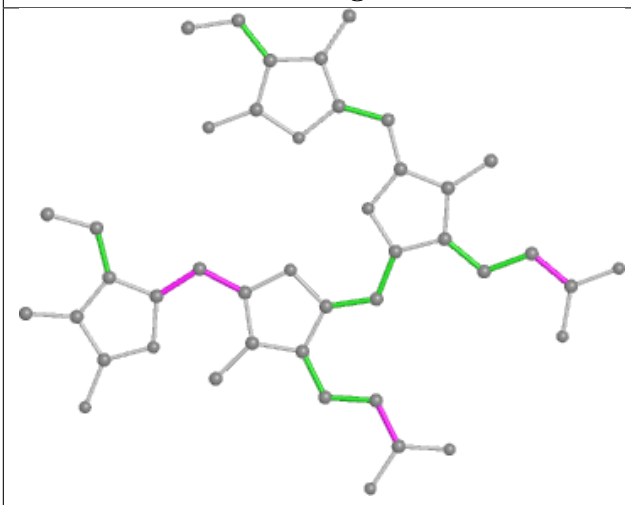

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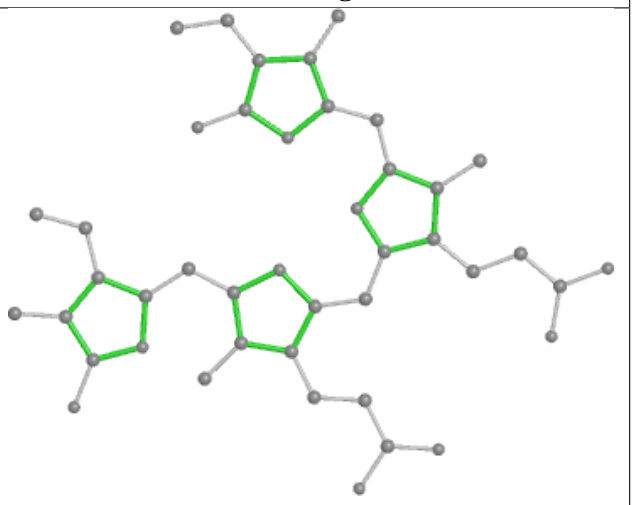

Rings

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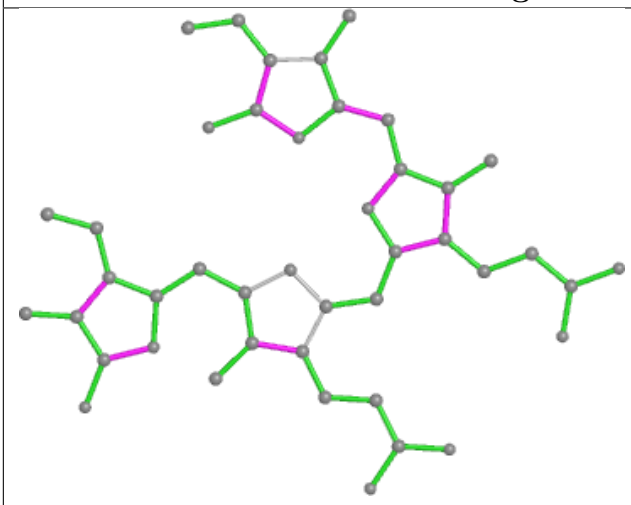

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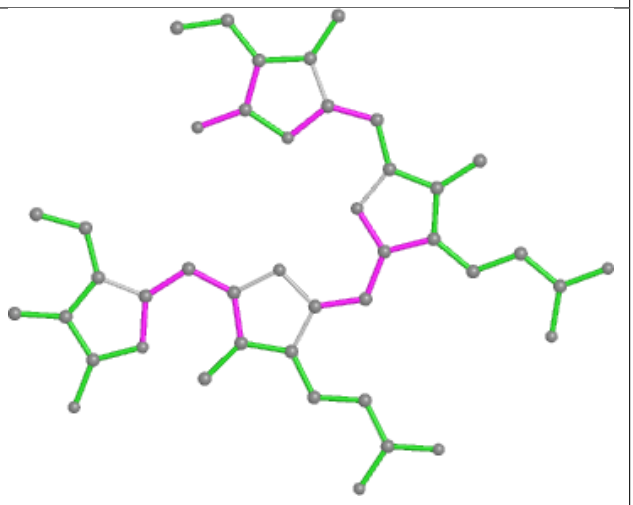

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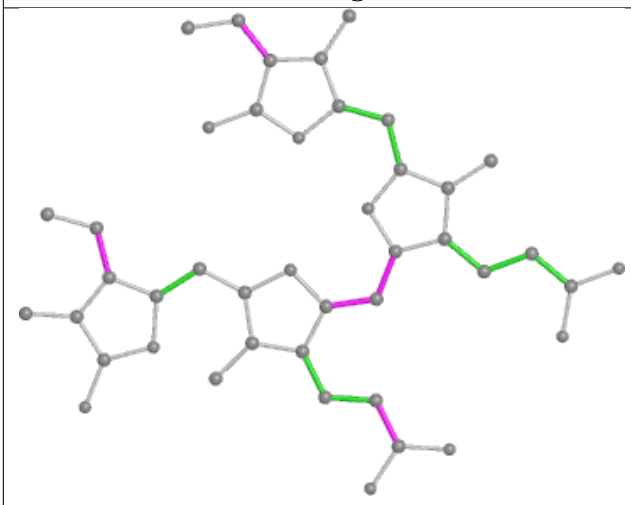

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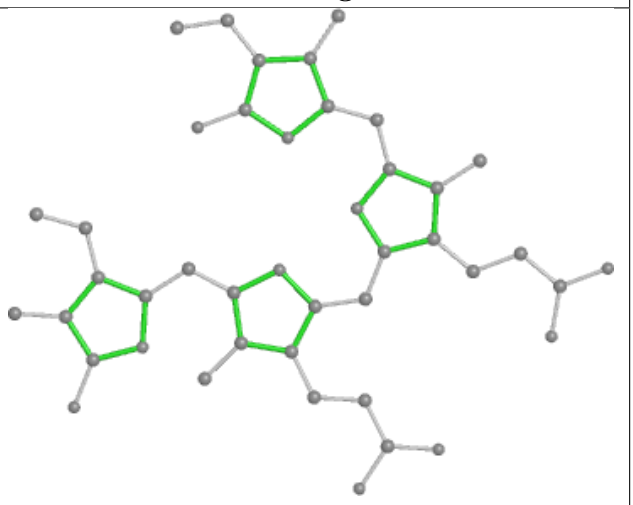
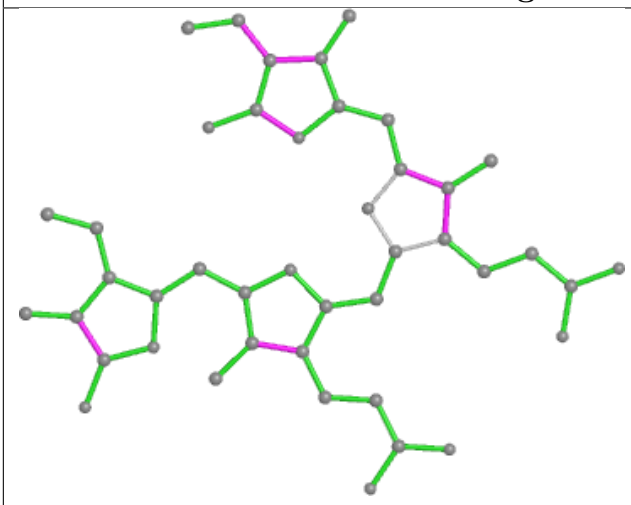


Rings

Ligand PEB F3 202



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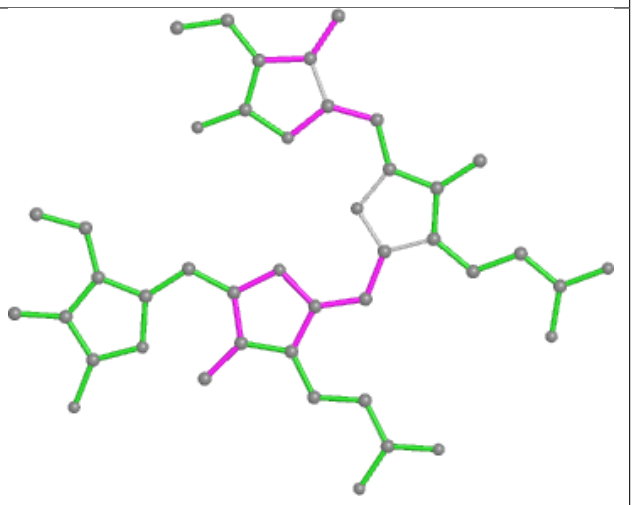

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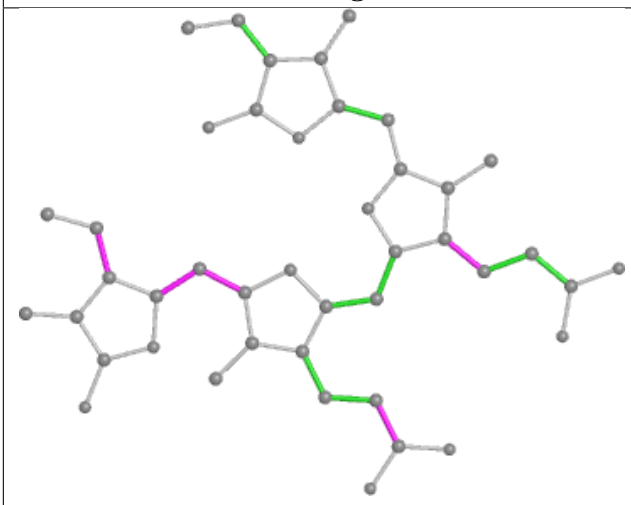

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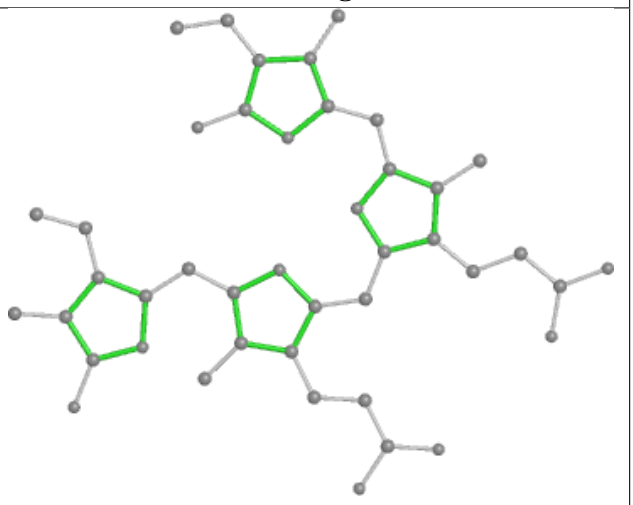

Rings

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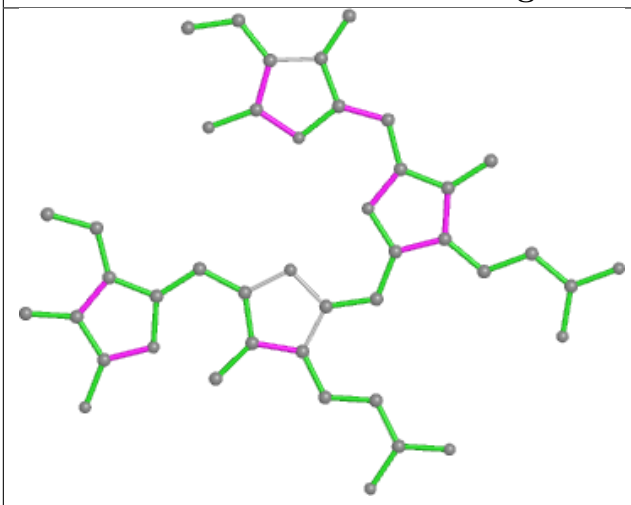

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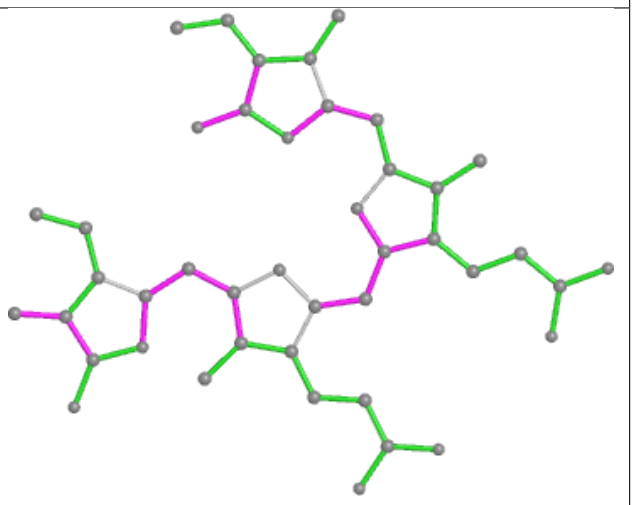

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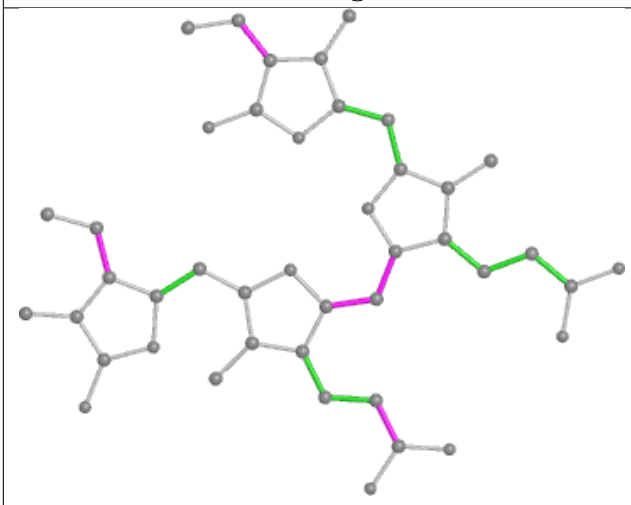

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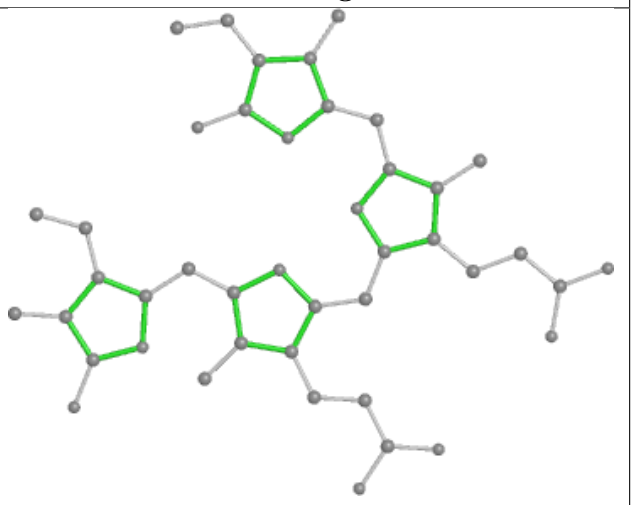
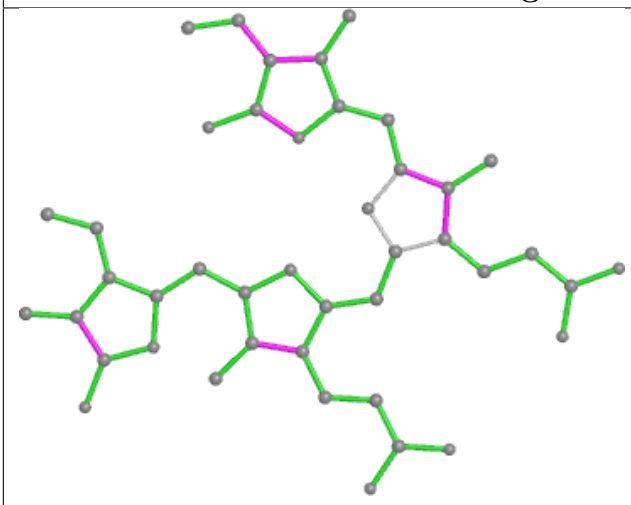


Rings

Ligand PEB t7 202



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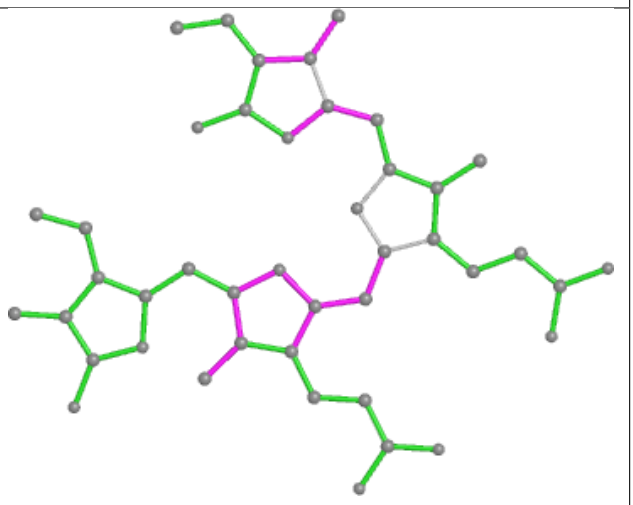

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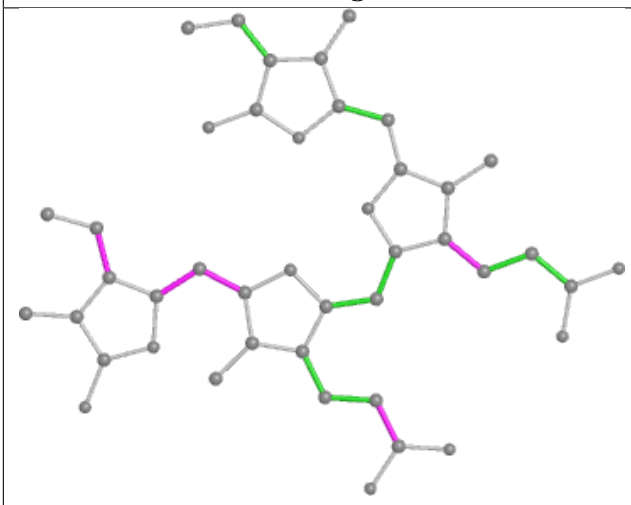

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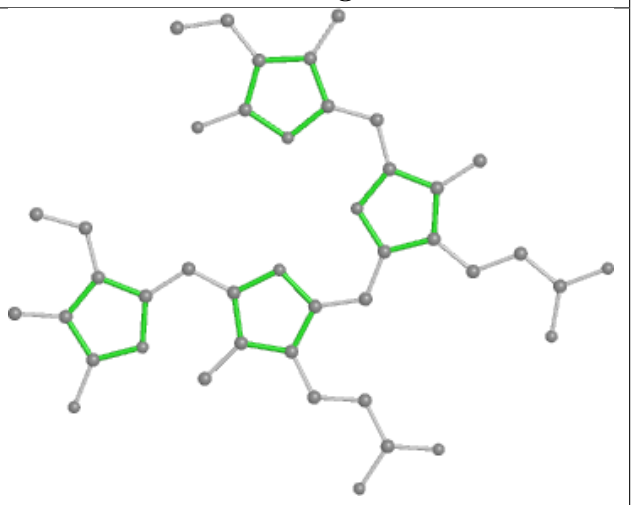
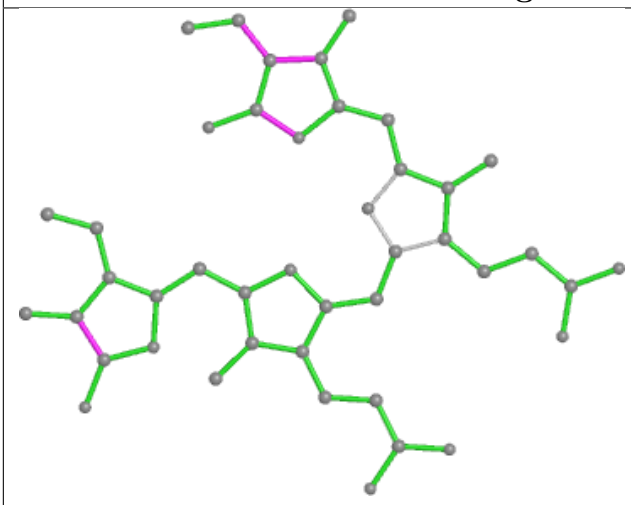


Rings

Ligand PEB eN 201



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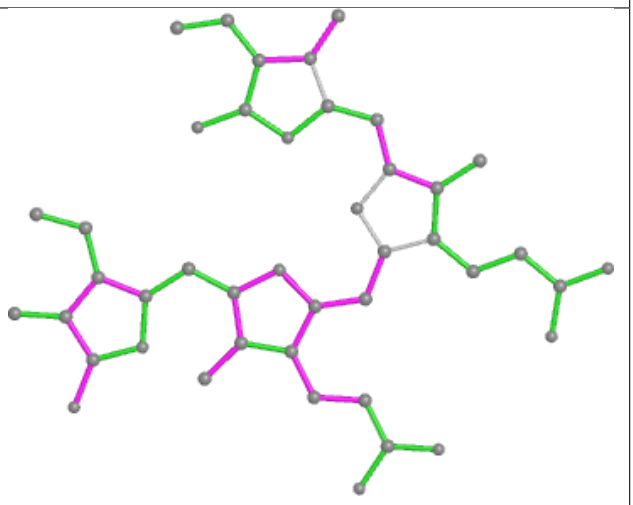

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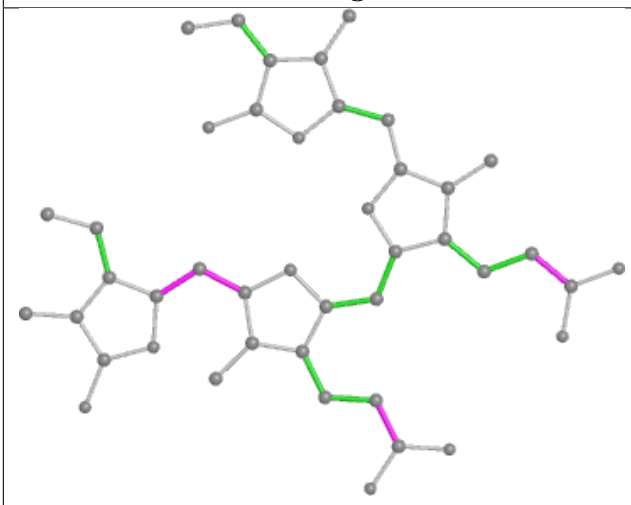
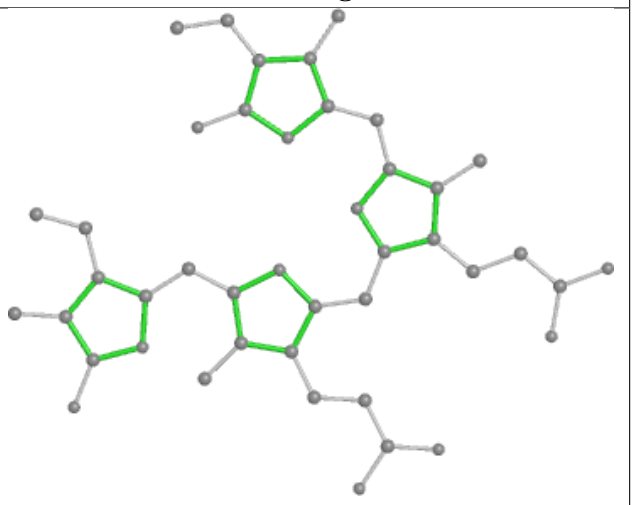
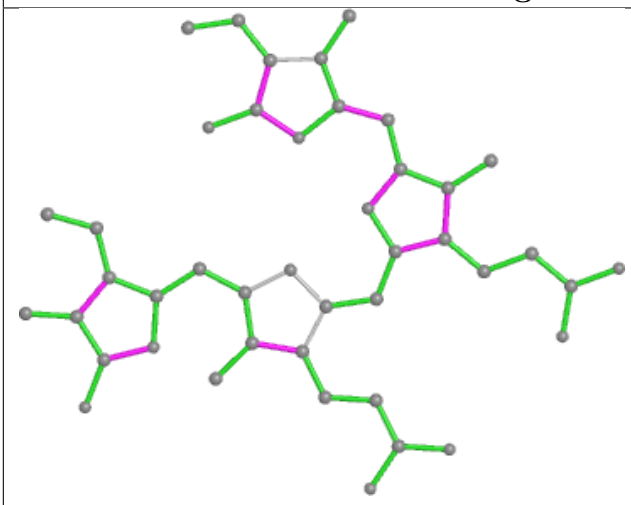


Torsions



Rings

Ligand PUB P6 203



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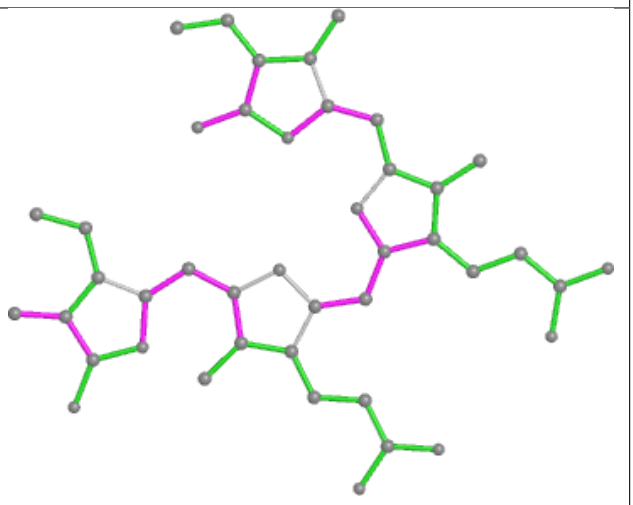
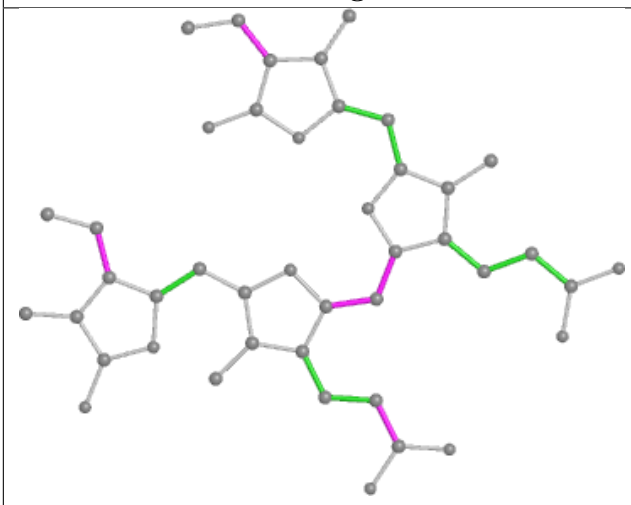


Bond angles



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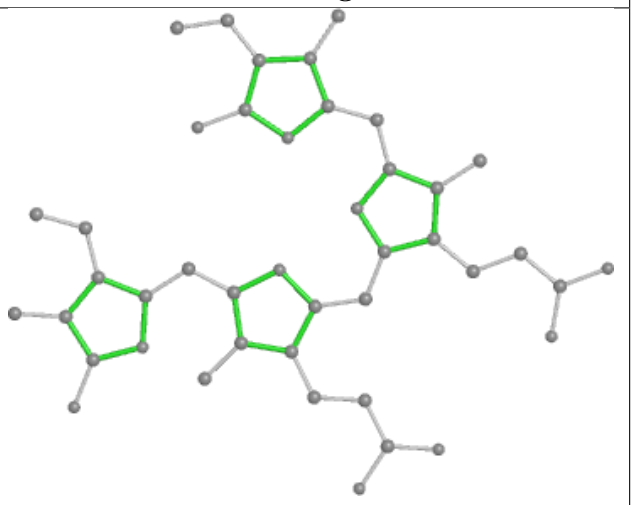
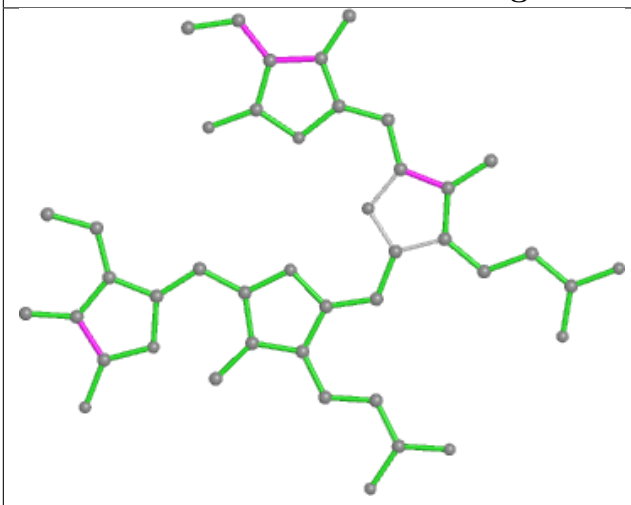


Rings

Ligand PEB W3 202



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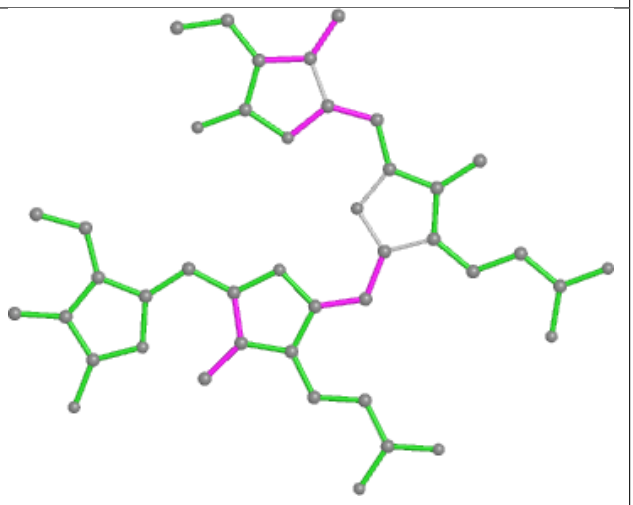

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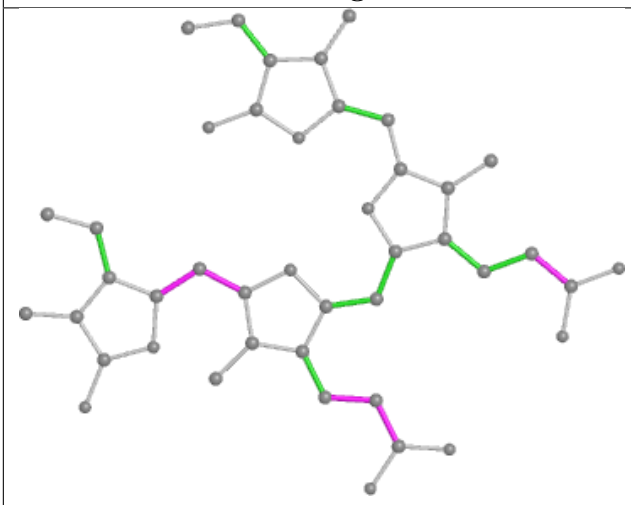

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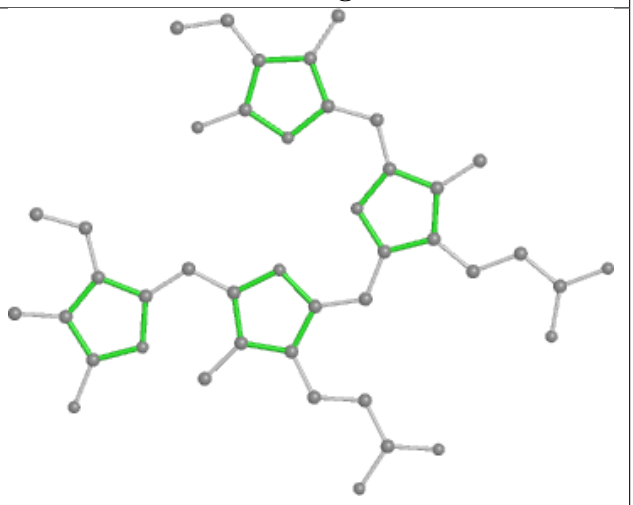
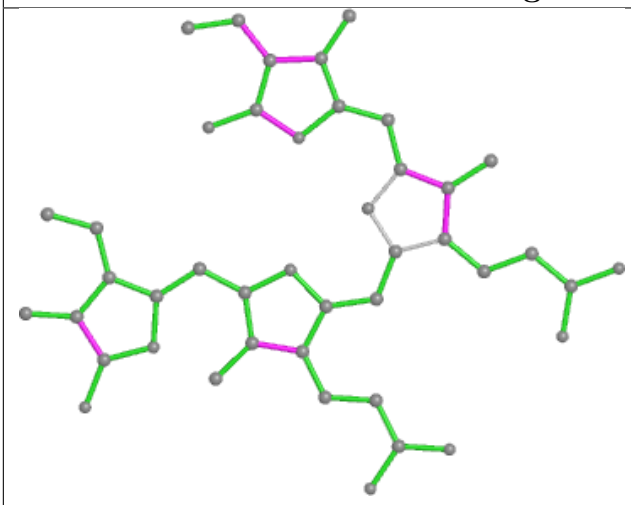


Rings

Ligand PEB j3 201



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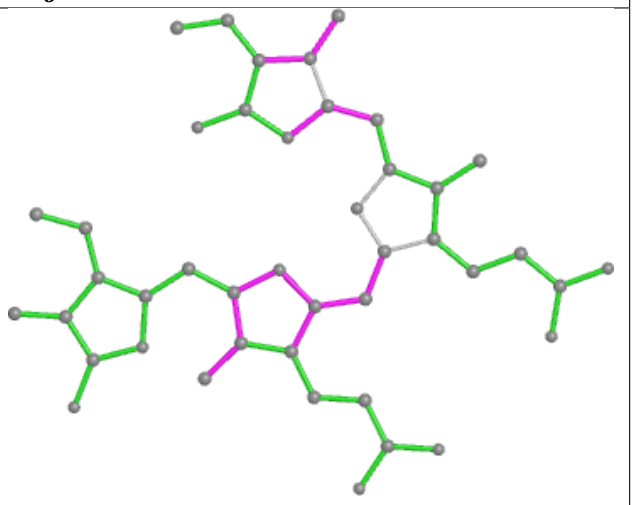
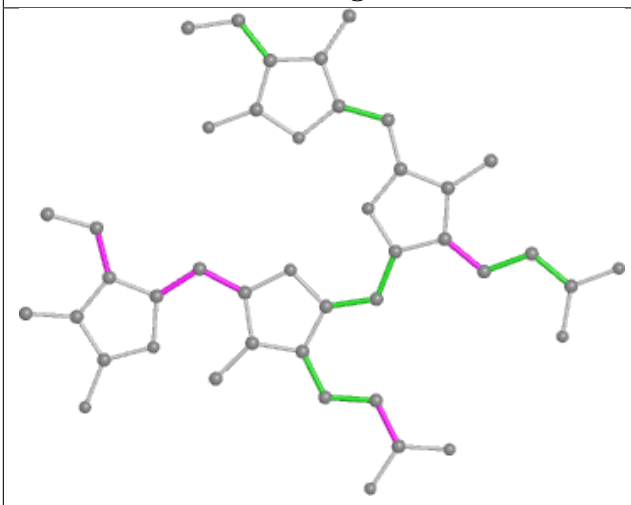


Bond angles



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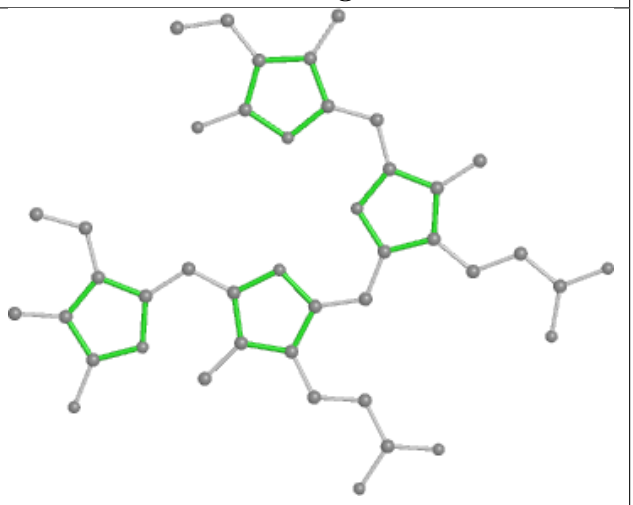
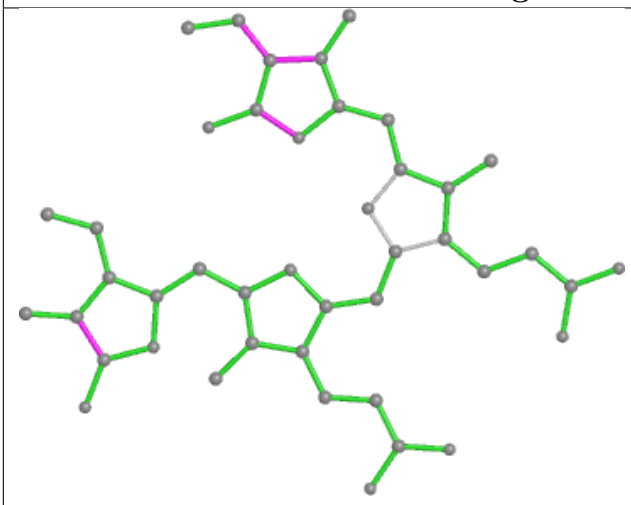


Rings

Ligand PEB bs 1003



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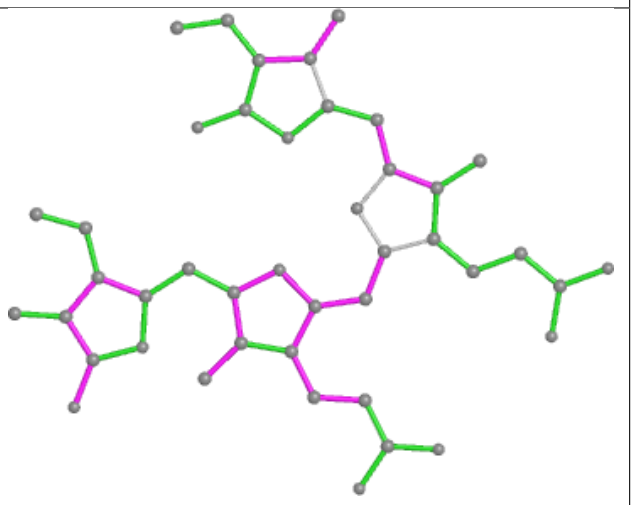
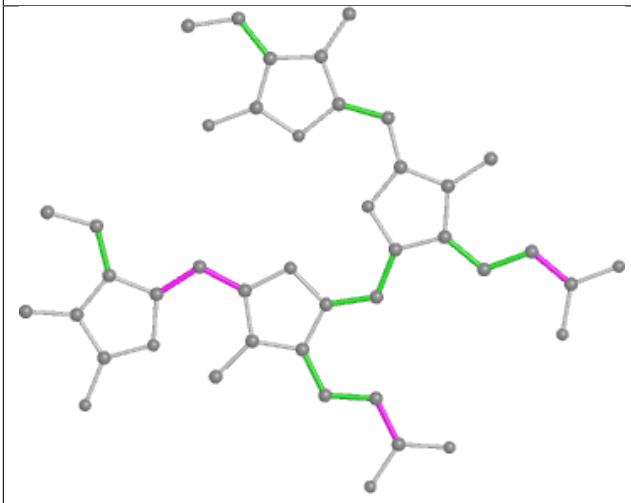


Bond angles



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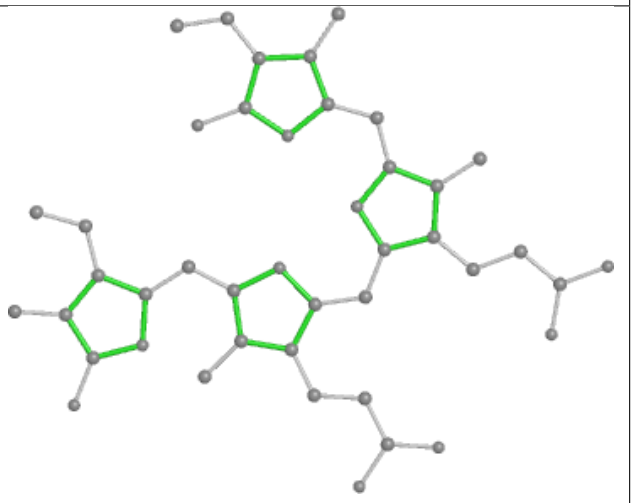
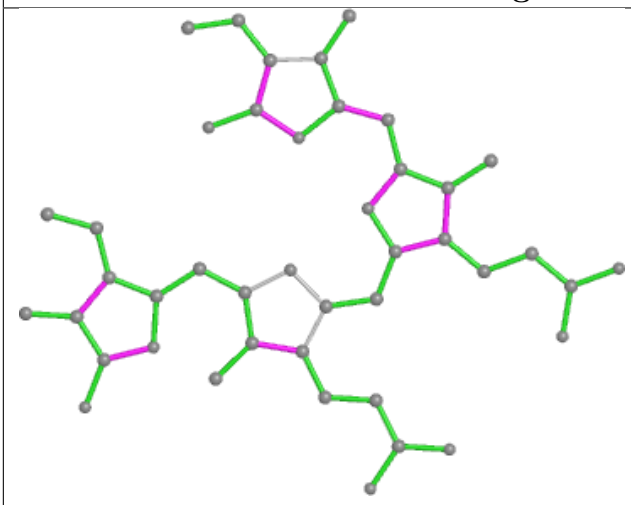


Rings

Ligand PUB H2 202



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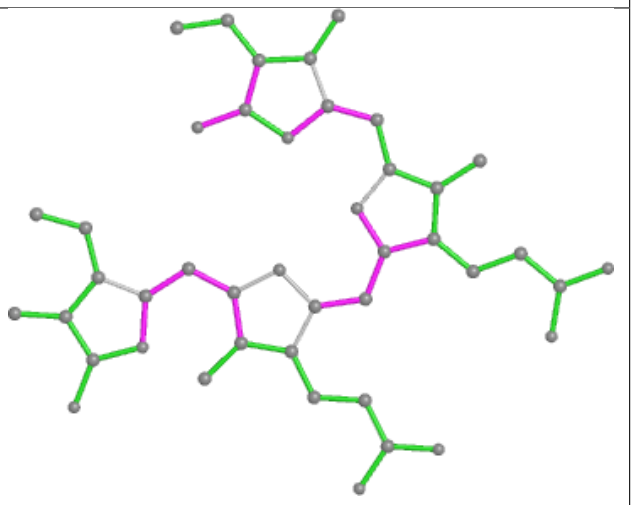
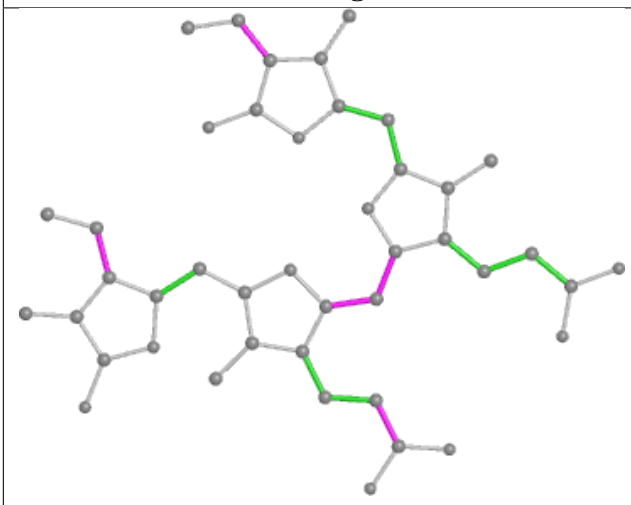


Bond angles



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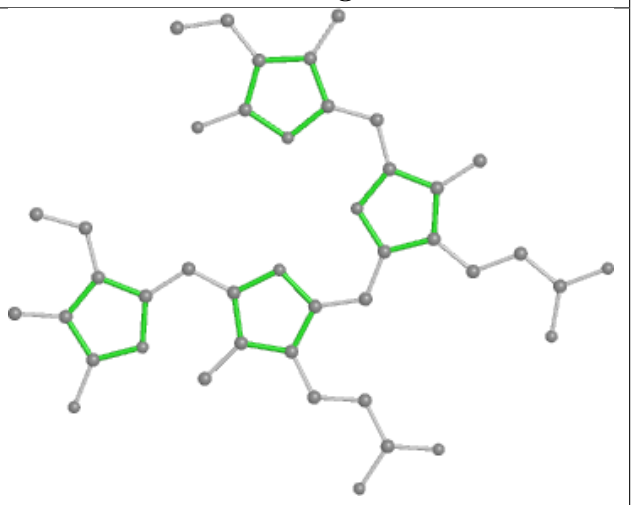

Rings

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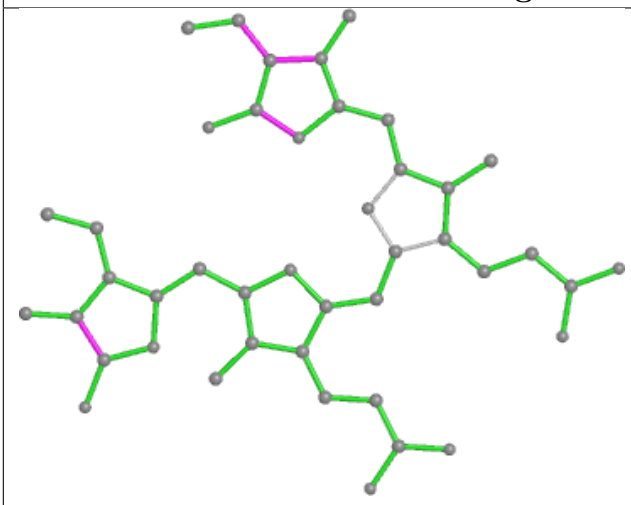

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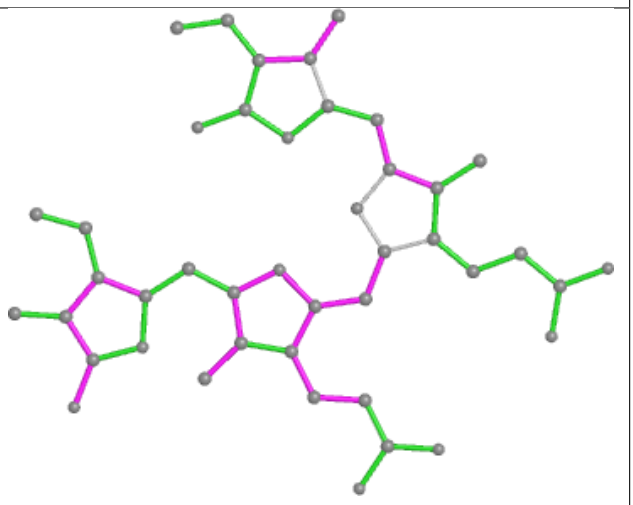

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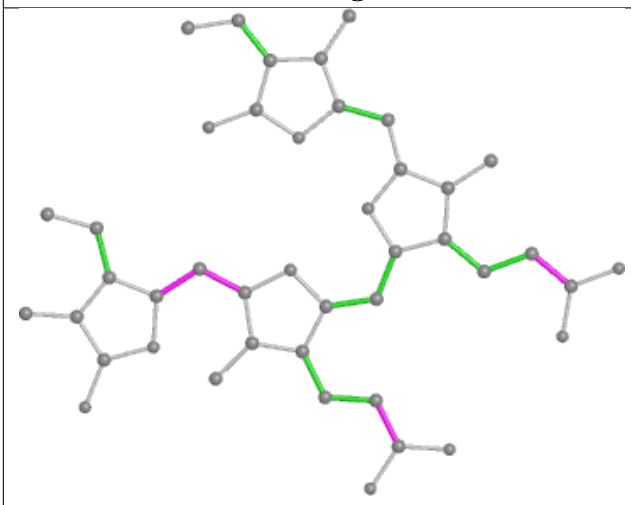

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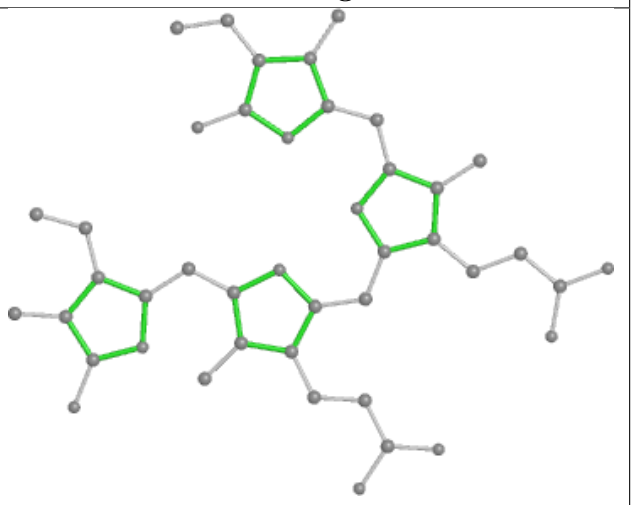
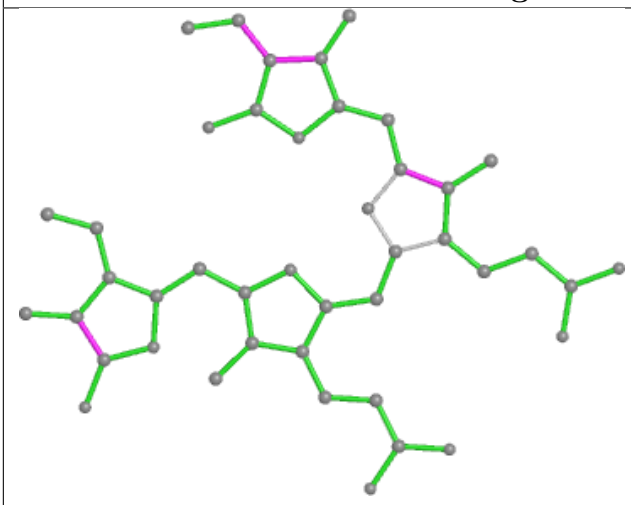


Rings

Ligand PEB ay 1002



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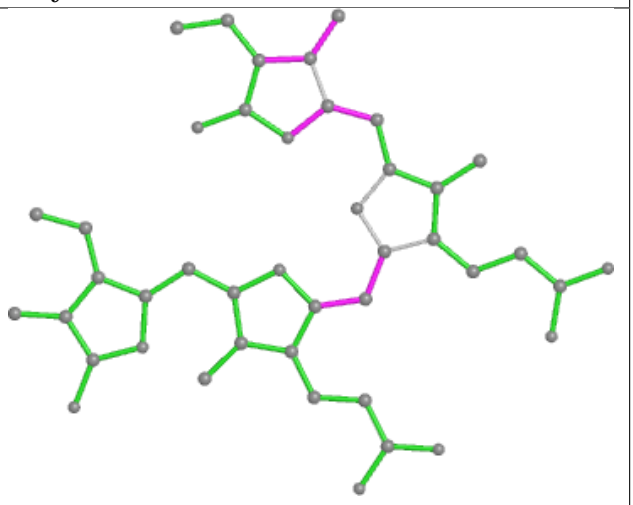

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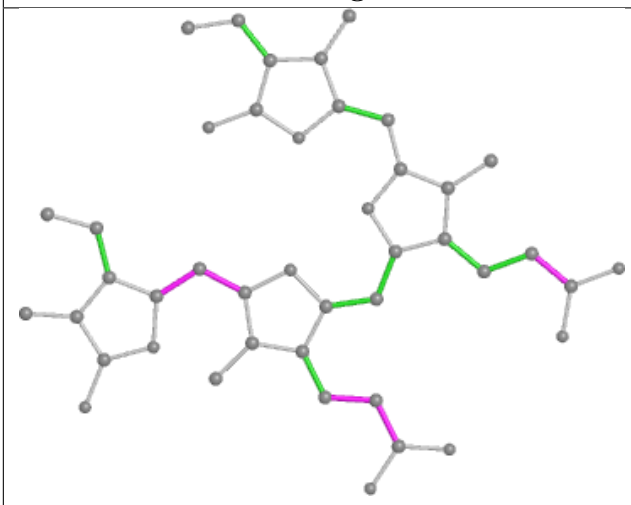

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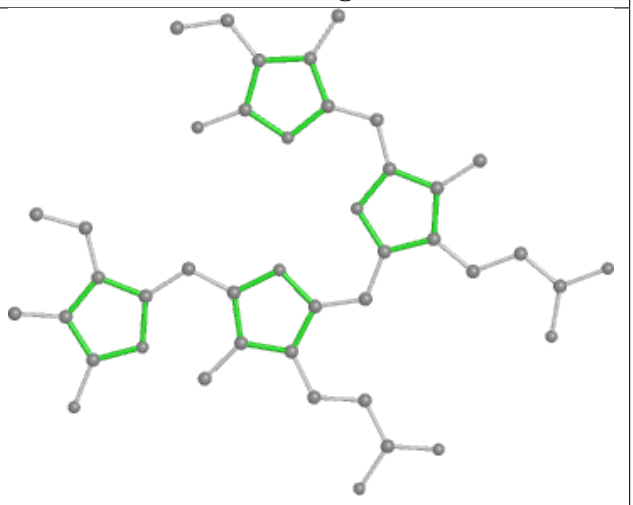
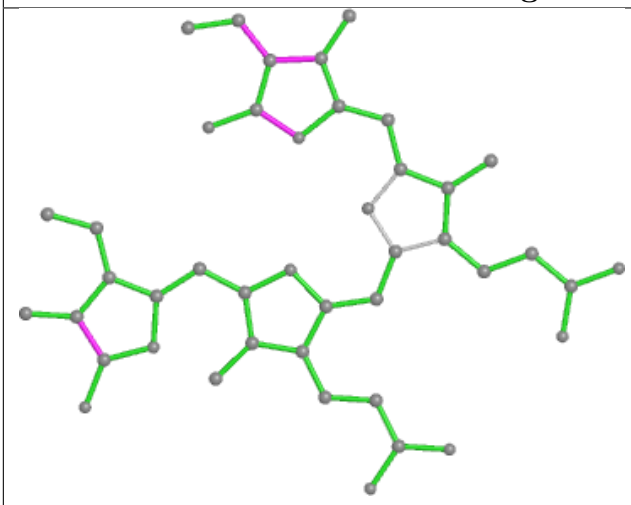


Rings

Ligand PEB z8 201



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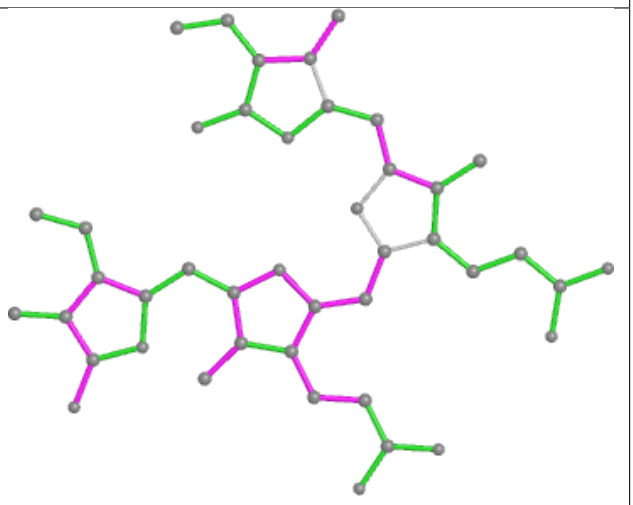

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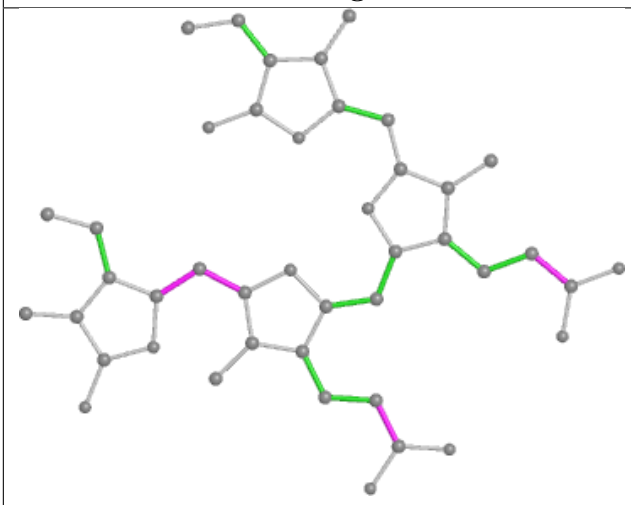

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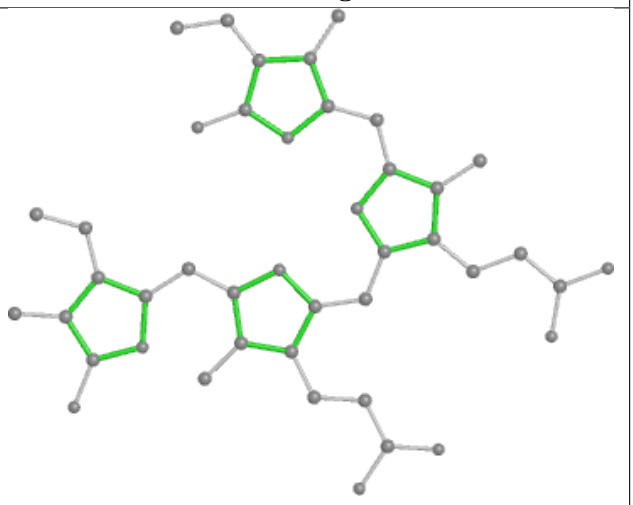
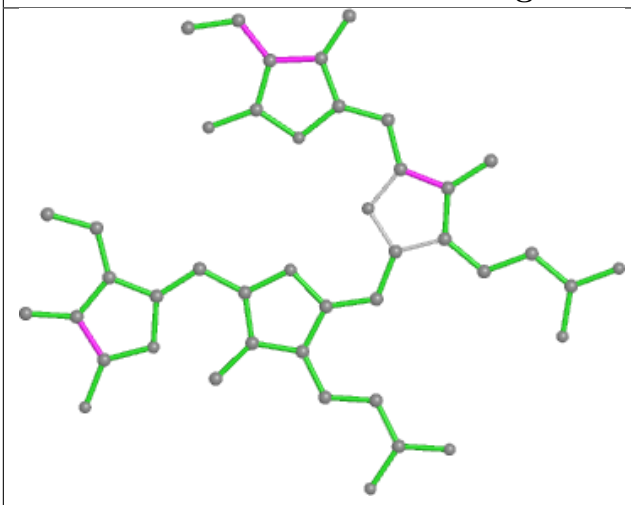


Rings

Ligand PEB cK 202



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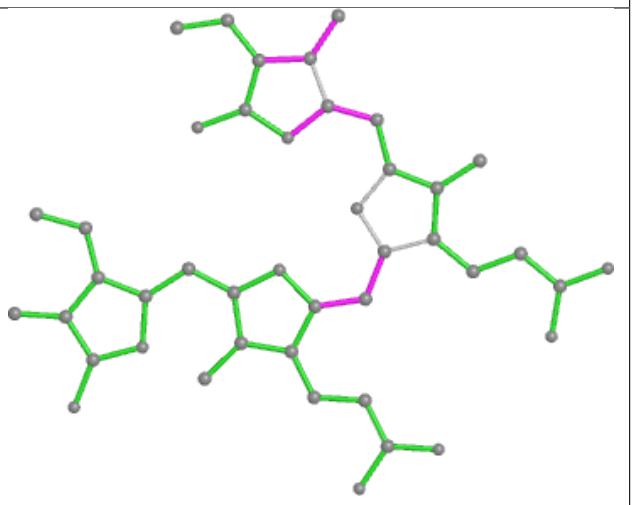

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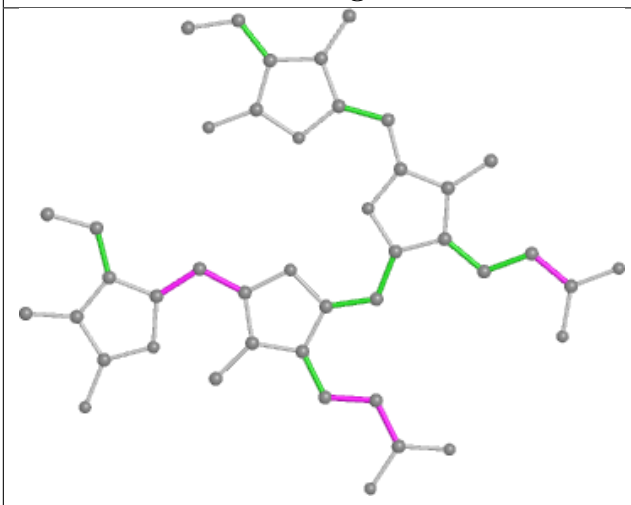

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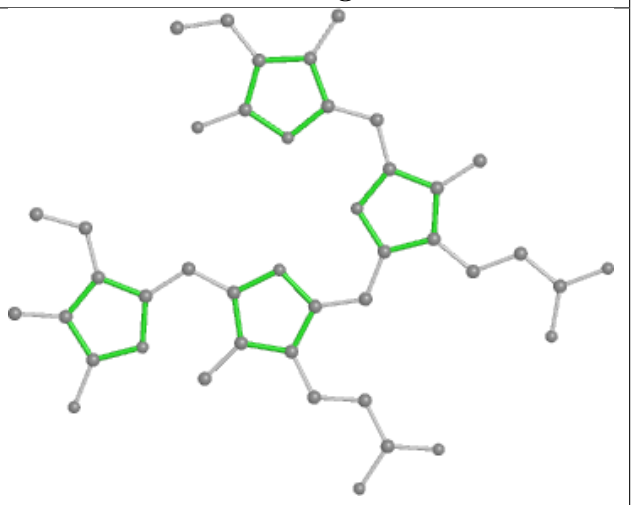
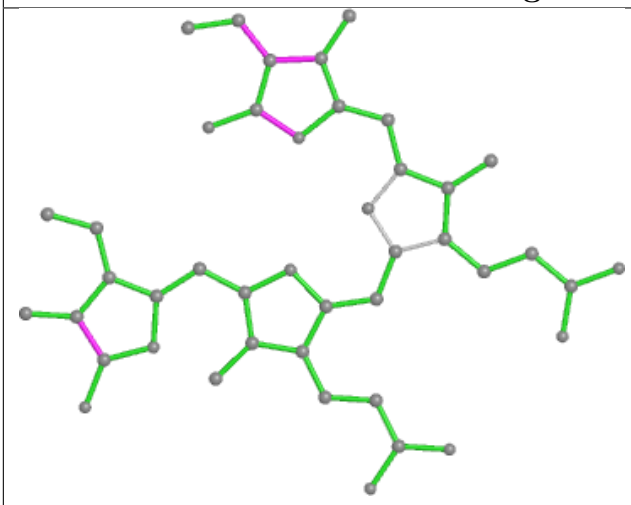


Rings

Ligand PEB f8 202



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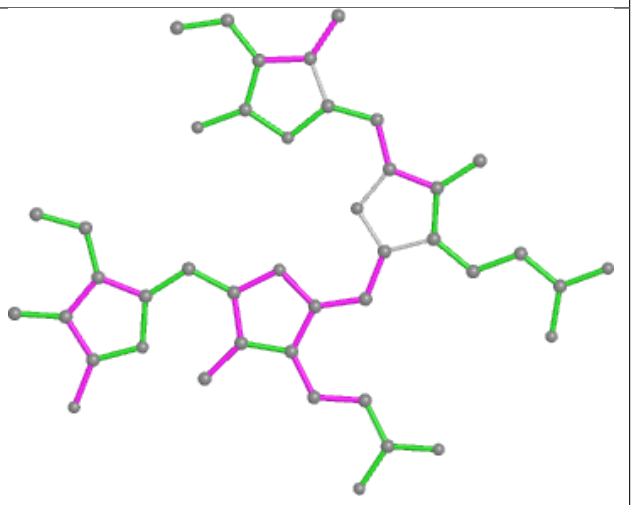

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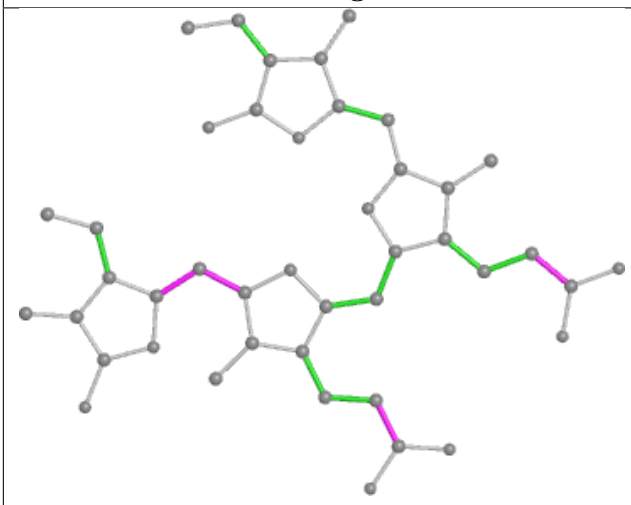

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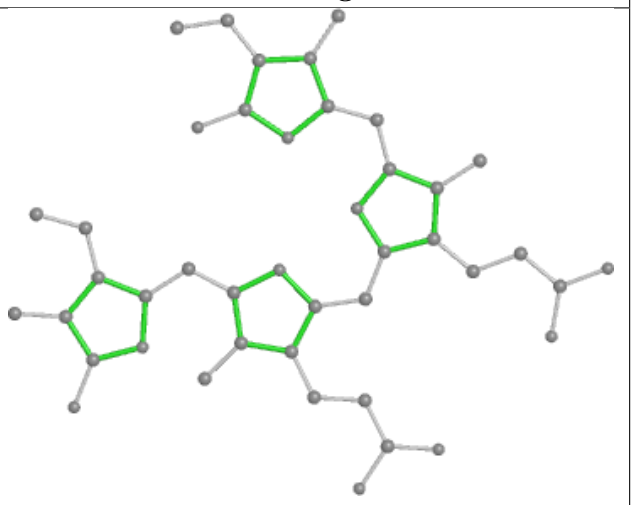
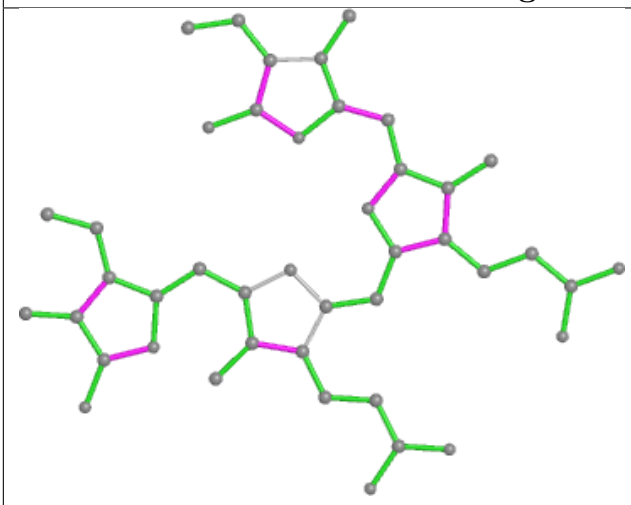


Rings

Ligand PUB gz 306



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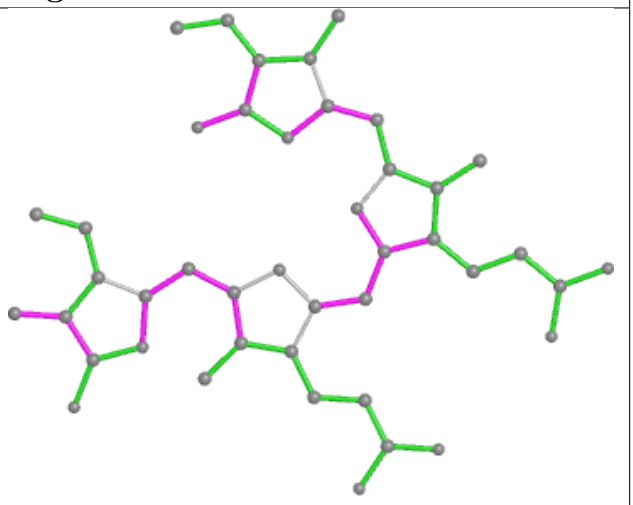

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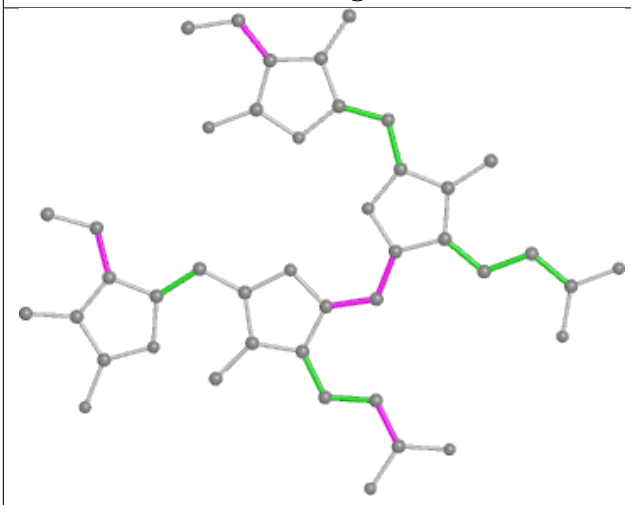

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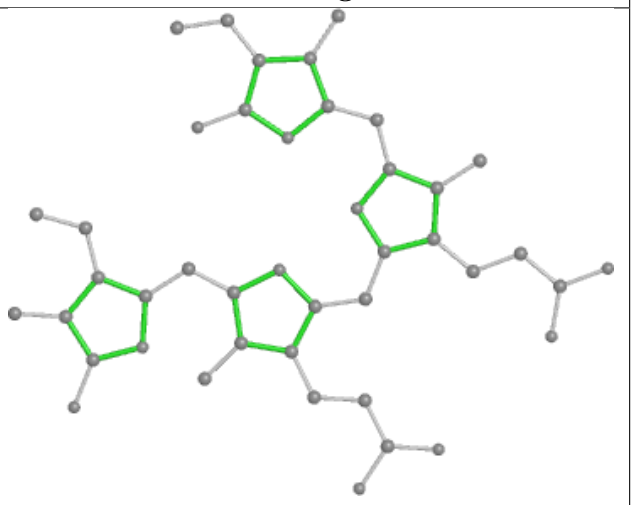
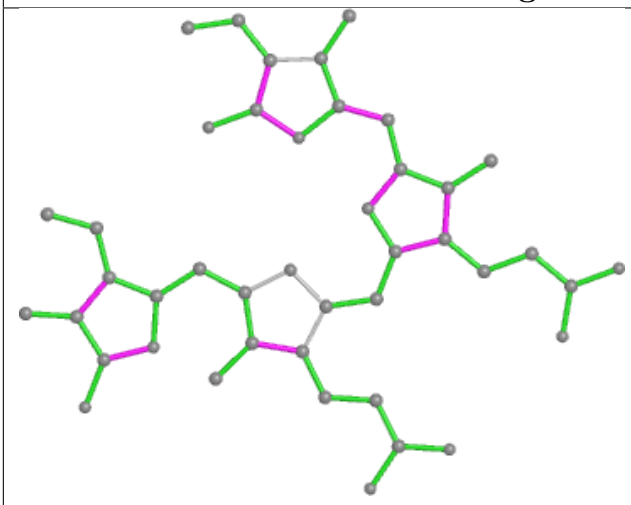


Rings

Ligand PUB c3 304



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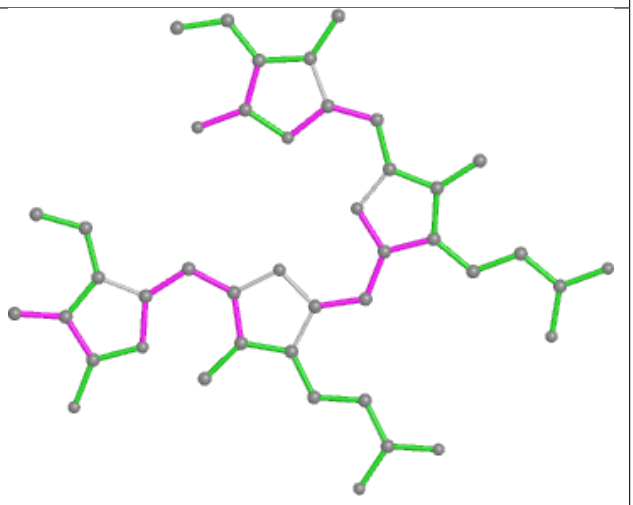
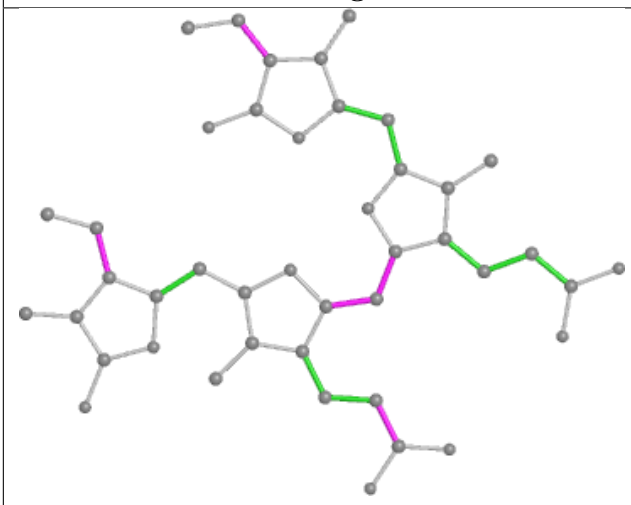


Bond angles



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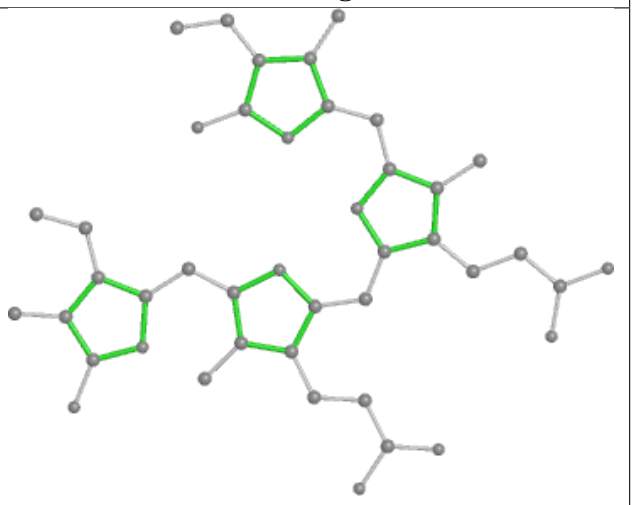
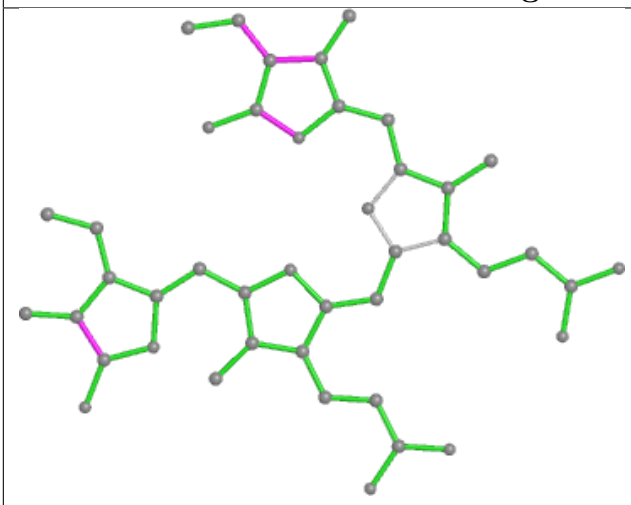


Rings

Ligand PEB s4 201



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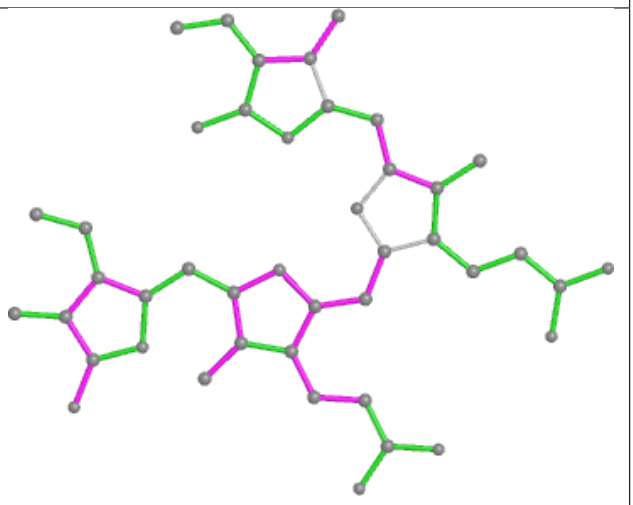
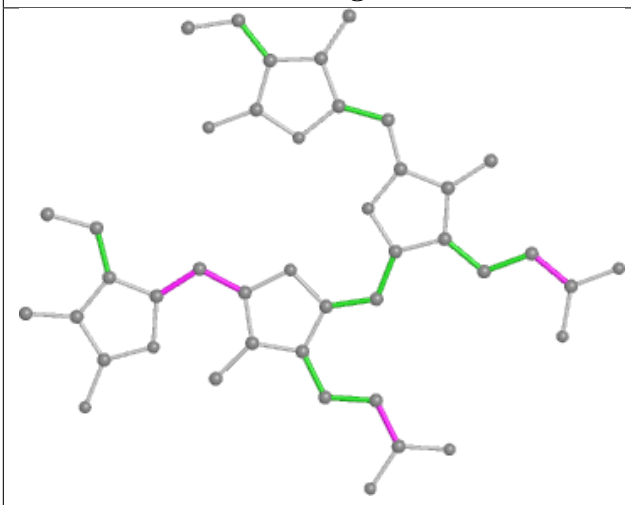


Bond angles



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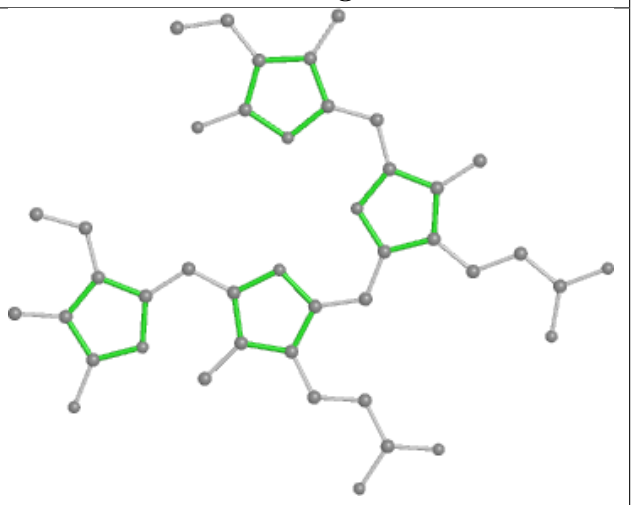
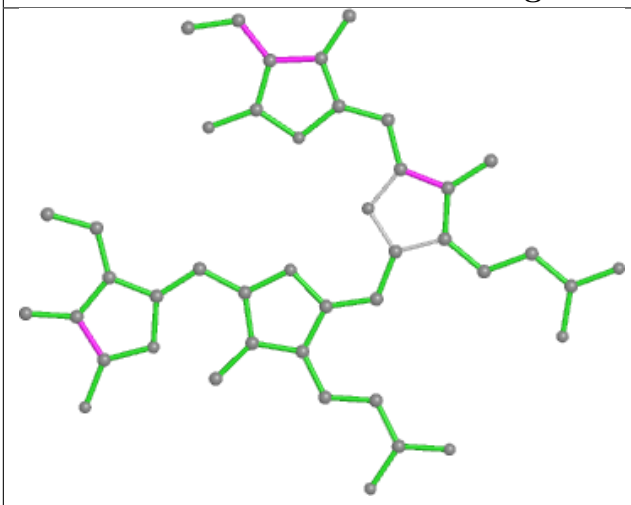


Rings

Ligand PEB fz 301



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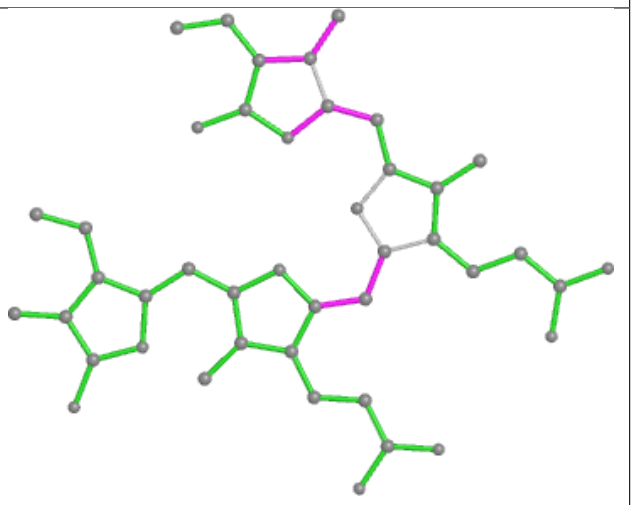

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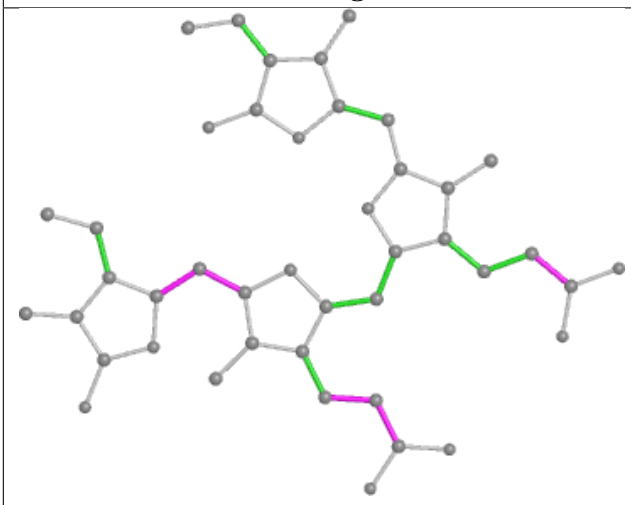

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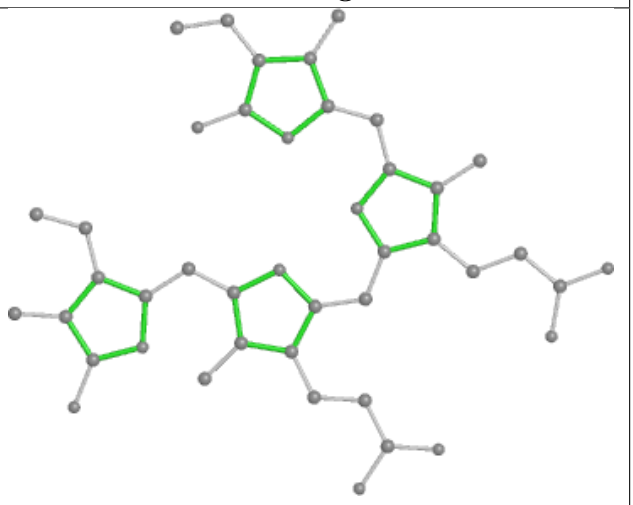
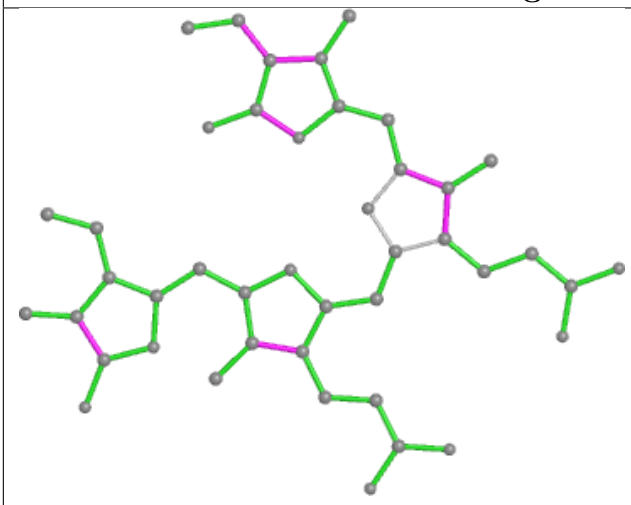


Rings

Ligand PEB i3 203



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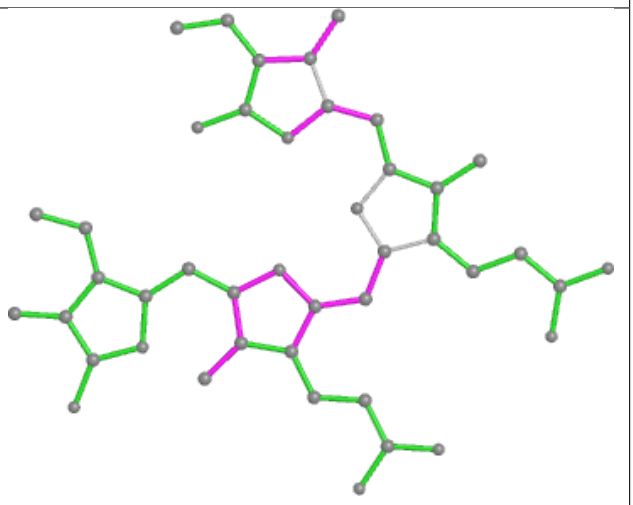

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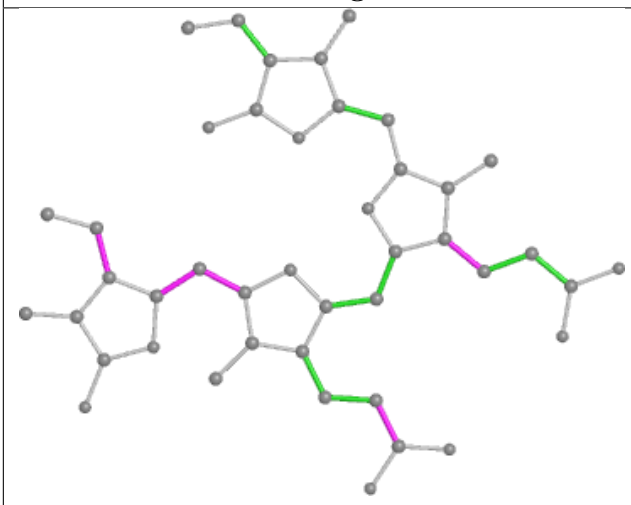

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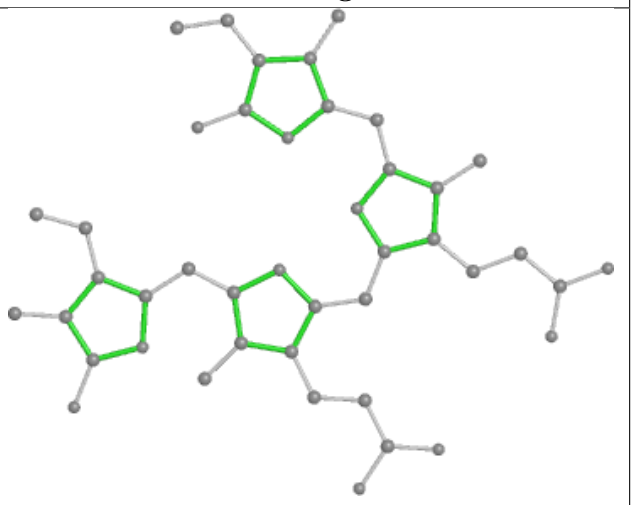
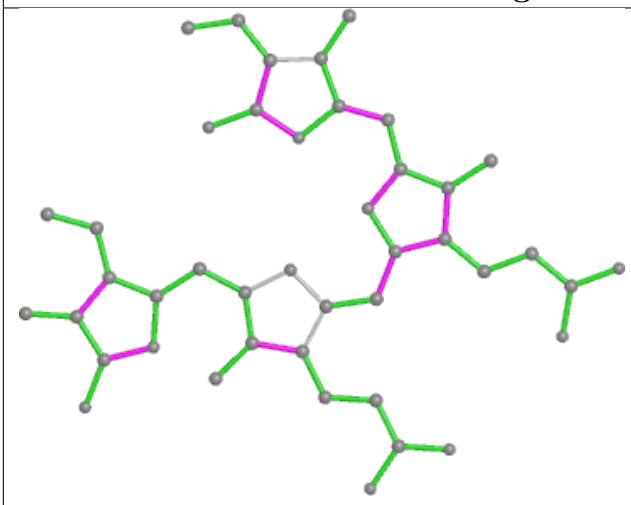


Rings

Ligand PUB D7 203



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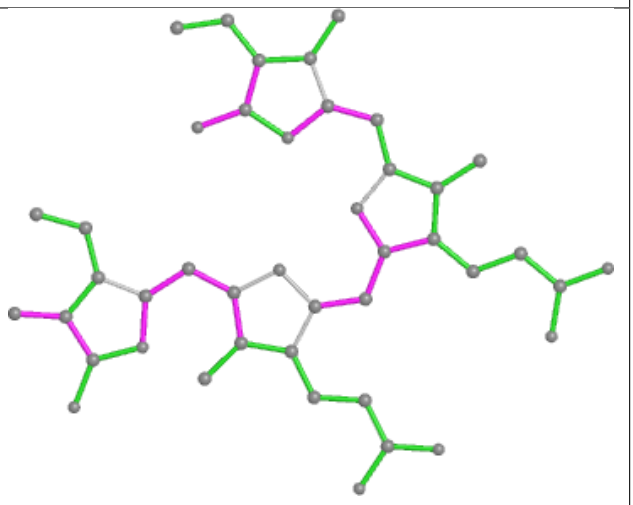

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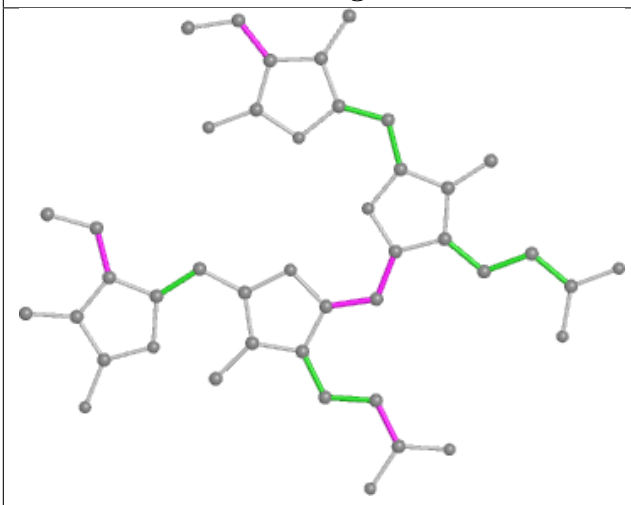

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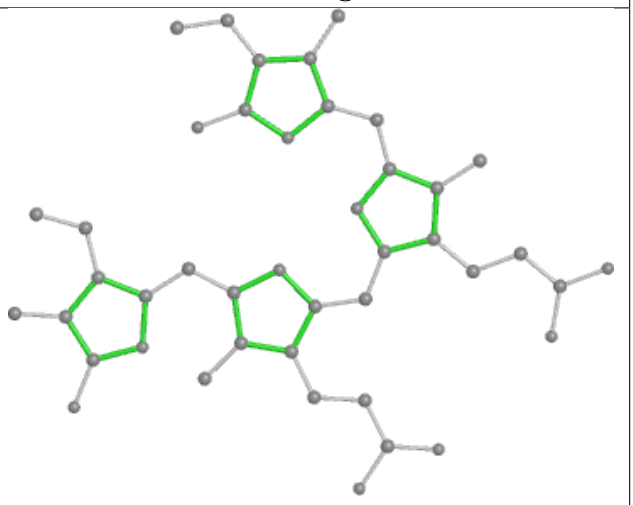

Rings

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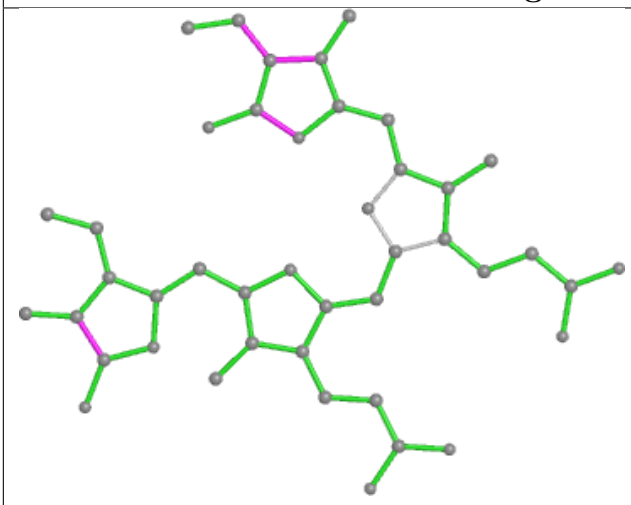

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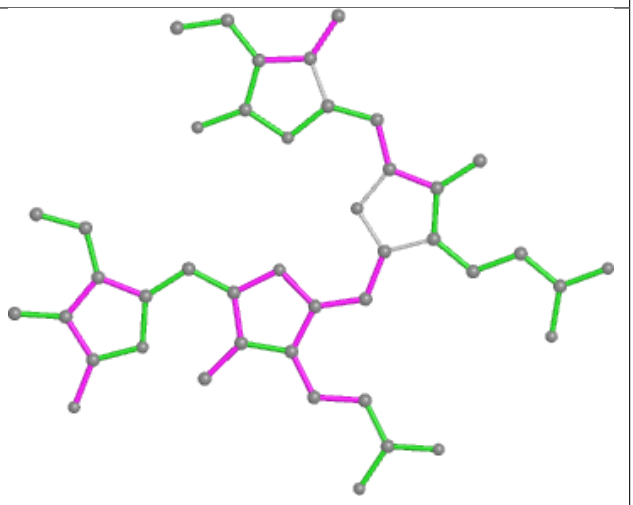

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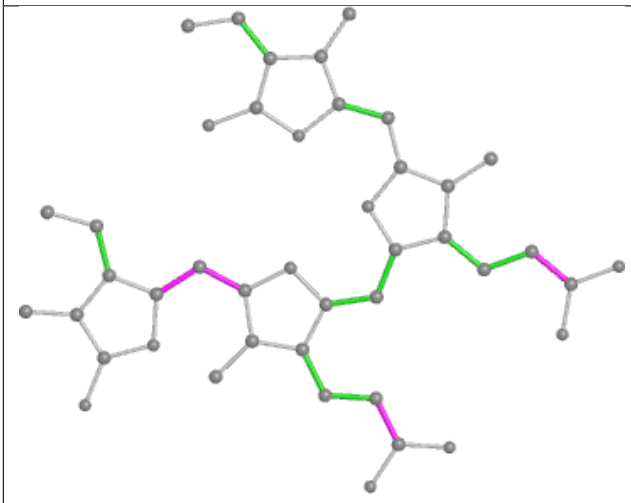

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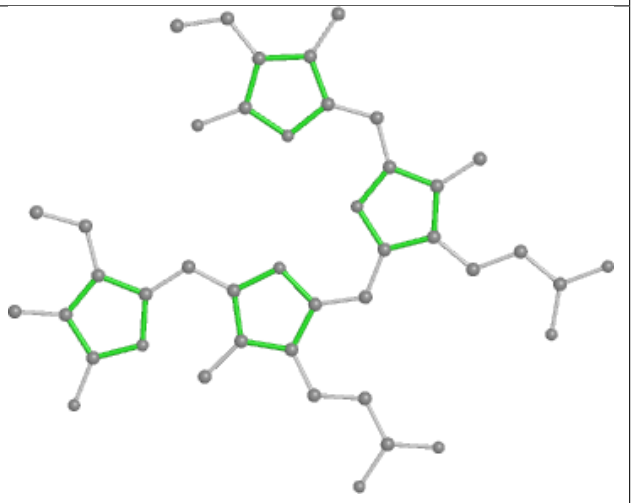

Rings

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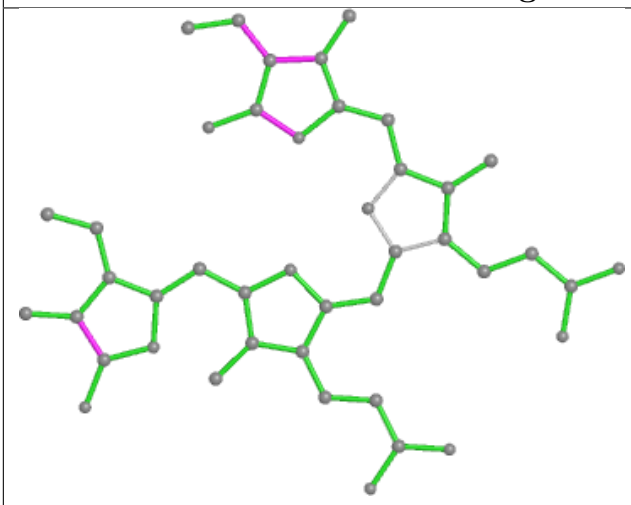

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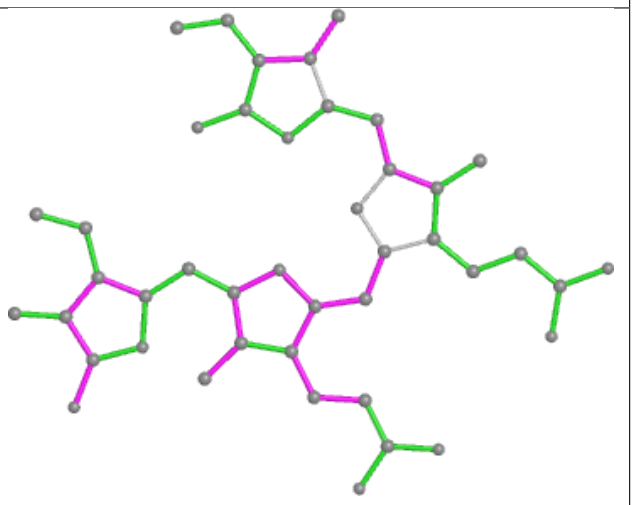

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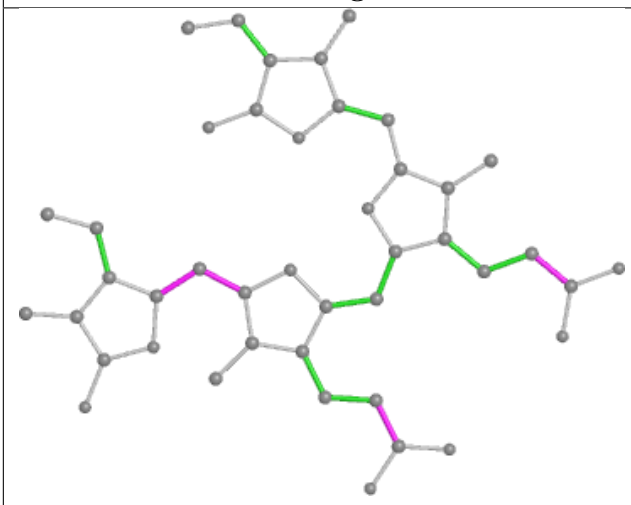

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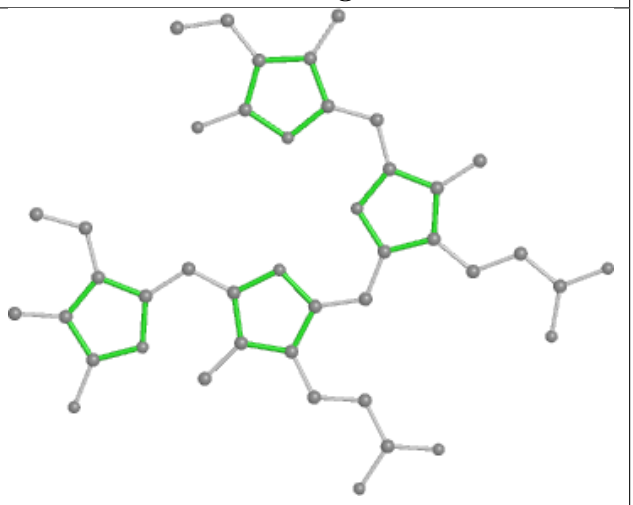

Rings

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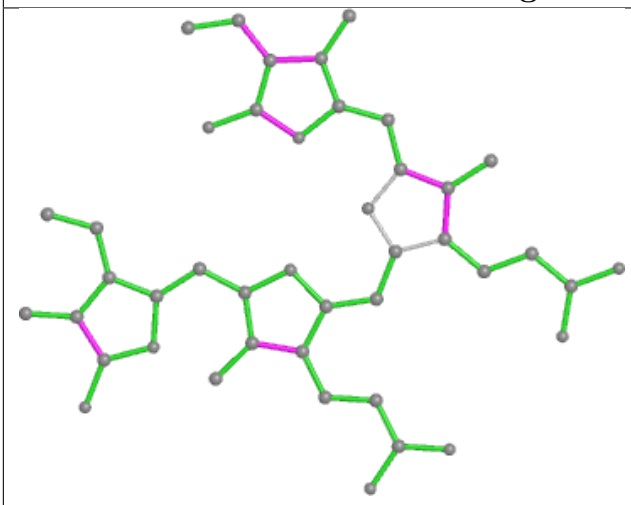

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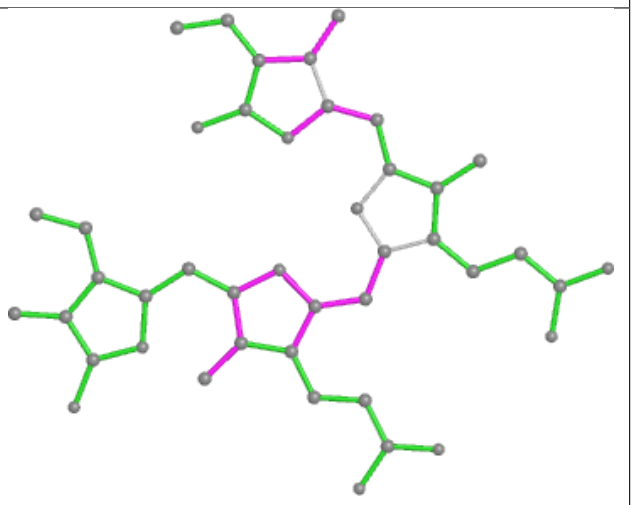

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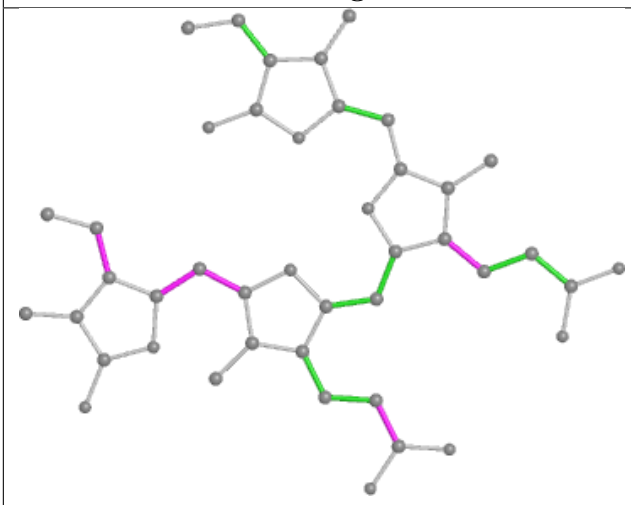

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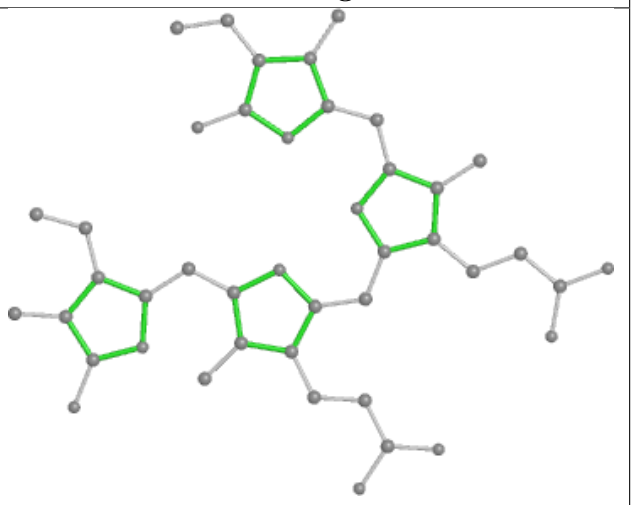

Rings

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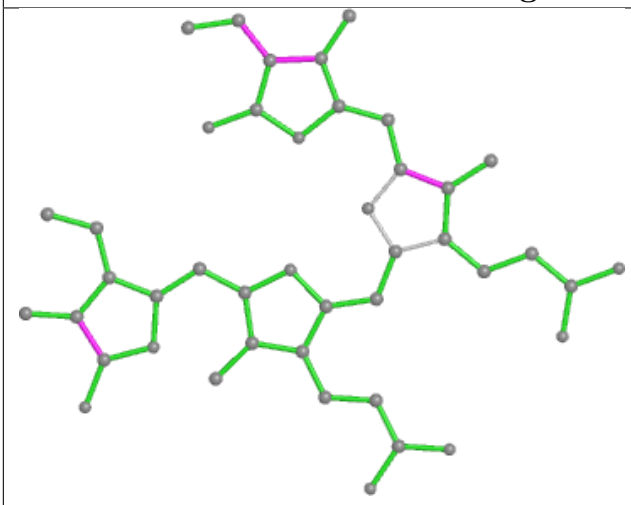

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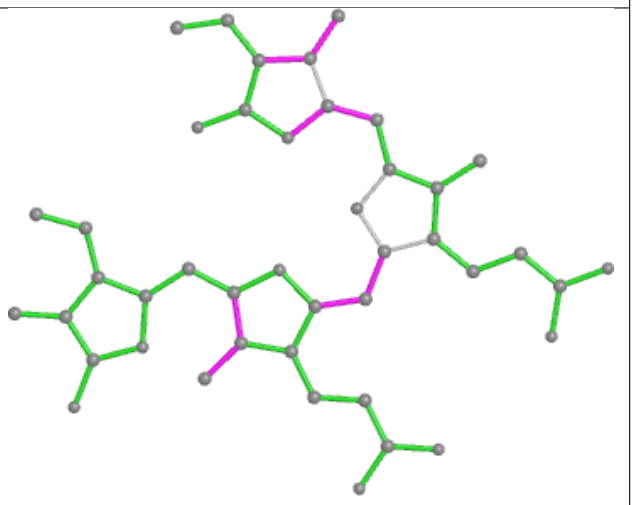

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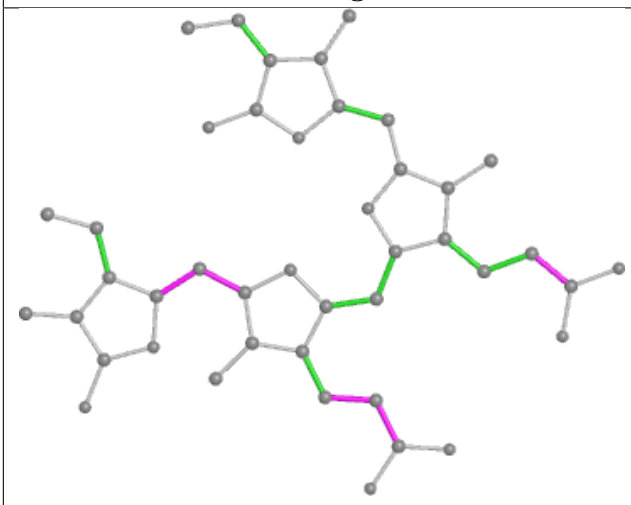

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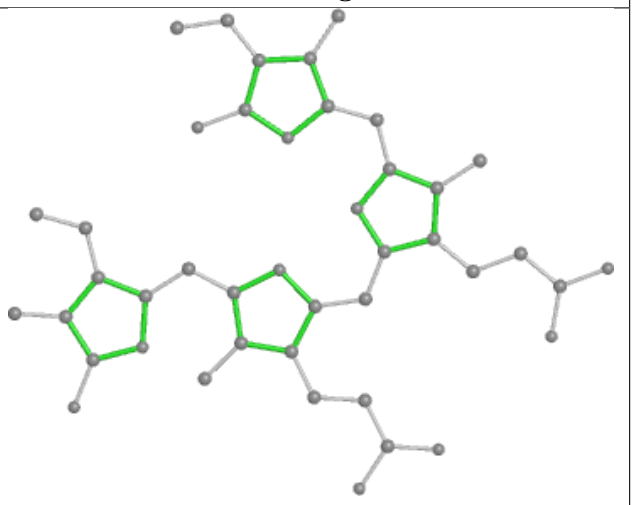

Rings

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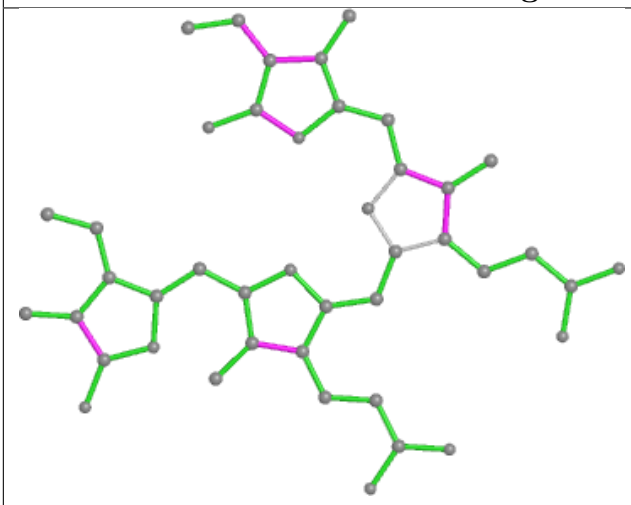

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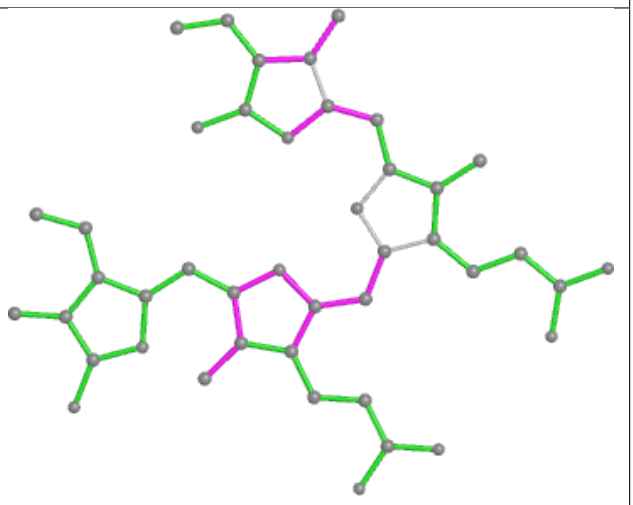

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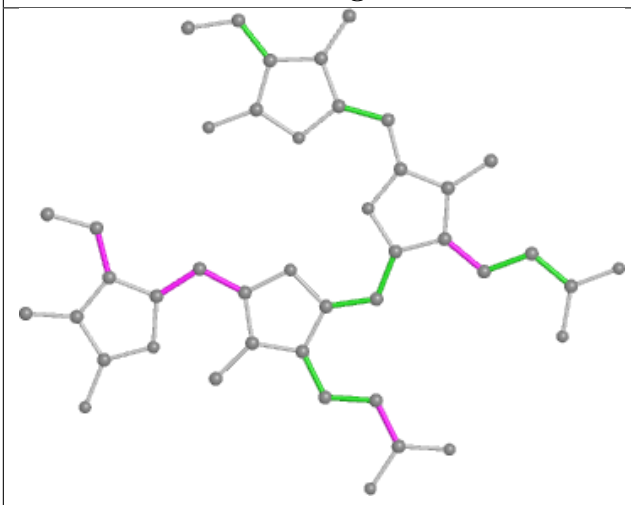

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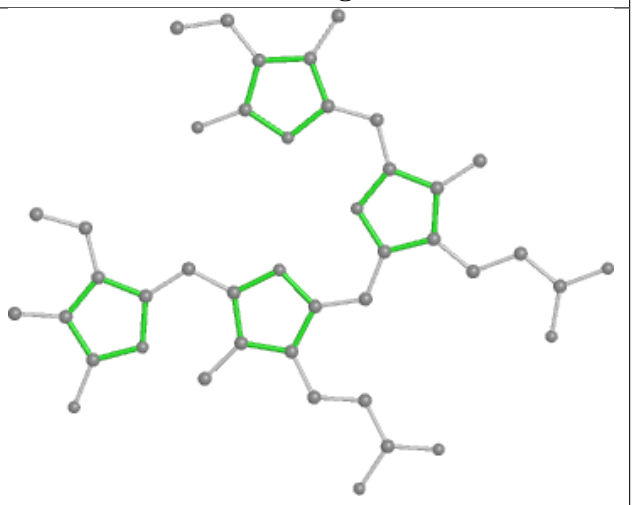

Rings

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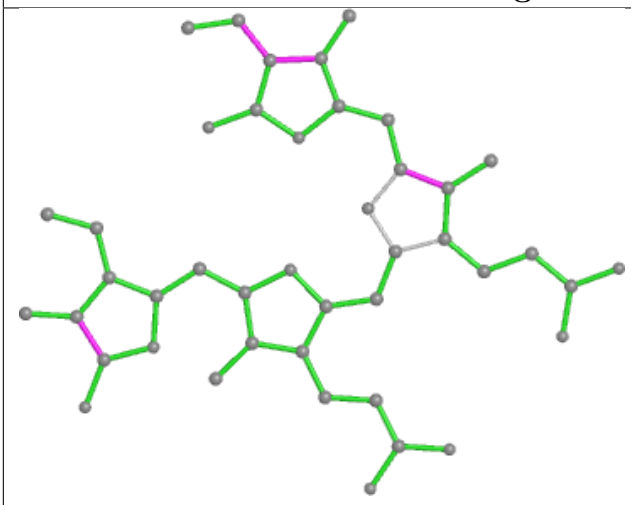

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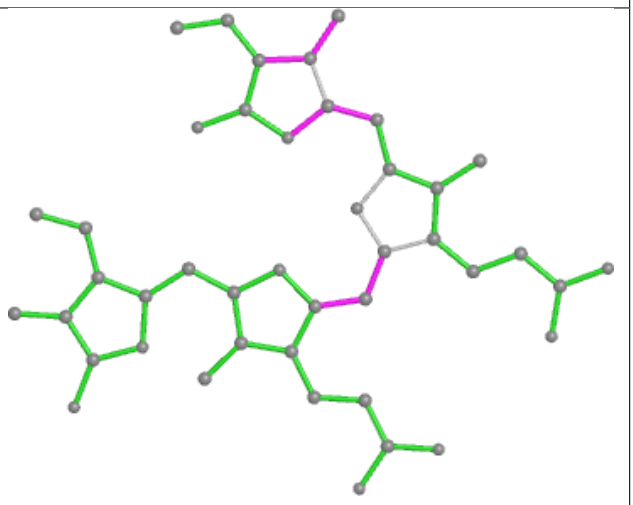

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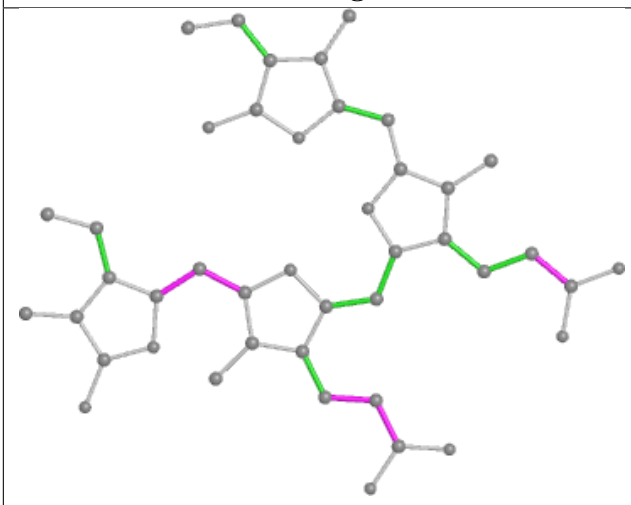

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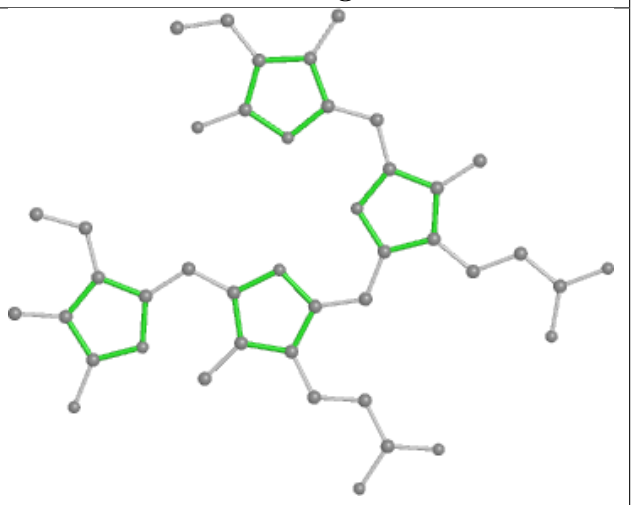

Rings

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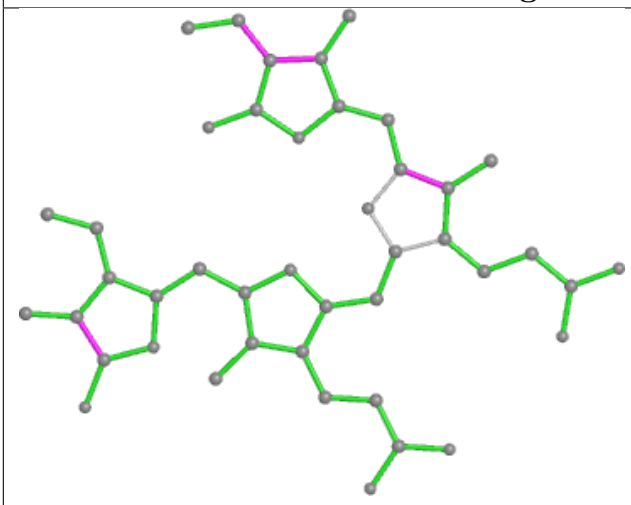

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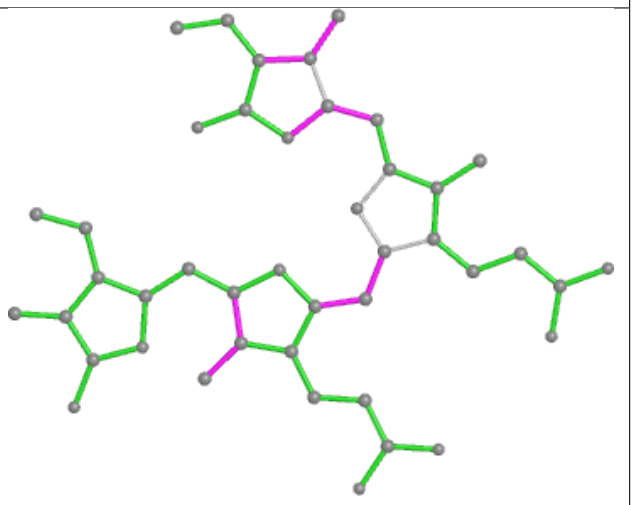

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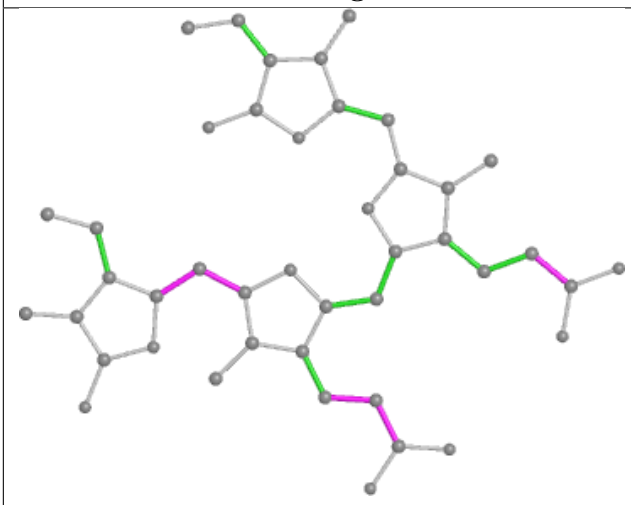

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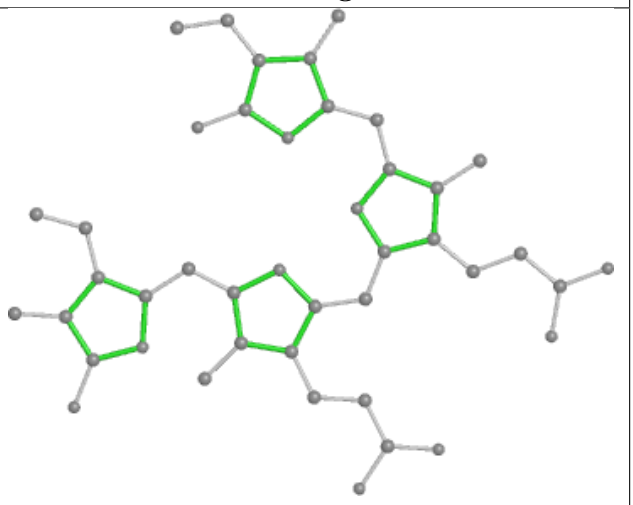

Rings

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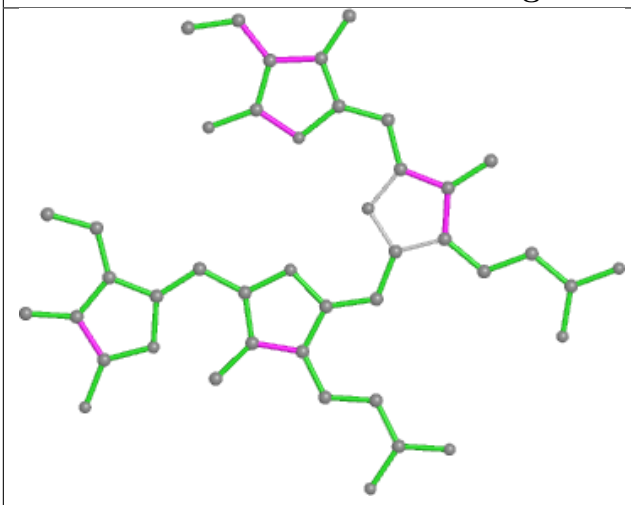

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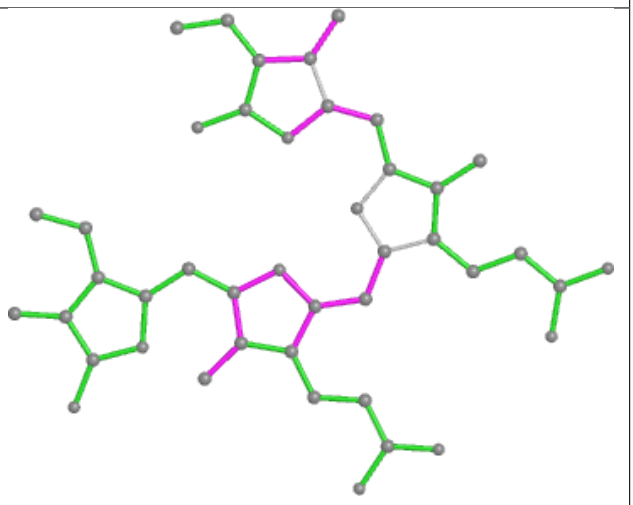

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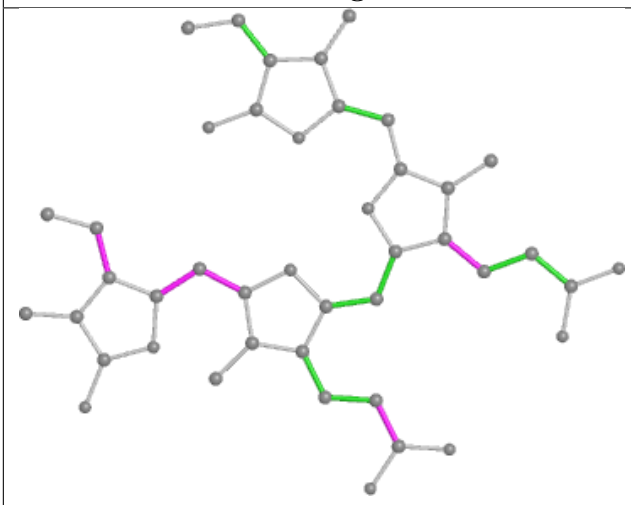

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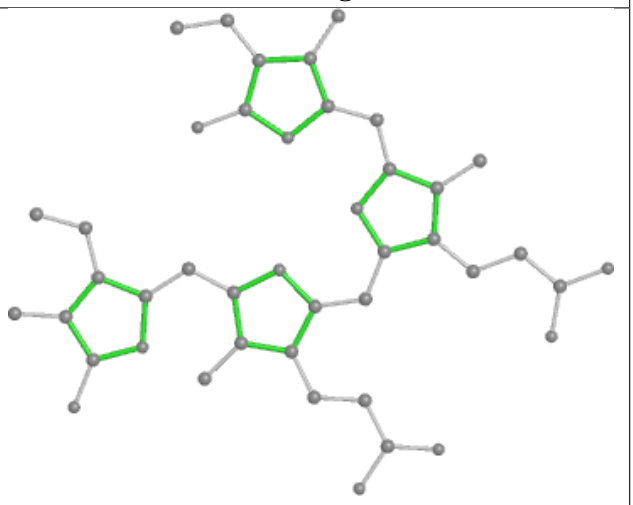

Rings

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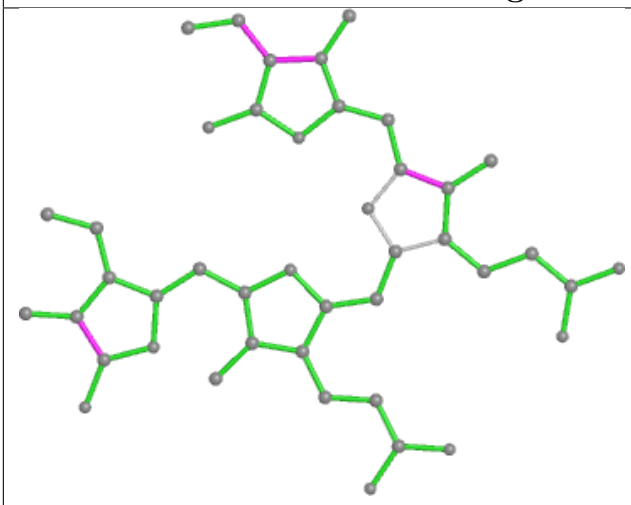

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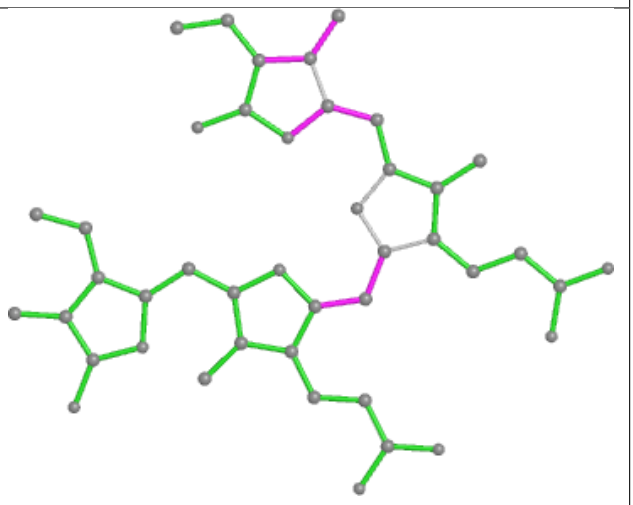

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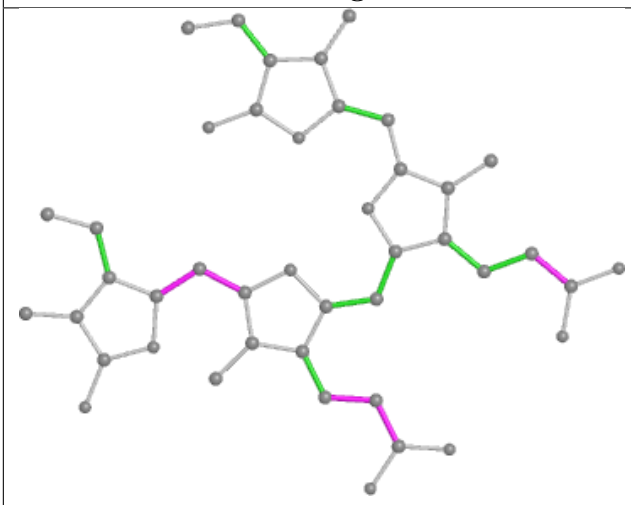

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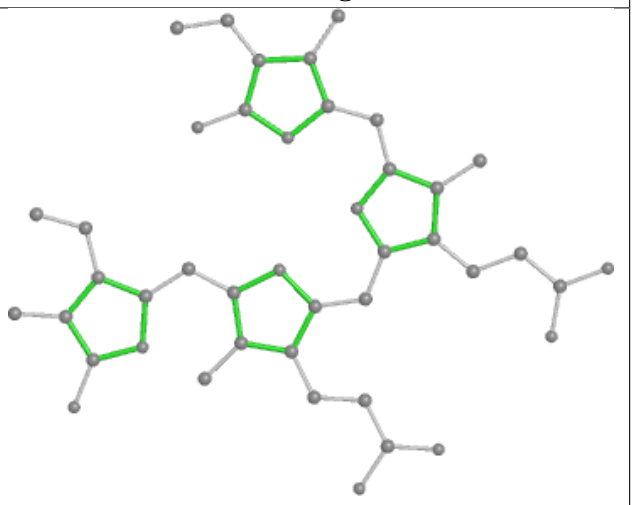
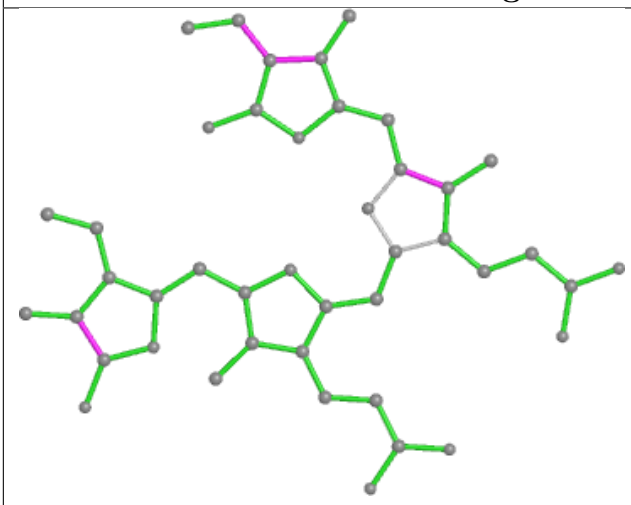


Rings

Ligand PEB M7 1003



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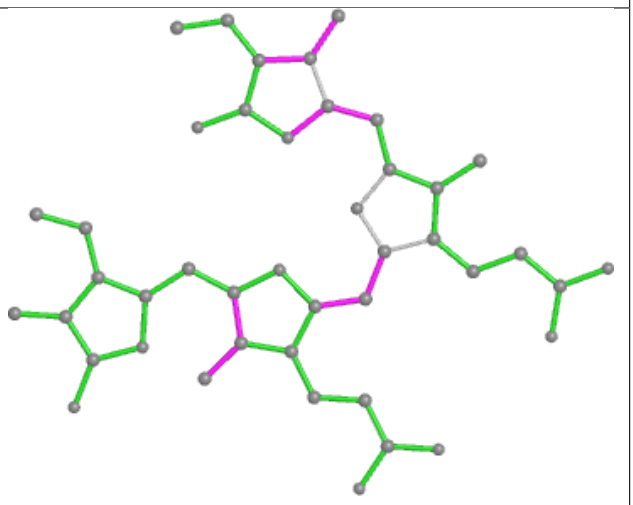

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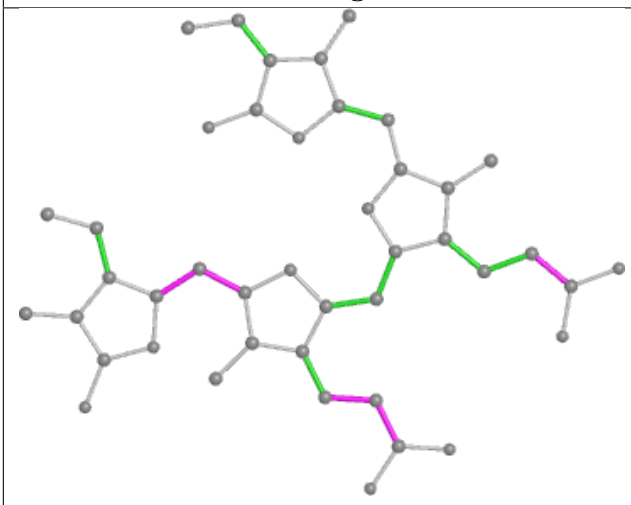

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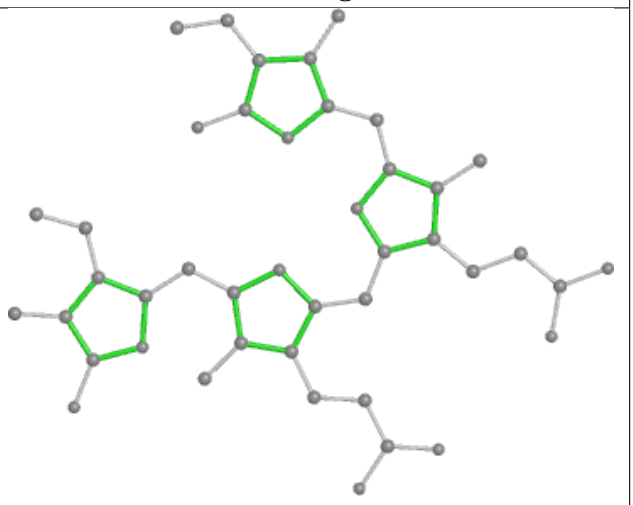

Rings

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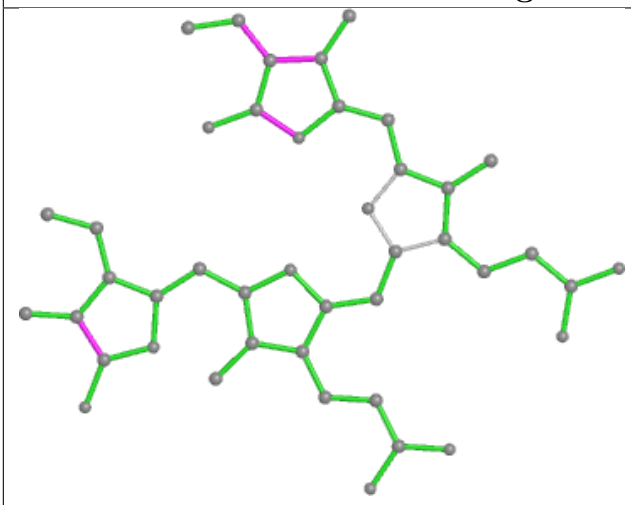

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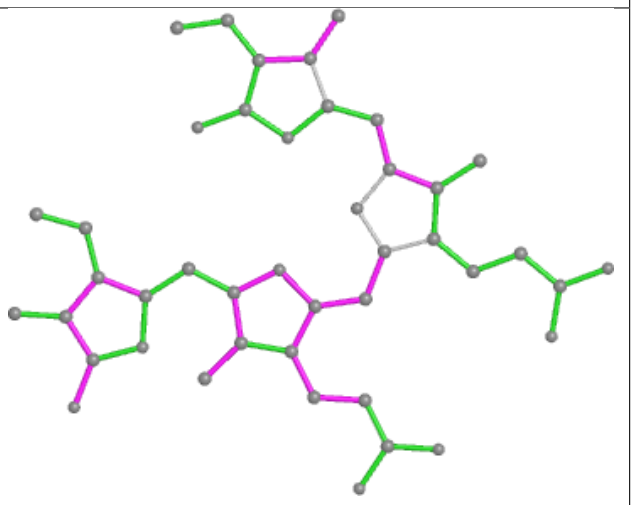
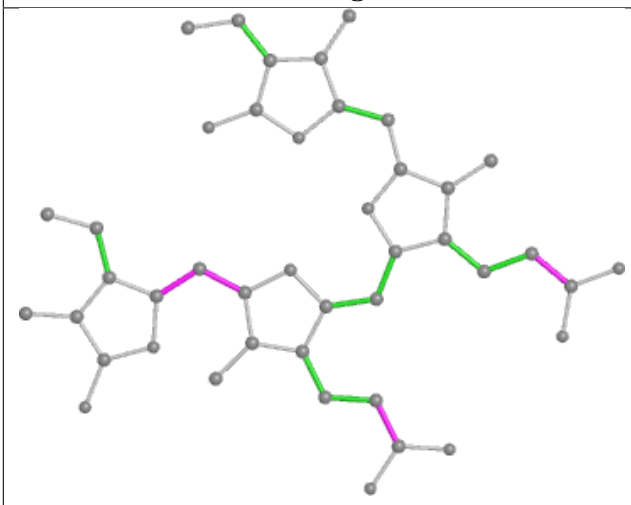
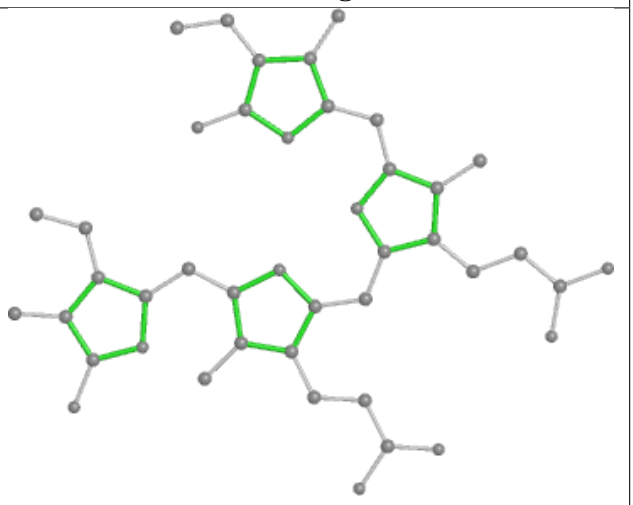


Bond angles

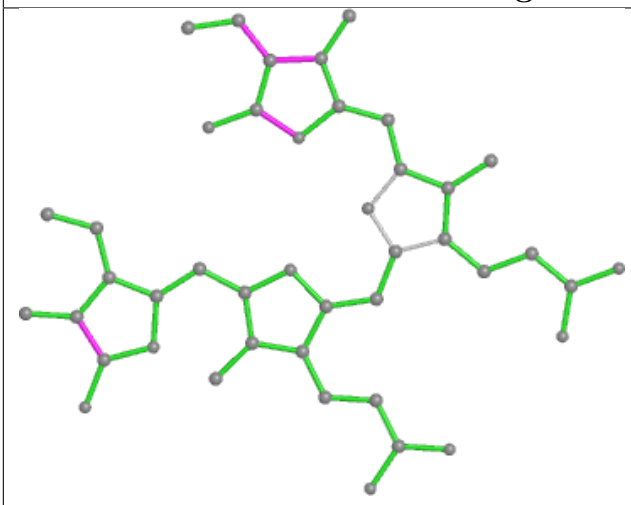


Torsions



Rings

Ligand PEB O8 202



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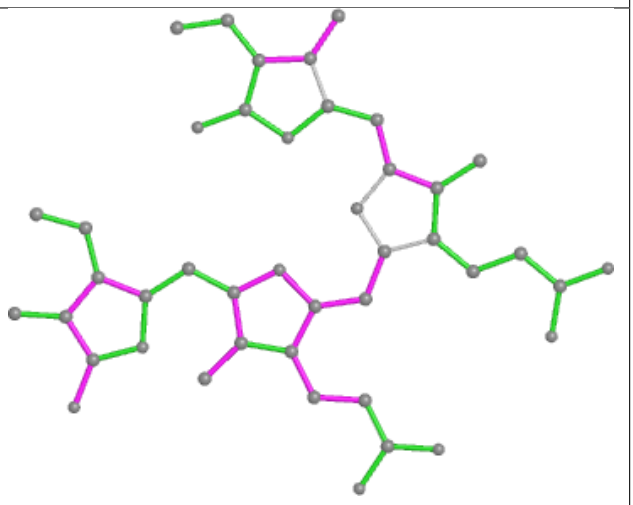

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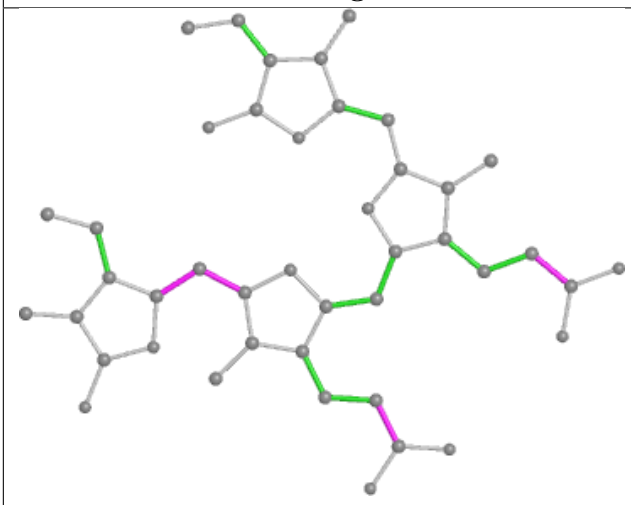

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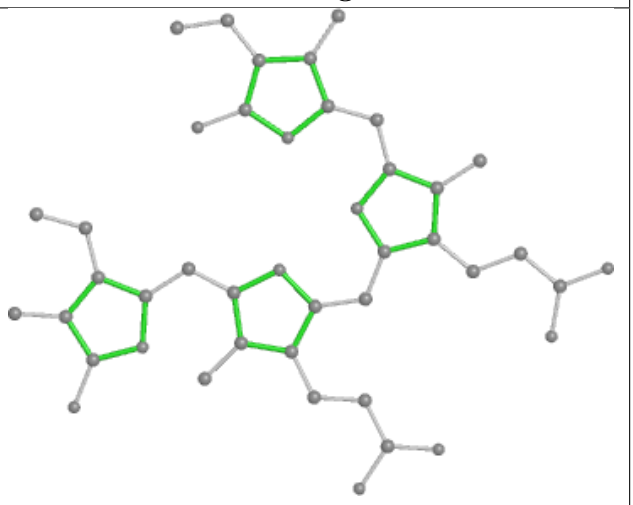
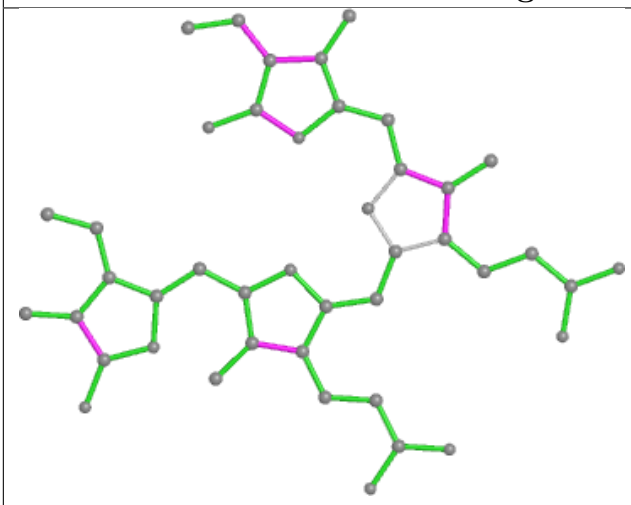


Rings

Ligand PEB cB 202



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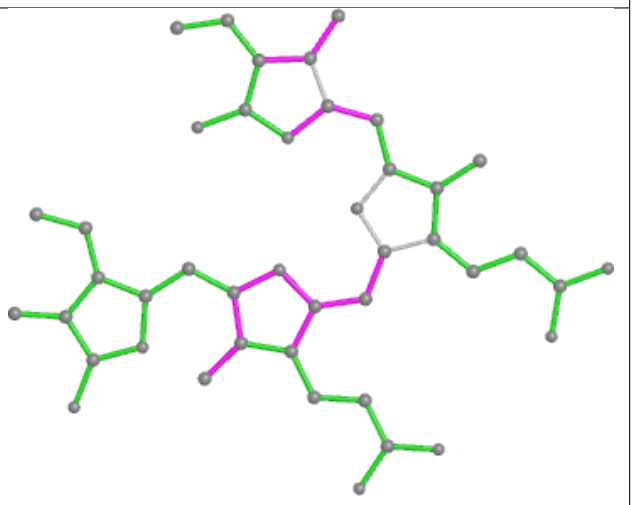

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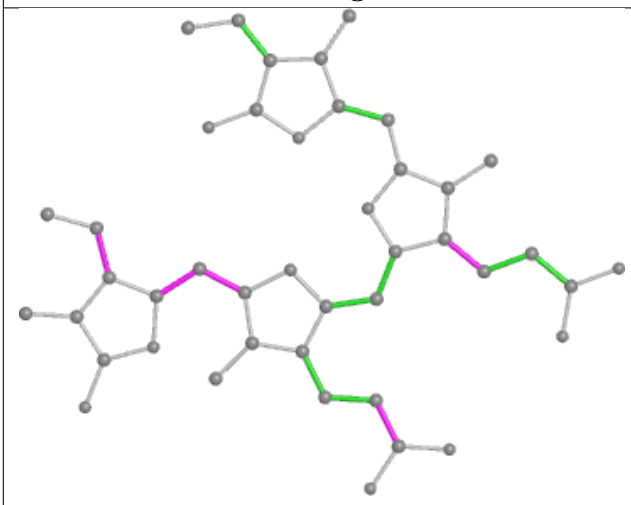

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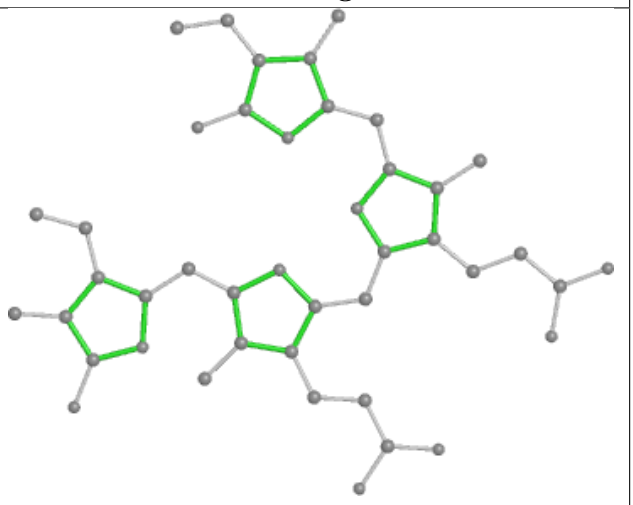
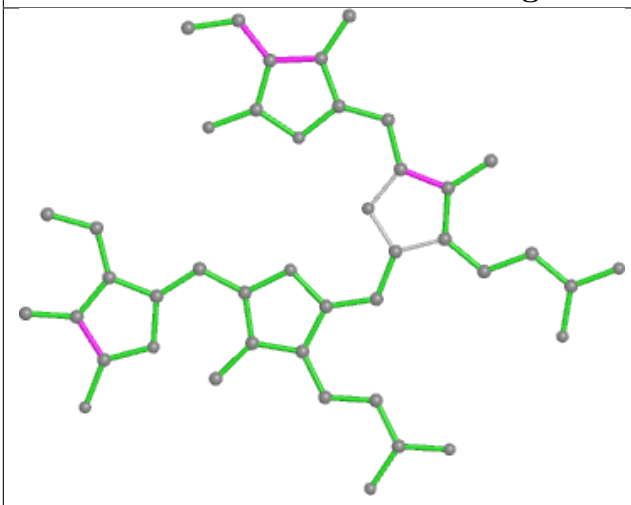


Rings

Ligand PEB s3 202



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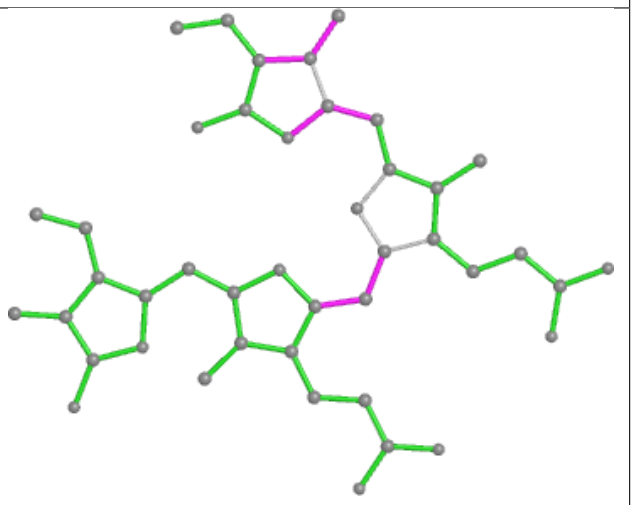

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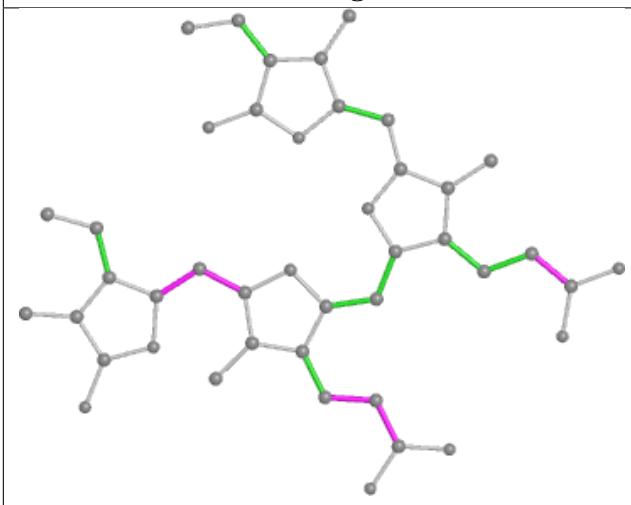

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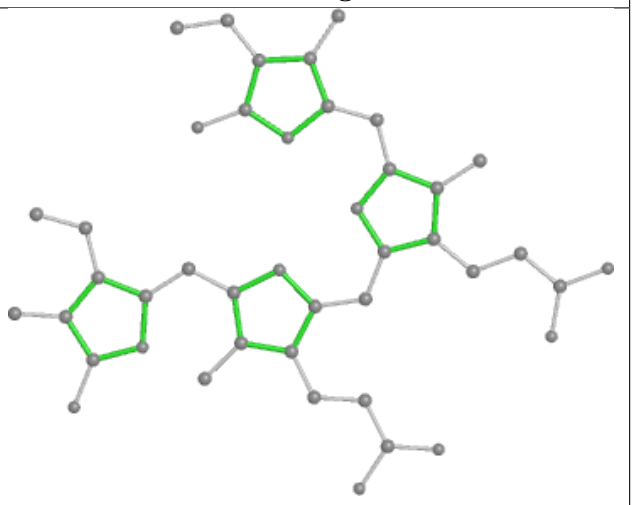
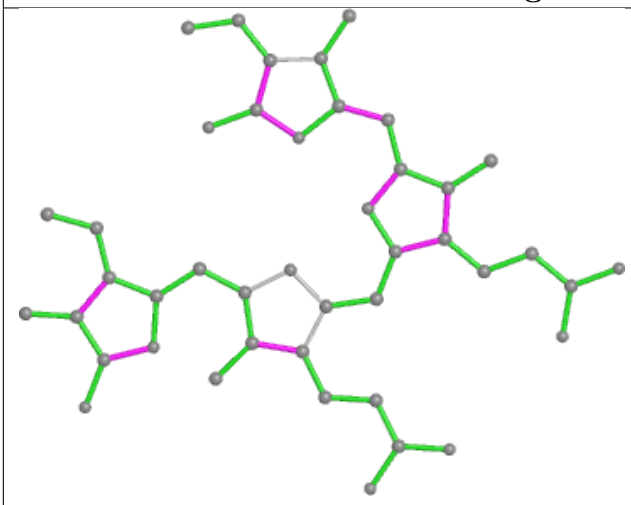


Rings

Ligand PUB fj 203



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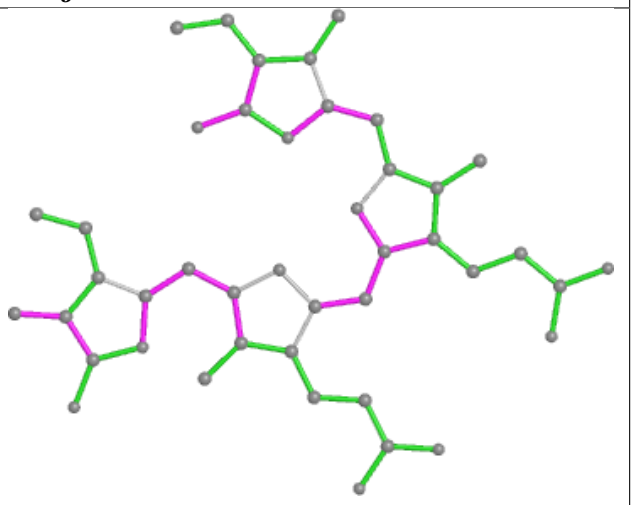

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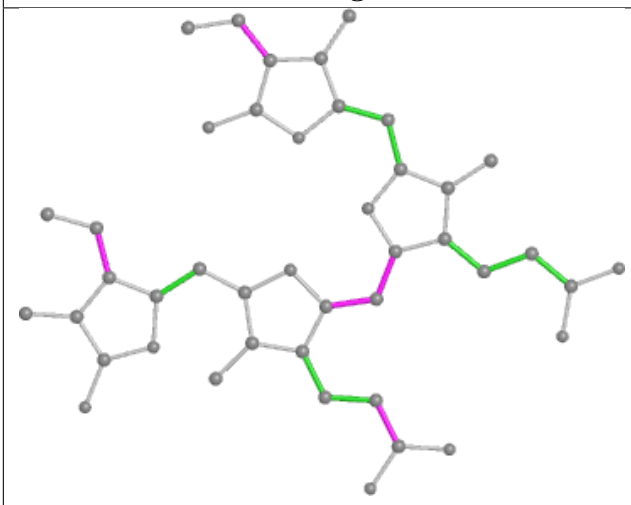

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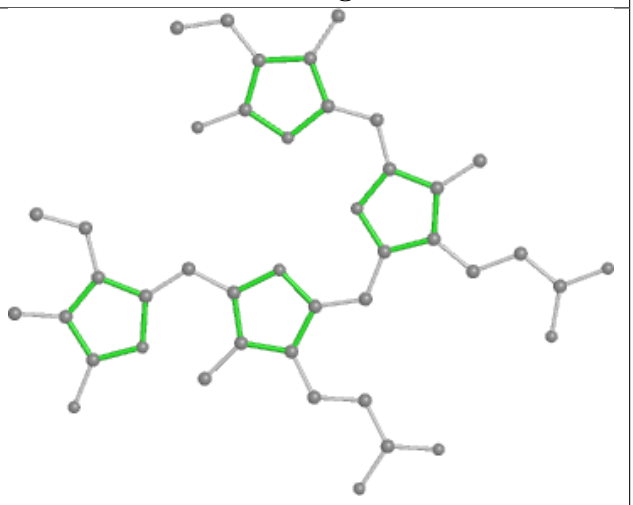
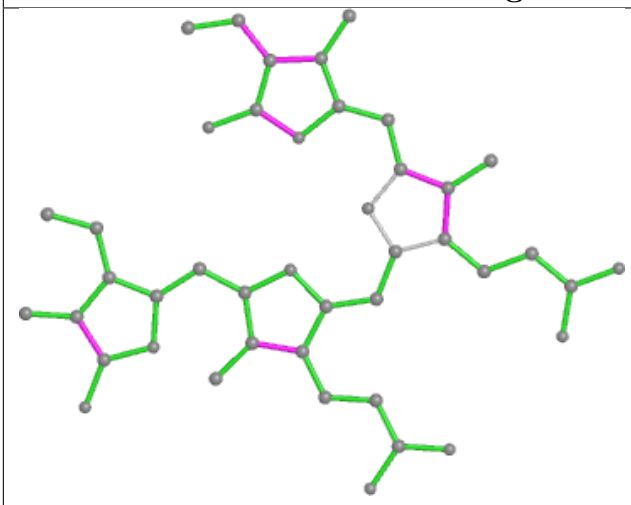


Rings

Ligand PEB kQ 1002



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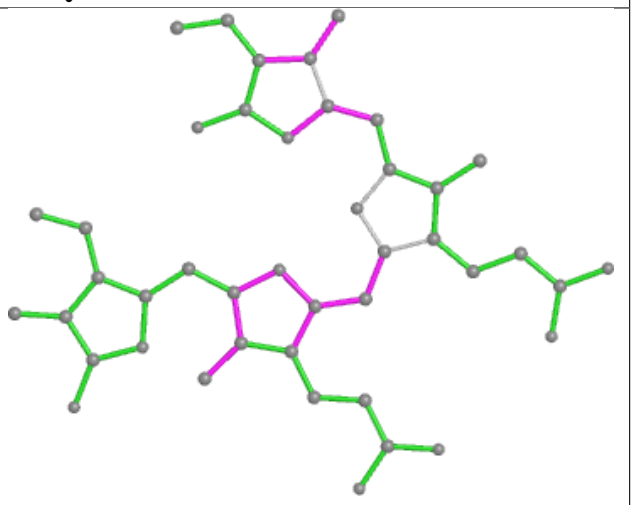

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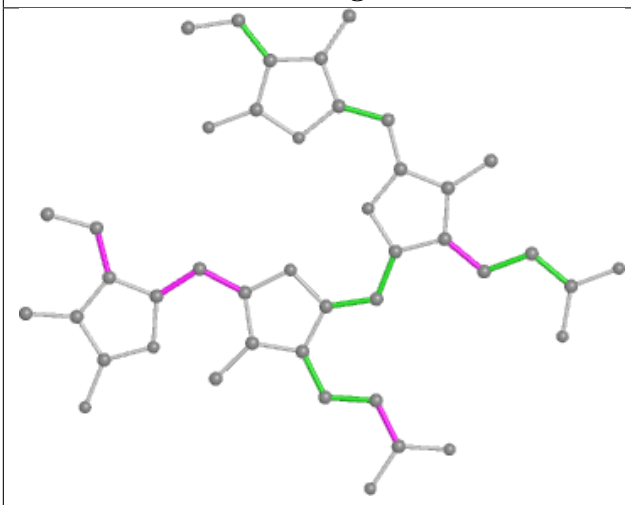

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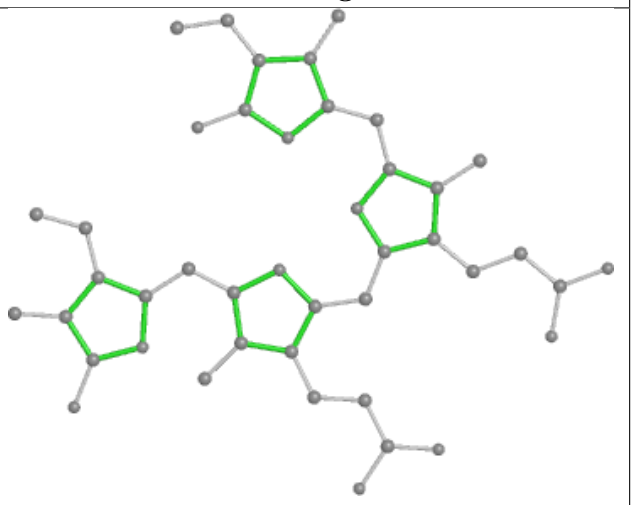

Rings

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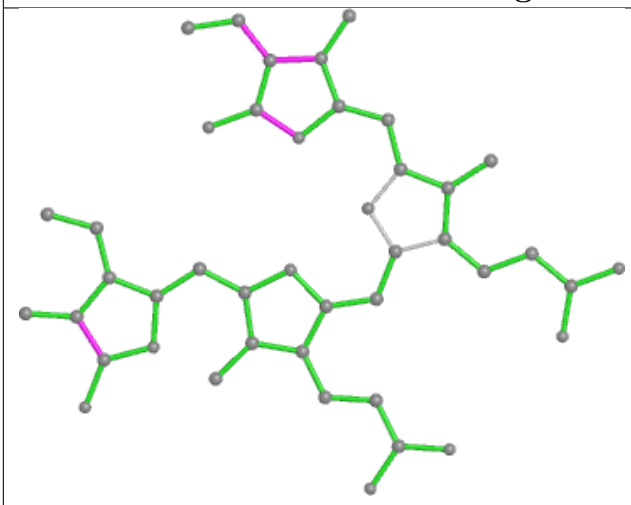

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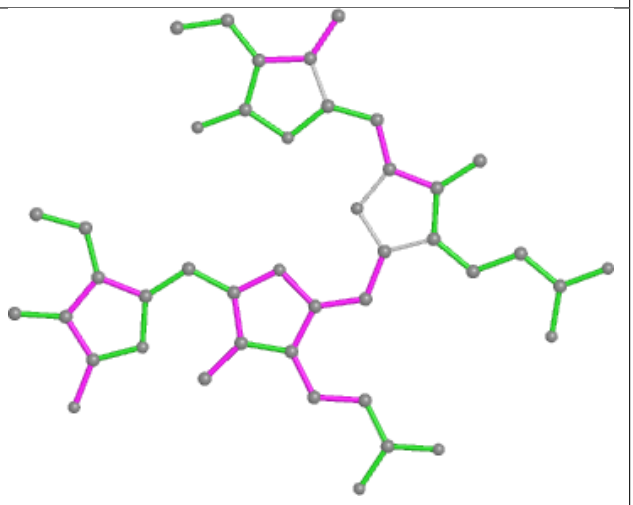

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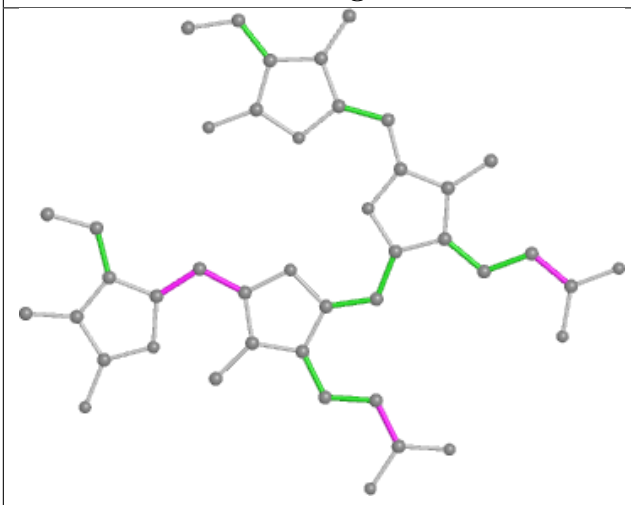

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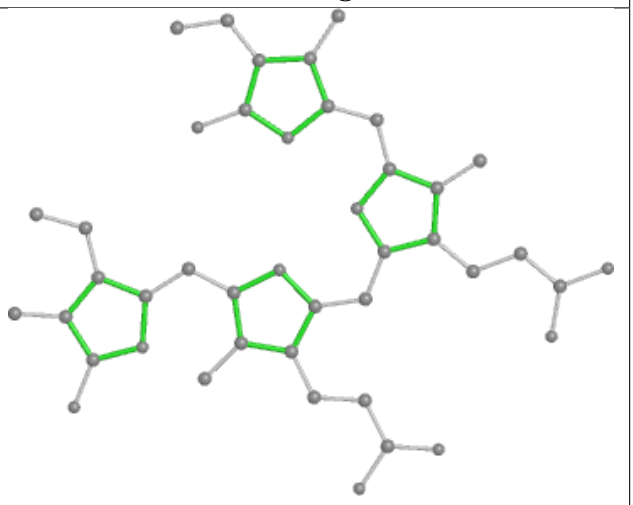
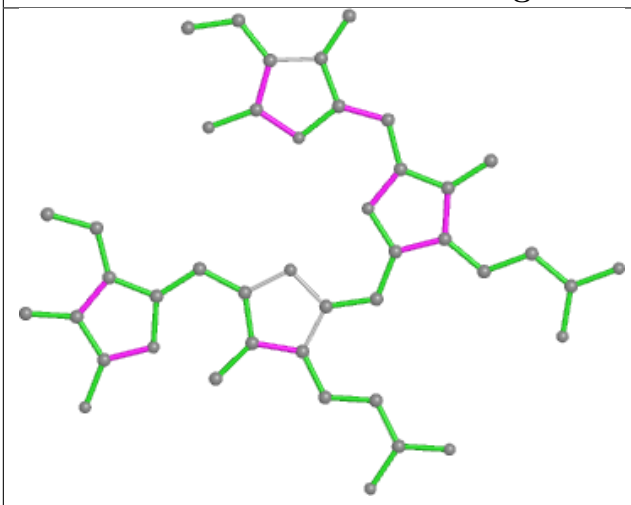


Rings

Ligand PUB R3 203



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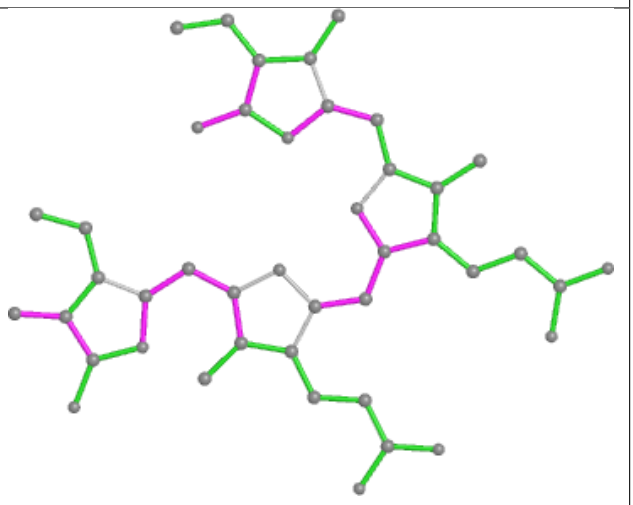

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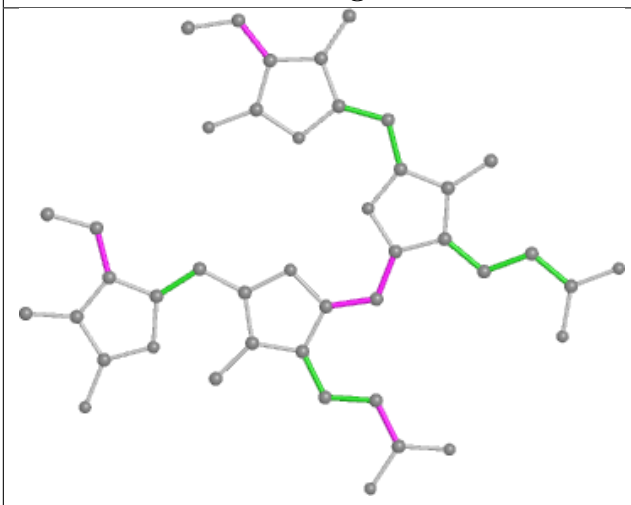

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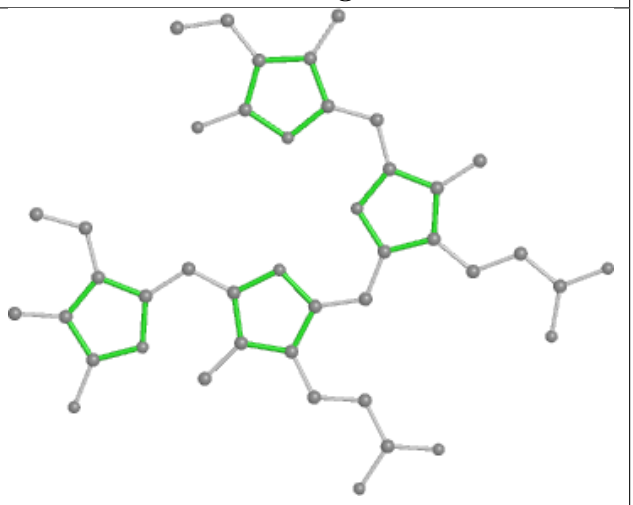
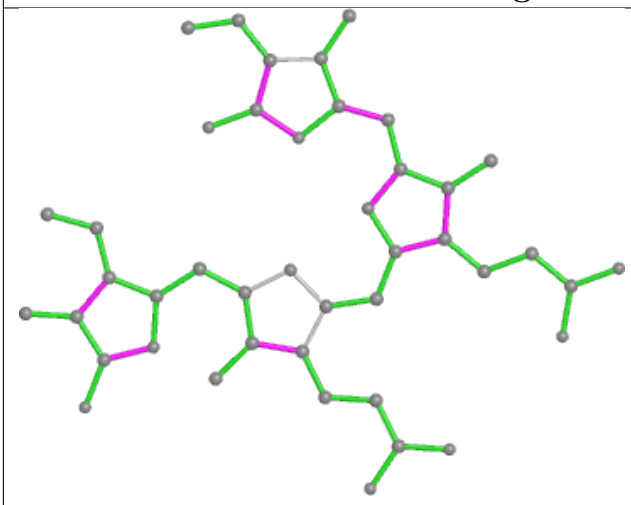


Rings

Ligand PUB X6 203



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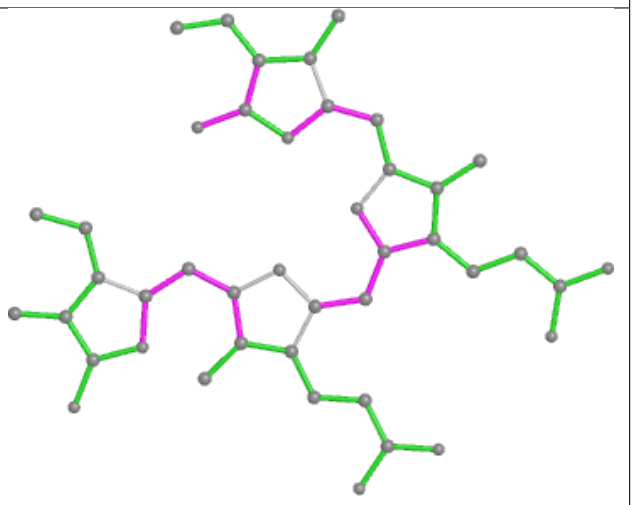

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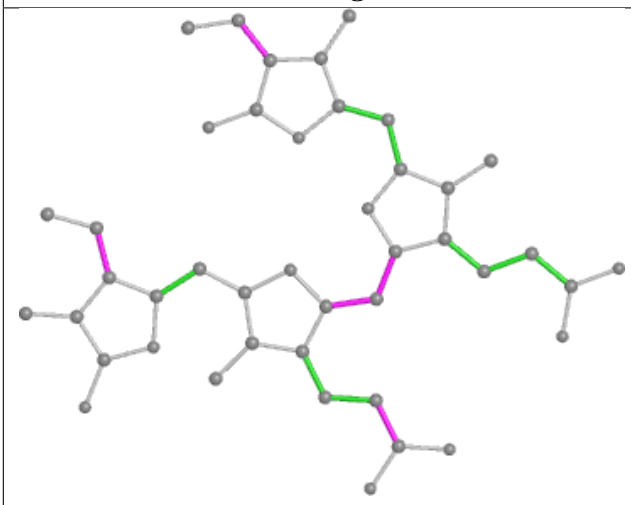

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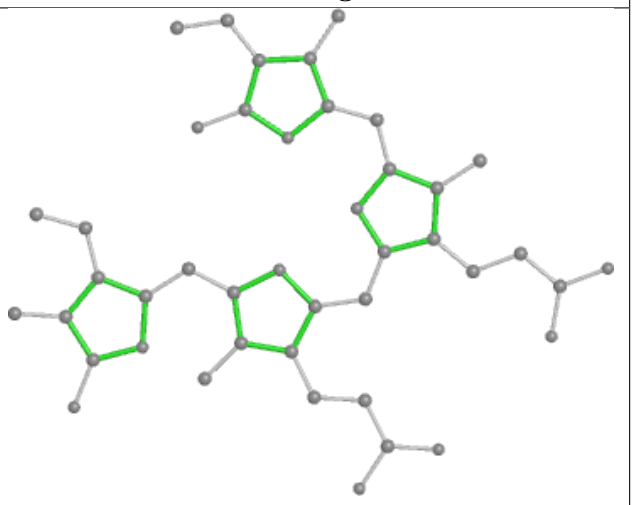
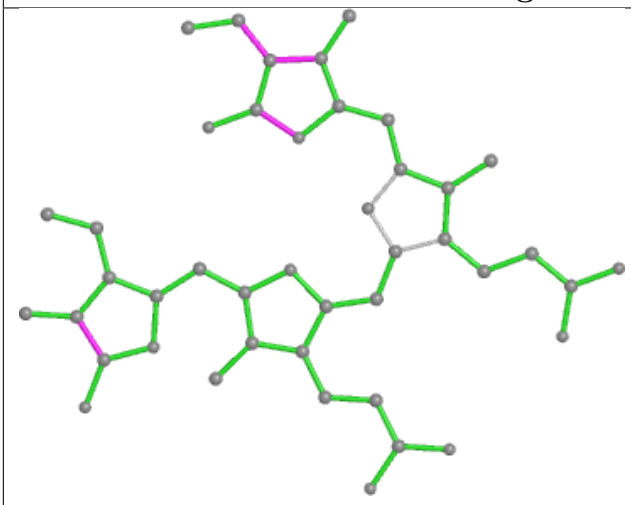


Rings

Ligand PEB cV 202



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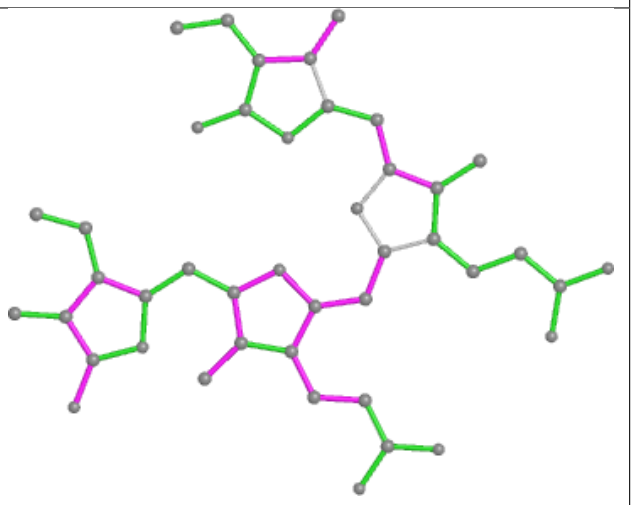

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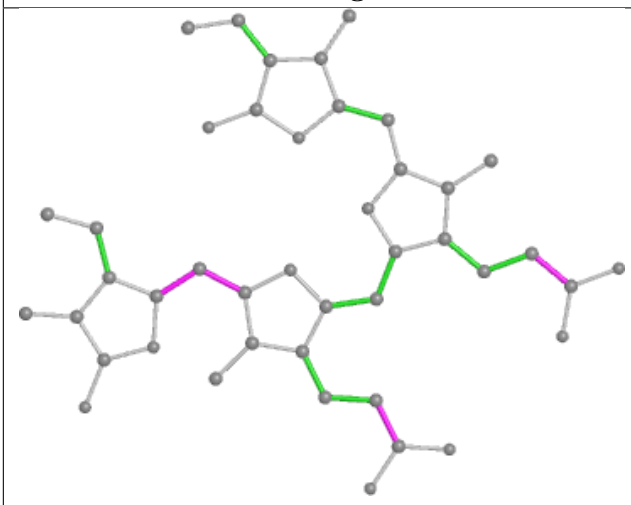

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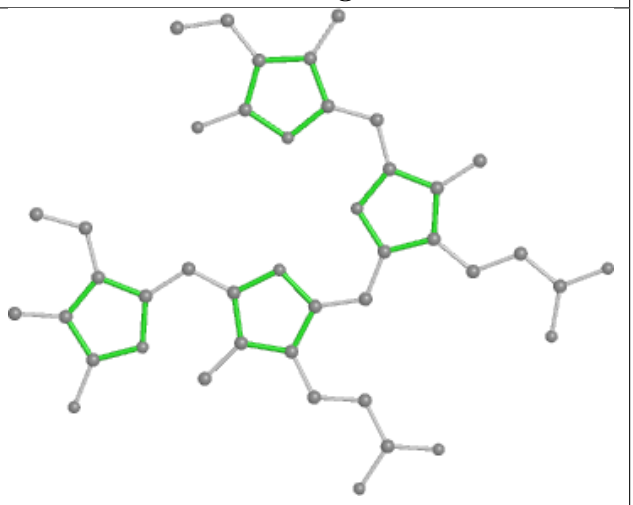
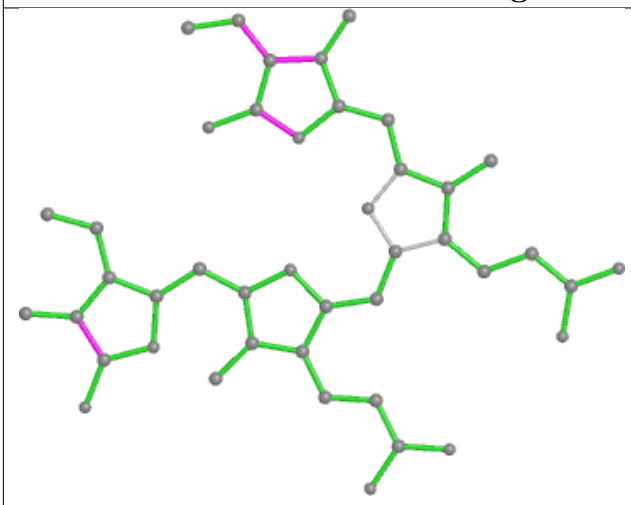


Rings

Ligand PEB aW 302



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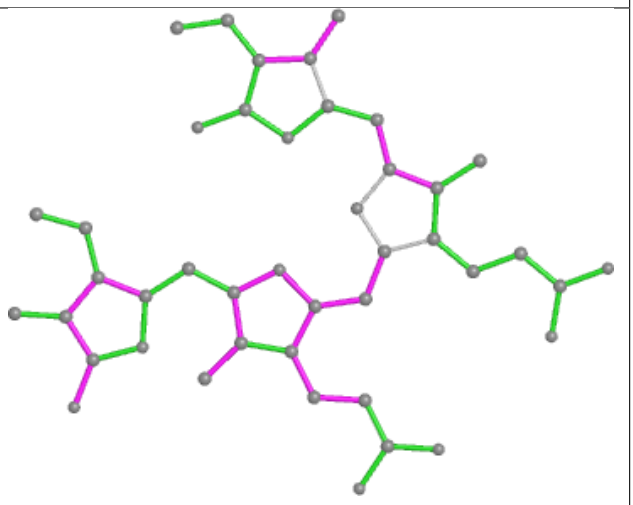

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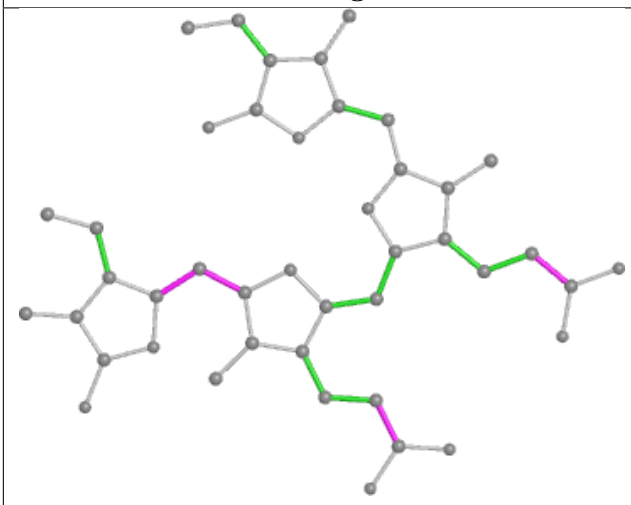

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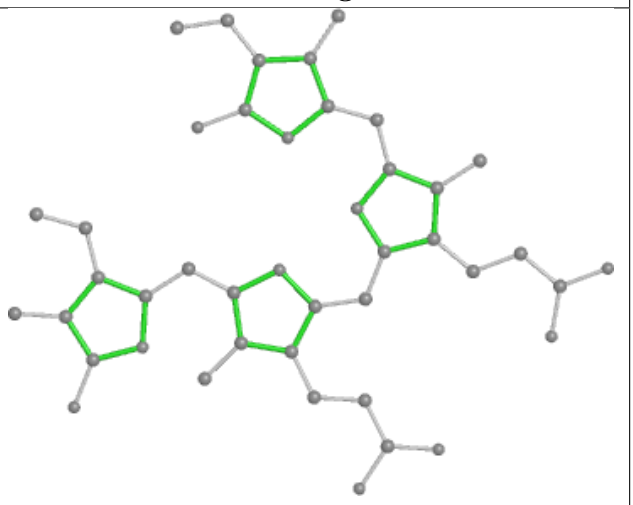

Rings

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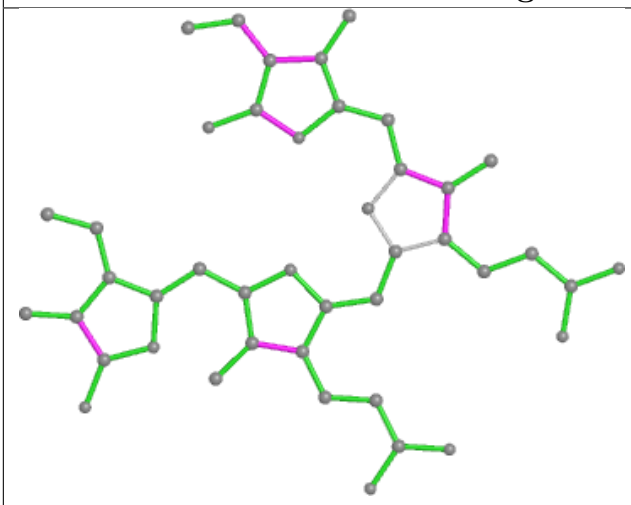

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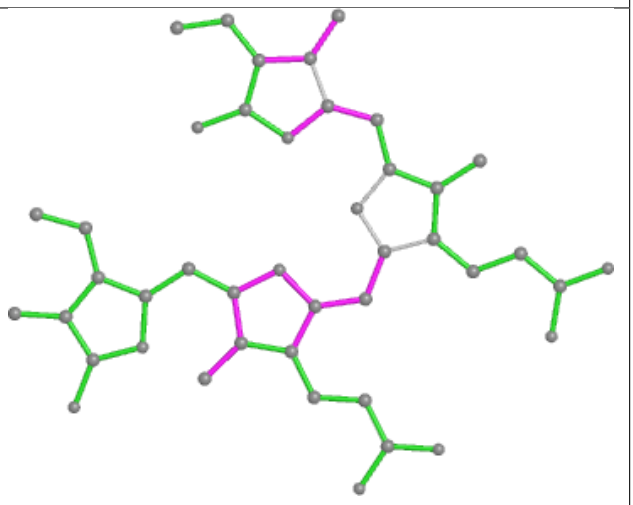
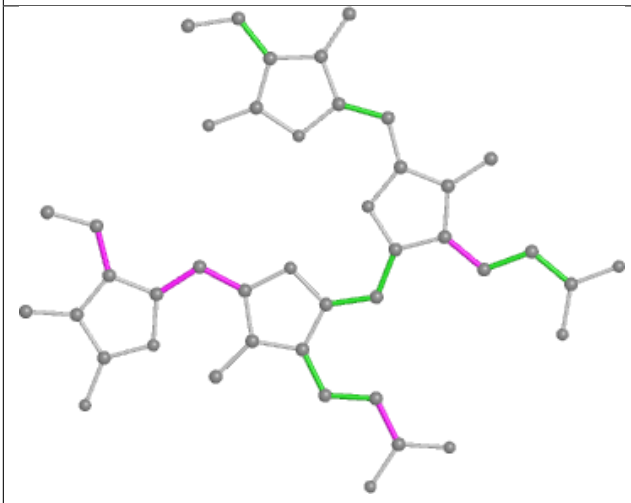


Bond angles



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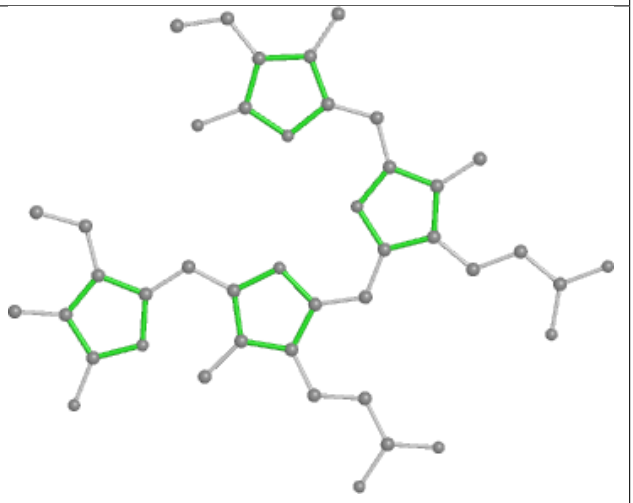

Rings

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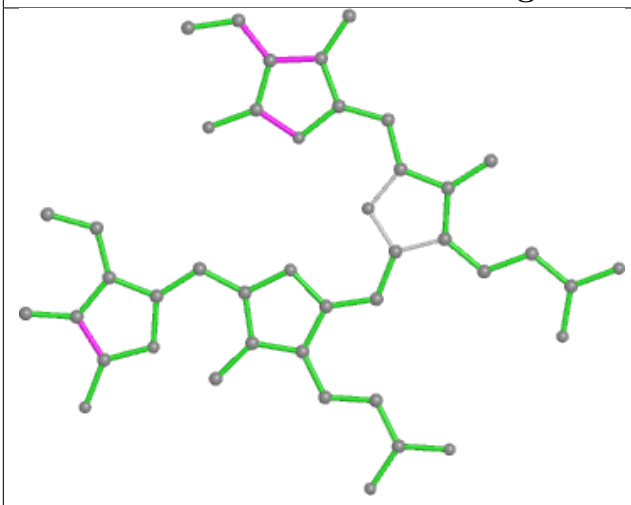

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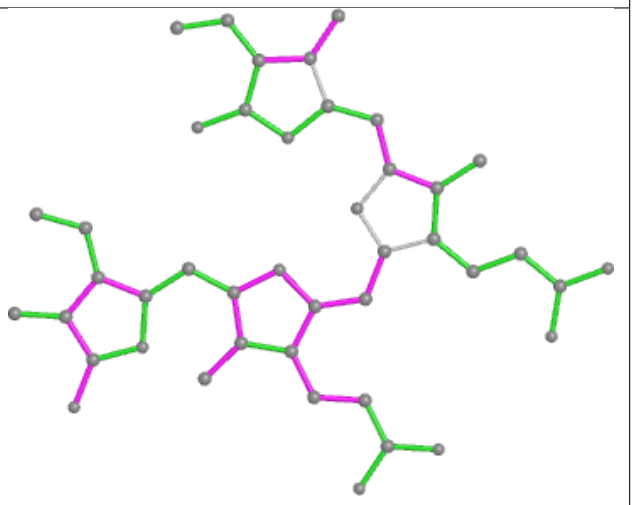

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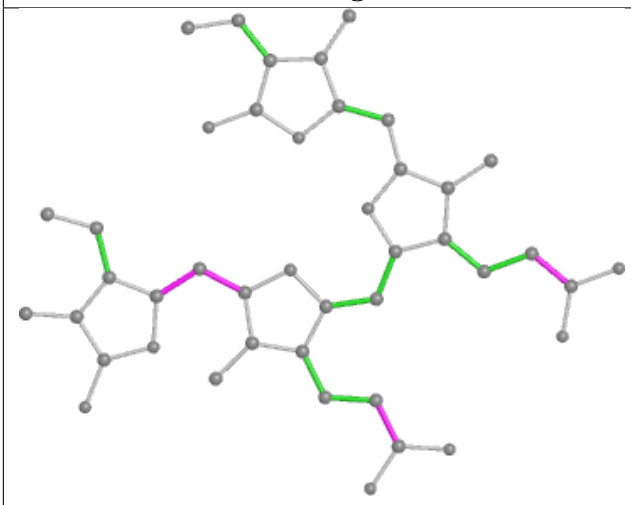

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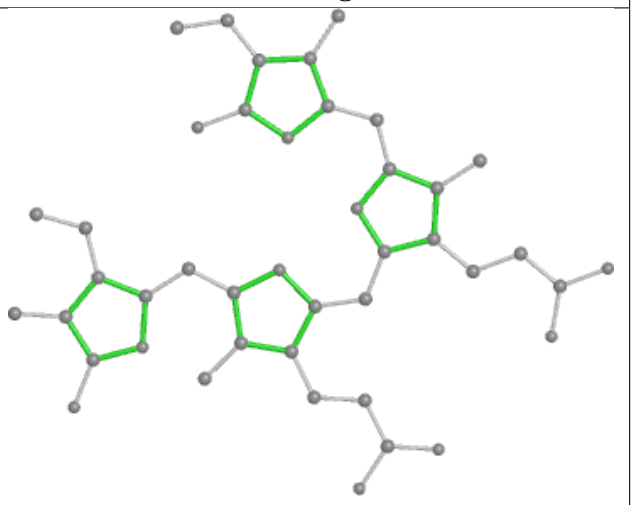
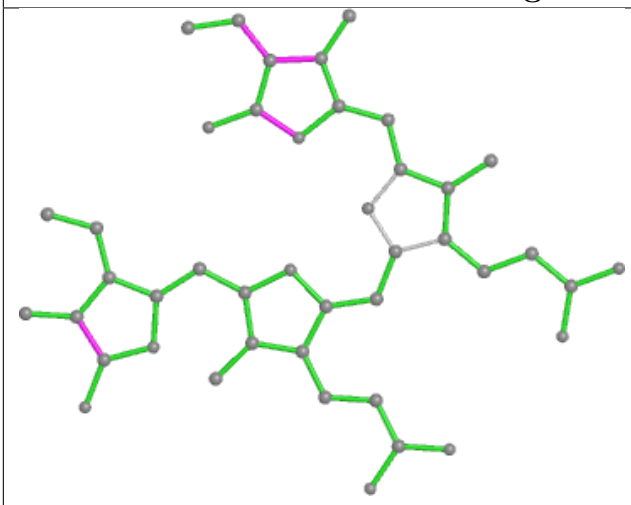


Rings

Ligand PEB ej 201



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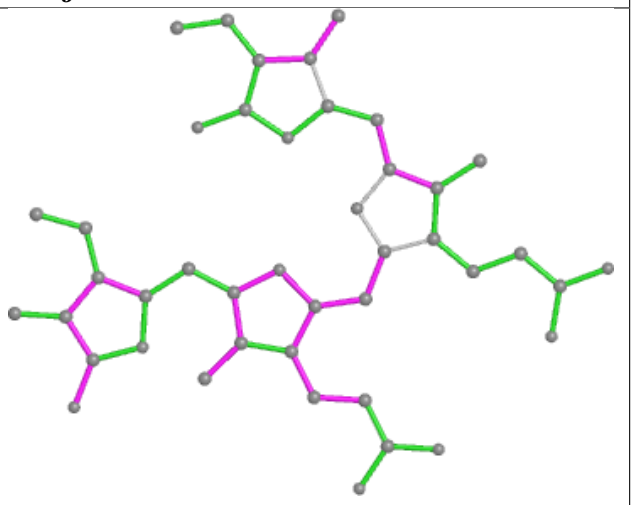
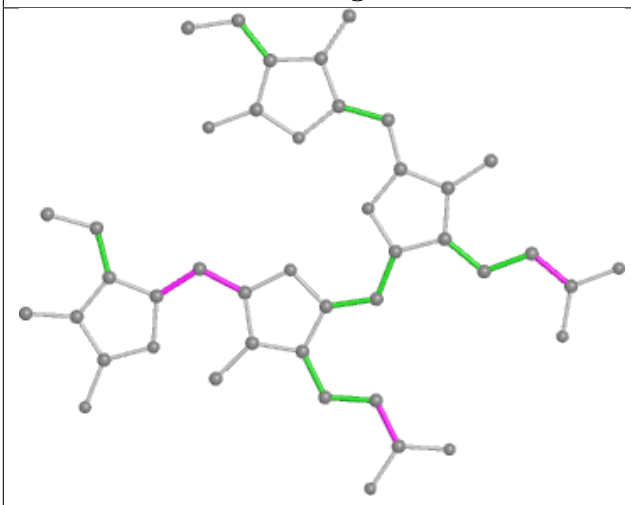
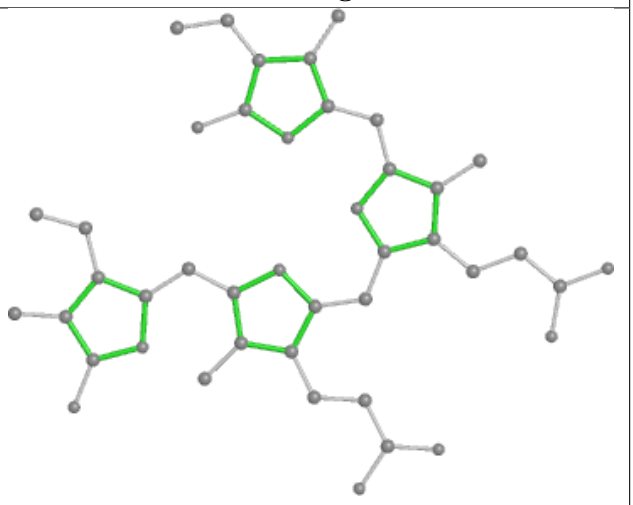


Bond angles



Torsions



Rings

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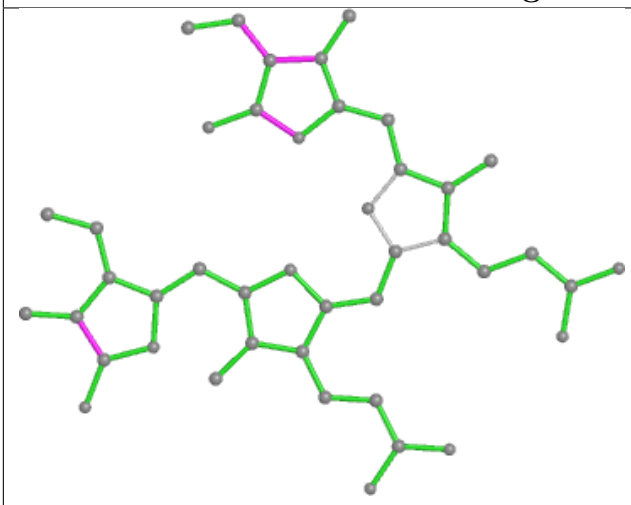

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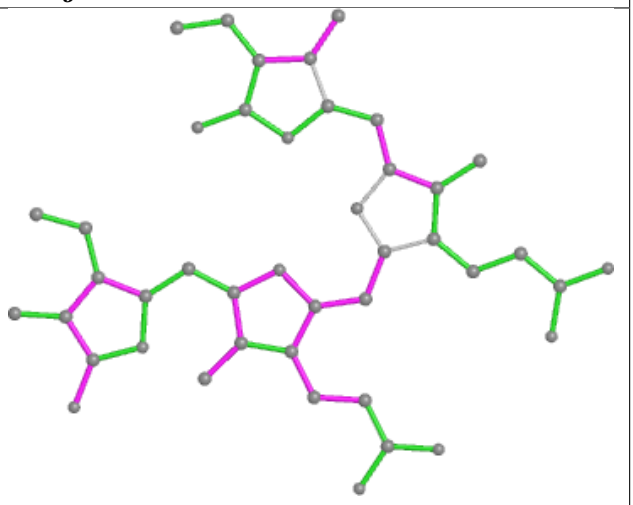

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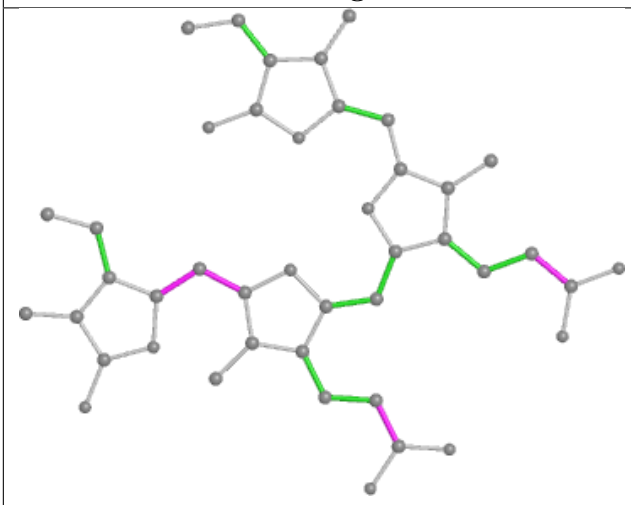

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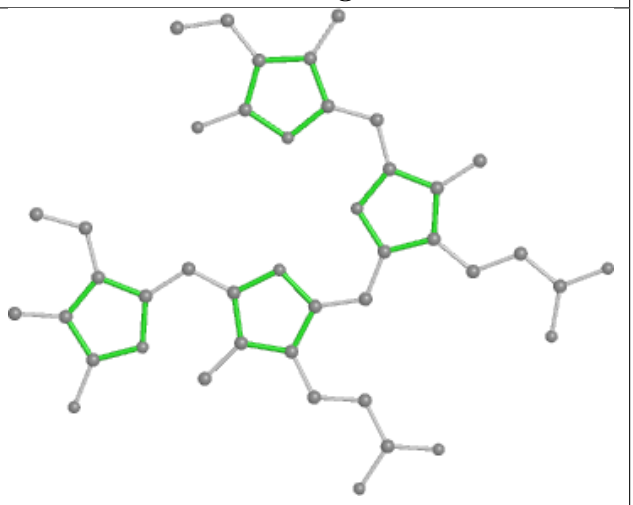

Rings

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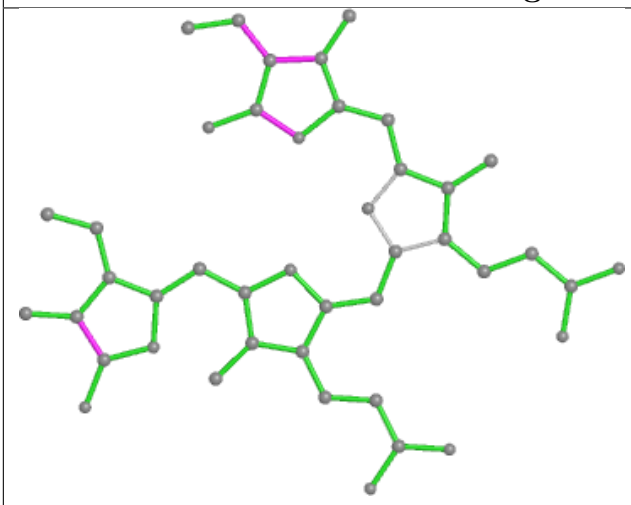

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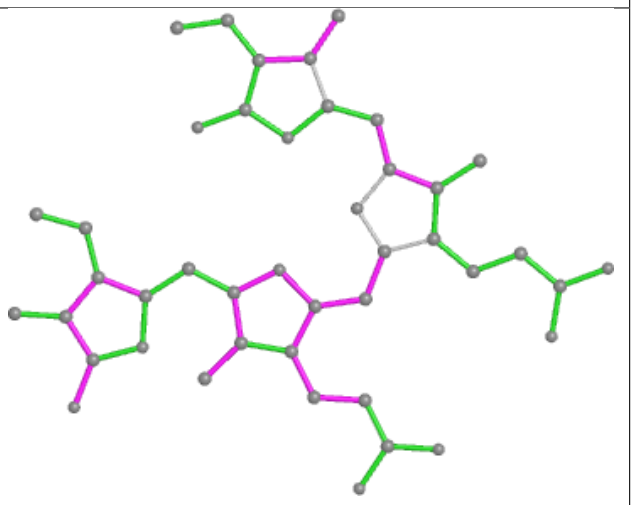

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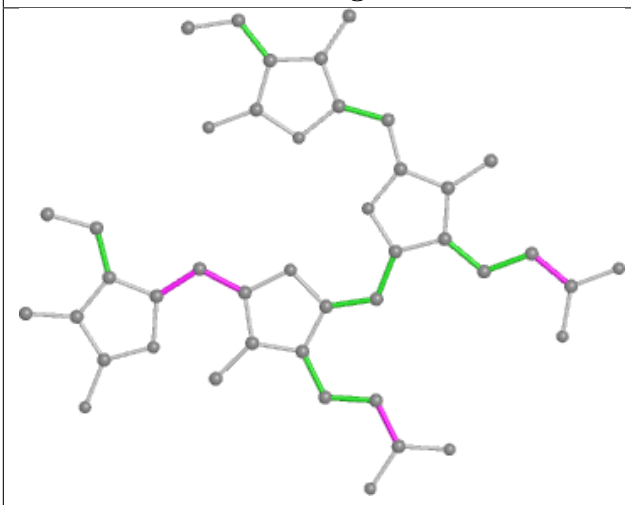

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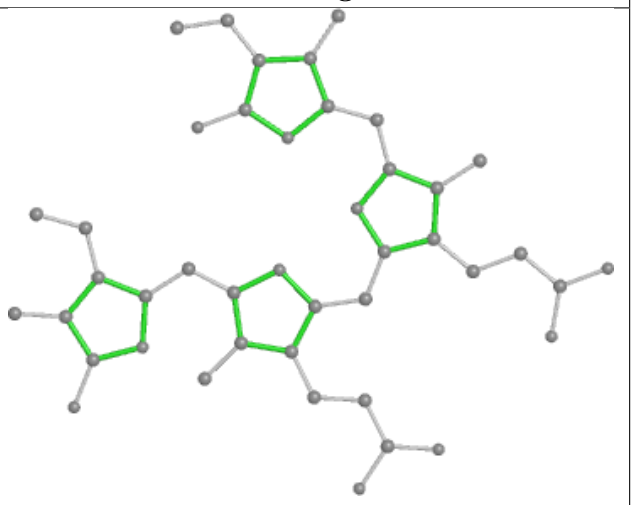

Rings

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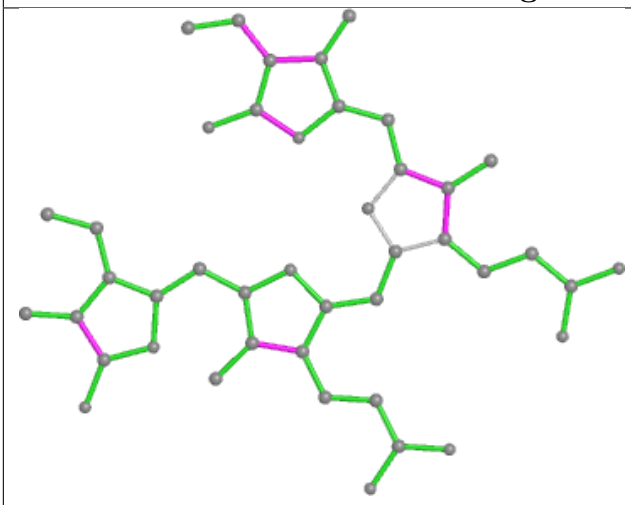

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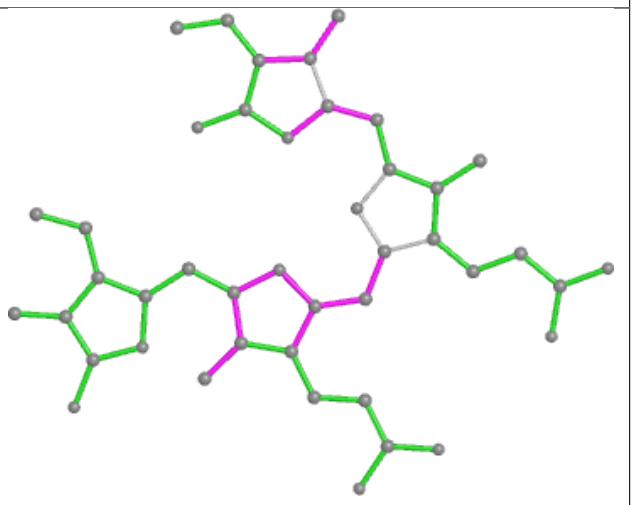

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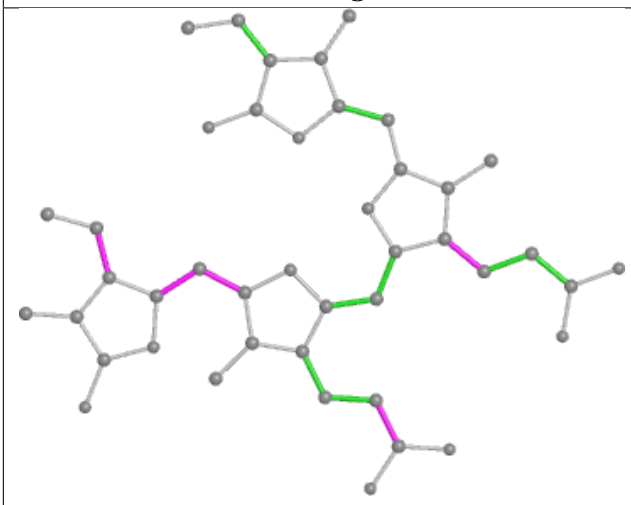

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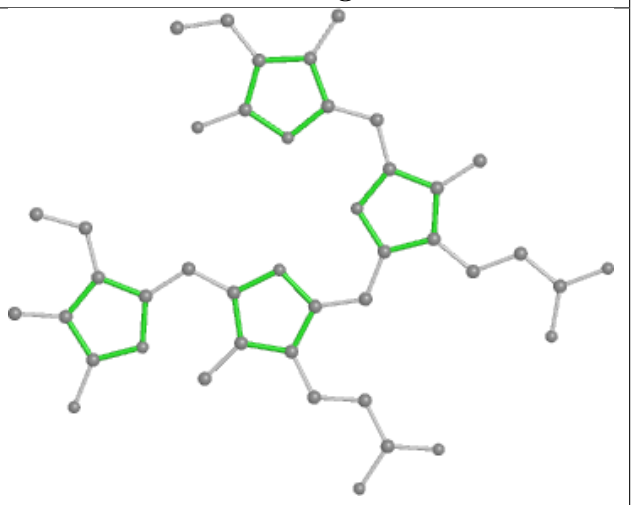

Rings

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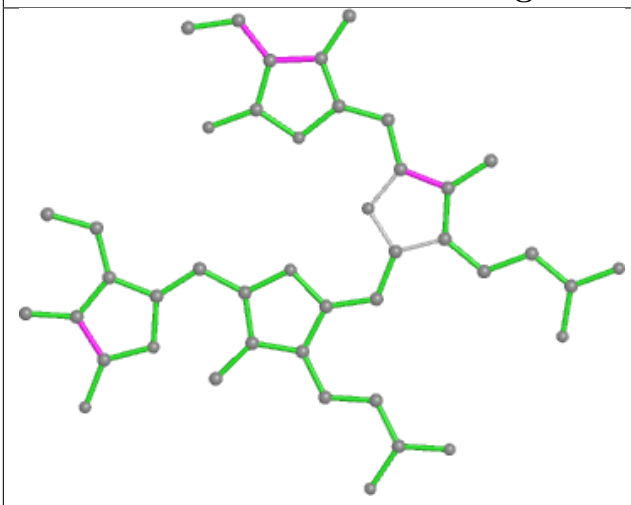

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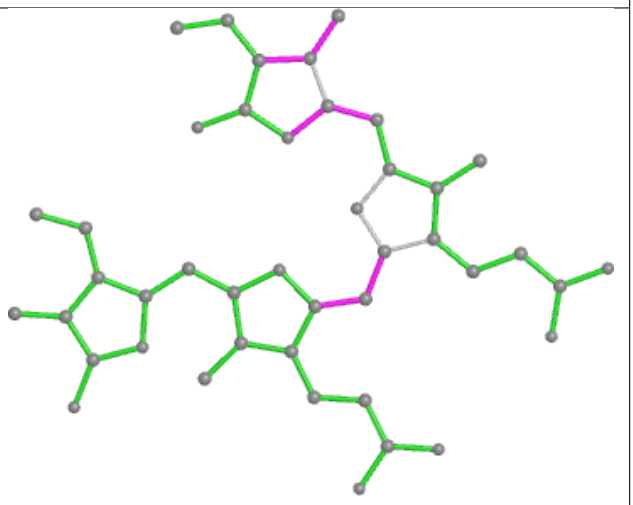

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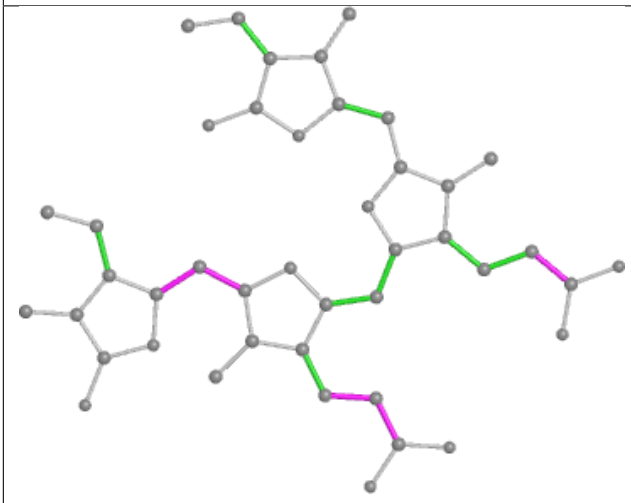

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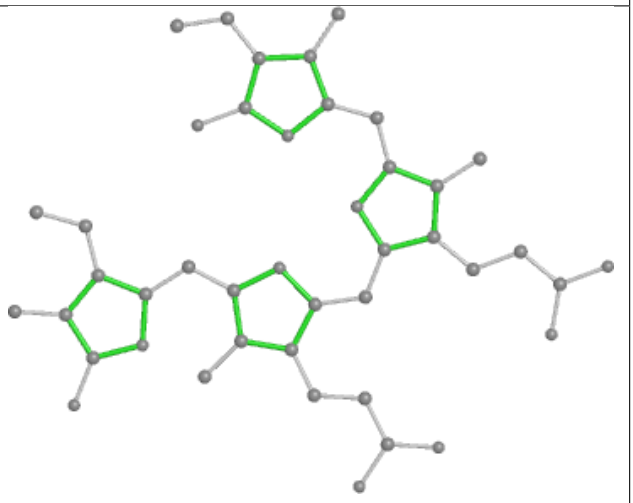

Rings

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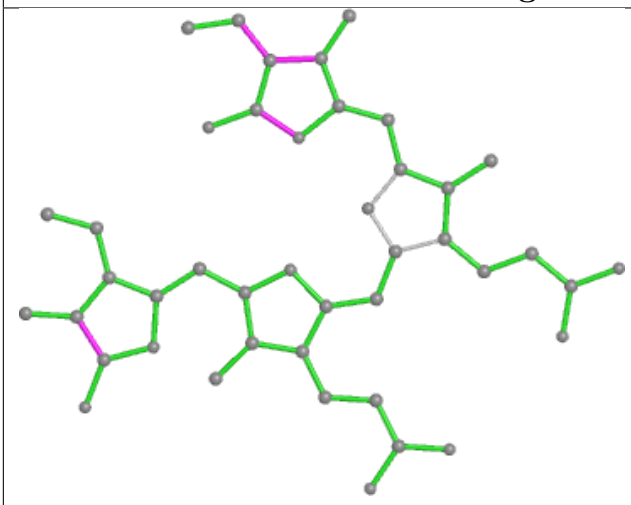

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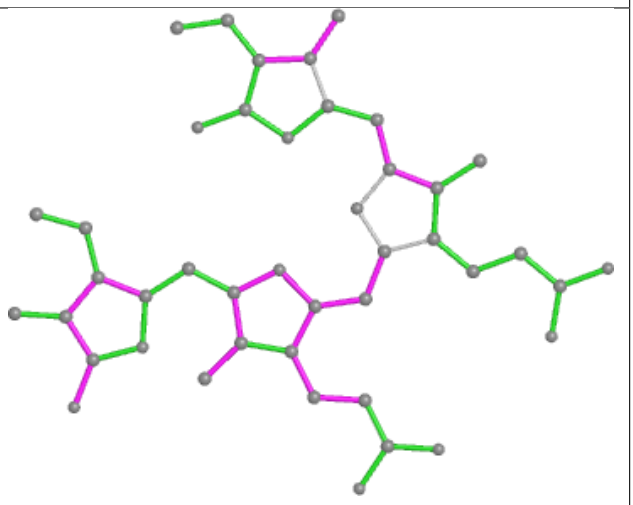

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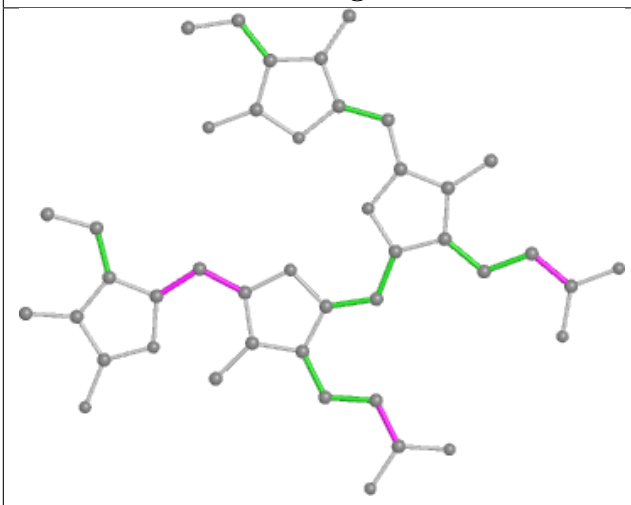

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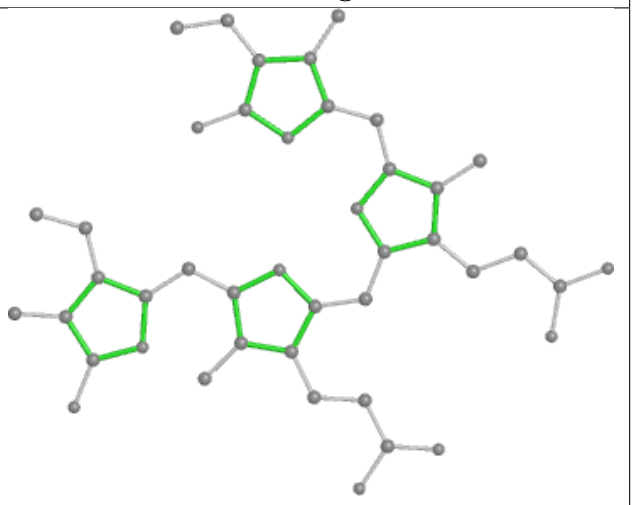

Rings

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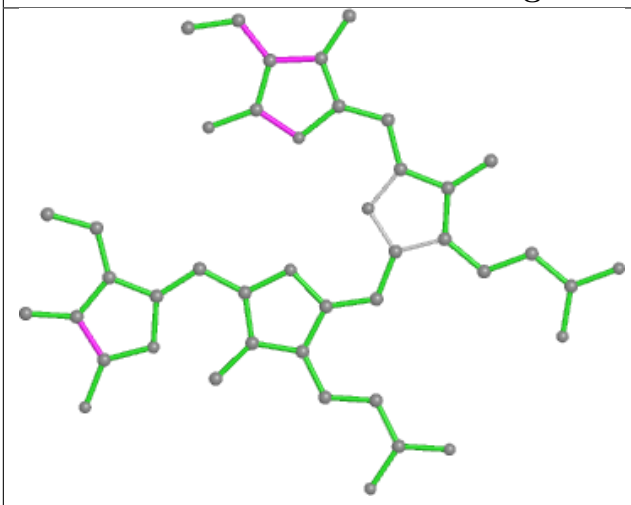

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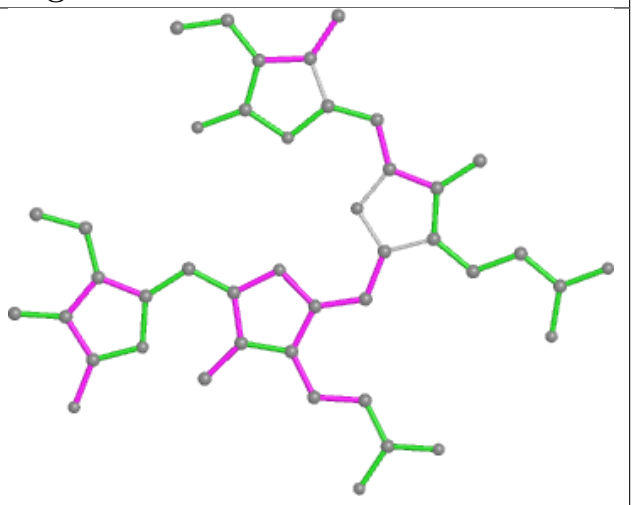

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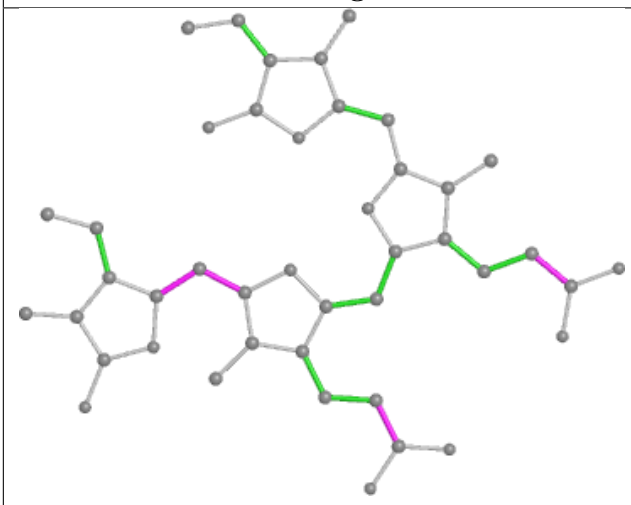

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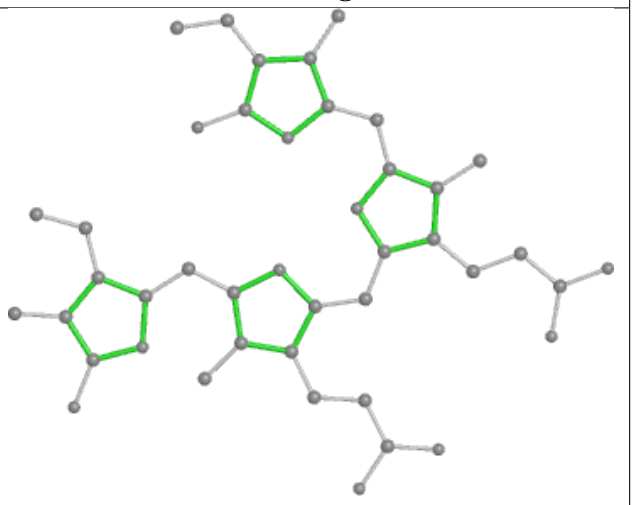

Rings

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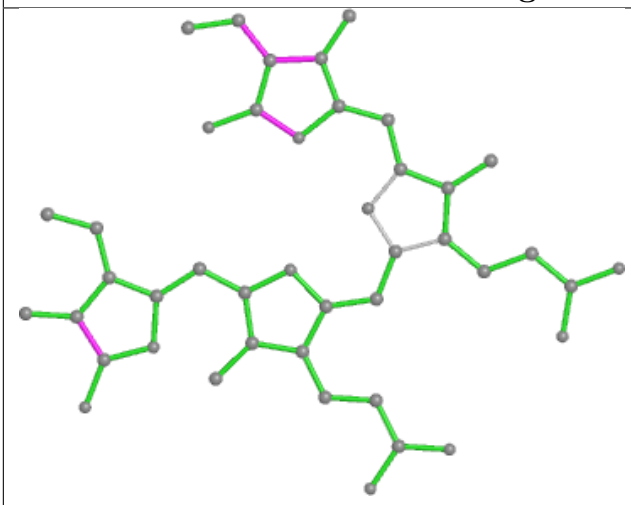

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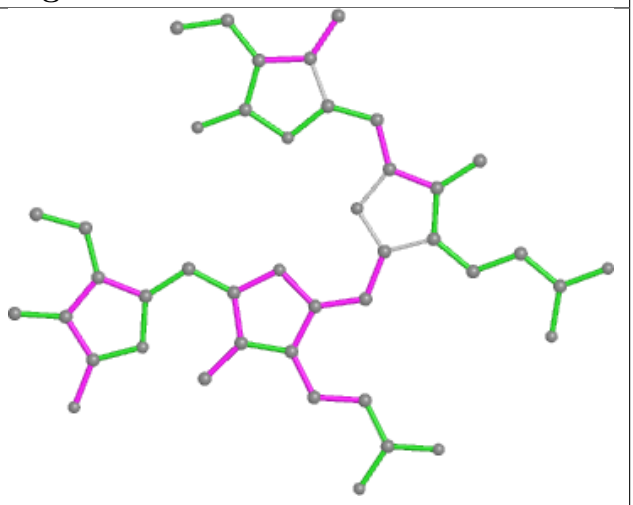

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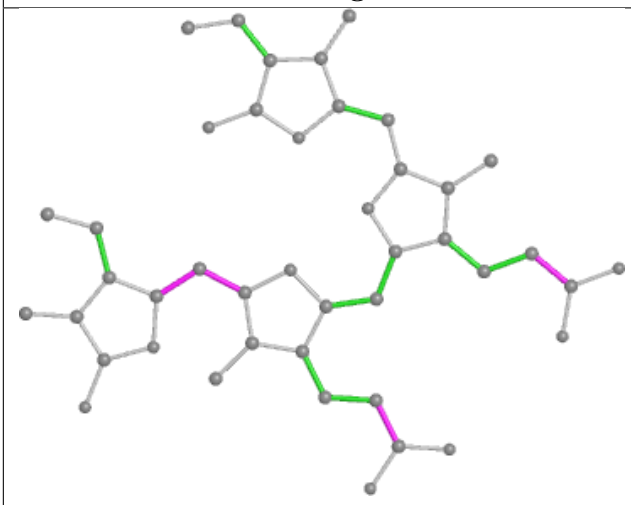

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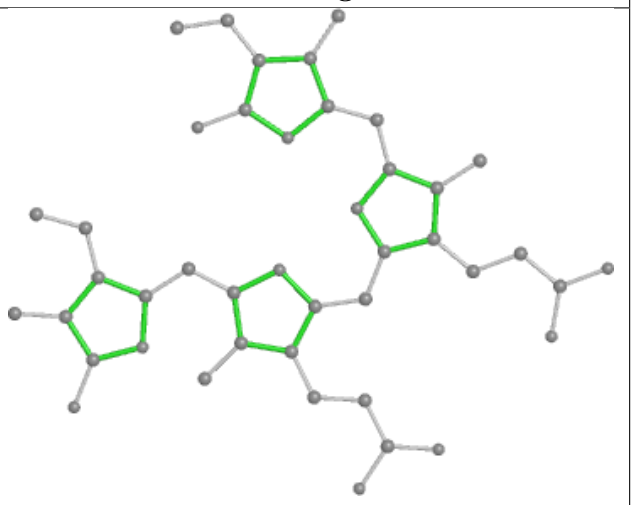

Rings

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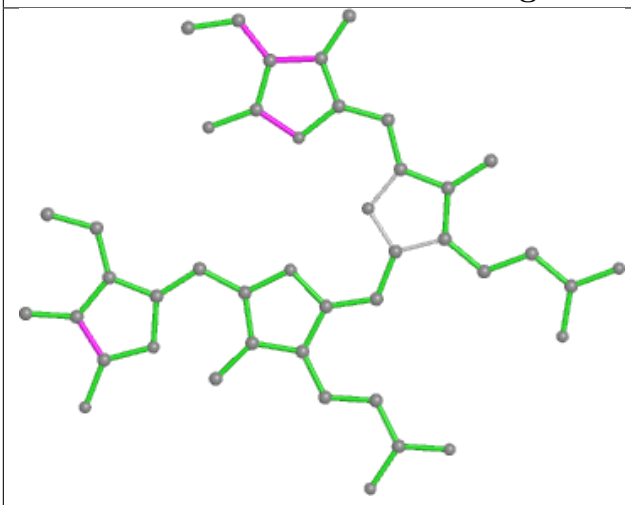

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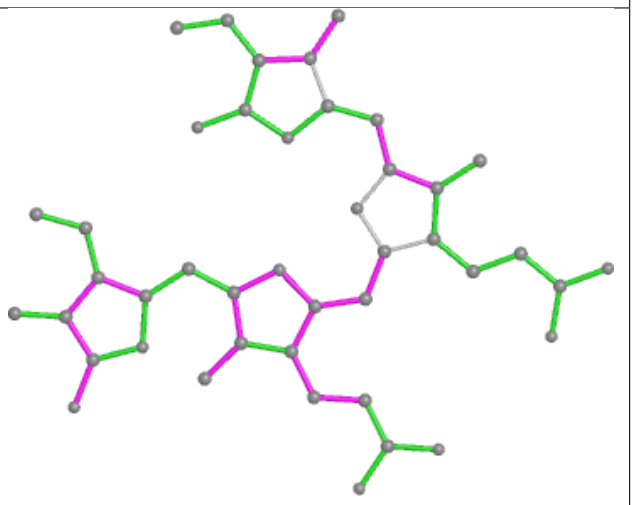

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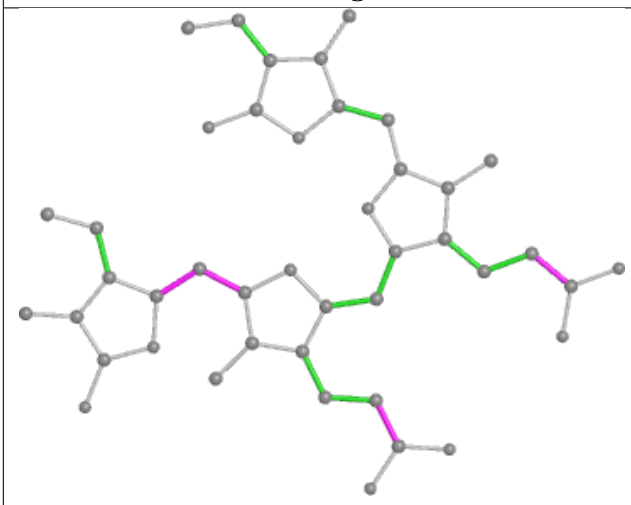

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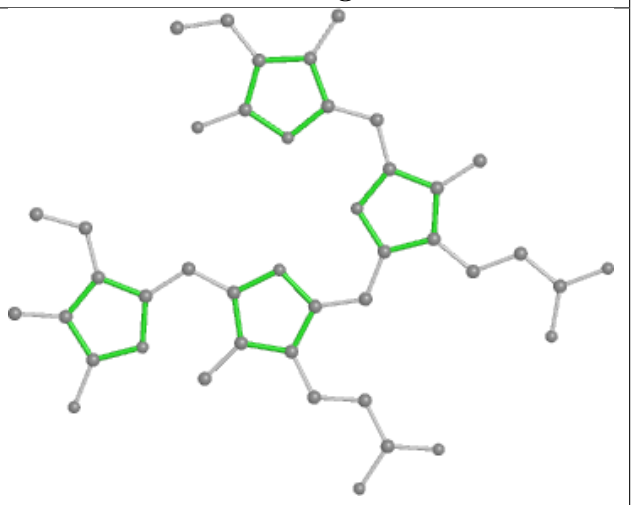

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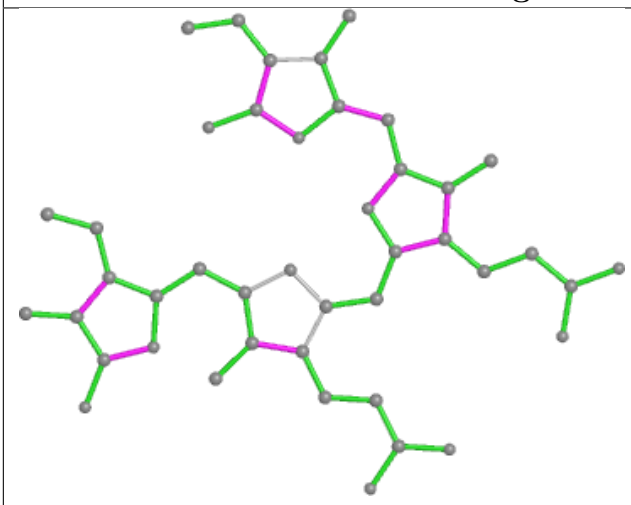

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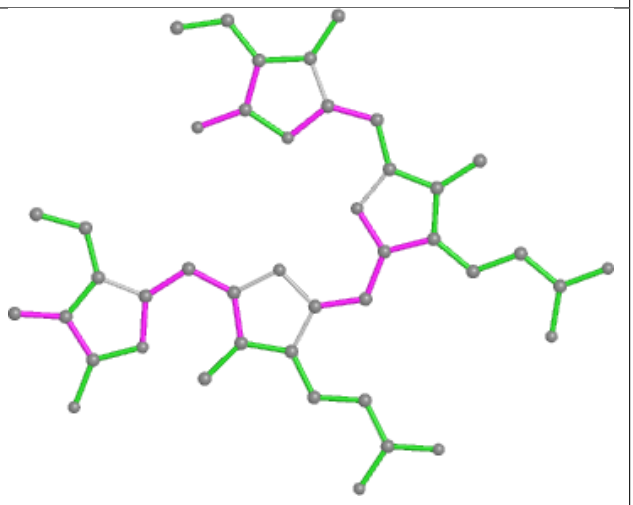

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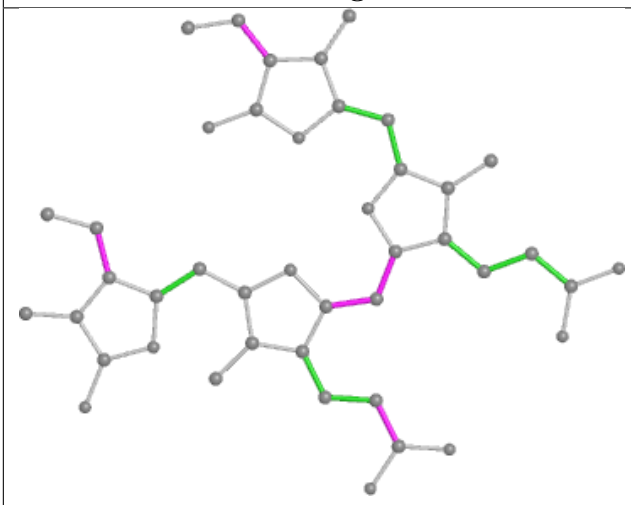

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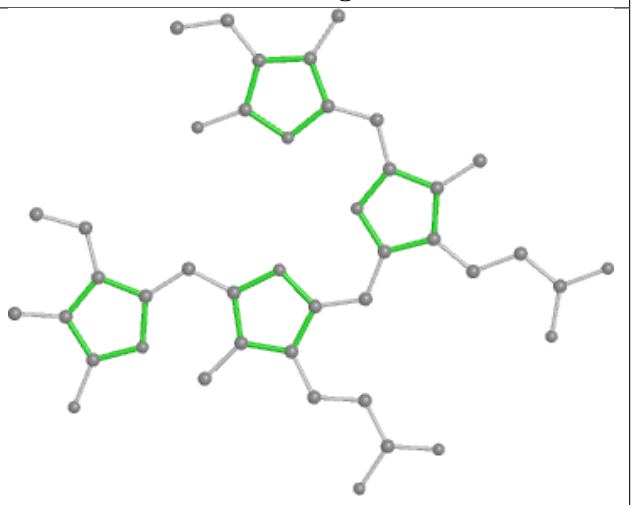

Rings

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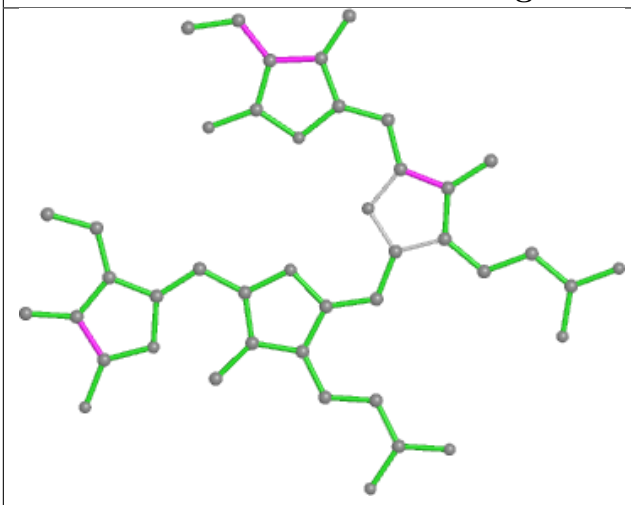

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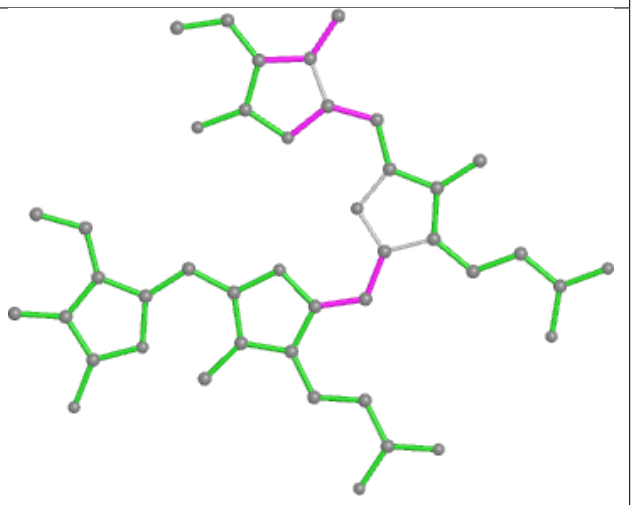

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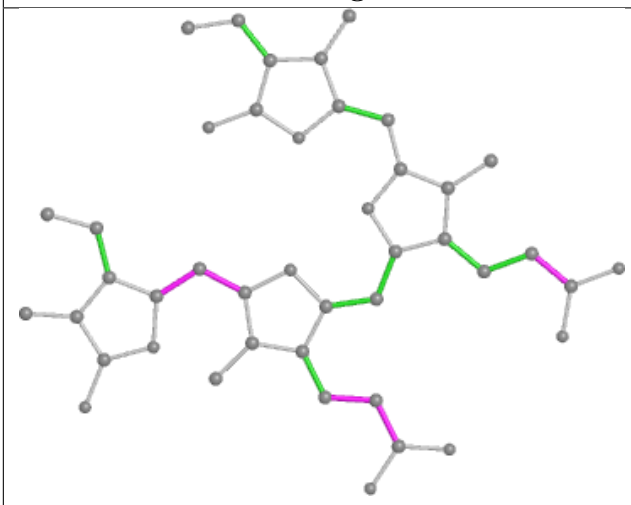

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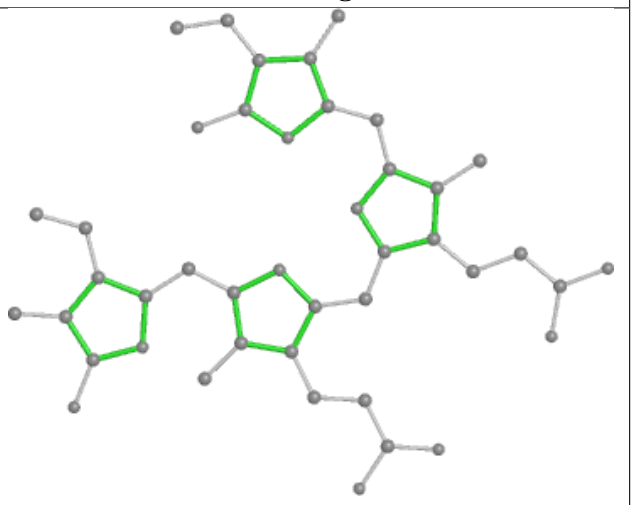

Rings

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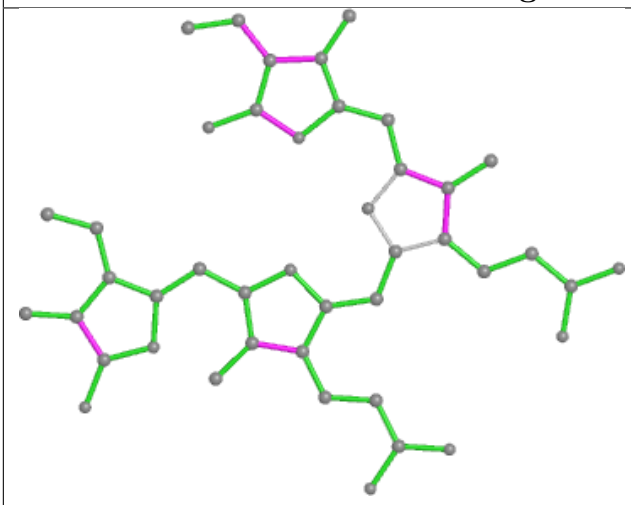

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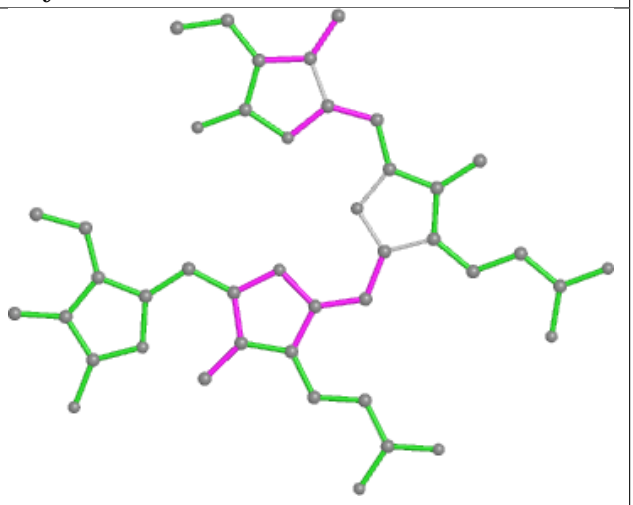

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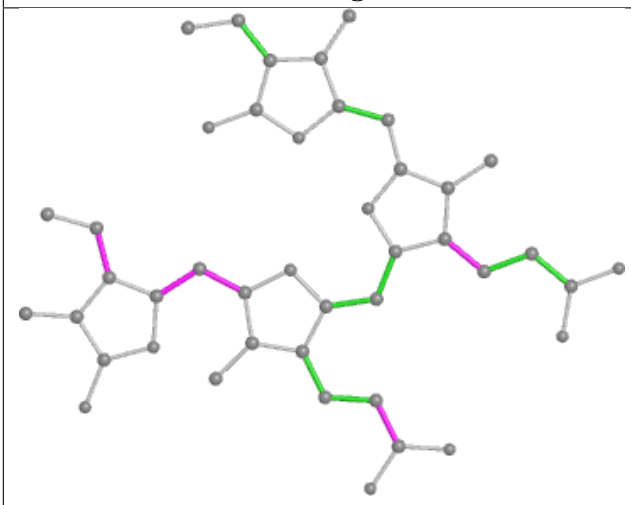

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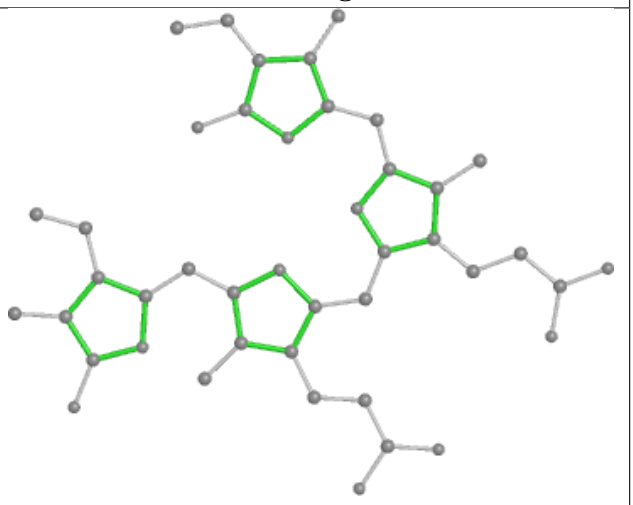
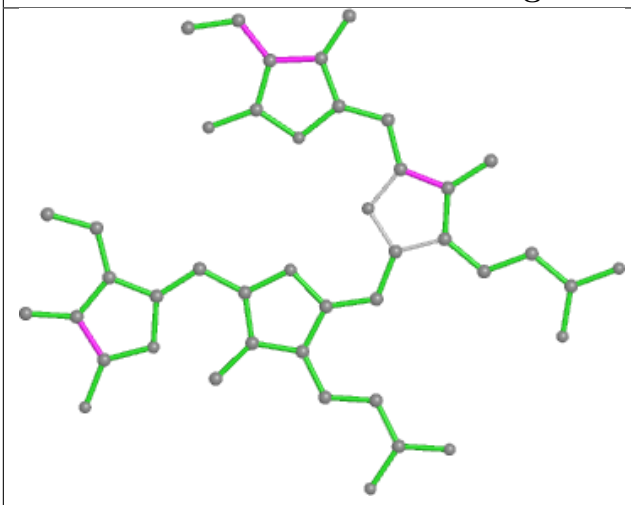


Rings

Ligand PEB lo 201



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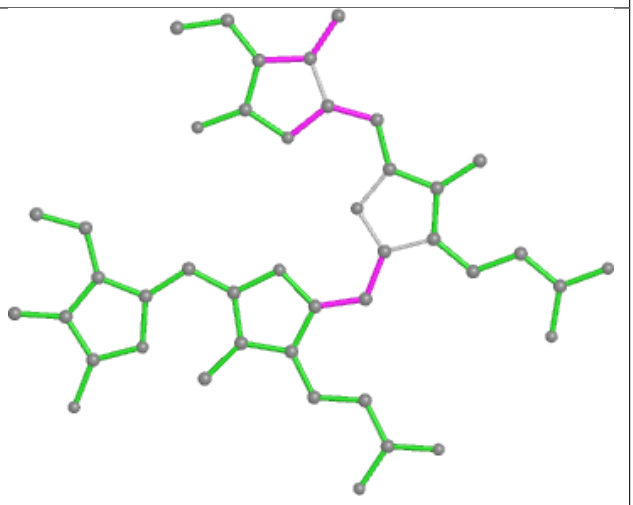

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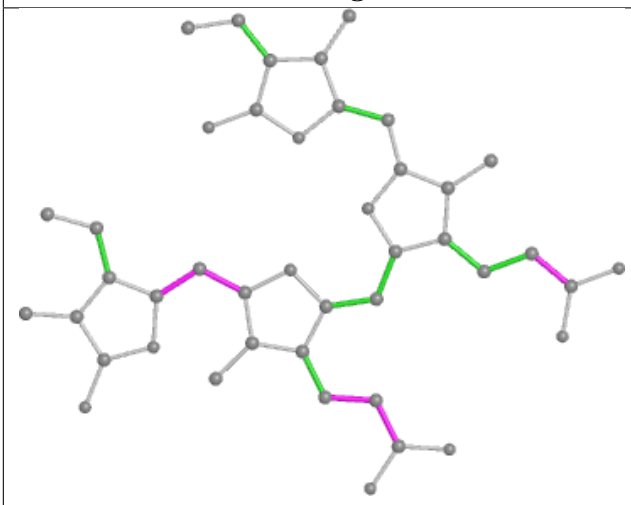

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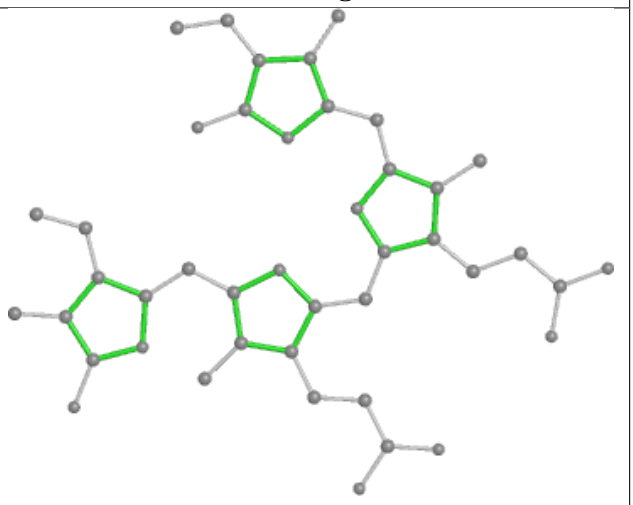
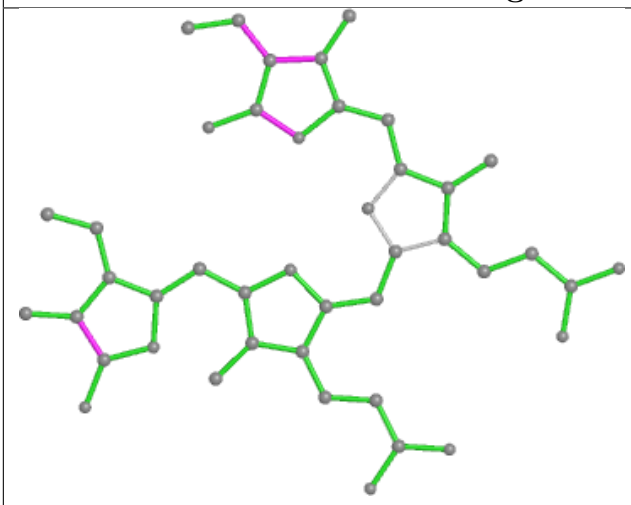


Rings

Ligand PEB w6 1001



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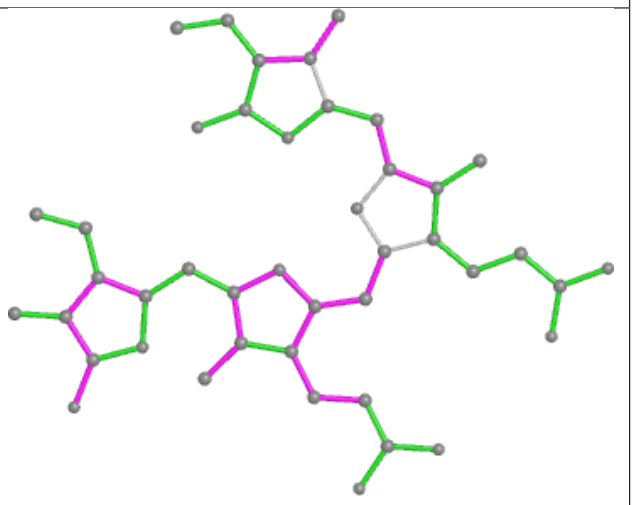

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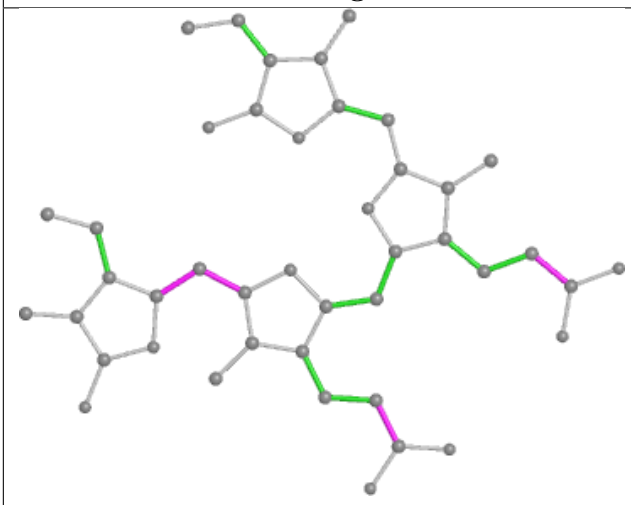

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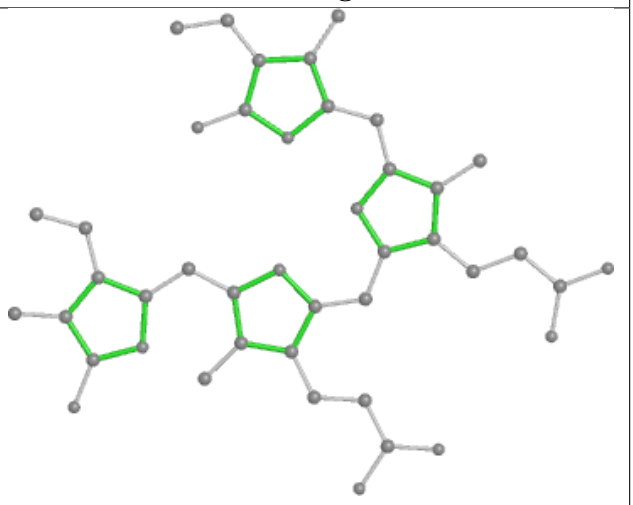
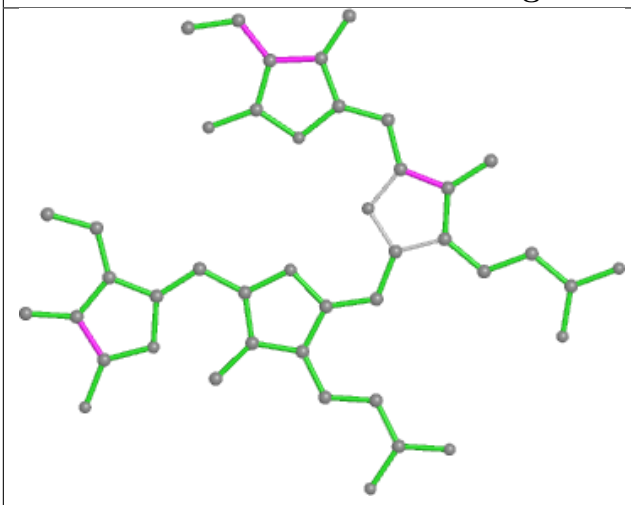
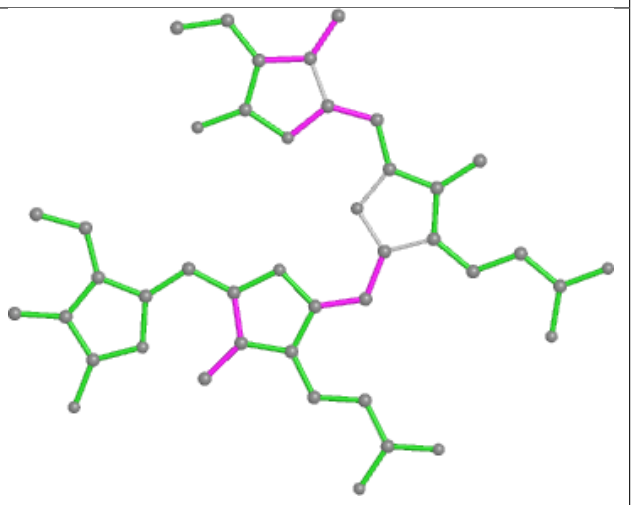


Rings

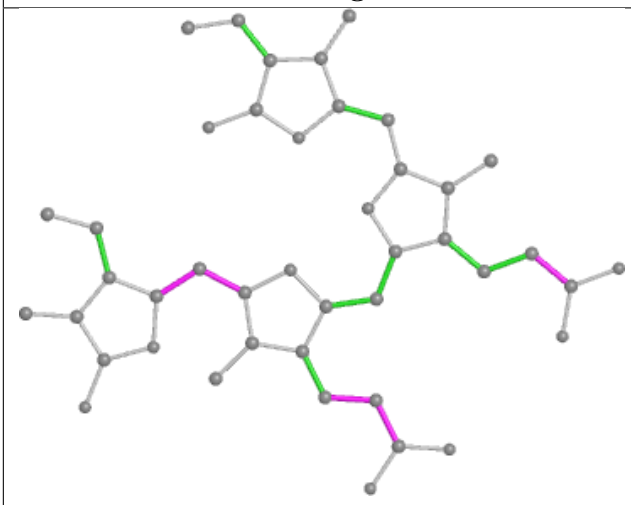
Ligand PEB lh 201



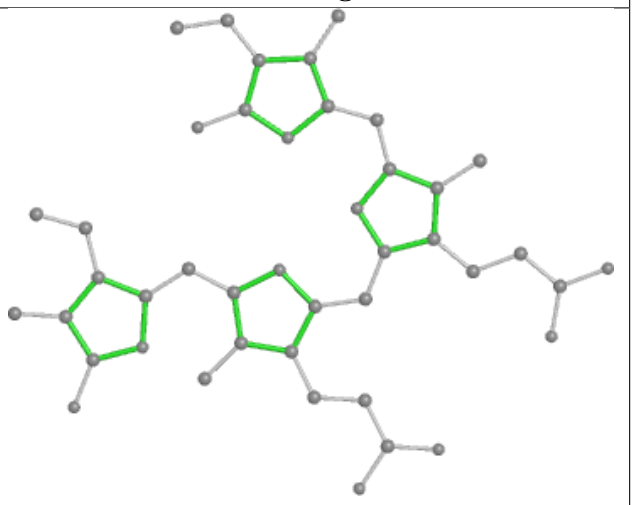
Bond lengths



Bond angles

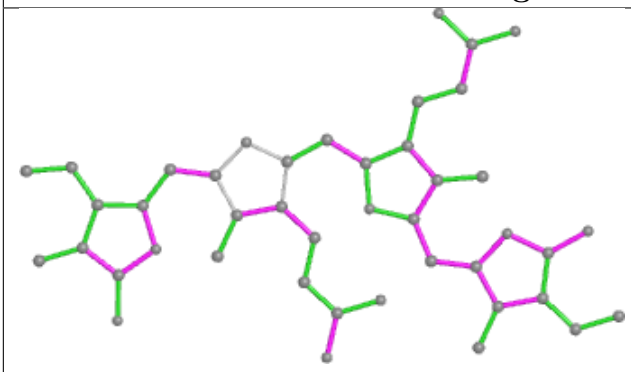


Torsions



Rings

Ligand CYC Y1 201



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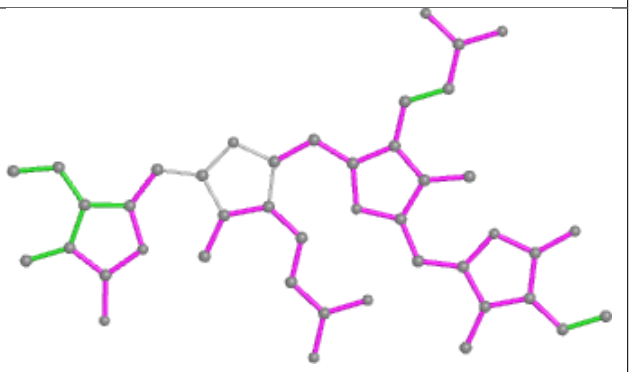

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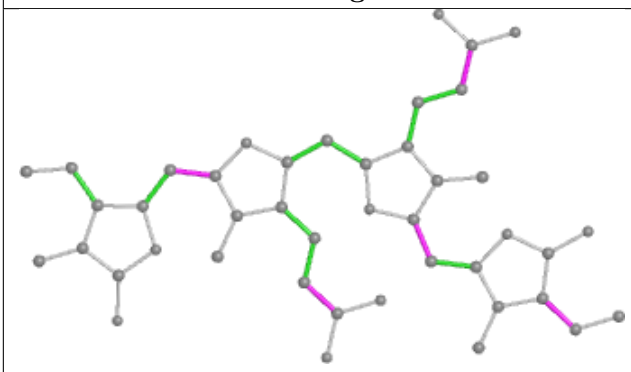

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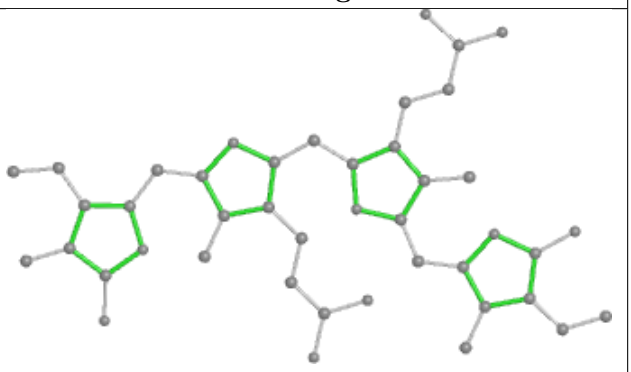
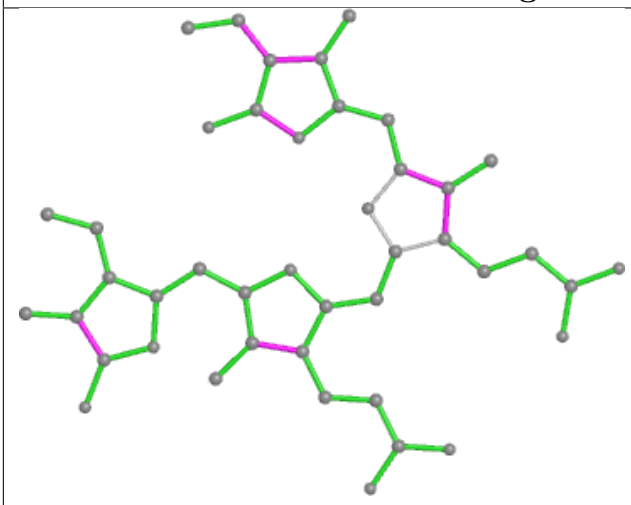


Rings

Ligand PEB gx 202



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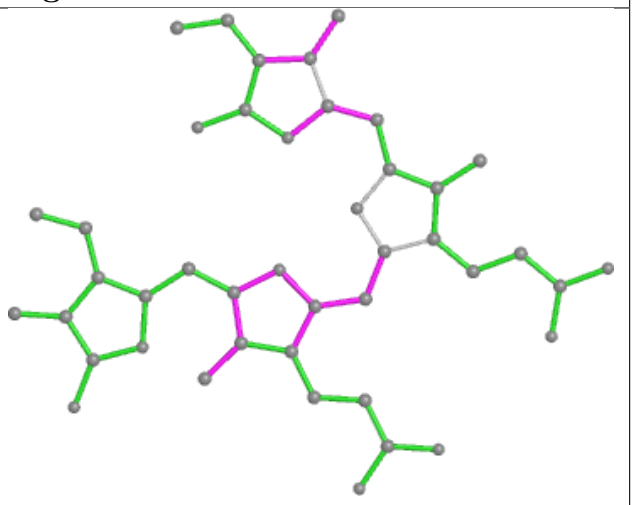

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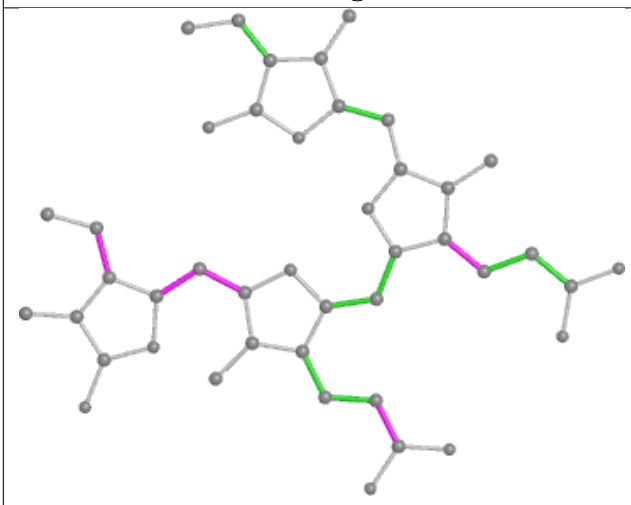

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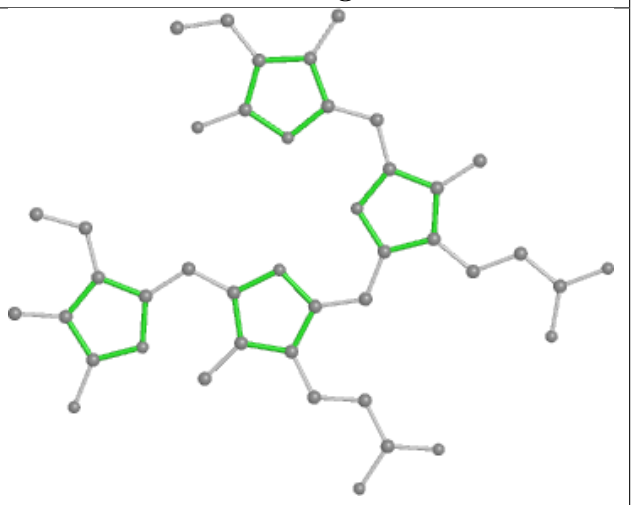
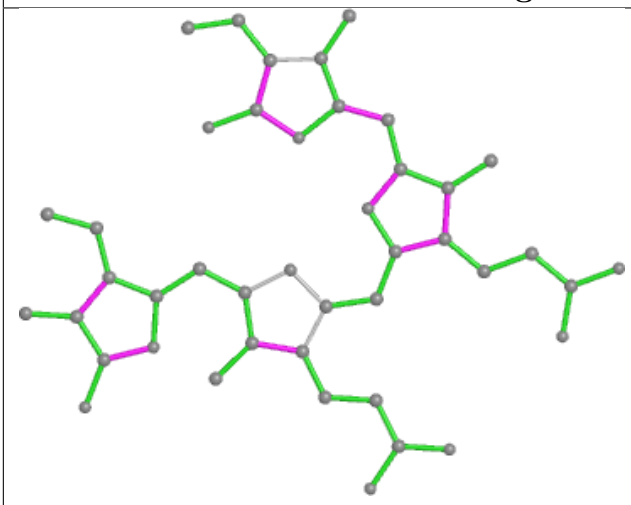


Rings

Ligand PUB cP 203



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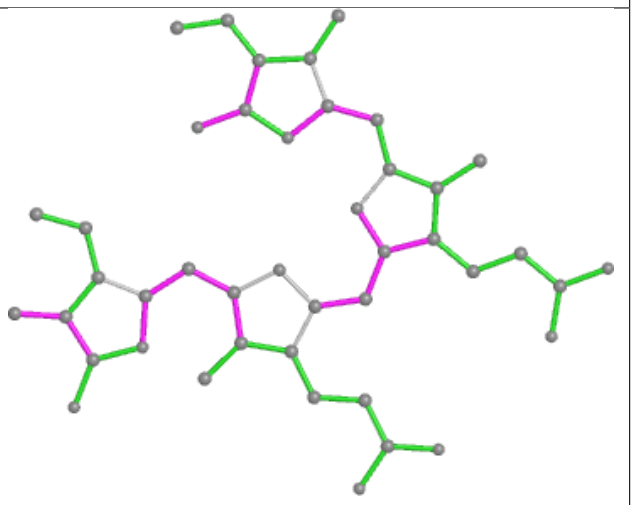

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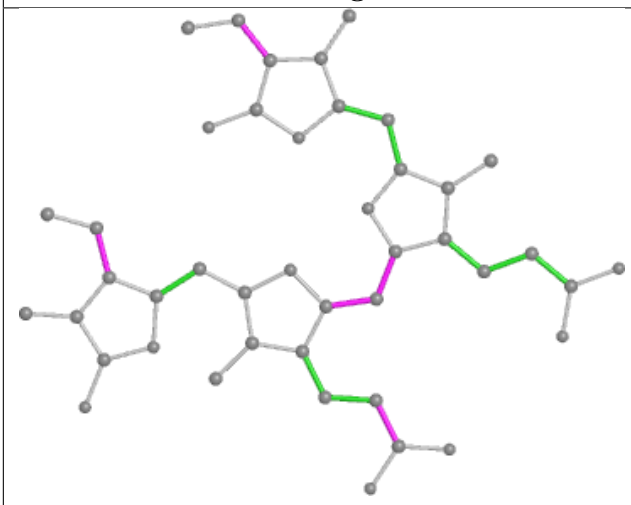

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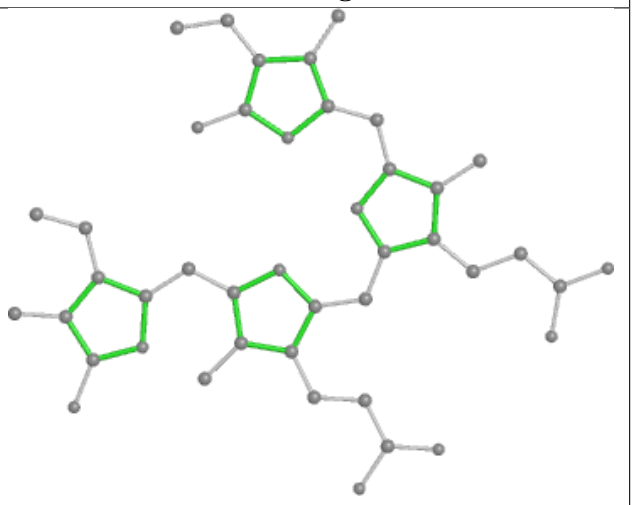
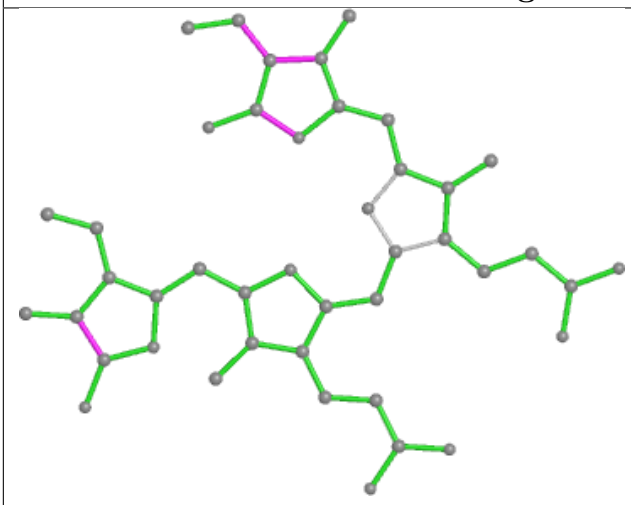


Rings

Ligand PEB Z8 201



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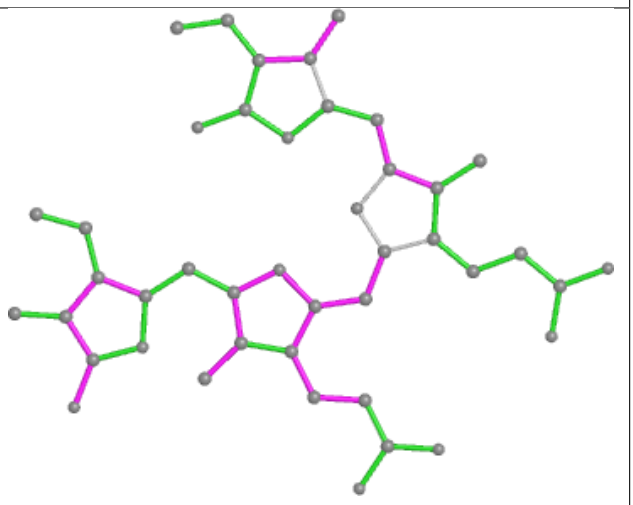

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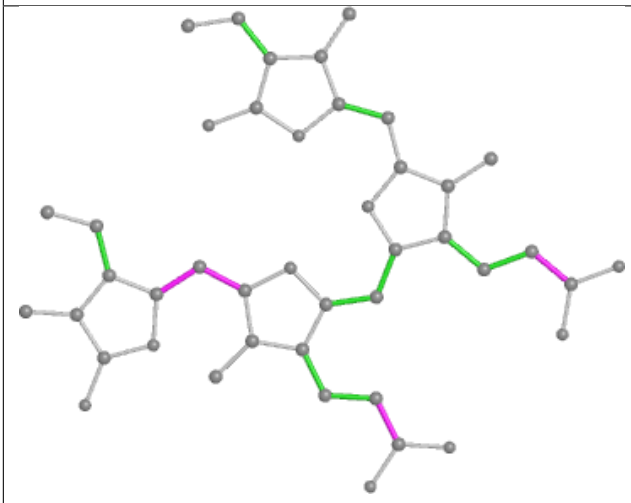

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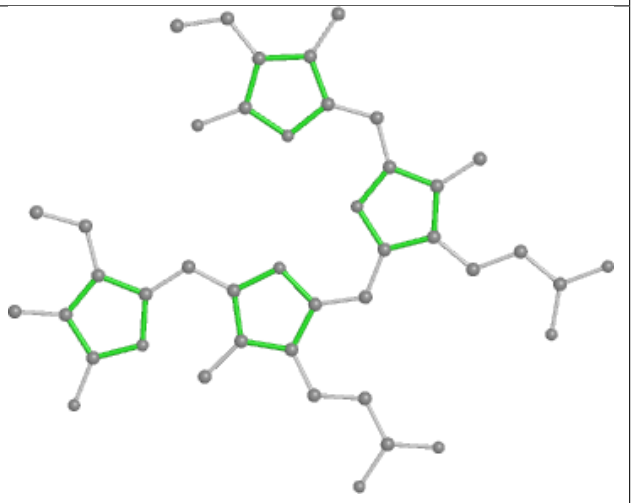

Rings

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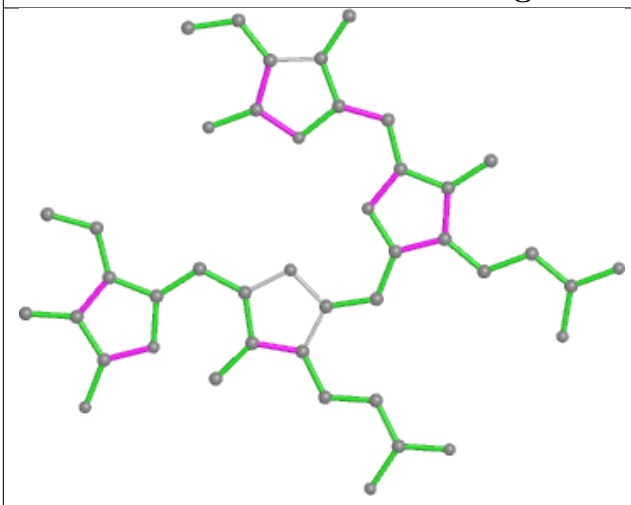

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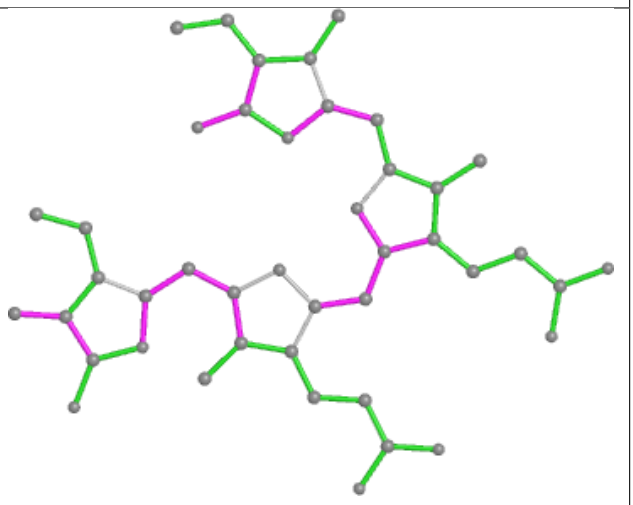

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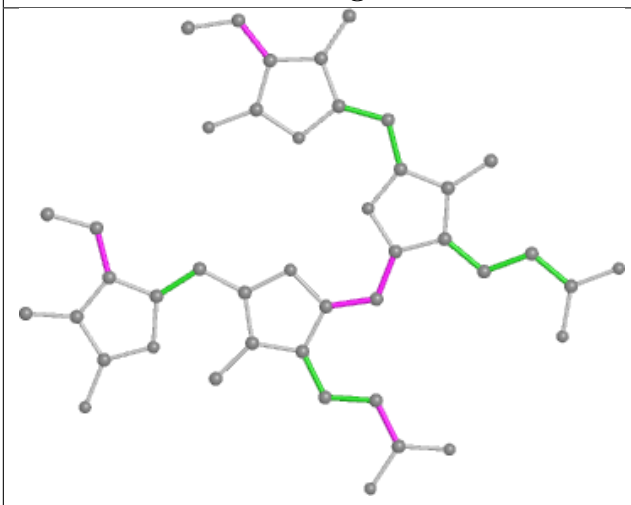

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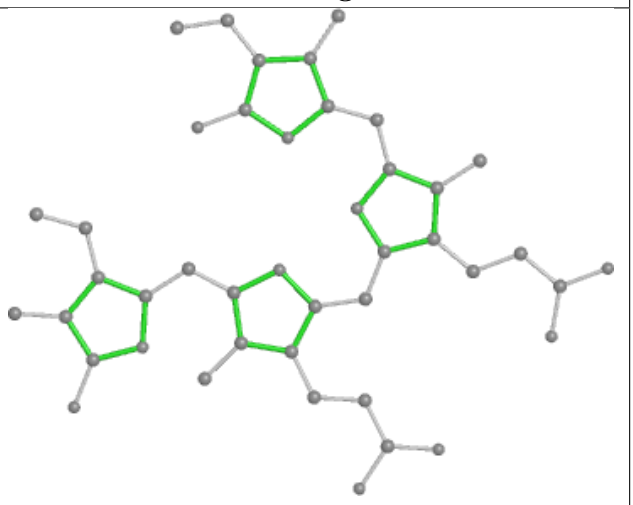

Rings

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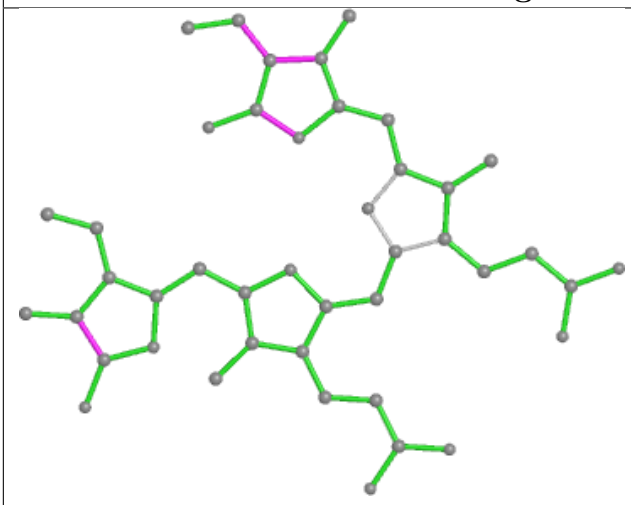

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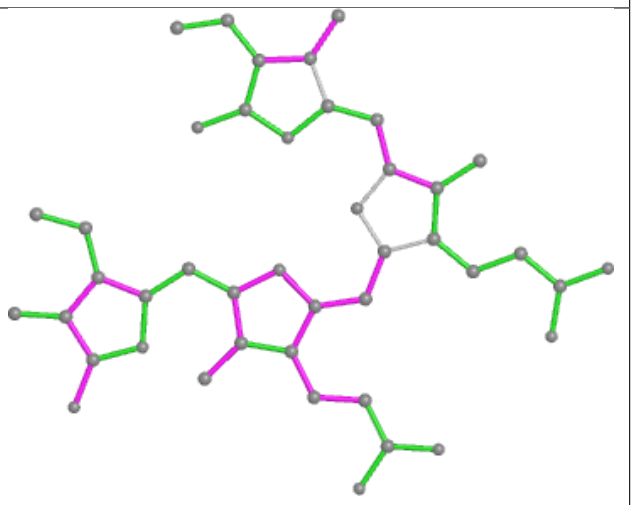

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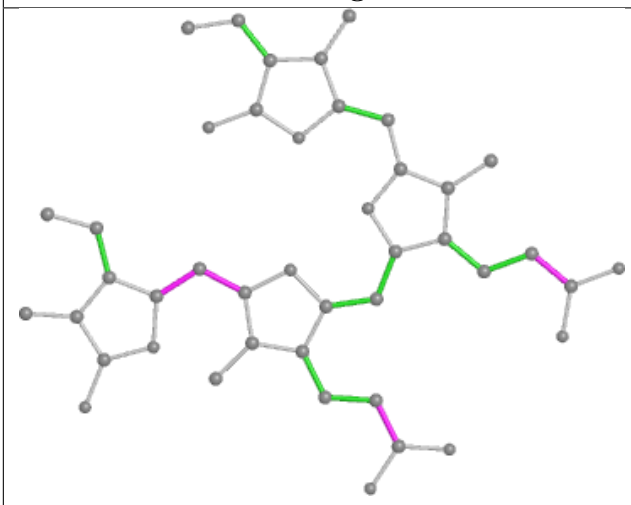

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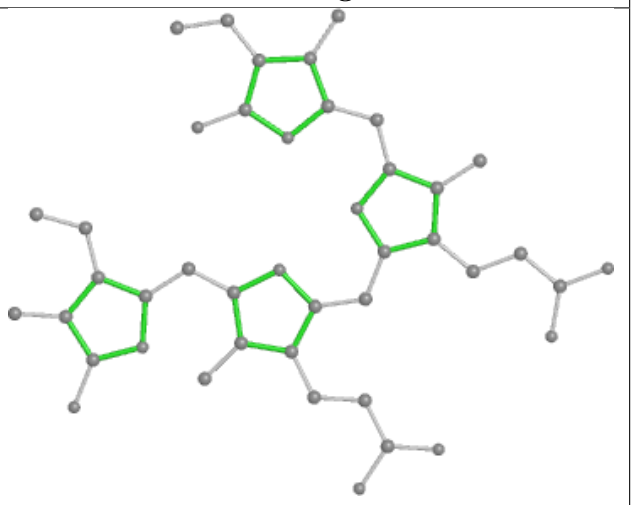
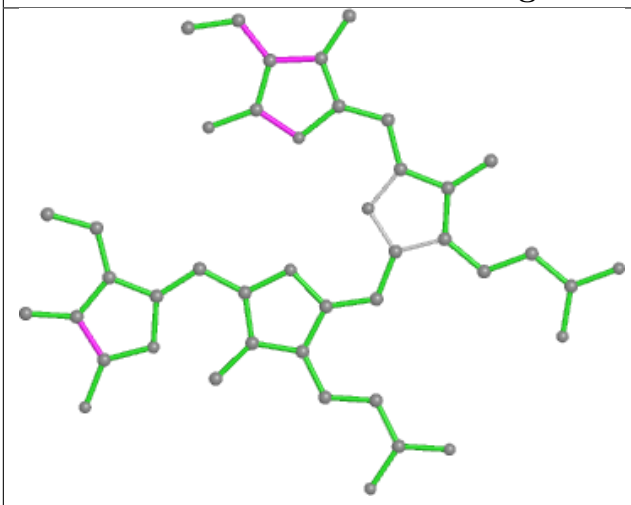


Rings

Ligand PEB h9 201



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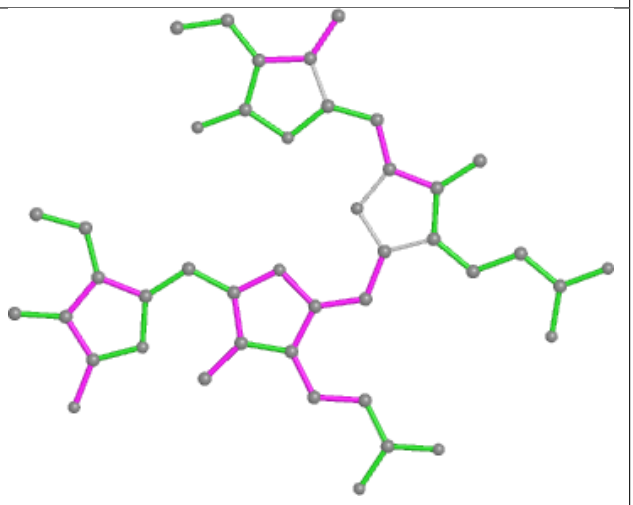

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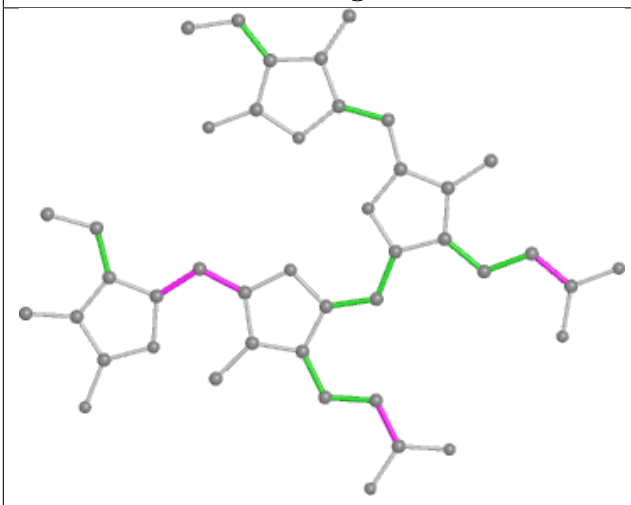

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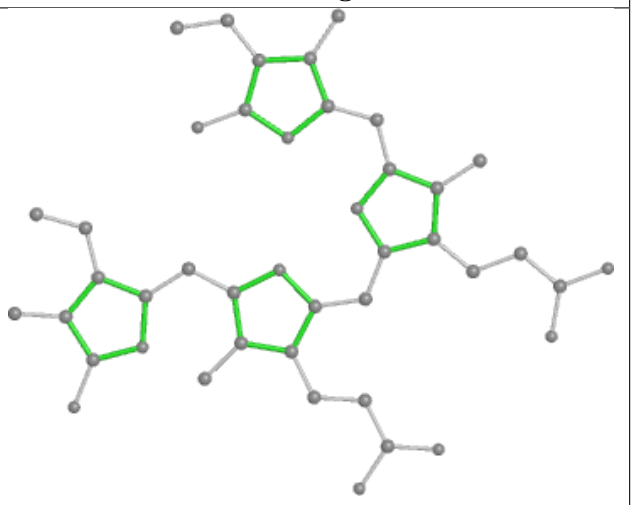
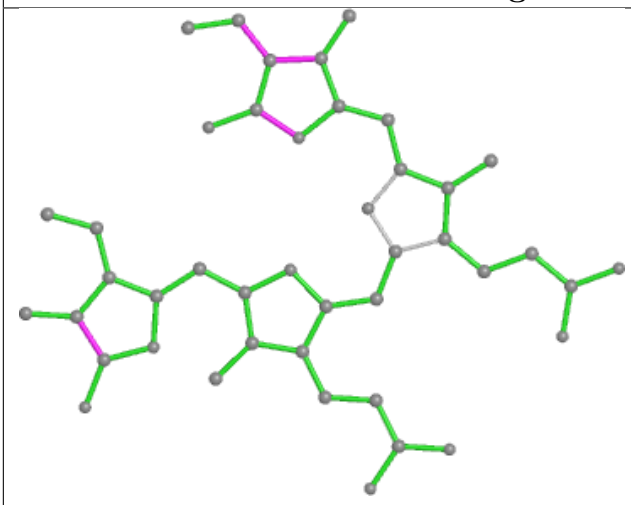


Rings

Ligand PEB Z9 1003



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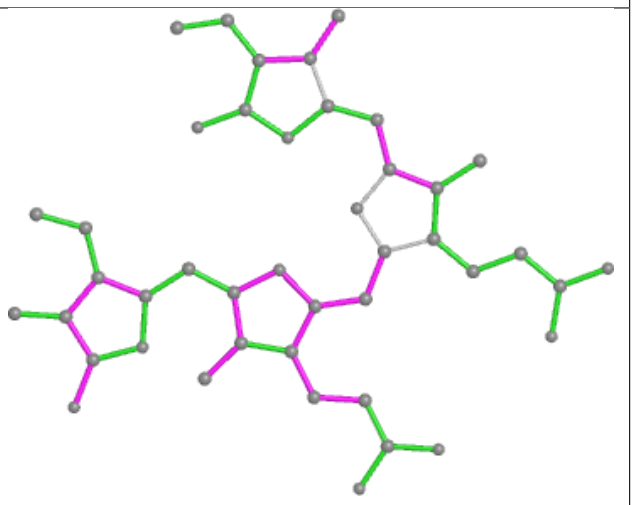

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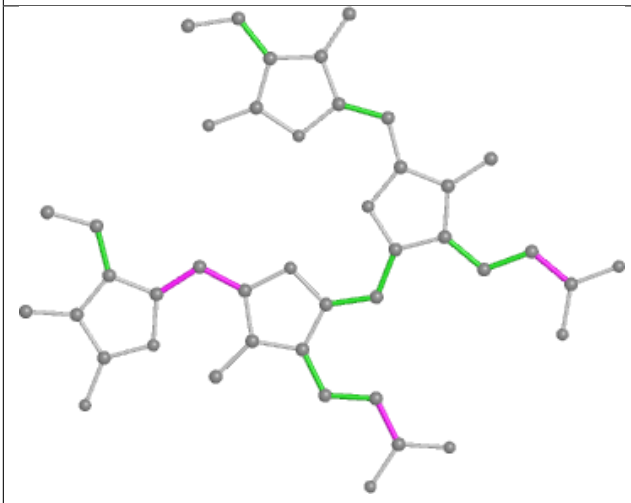

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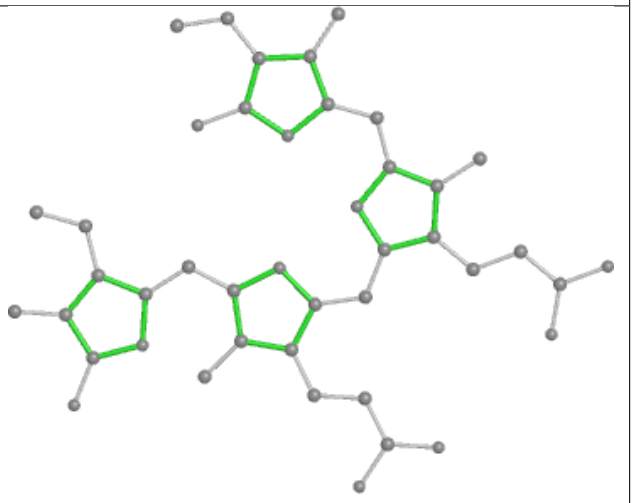

Rings

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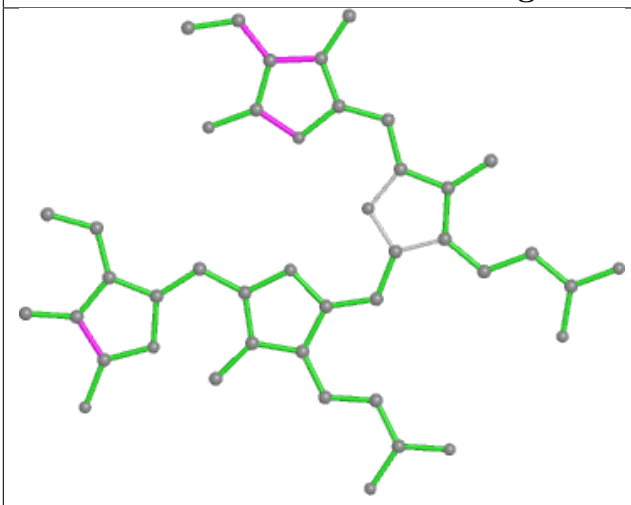

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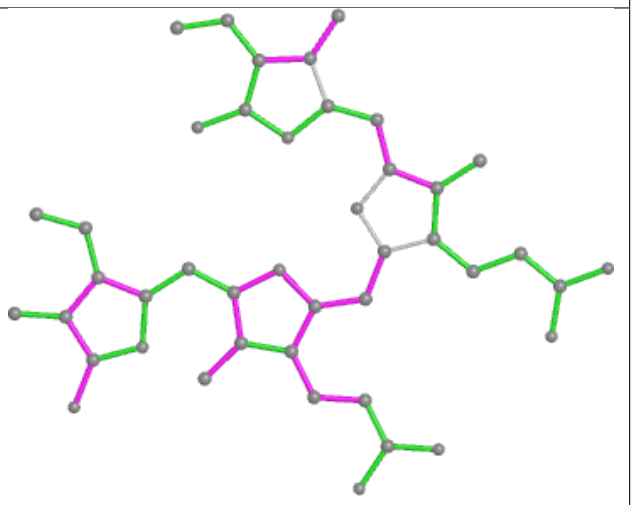

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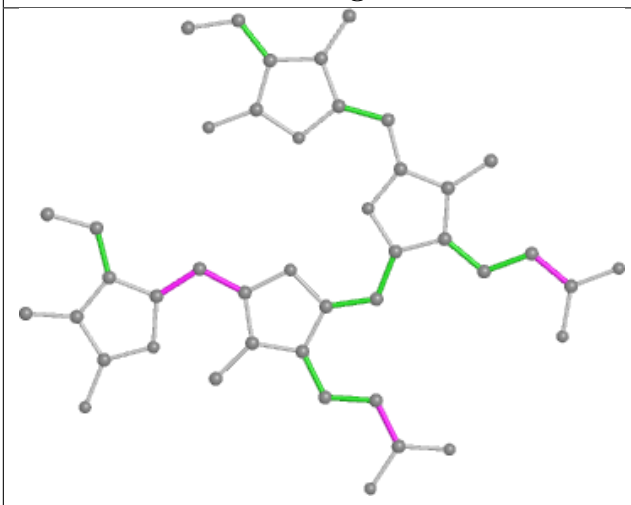

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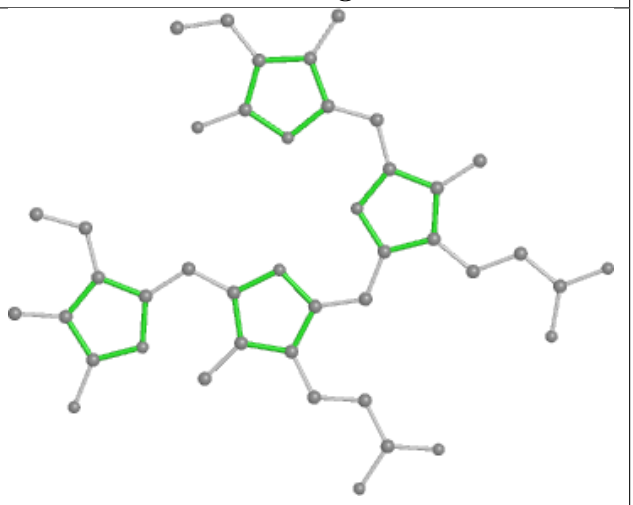
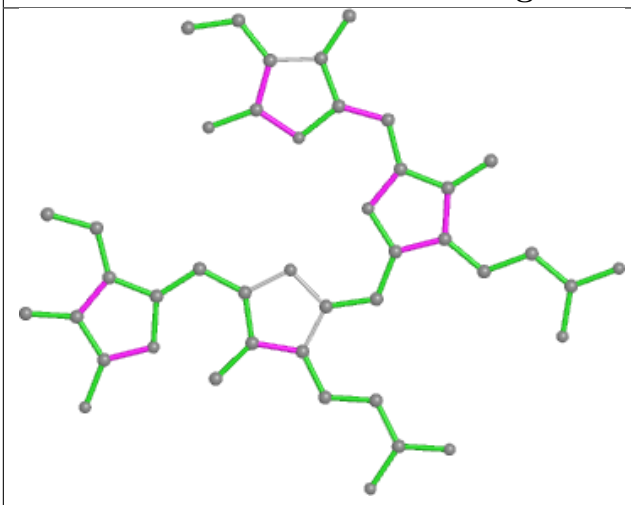


Rings

Ligand PUB cE 203



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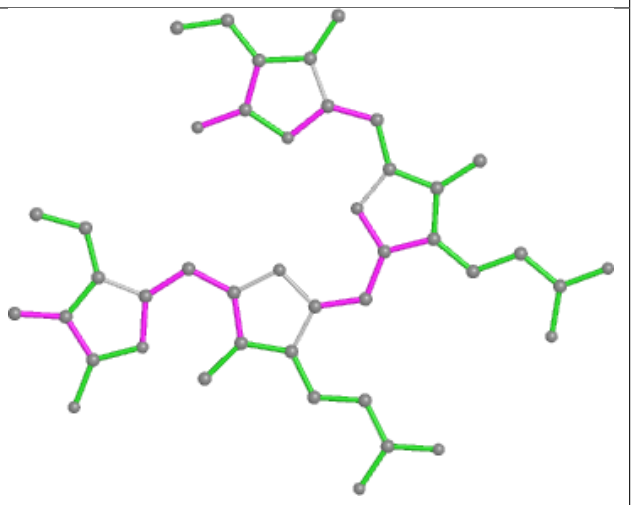

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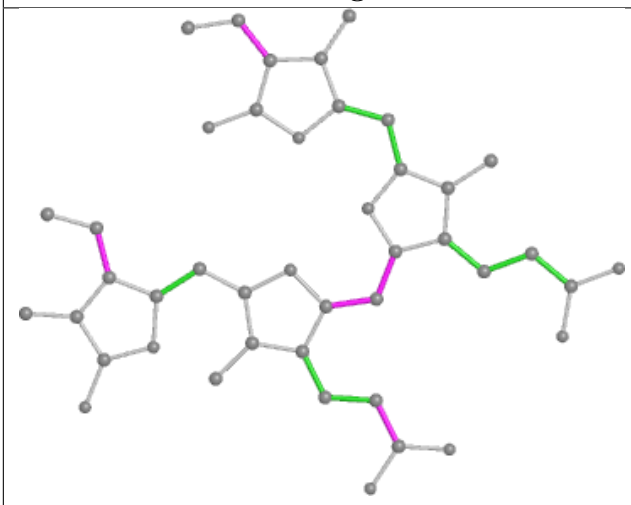

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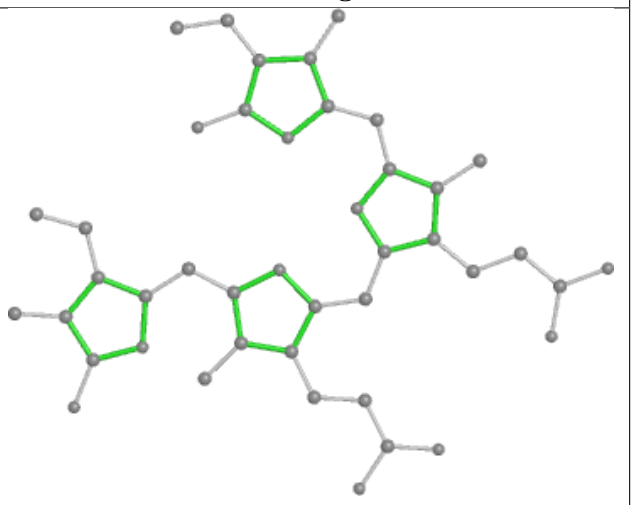

Rings

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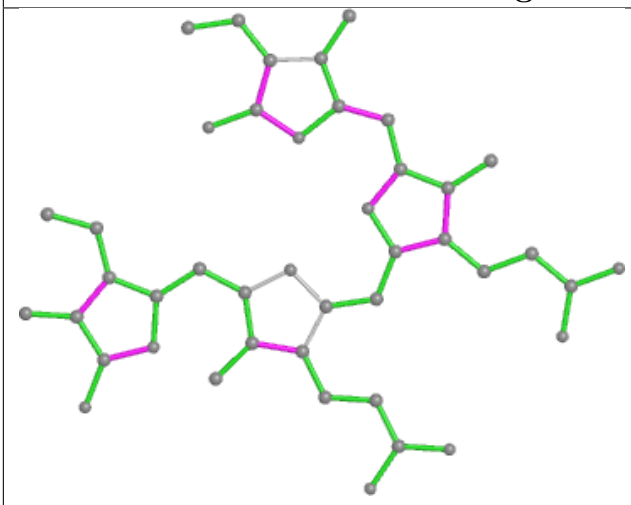

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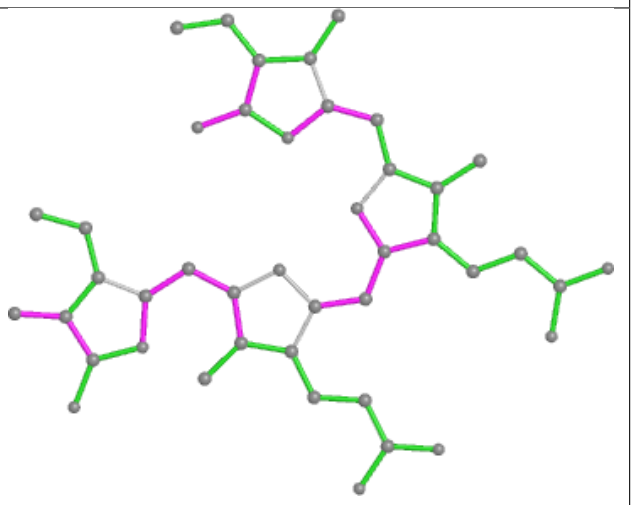

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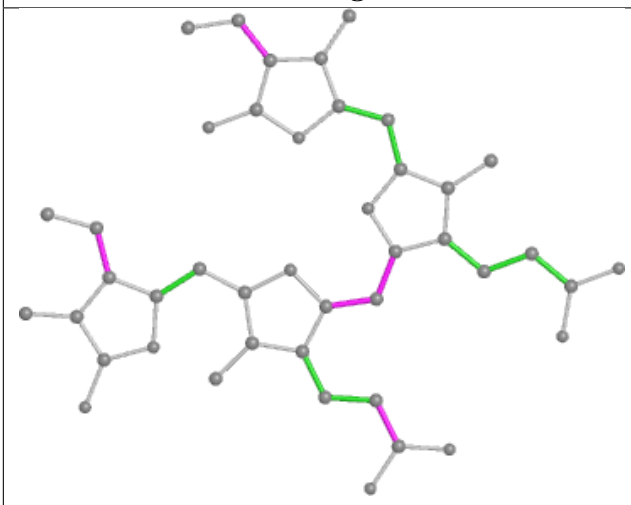

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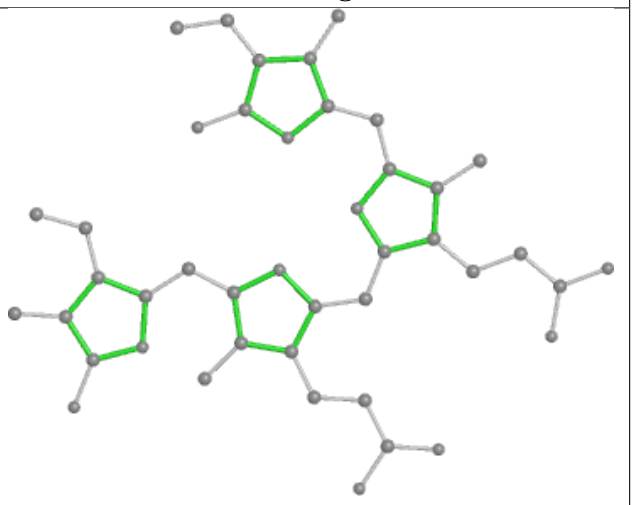
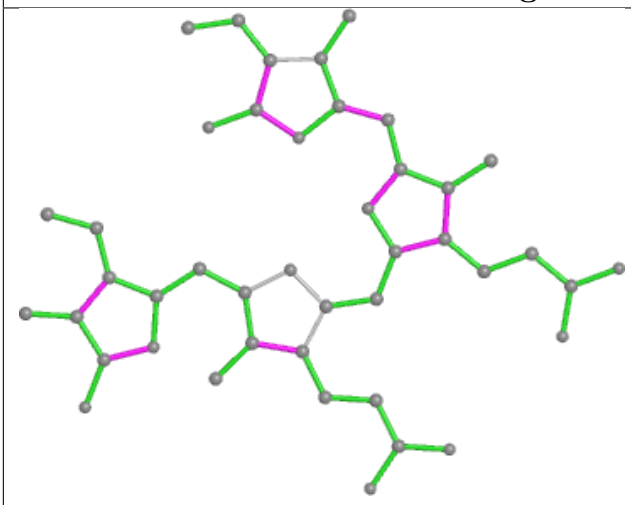


Rings

Ligand PUB ar 203



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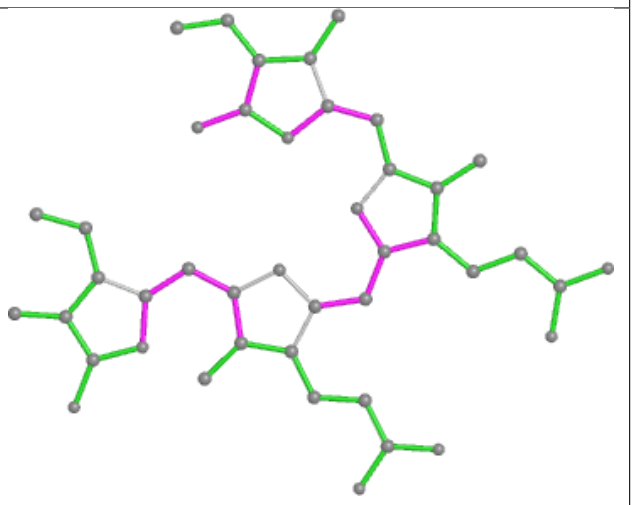

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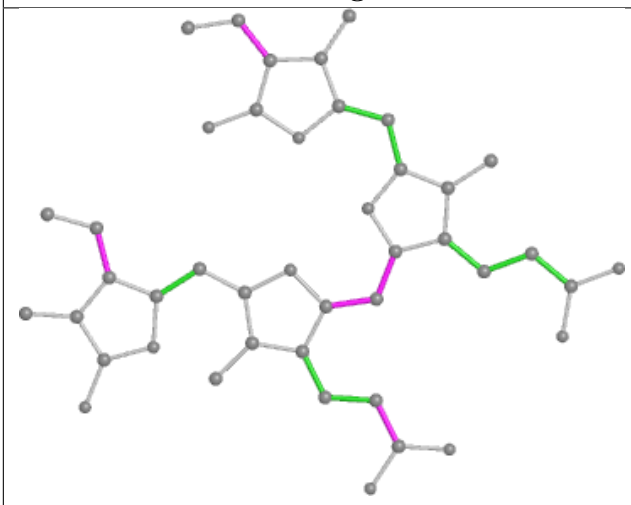

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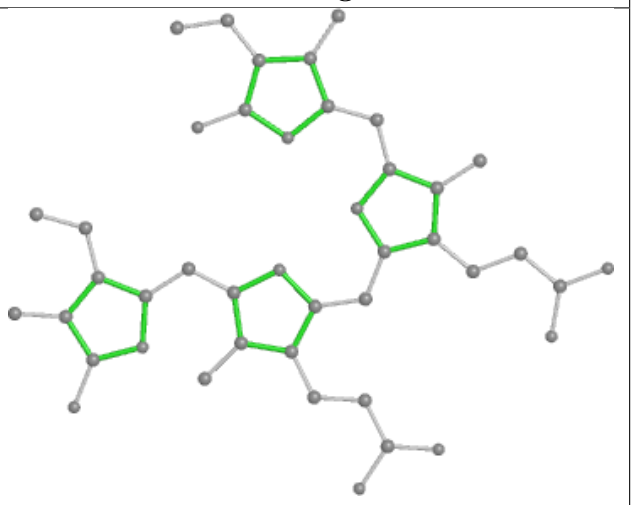
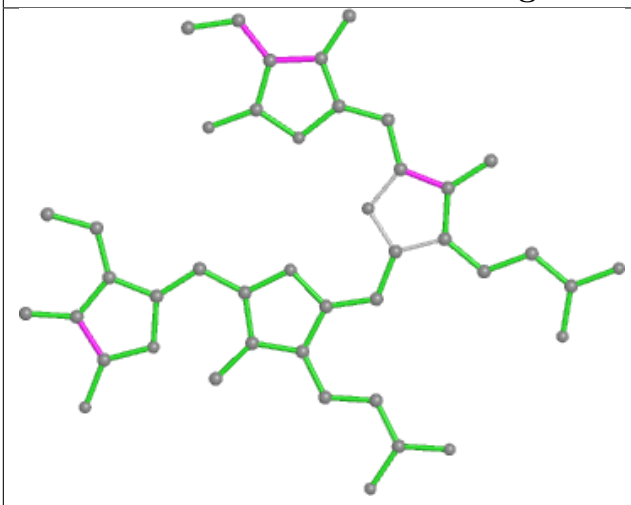


Rings

Ligand PEB cZ 202



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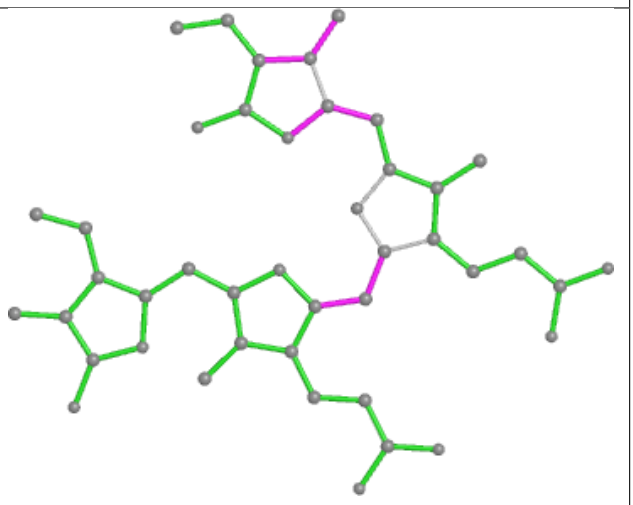
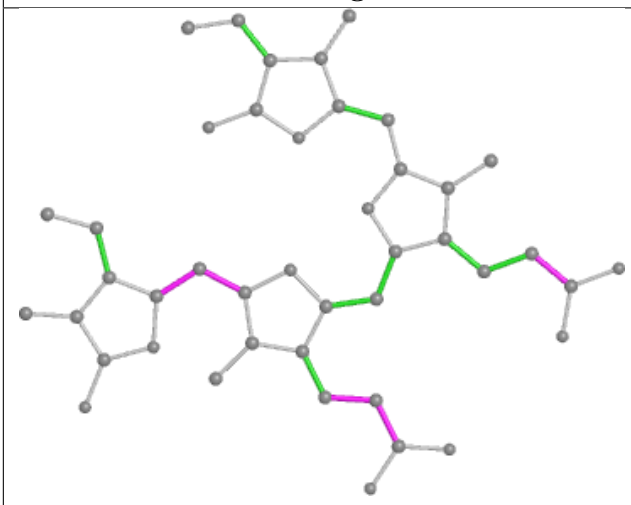
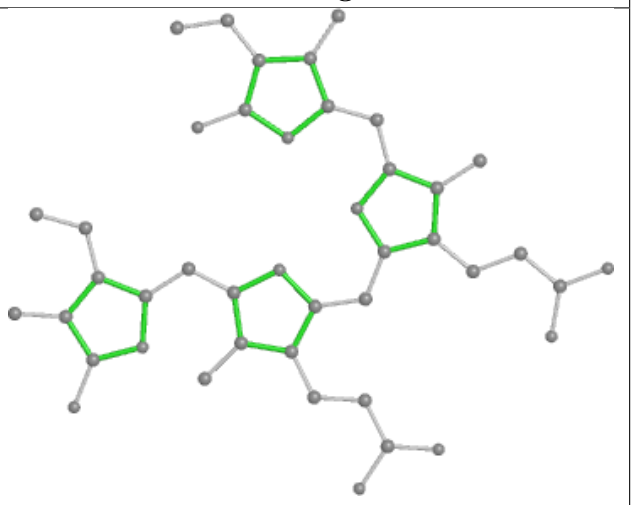


Bond angles

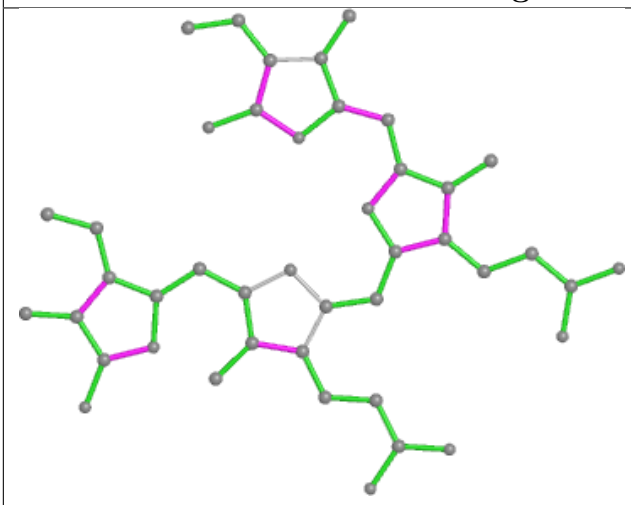


Torsions



Rings

Ligand PUB bD 203



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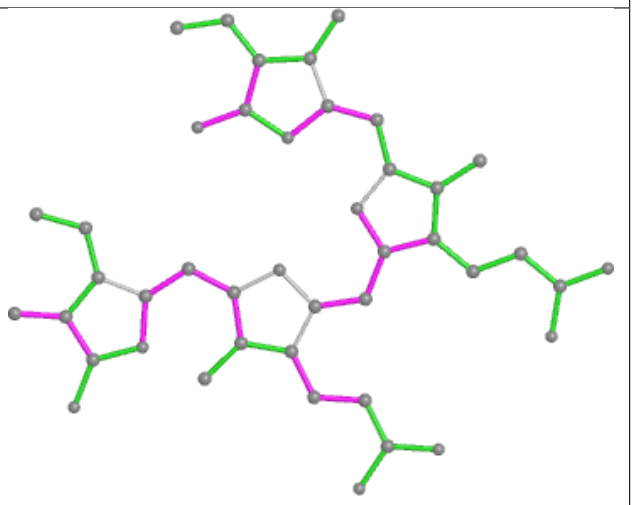

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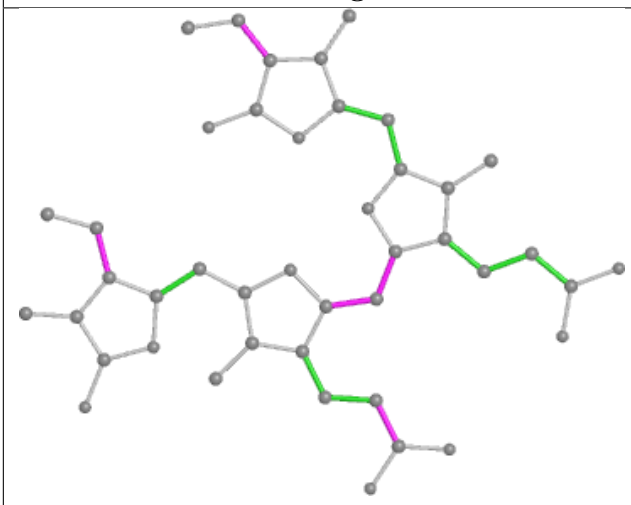

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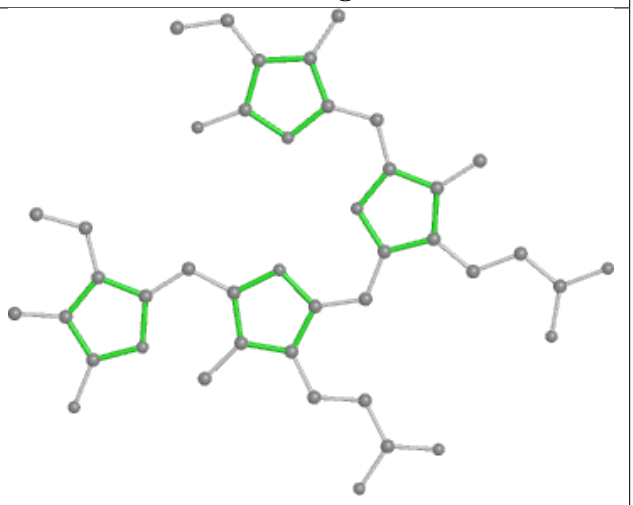
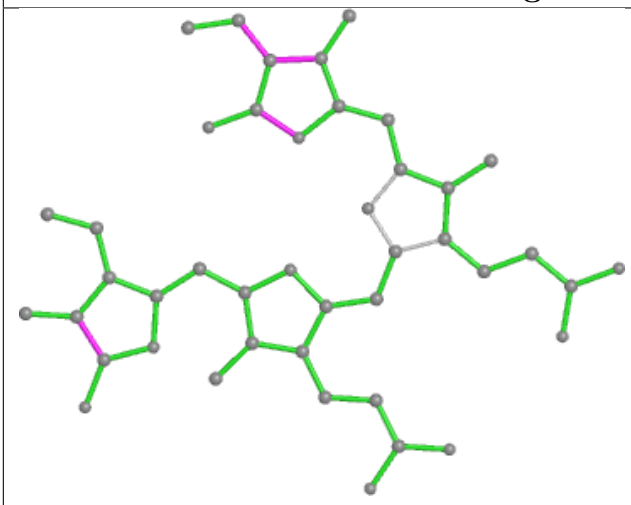


Rings

Ligand PEB i5 201



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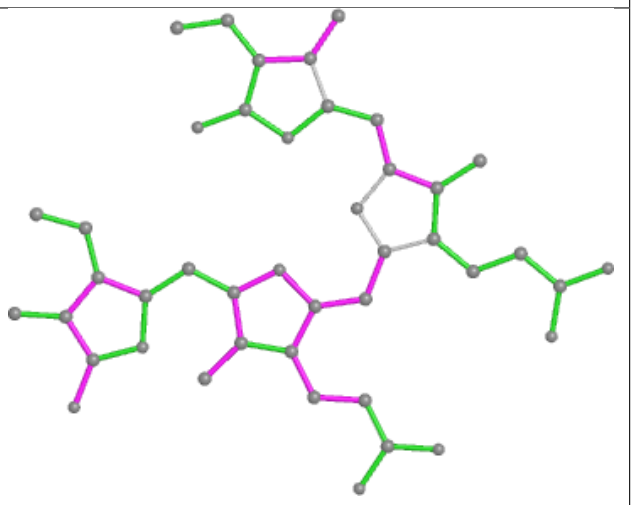

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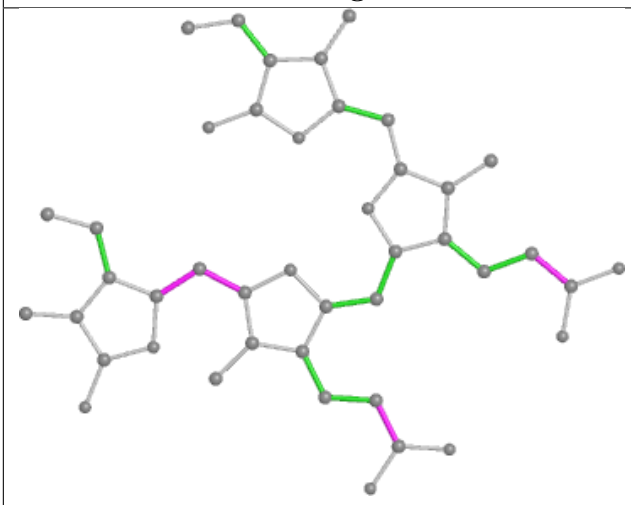

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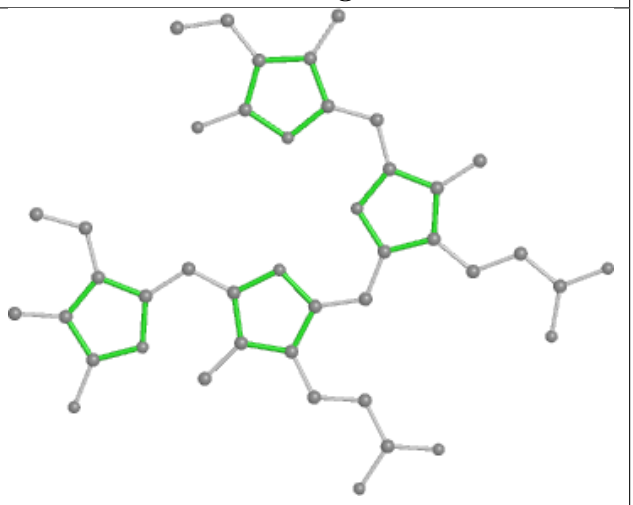
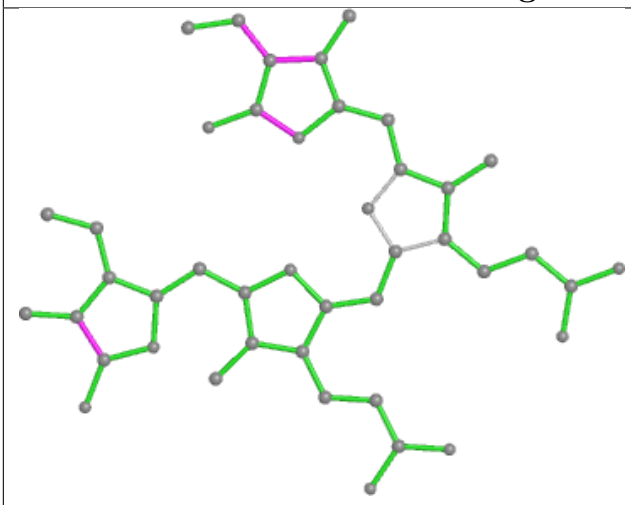


Rings

Ligand PEB p3 201



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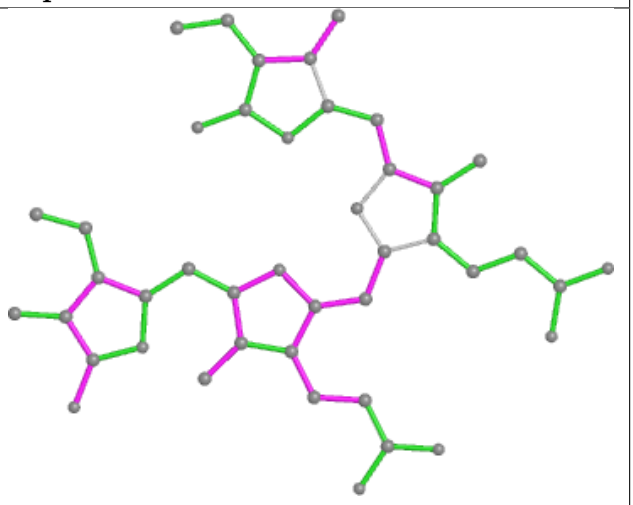
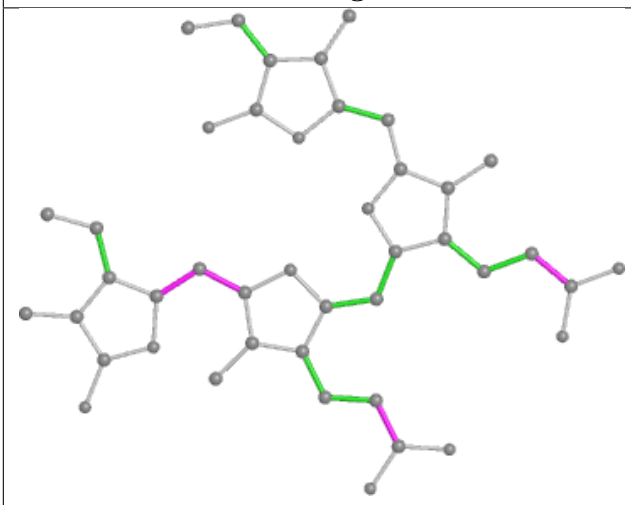


Bond angles



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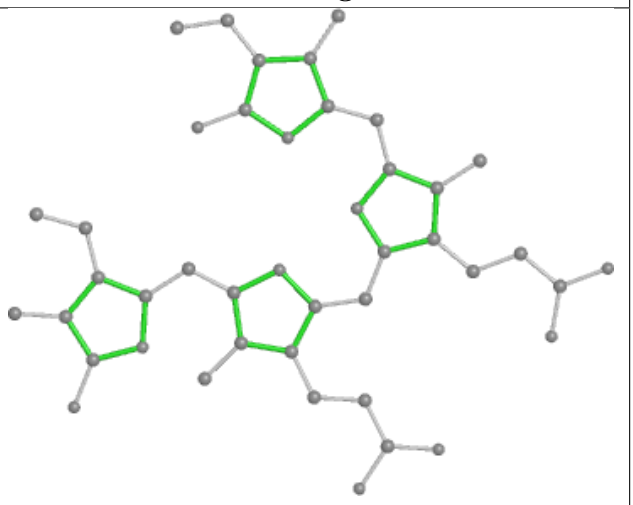
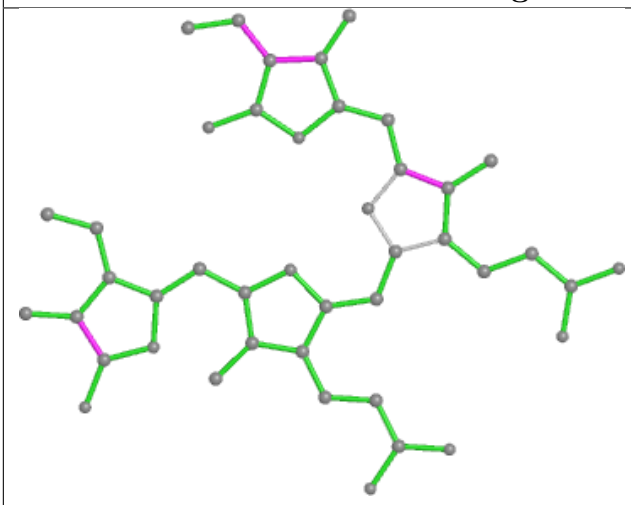


Rings

Ligand PEB cy 1002



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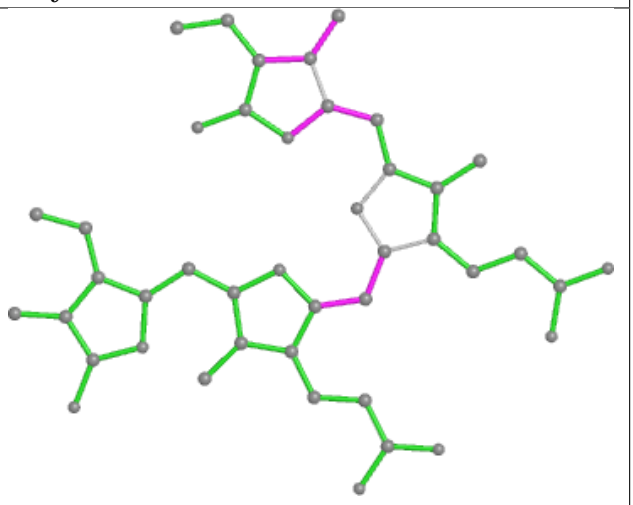

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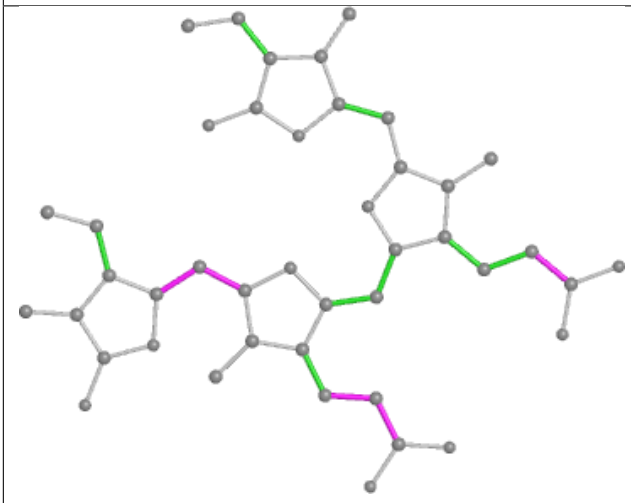

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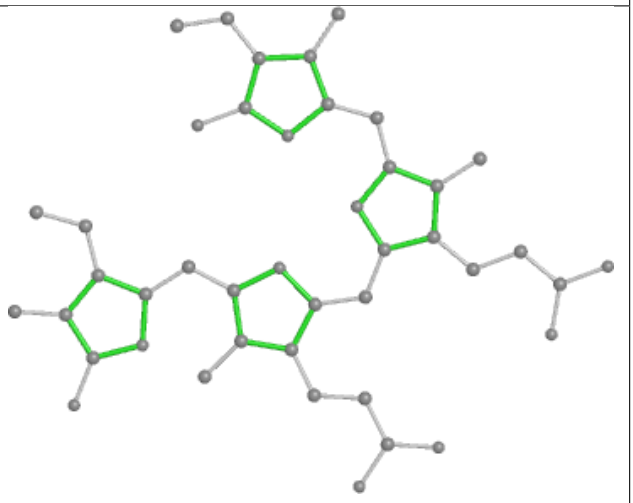
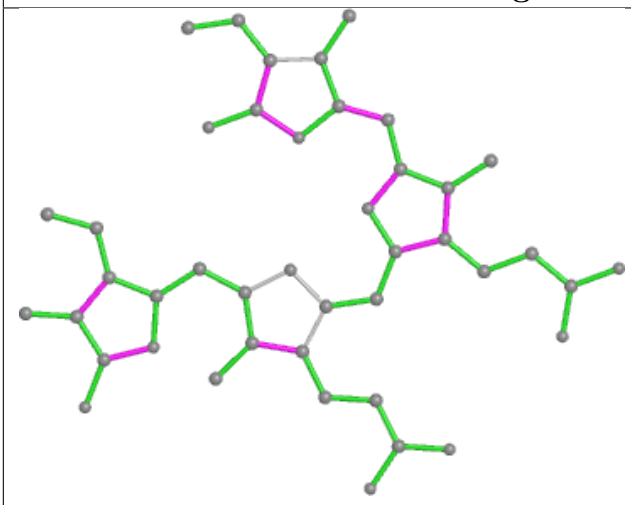


Rings

Ligand PUB H9 203



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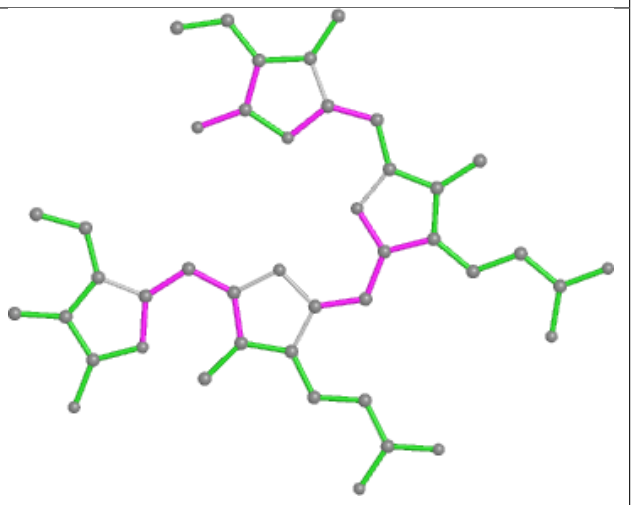

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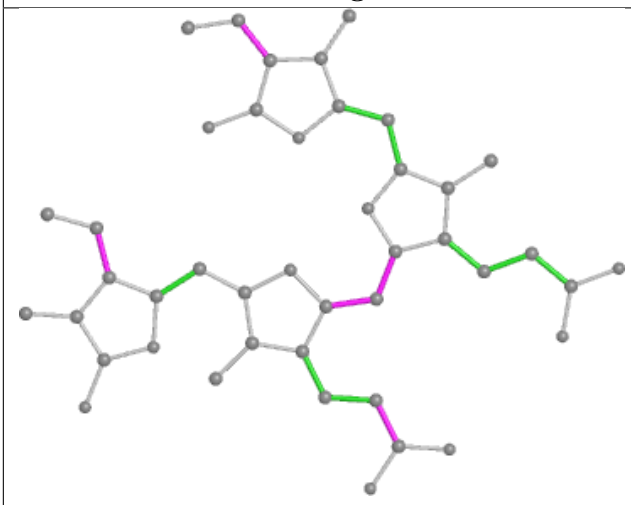

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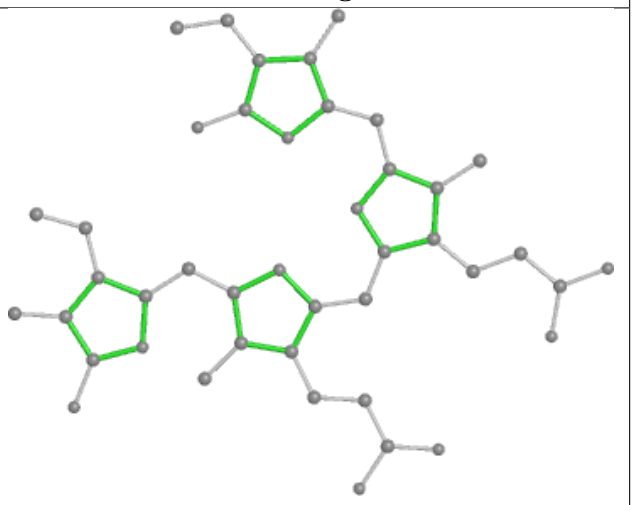
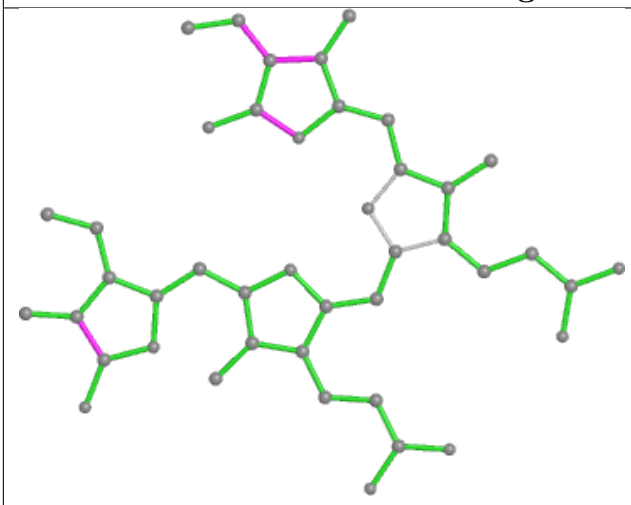


Rings

Ligand PEB db 201



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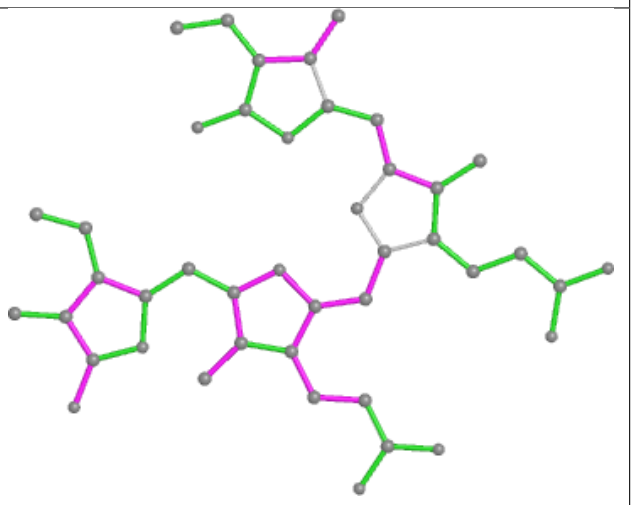

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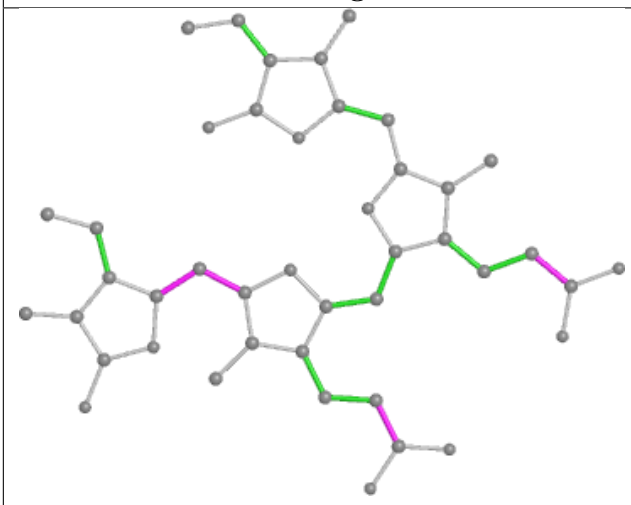

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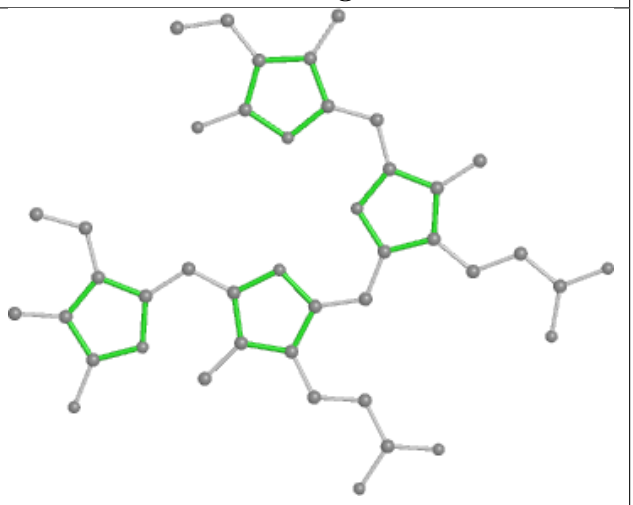

Rings

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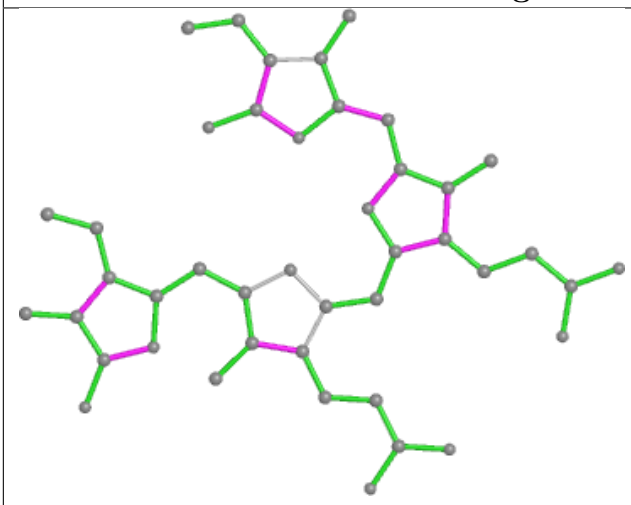

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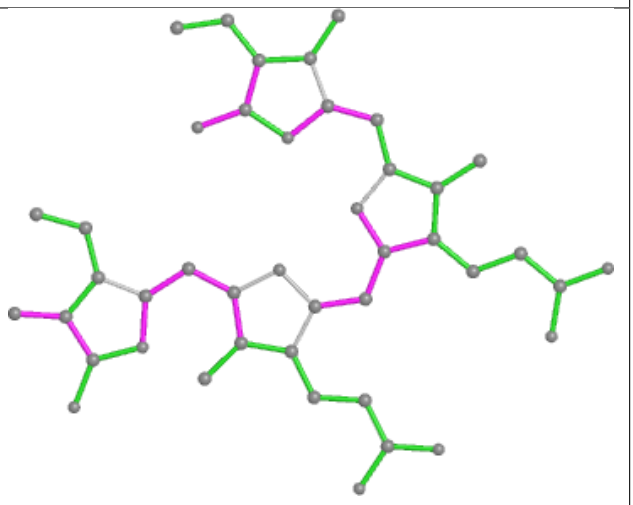

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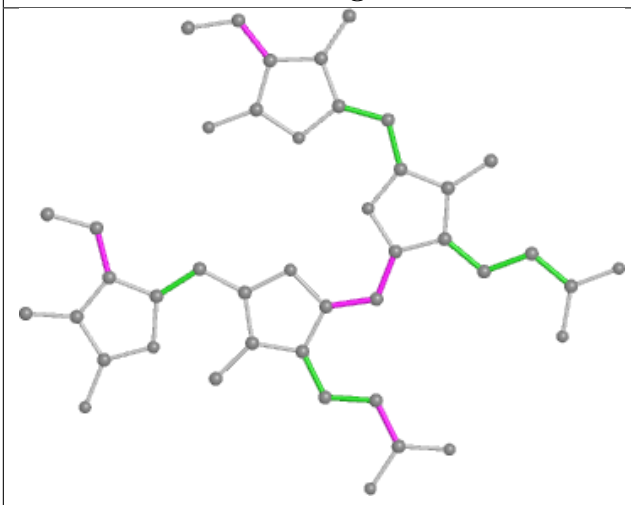

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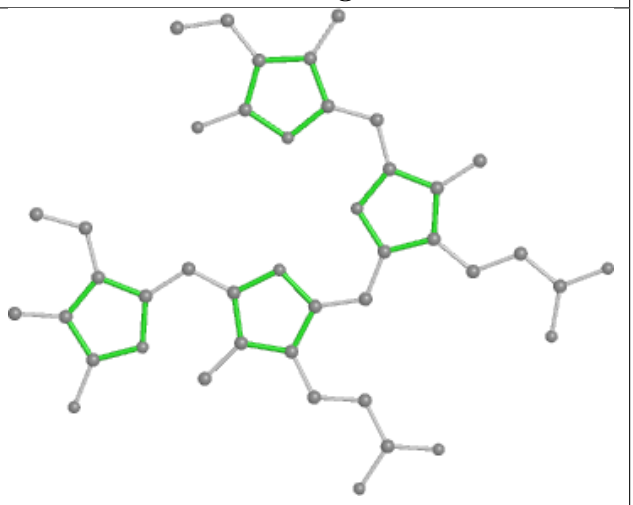
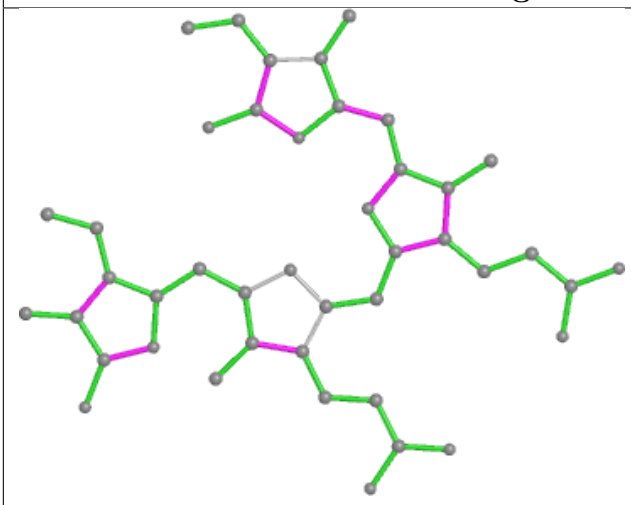


Rings

Ligand PUB H7 203



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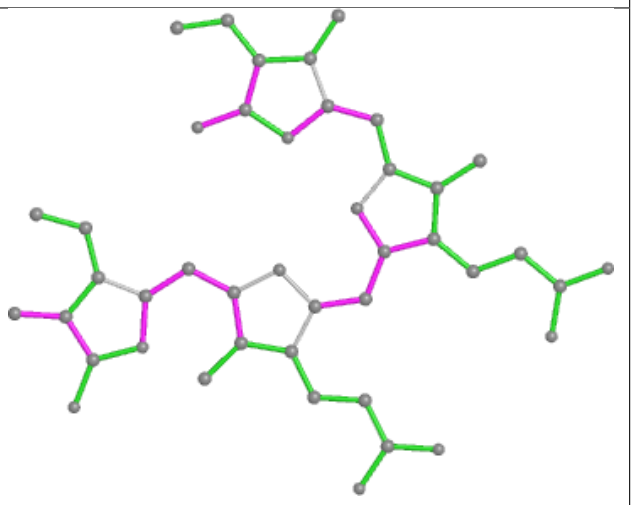

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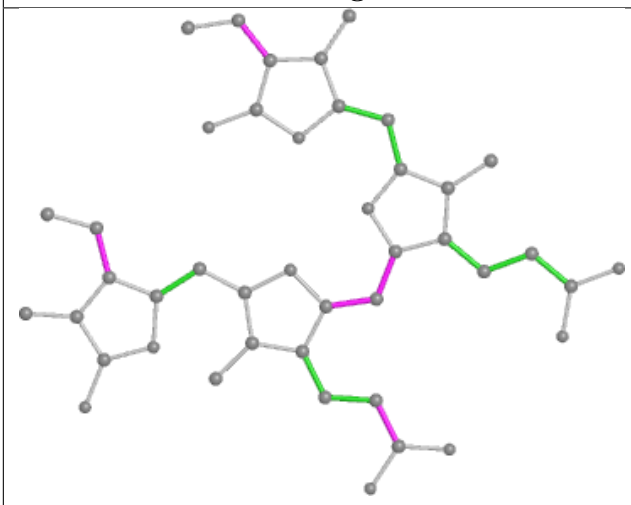

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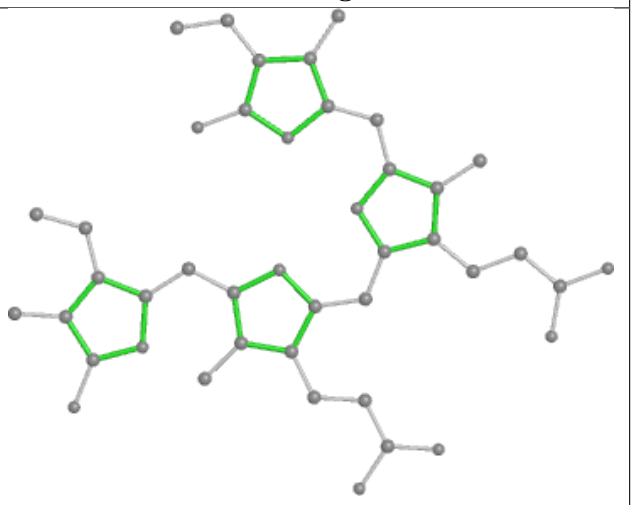

Rings

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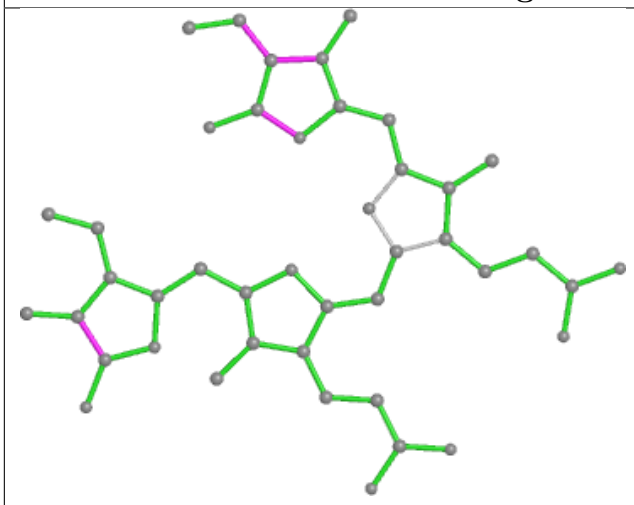

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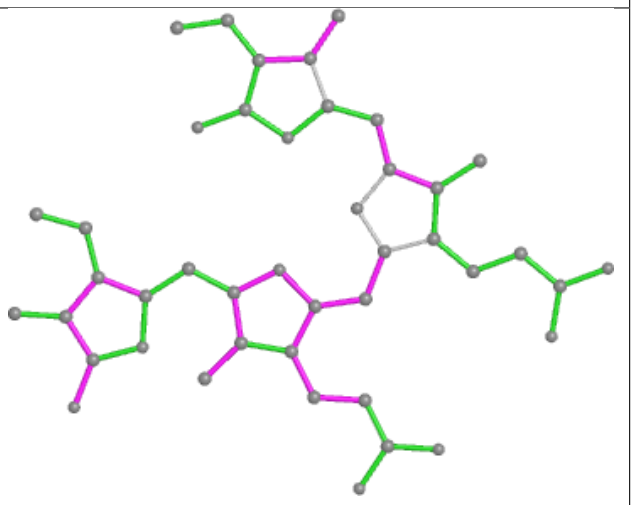

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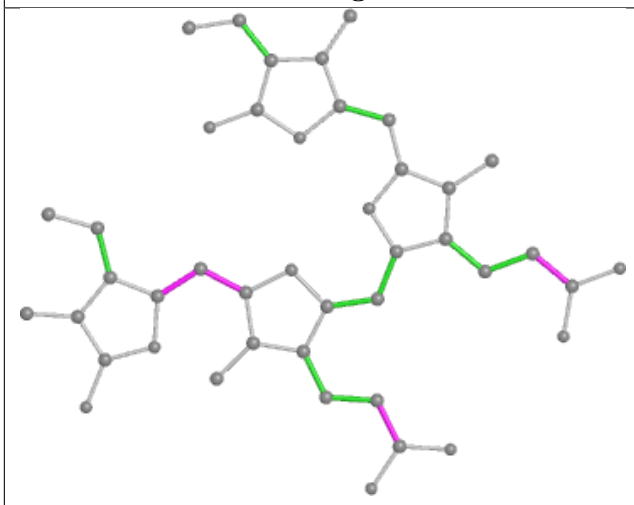

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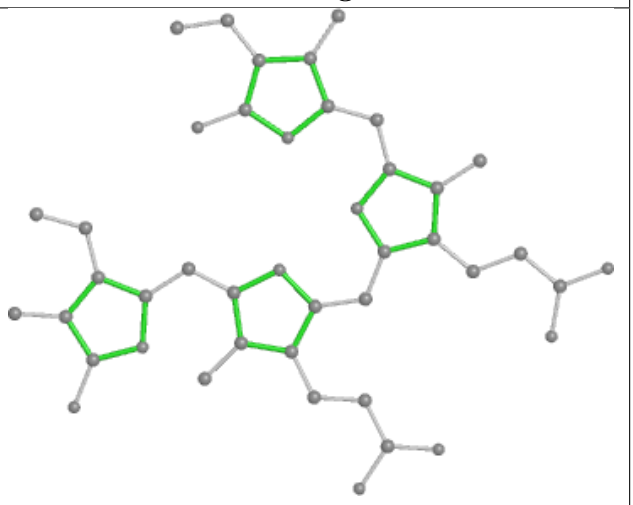

Rings

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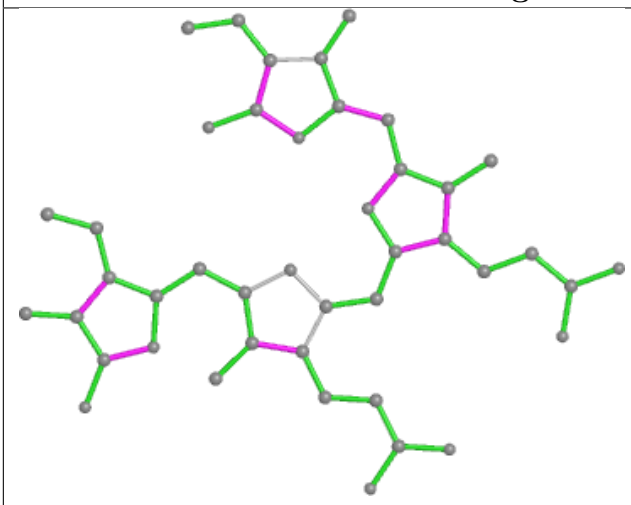

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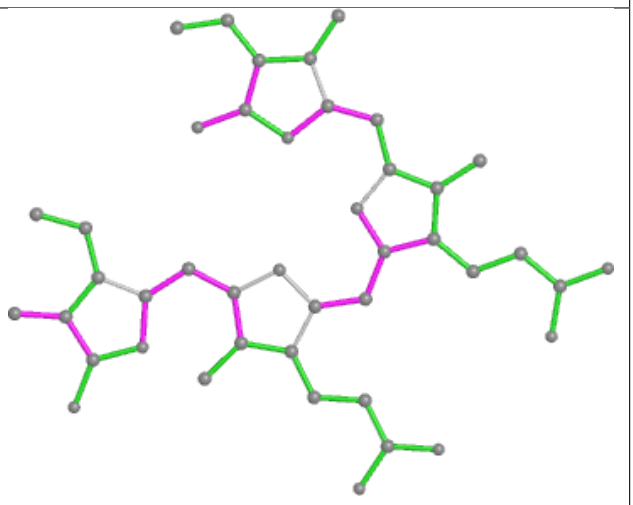

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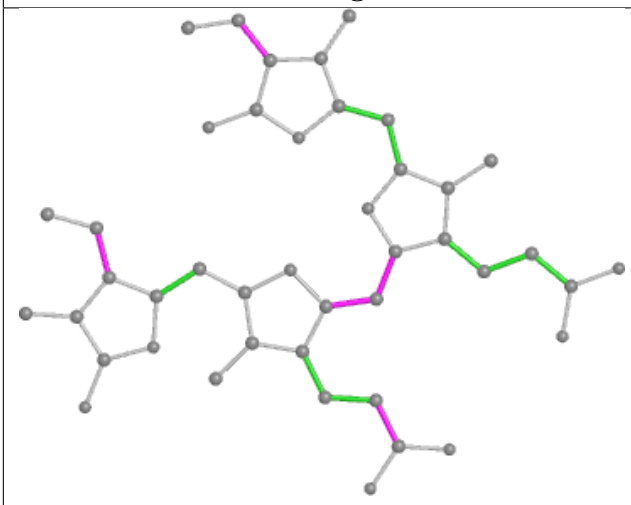

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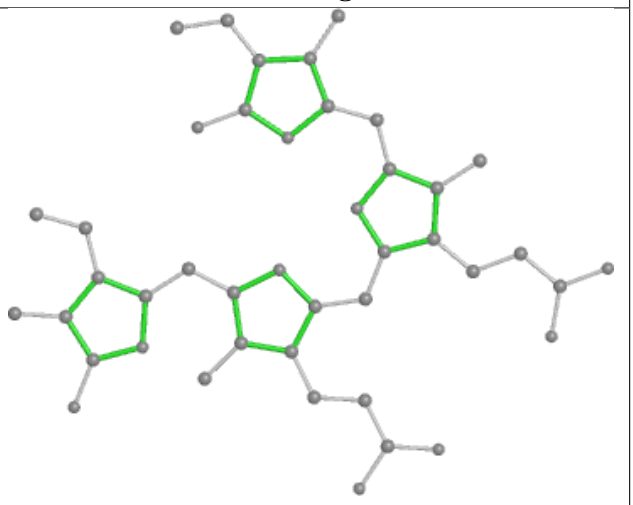

Rings

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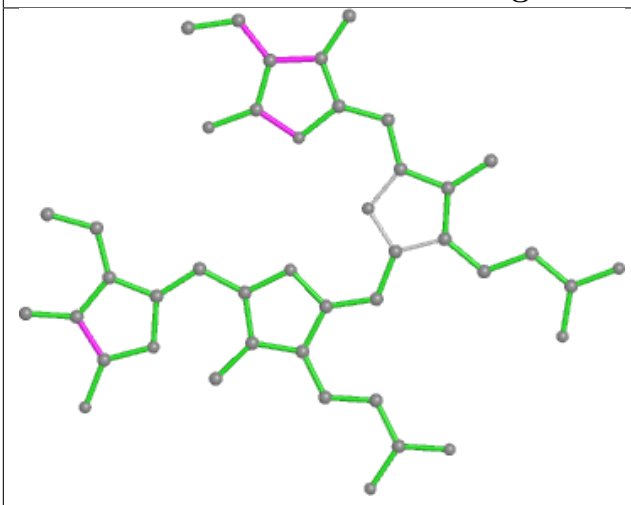

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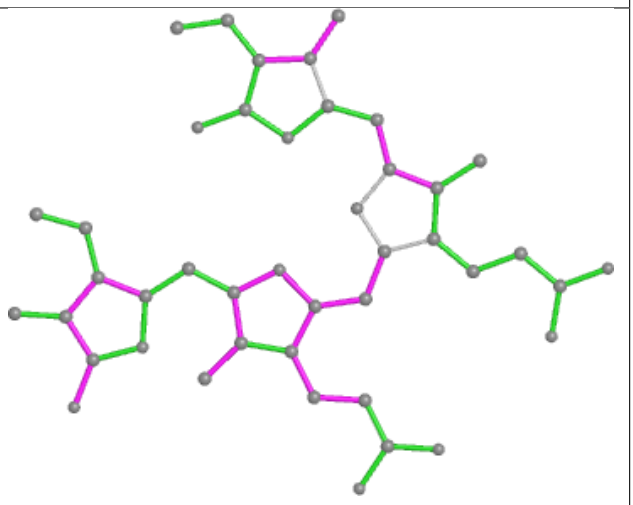

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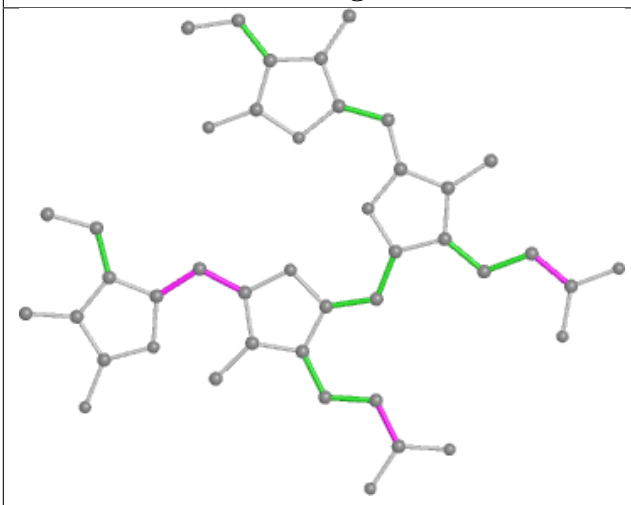

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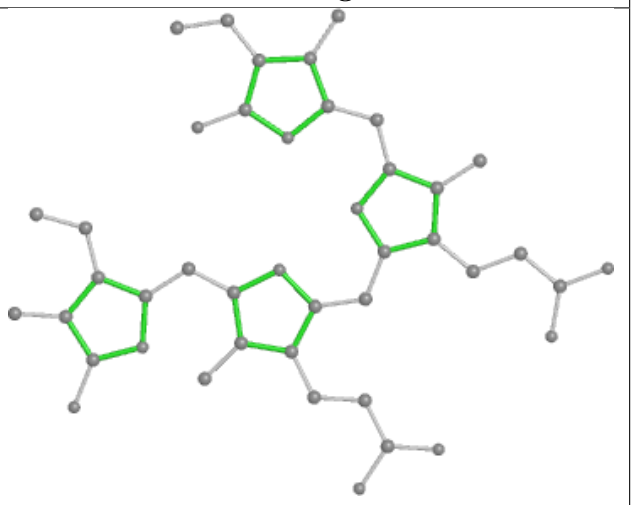
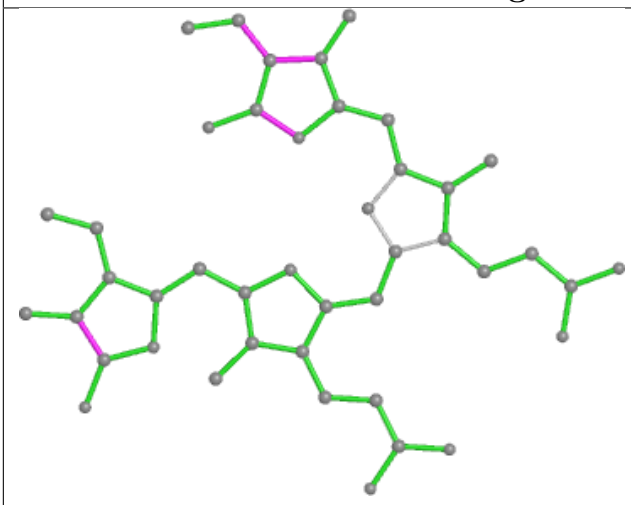


Rings

Ligand PEB Z9 1001



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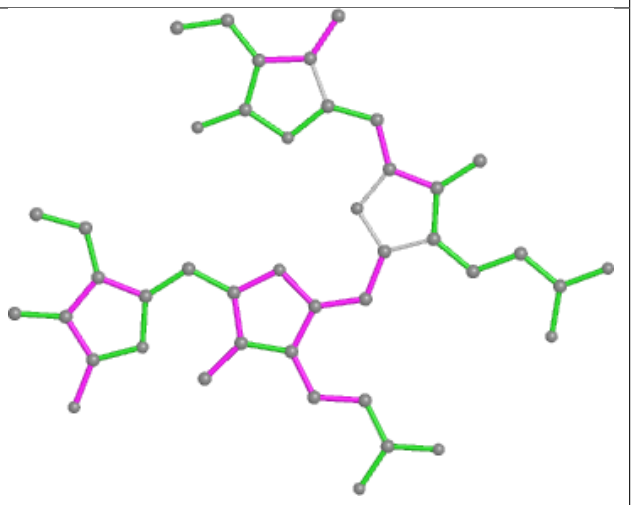

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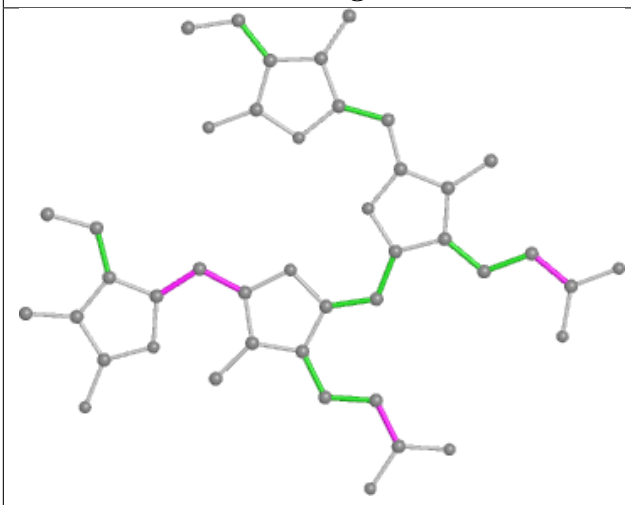

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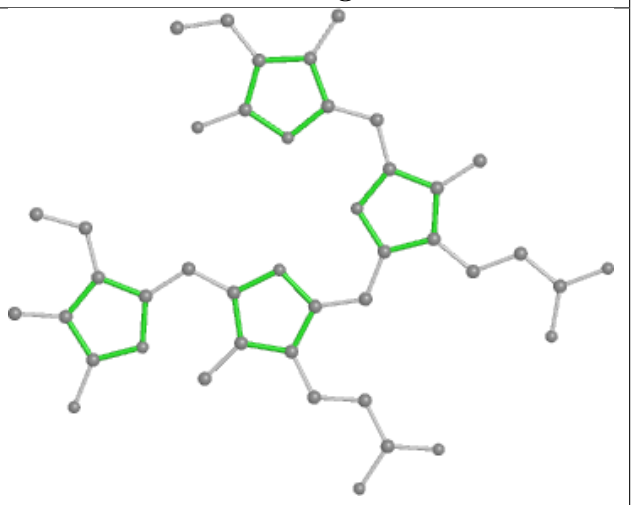
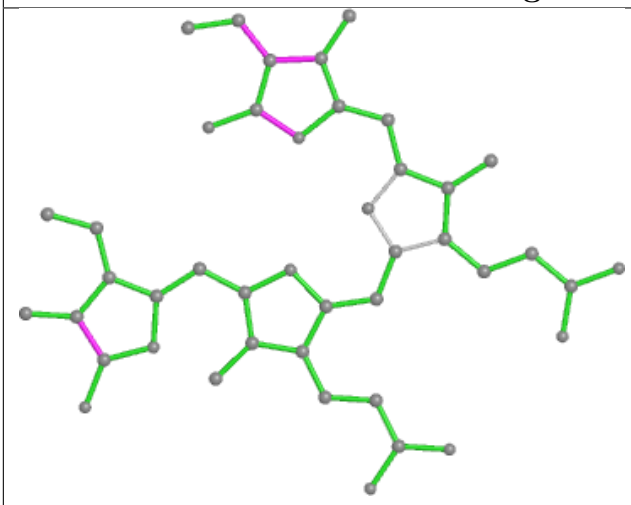


Rings

Ligand PEB fo 201



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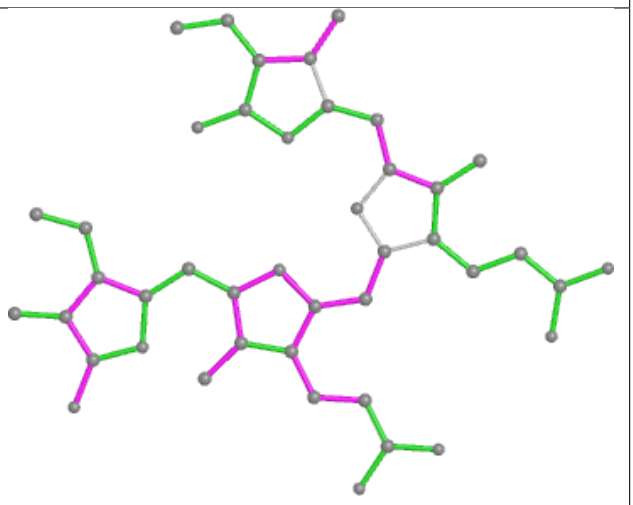

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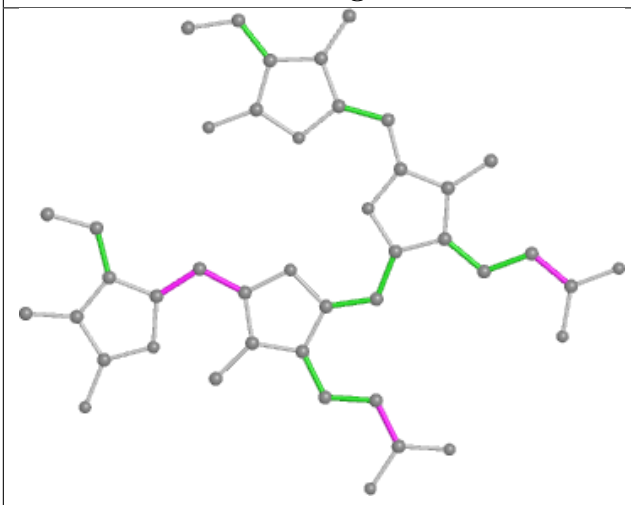
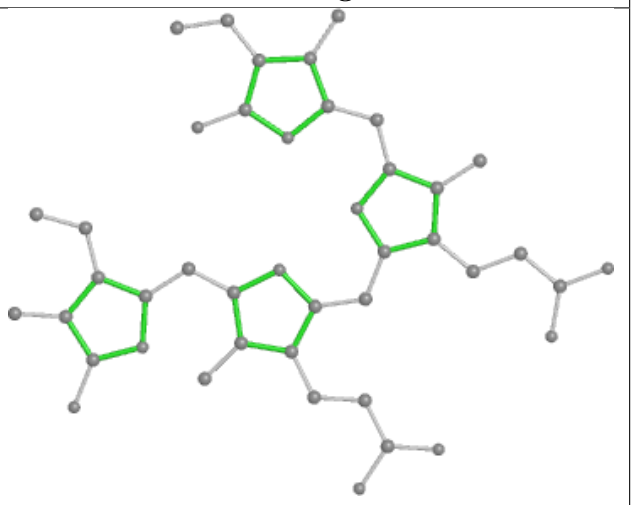
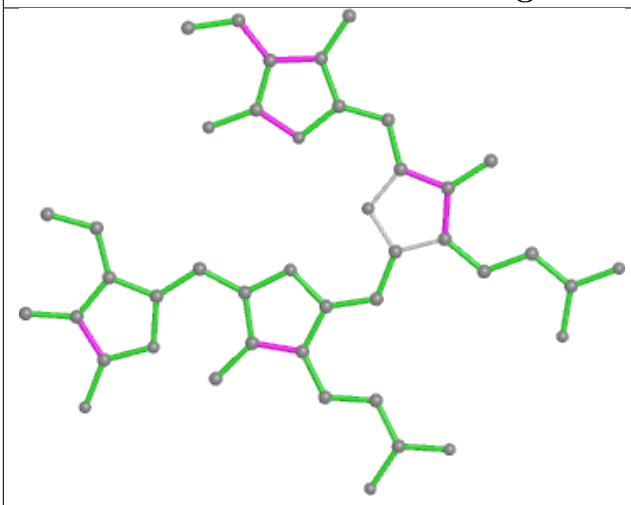


Torsions



Rings

Ligand PEB T9 202



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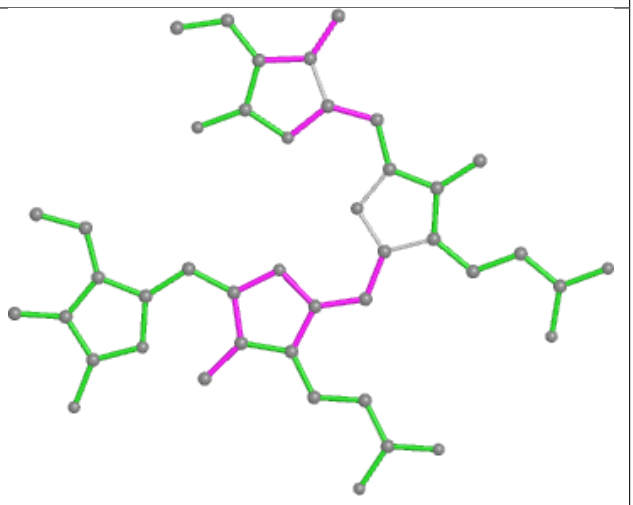

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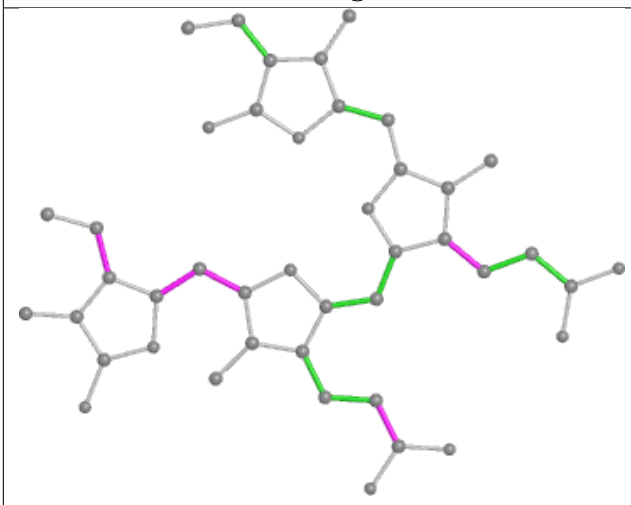

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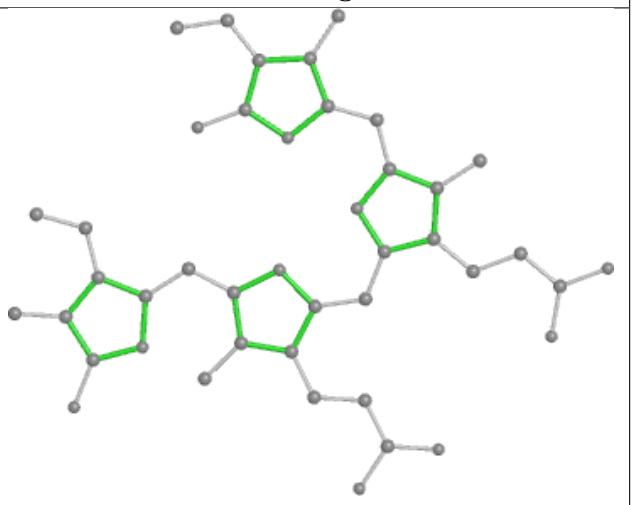
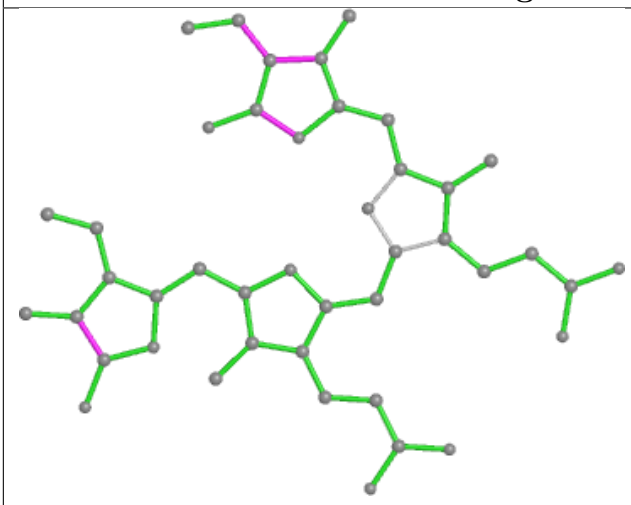


Rings

Ligand PEB B6 201



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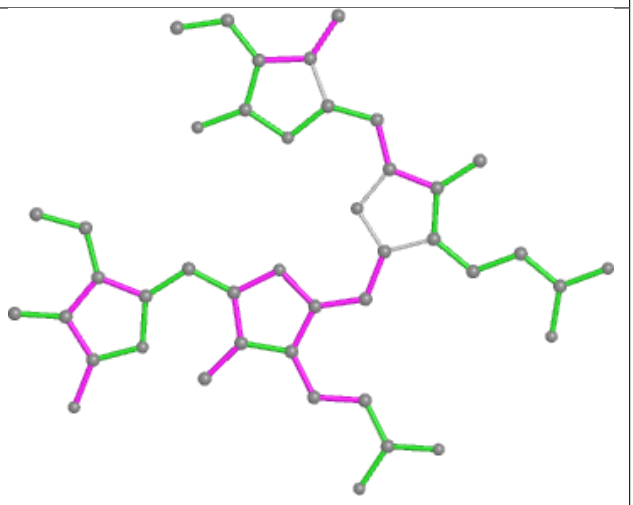

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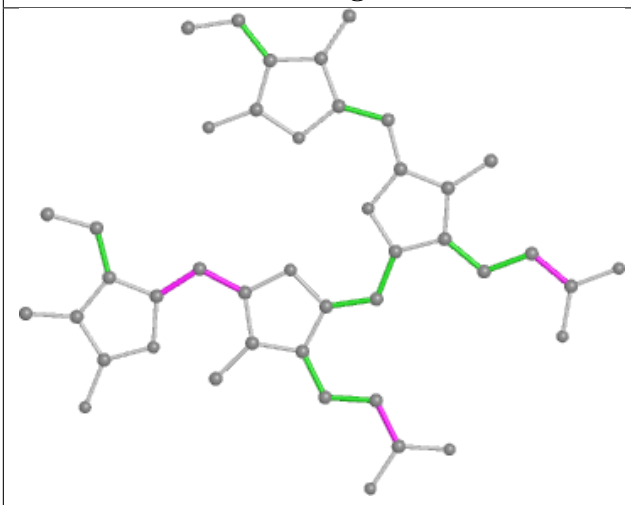

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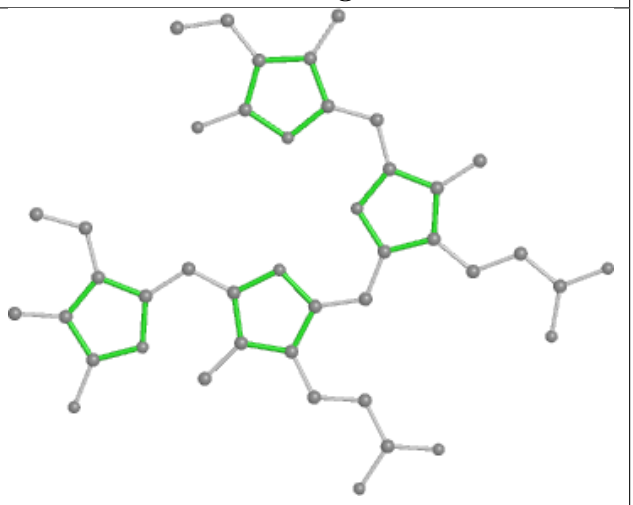
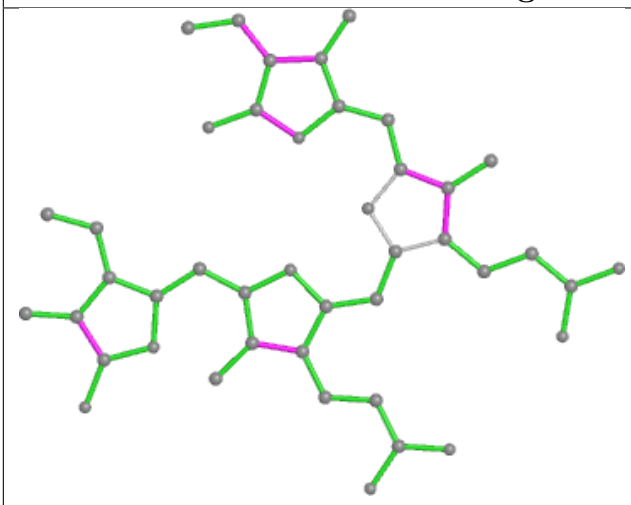


Rings

Ligand PEB Z3 202



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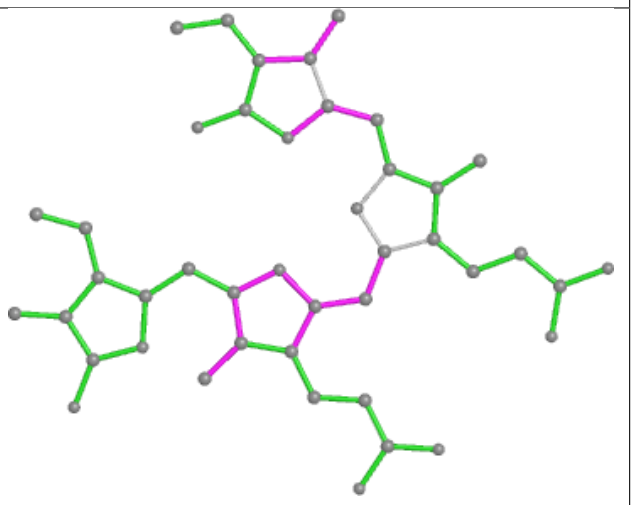

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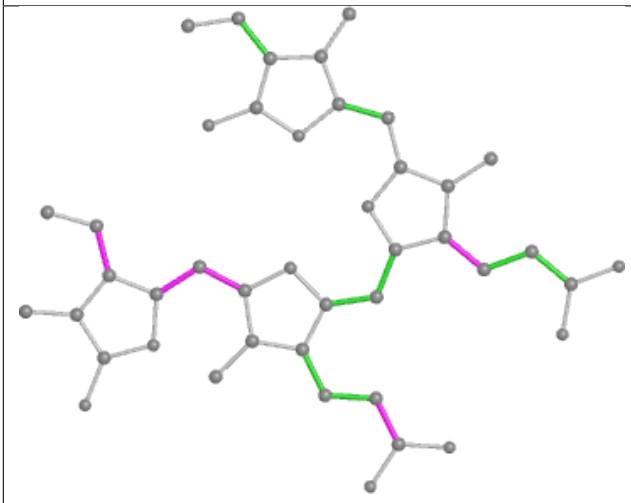

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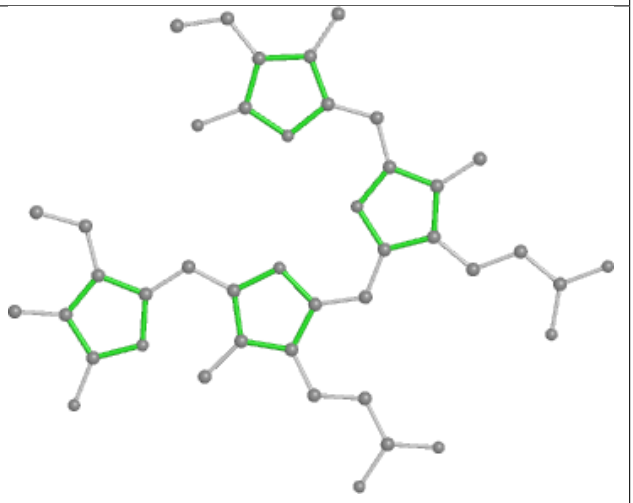
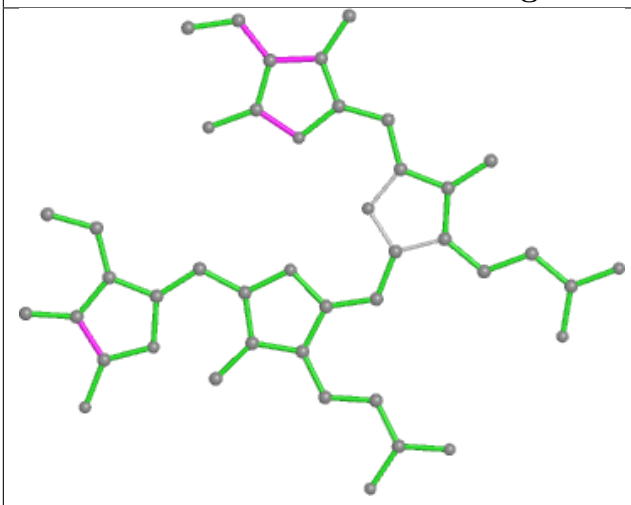


Rings

Ligand PEB z2 202



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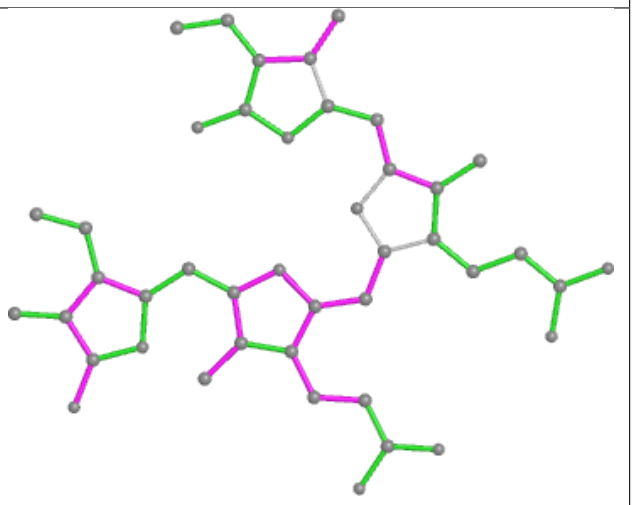

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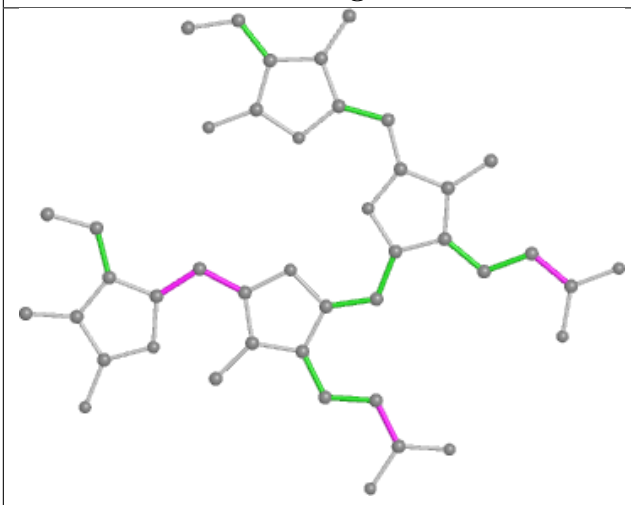

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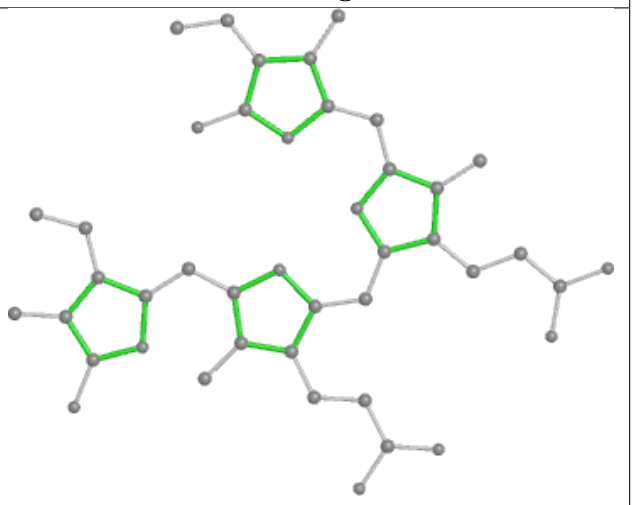
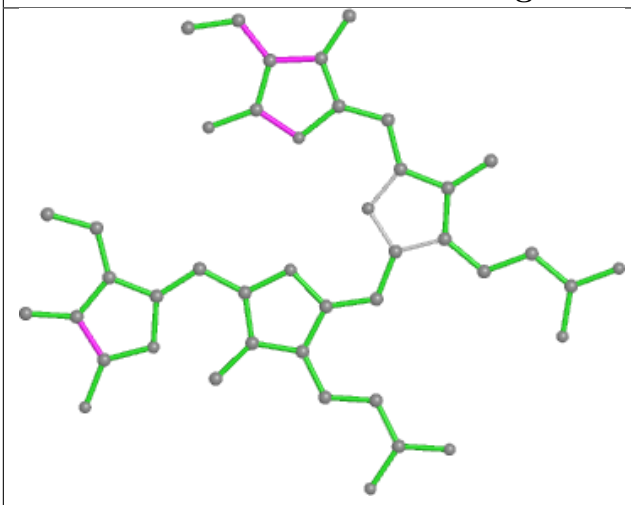


Rings

Ligand PEB aA 201



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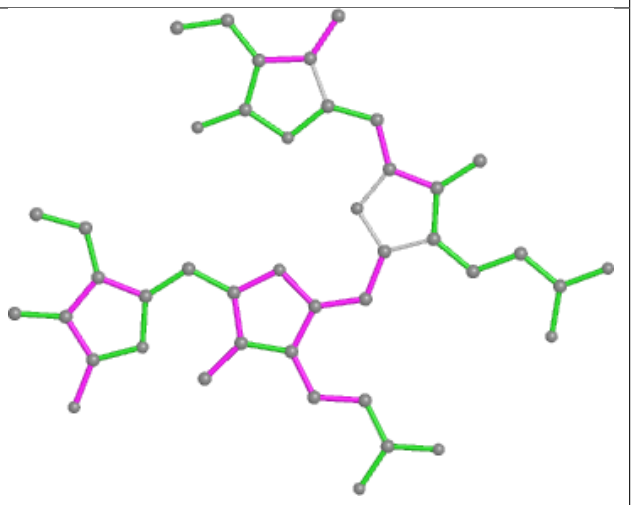

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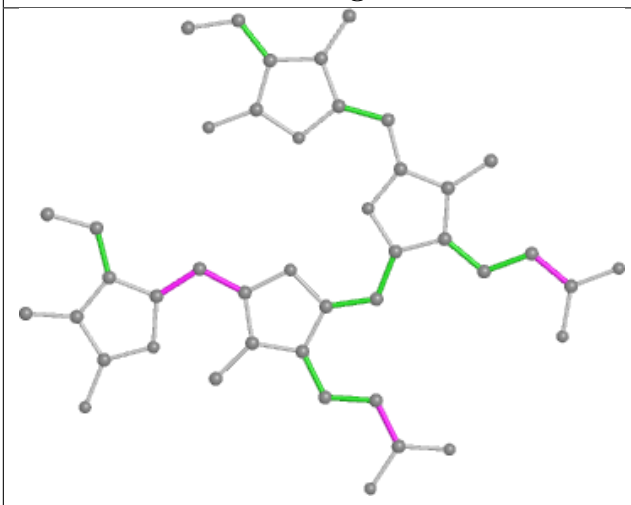

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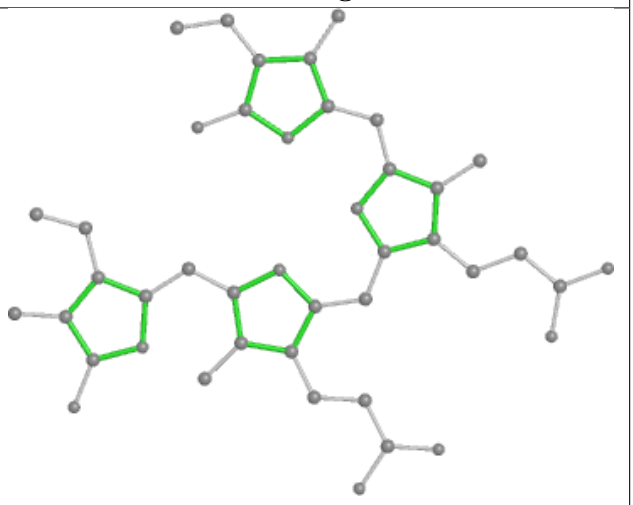

Rings

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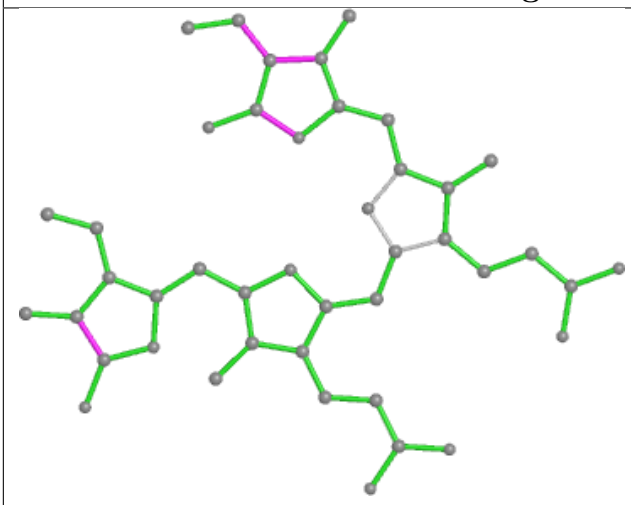

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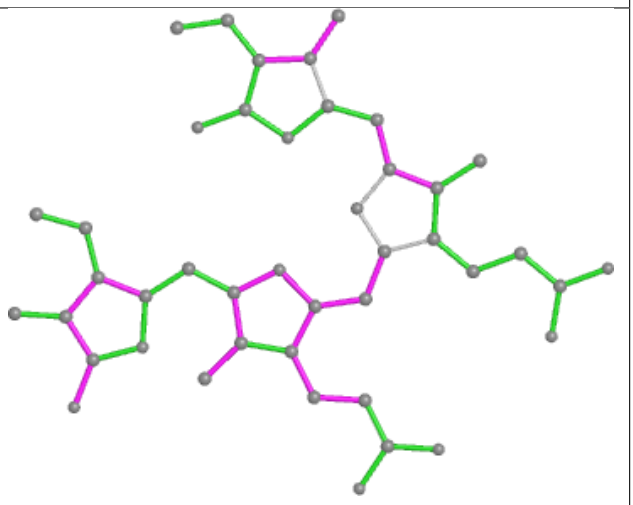

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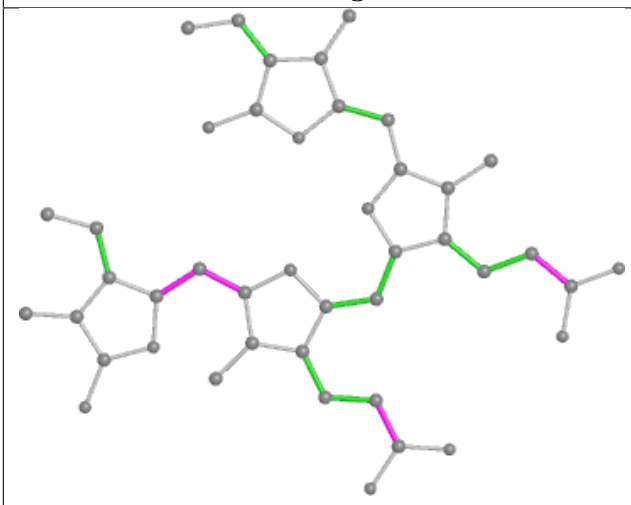

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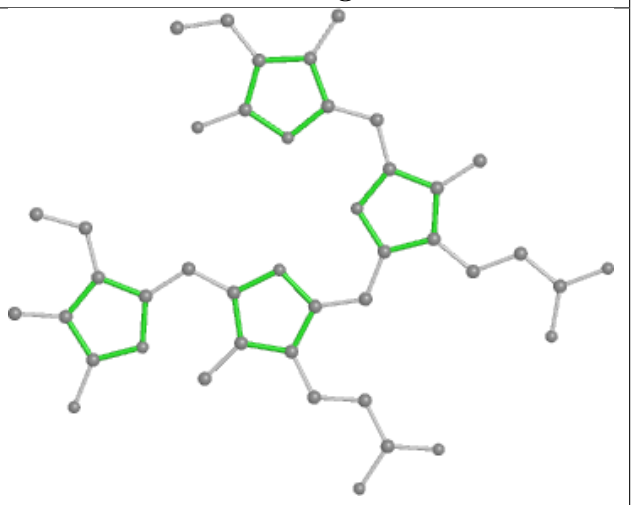

Rings

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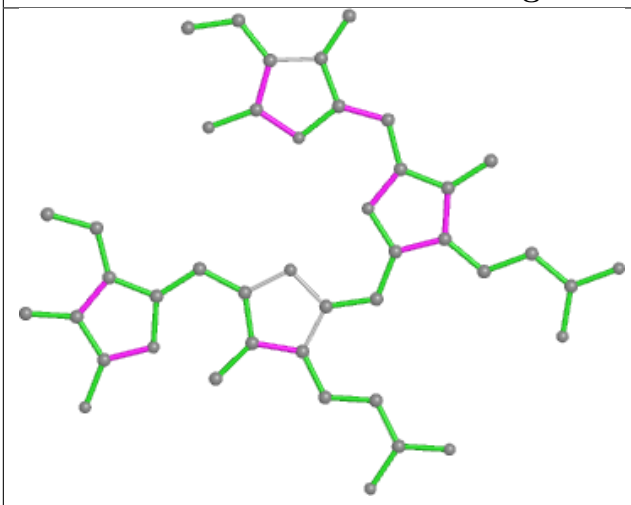

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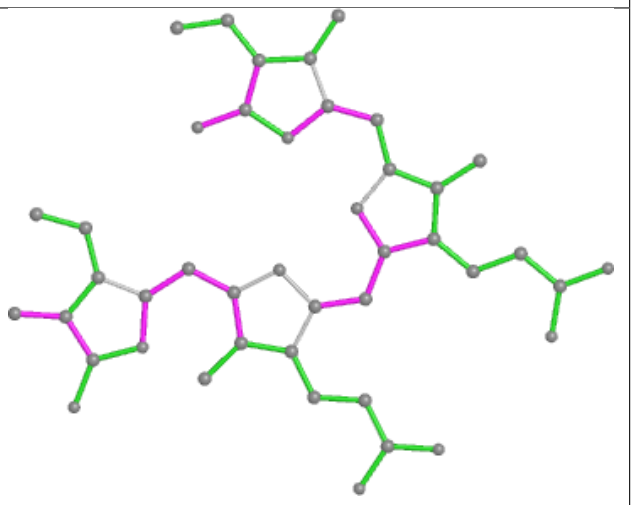

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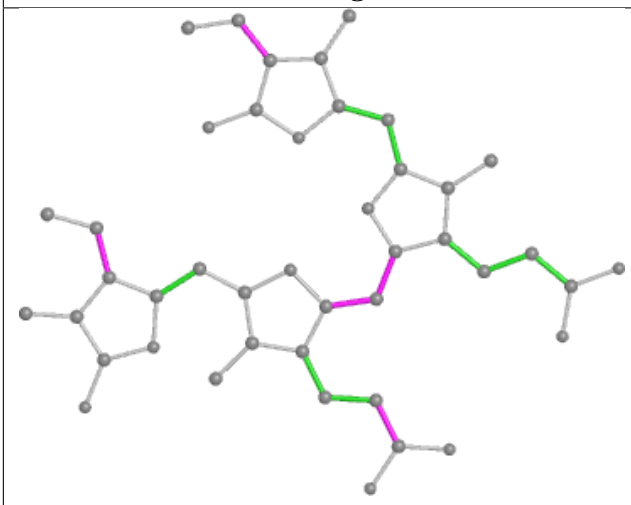

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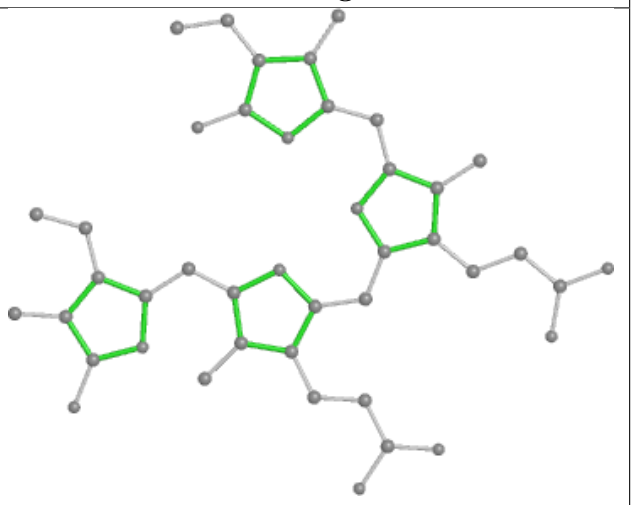
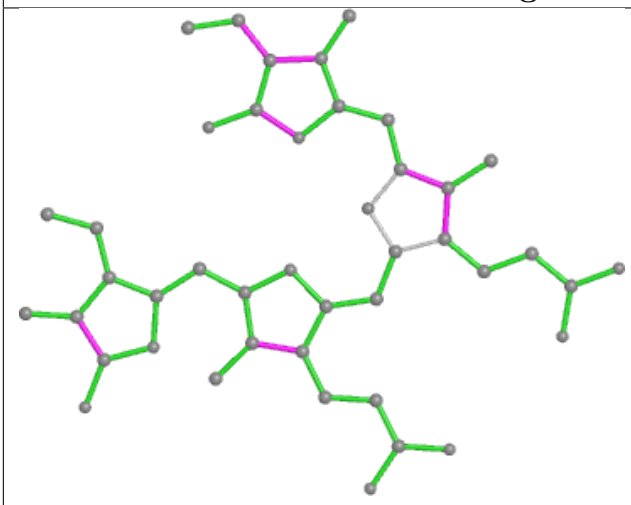


Rings

Ligand PEB g5 202



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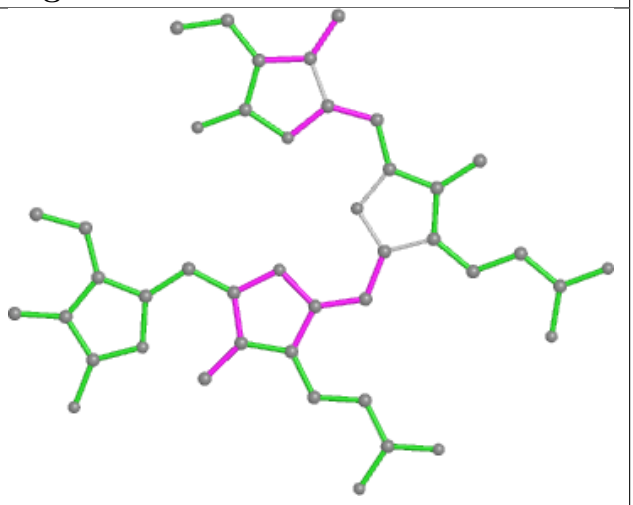

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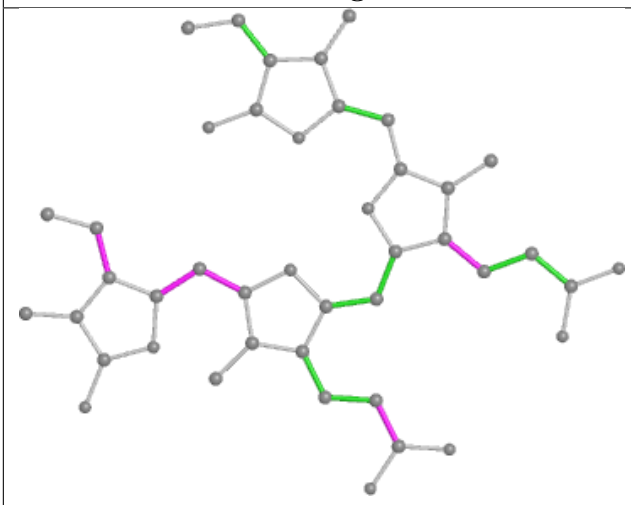

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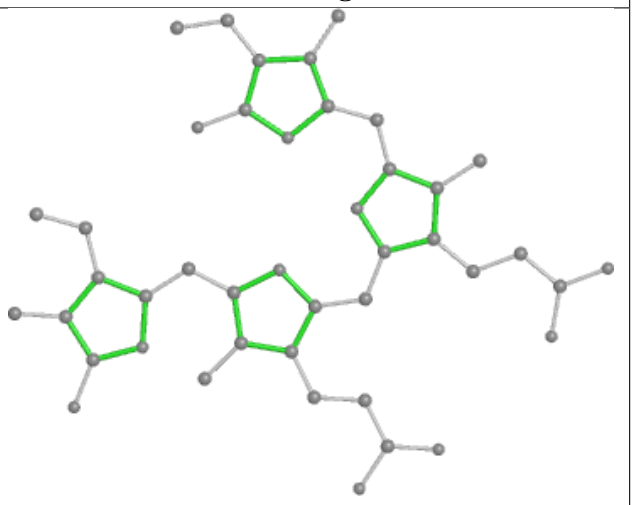

Rings

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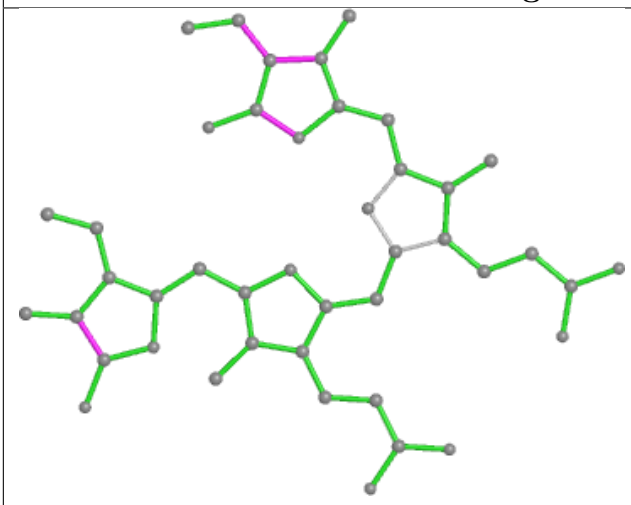

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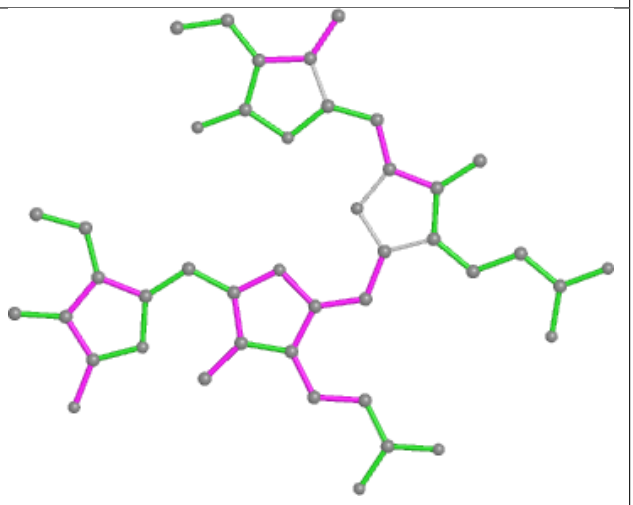

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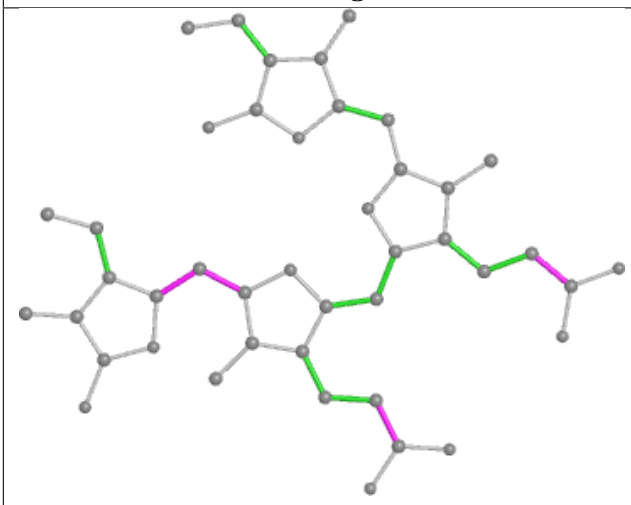

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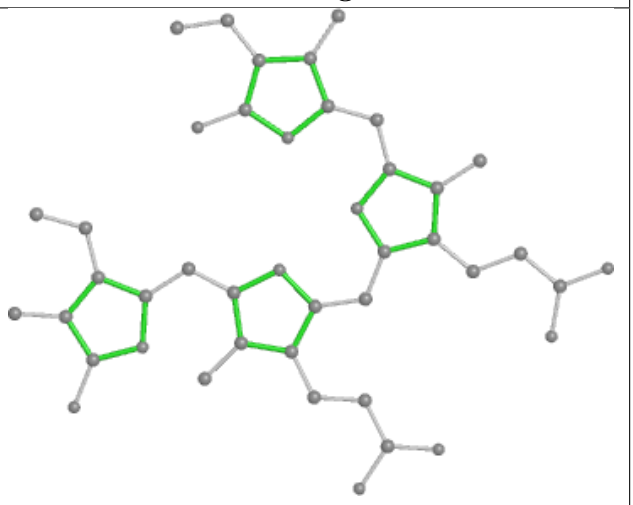
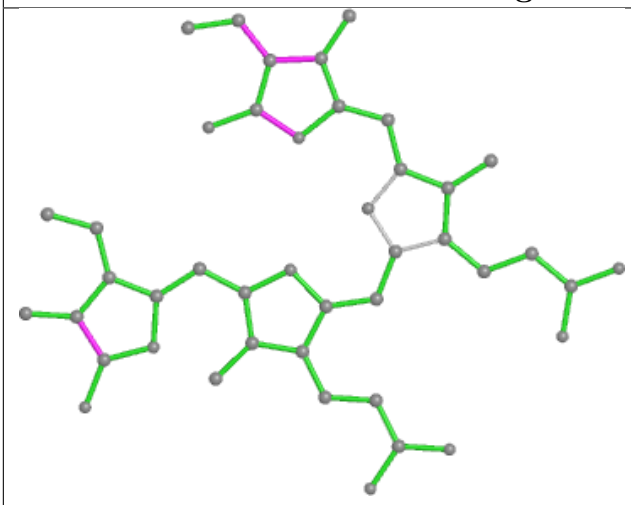


Rings

Ligand PEB Q3 201



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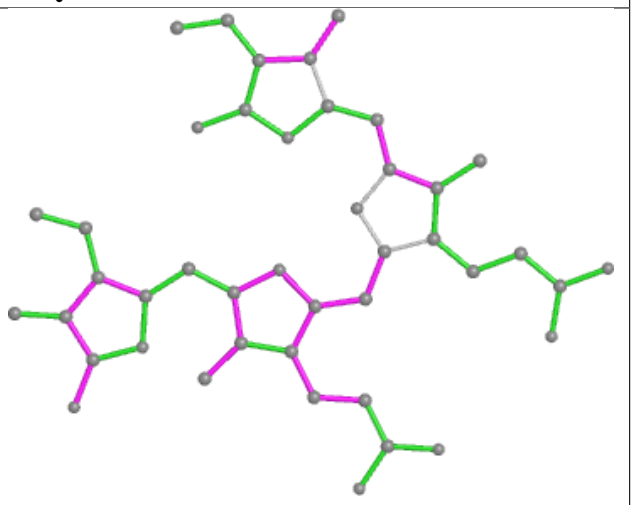

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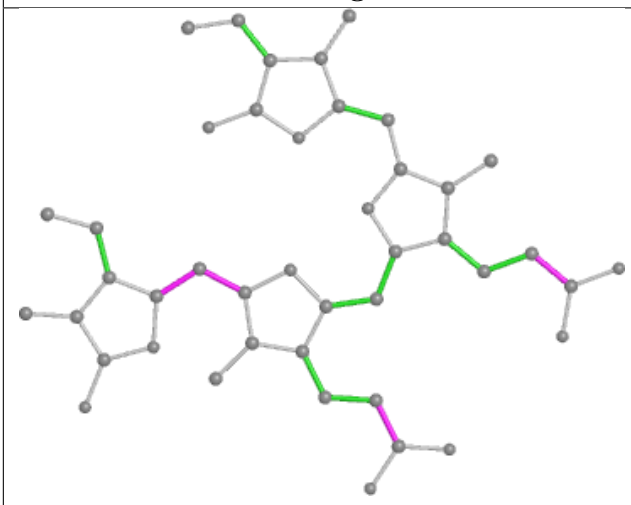

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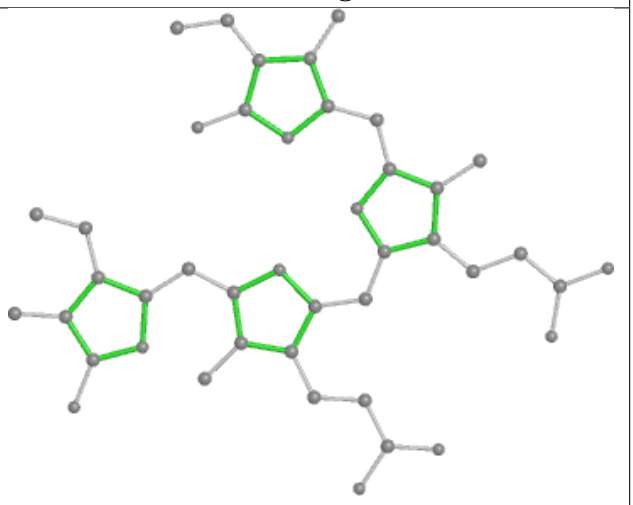
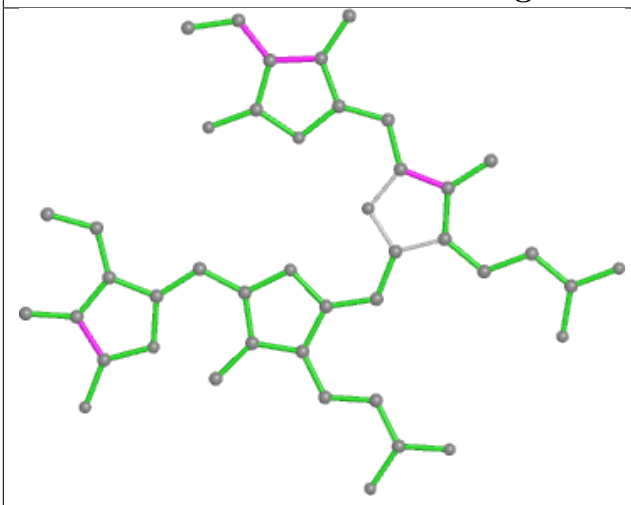


Rings

Ligand PEB bC 202



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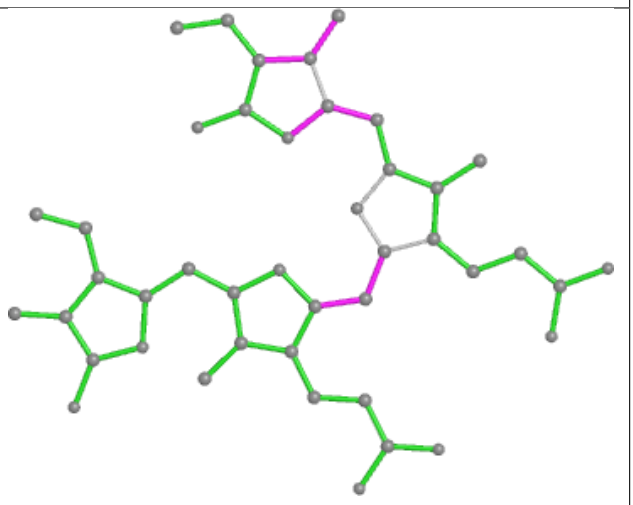

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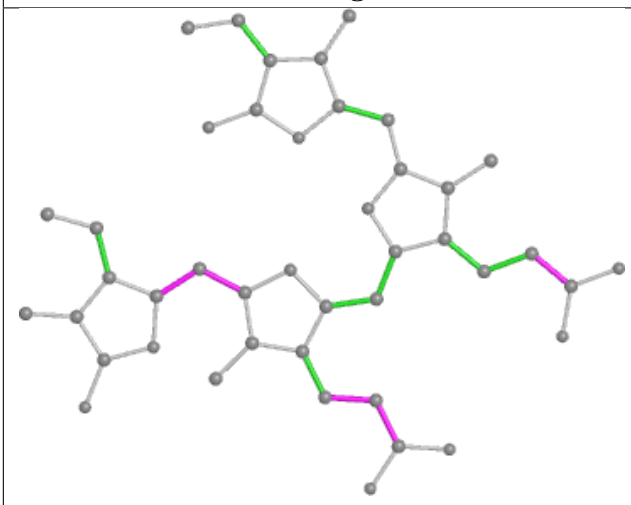

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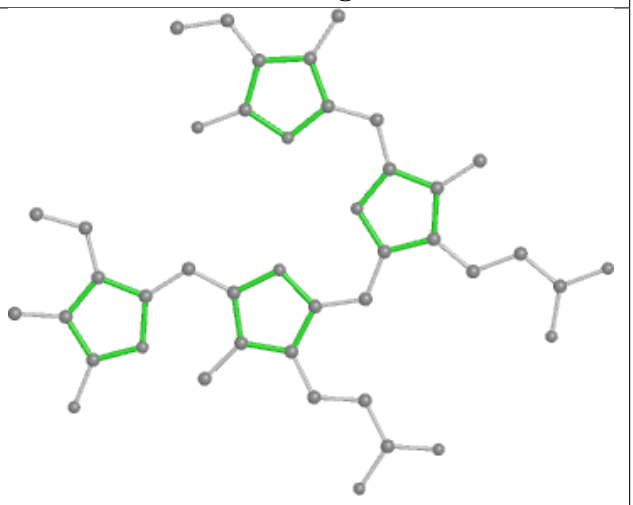

Rings

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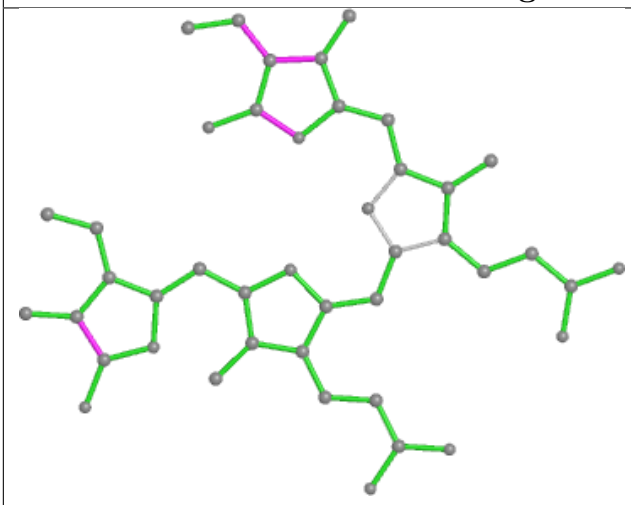

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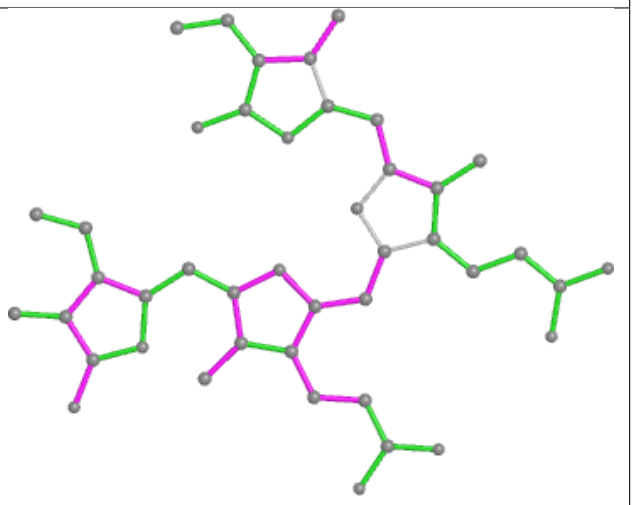

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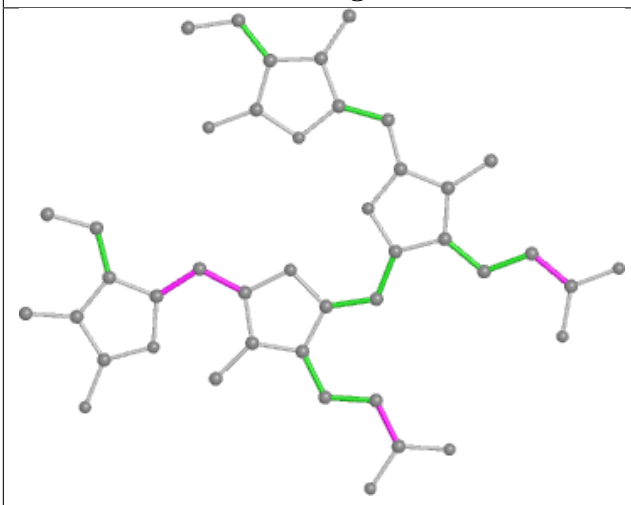

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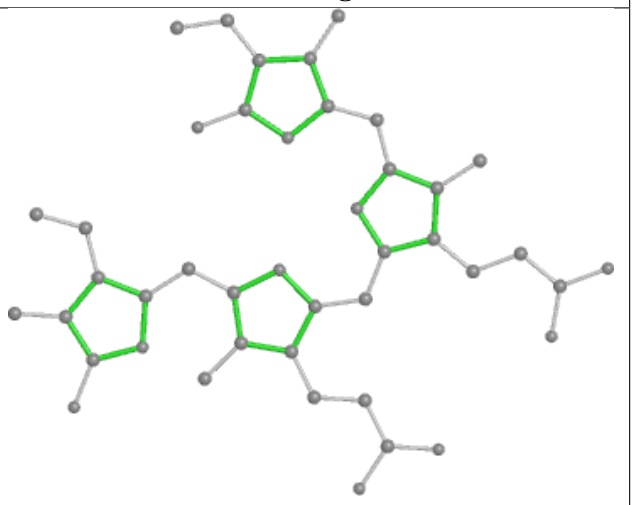
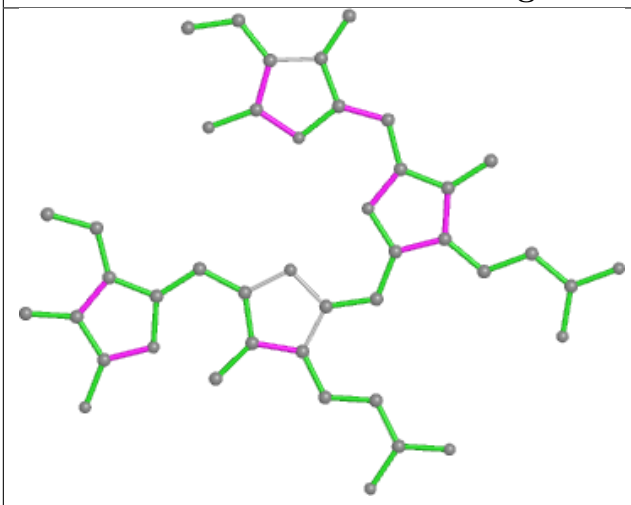


Rings

Ligand PUB 44 304



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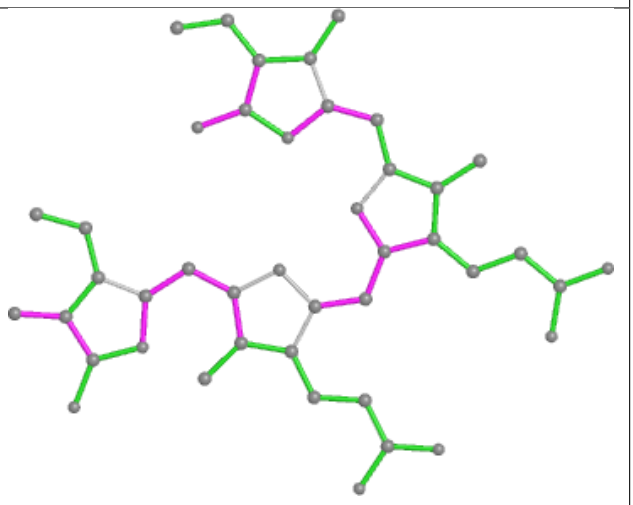

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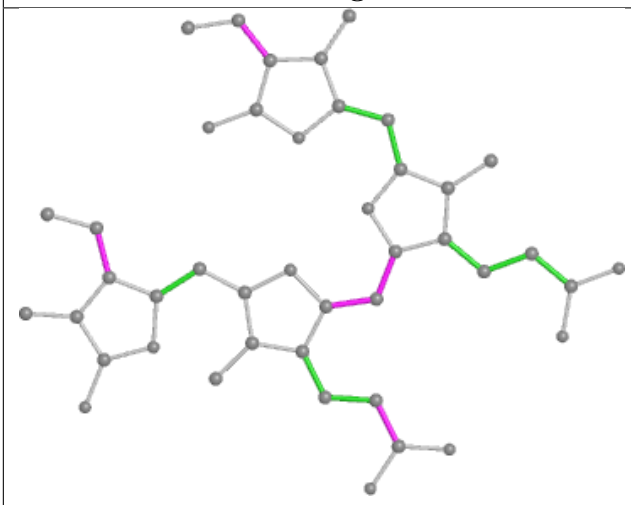

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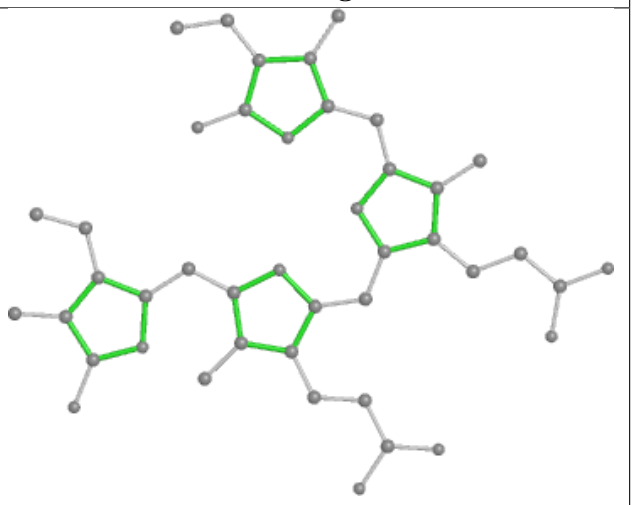
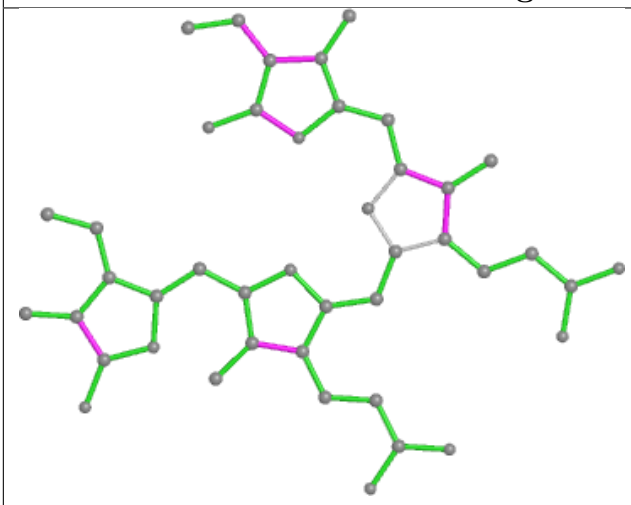


Rings

Ligand PEB T2 202



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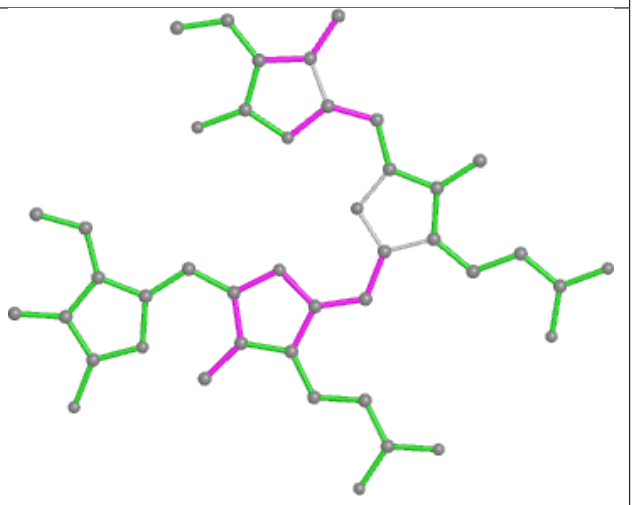

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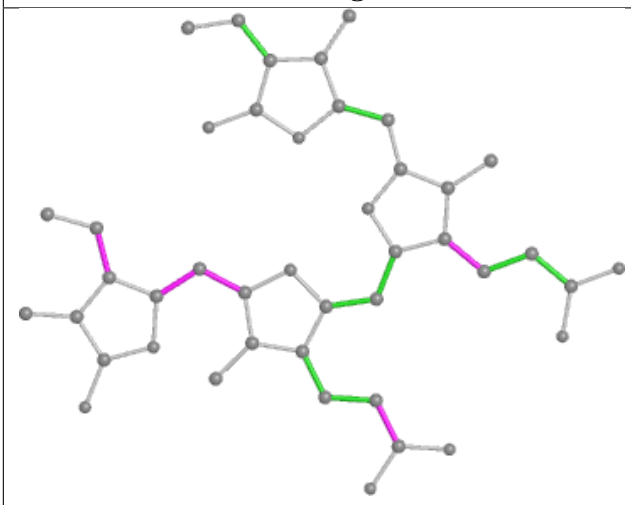
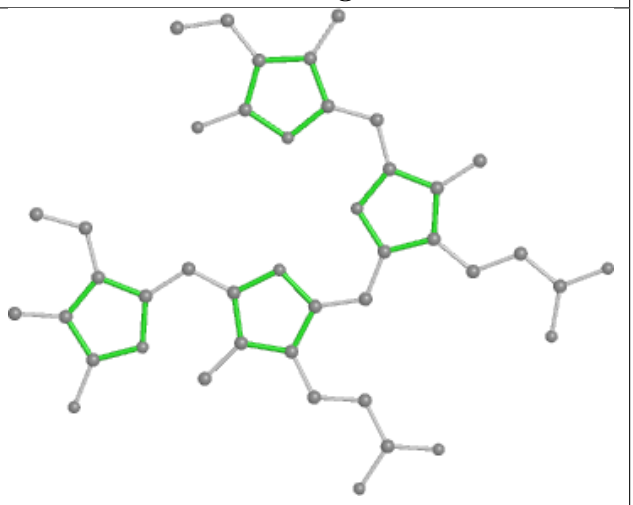
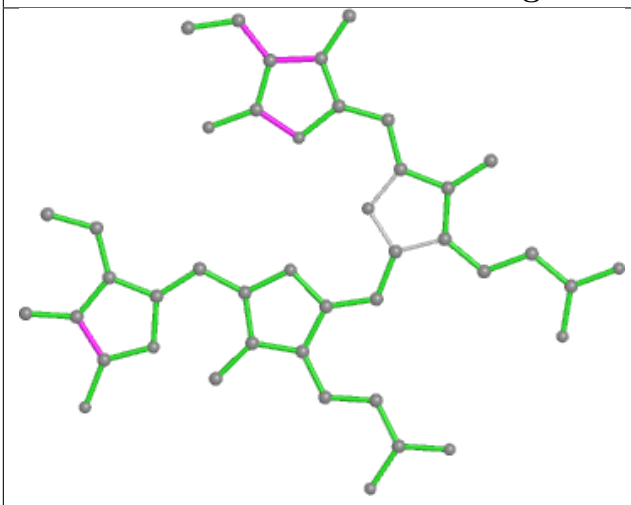


Torsions



Rings

Ligand PEB fq 201



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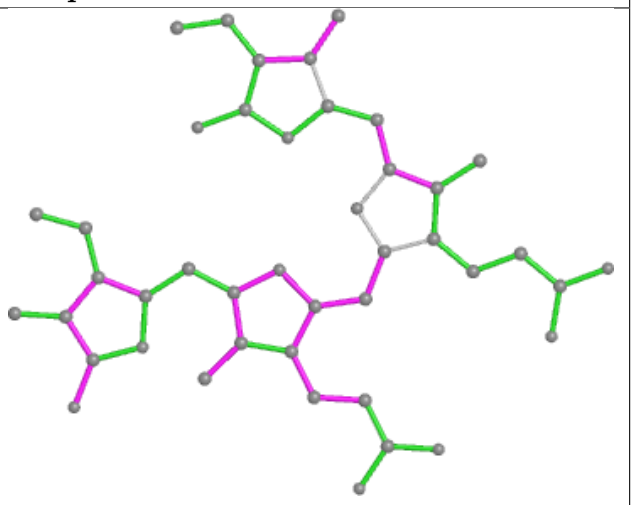

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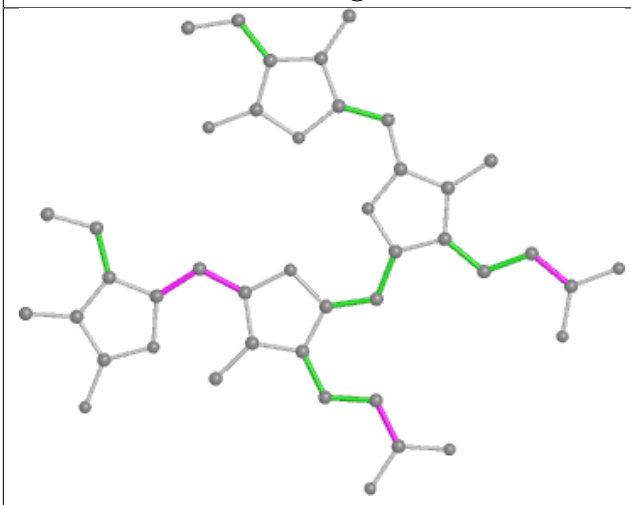

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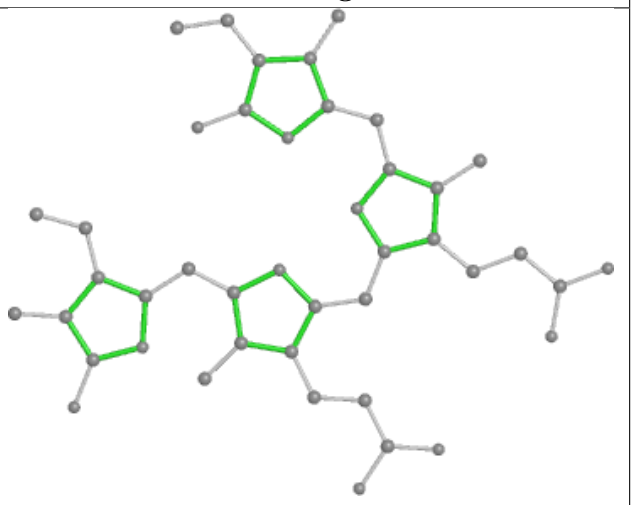
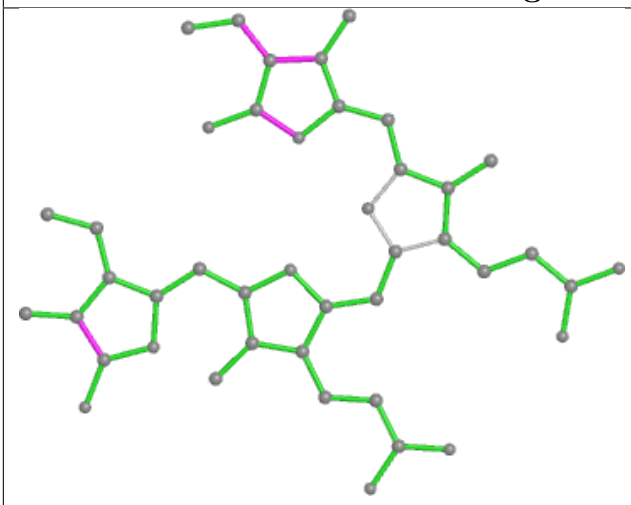


Rings

Ligand PEB l6 201



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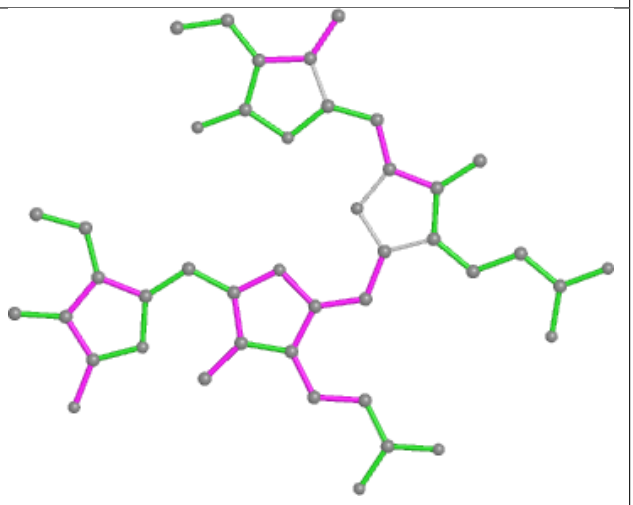

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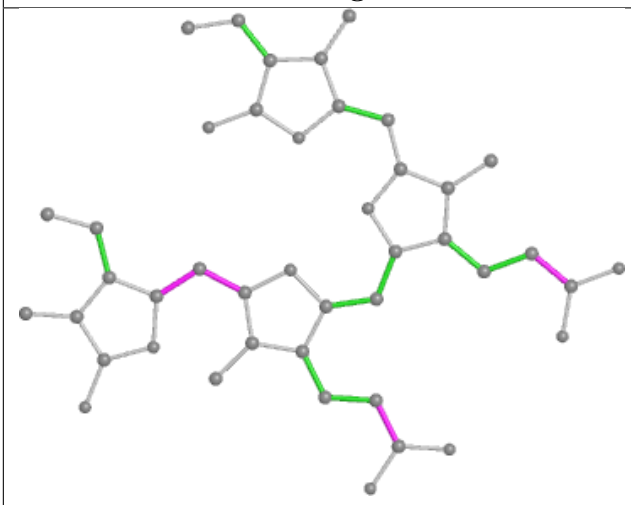

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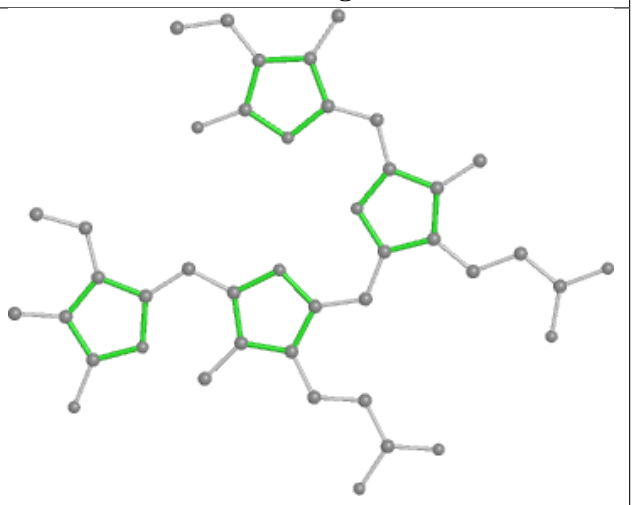
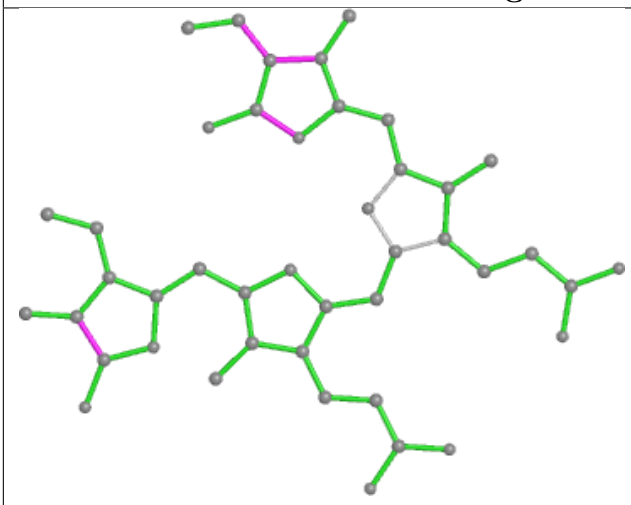


Rings

Ligand PEB K5 1001



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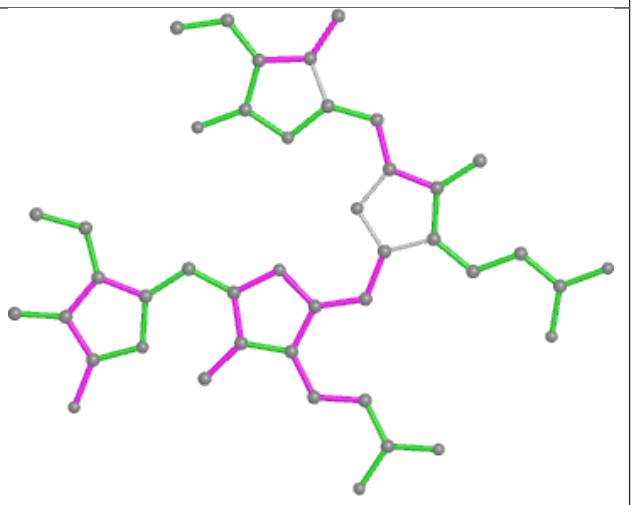

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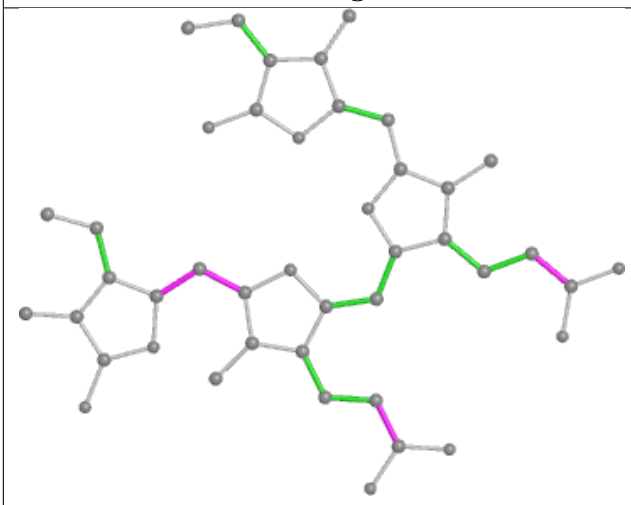

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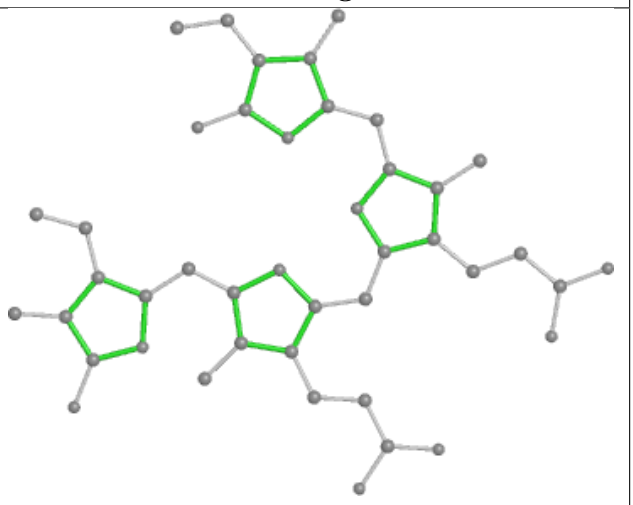
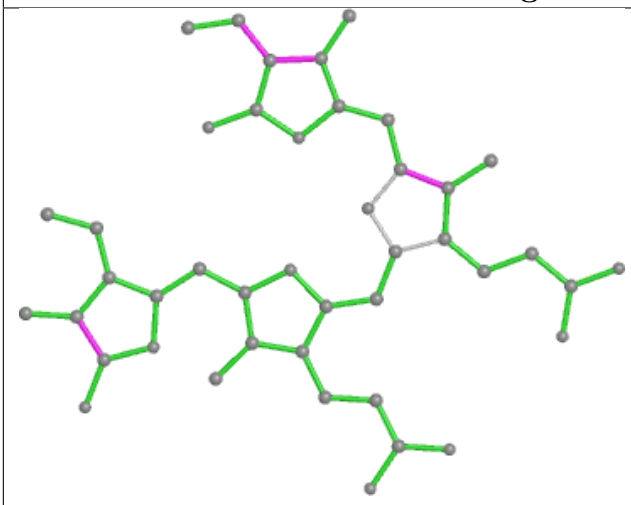


Rings

Ligand PEB e6 202



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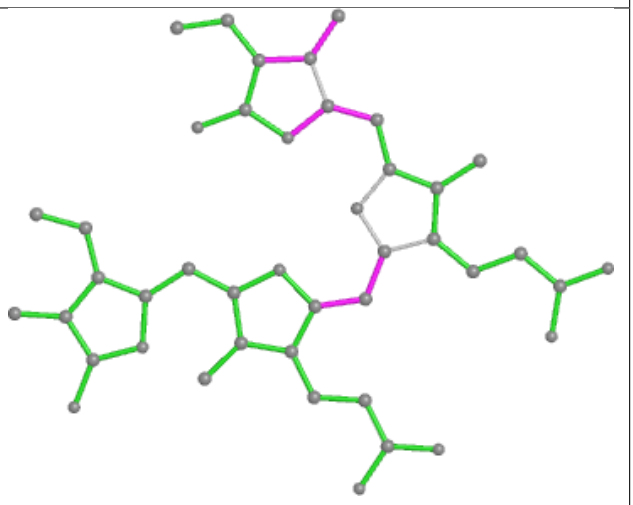

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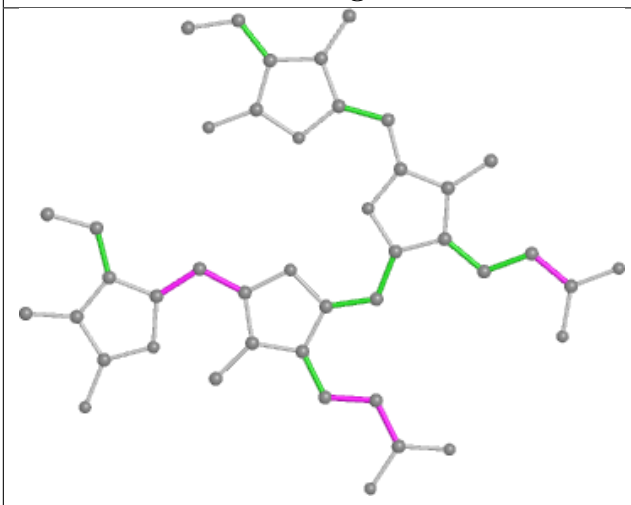

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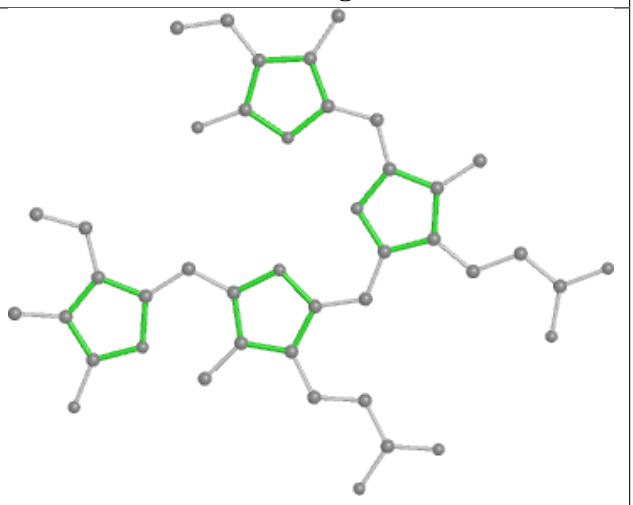

Rings

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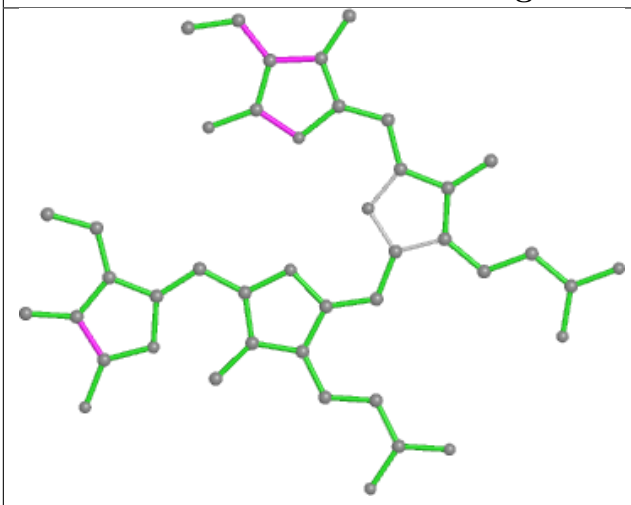

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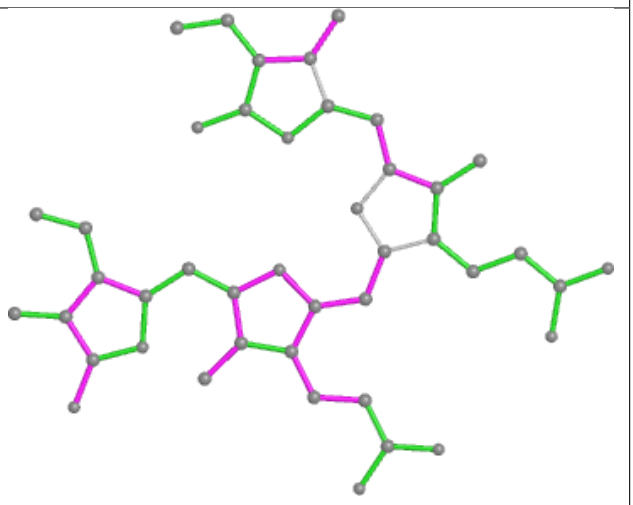

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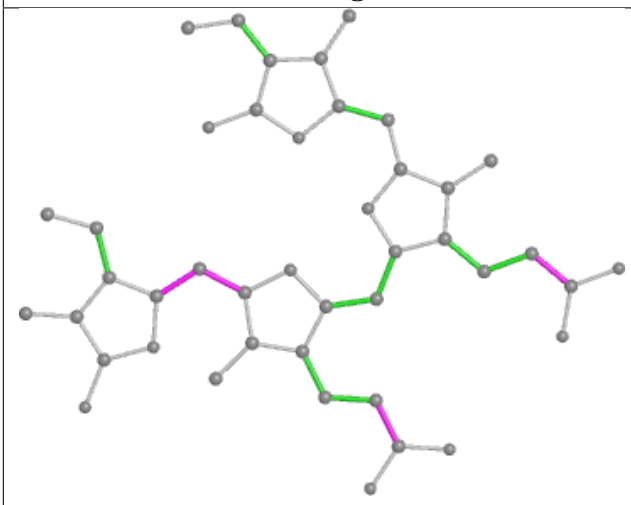

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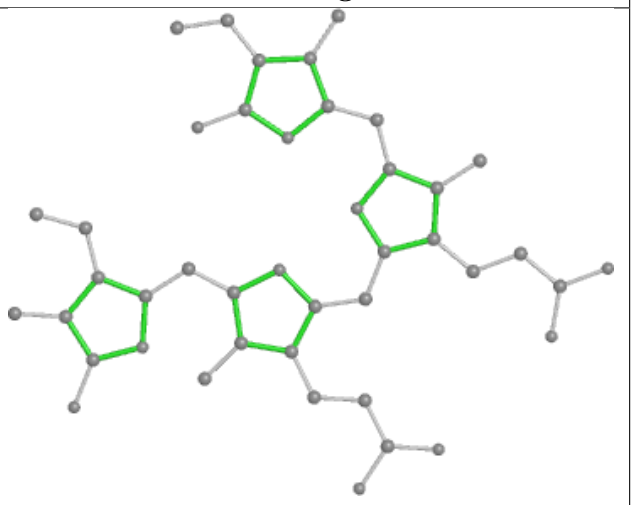

Rings

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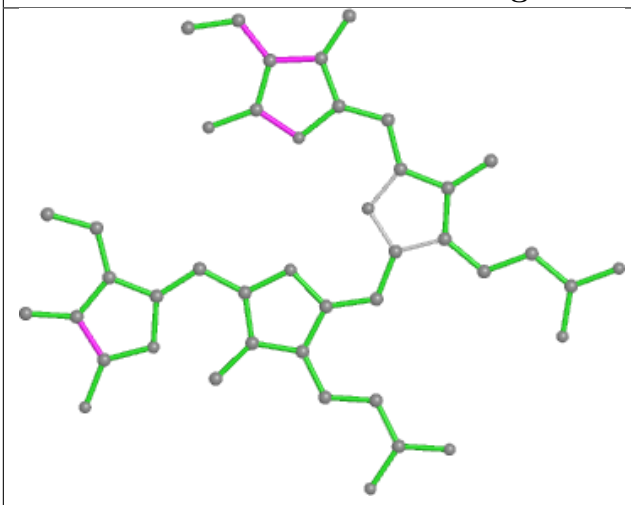

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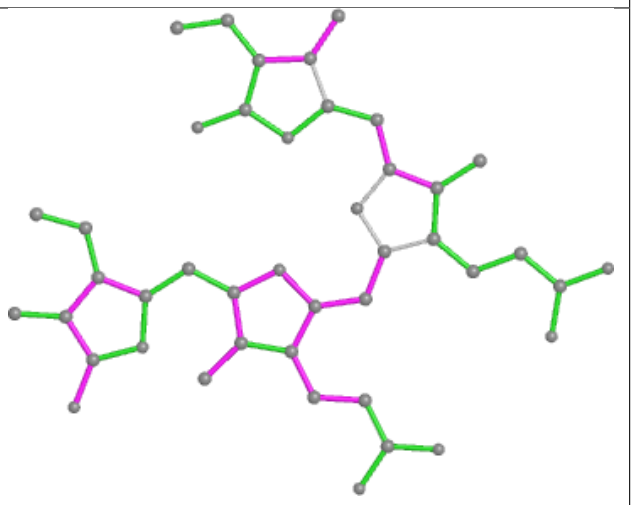

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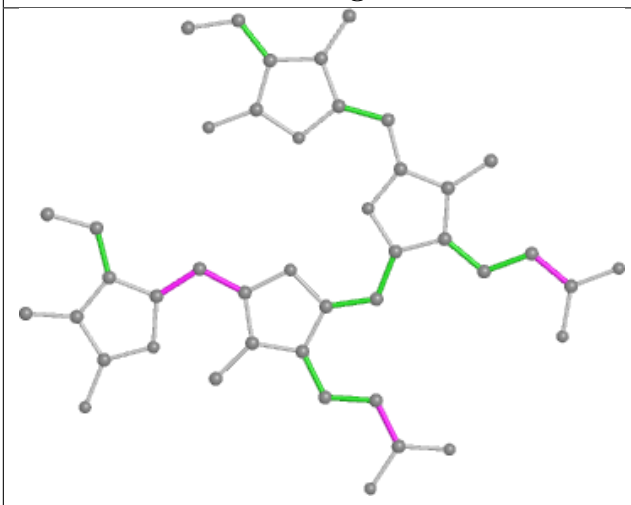

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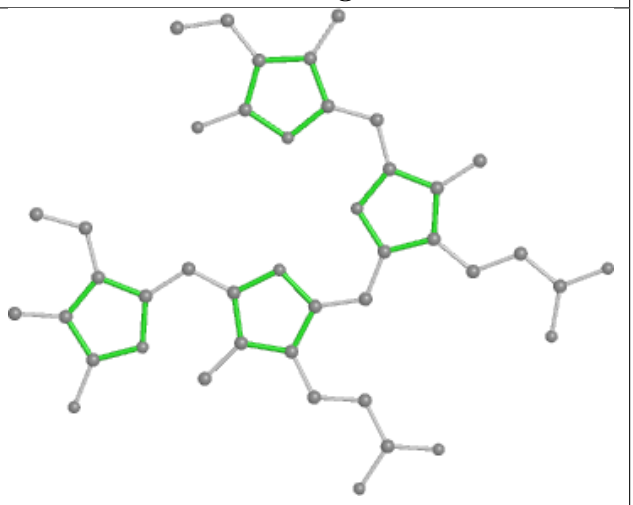

Rings

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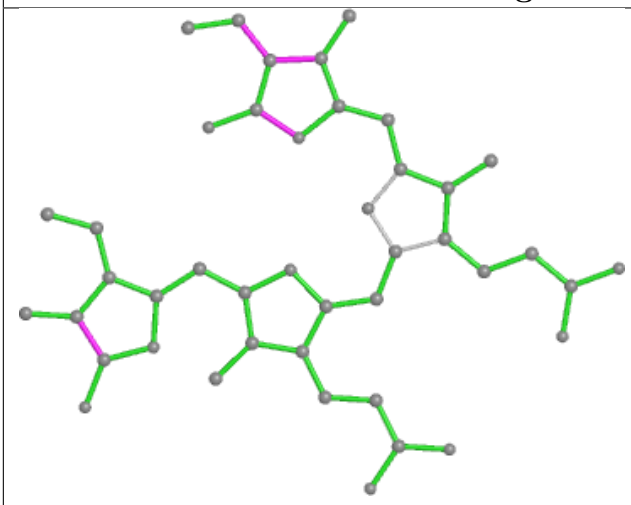

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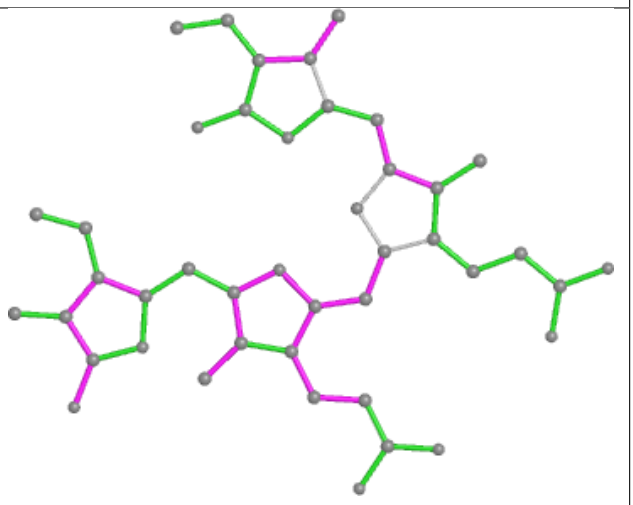

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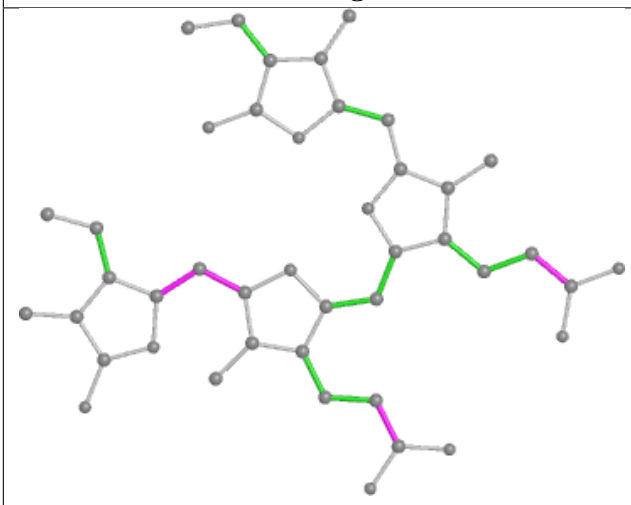

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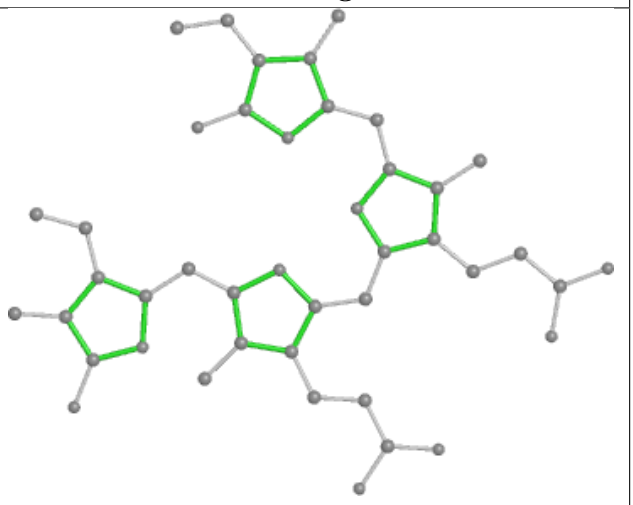
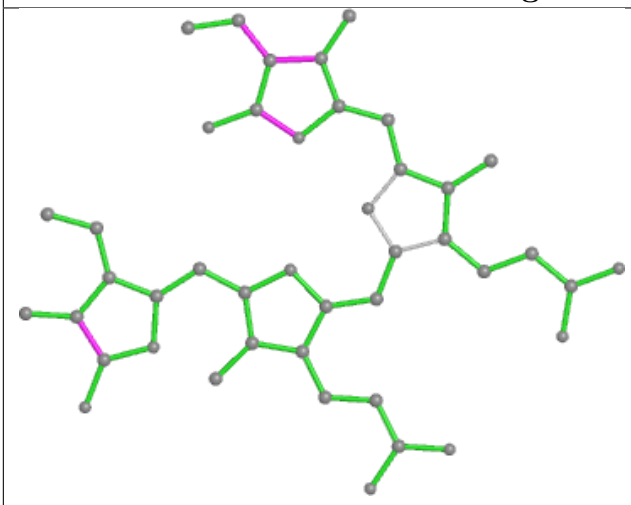


Rings

Ligand PEB t8 201



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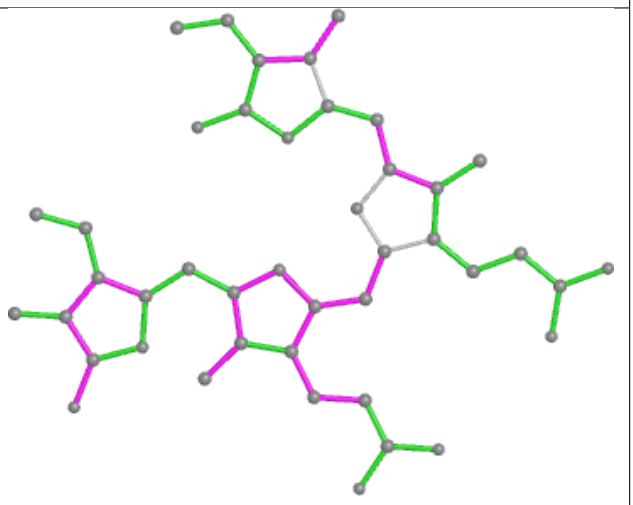

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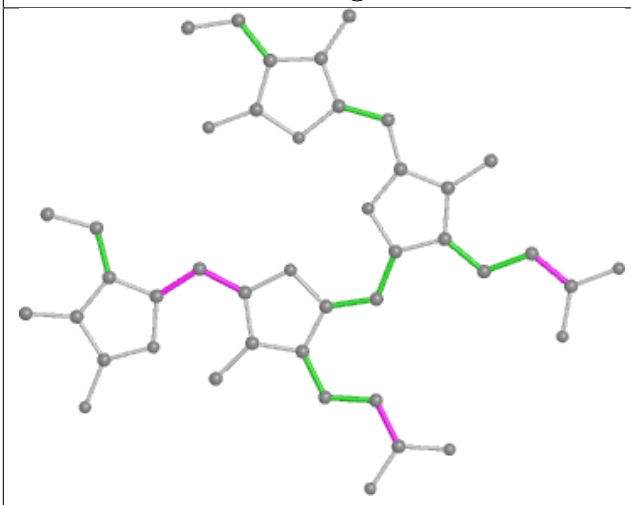

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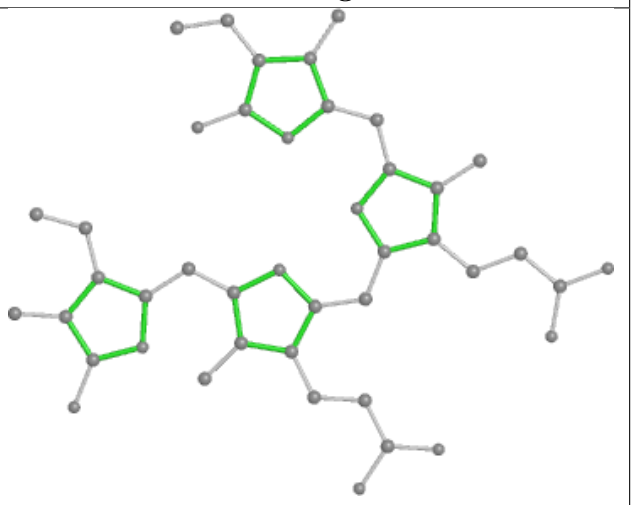

Rings

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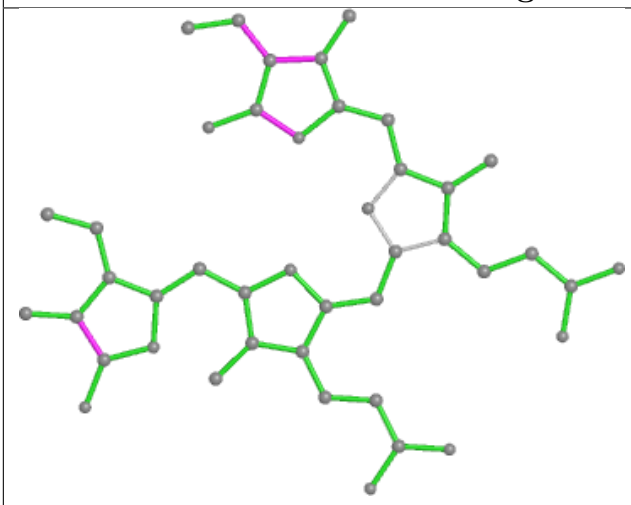

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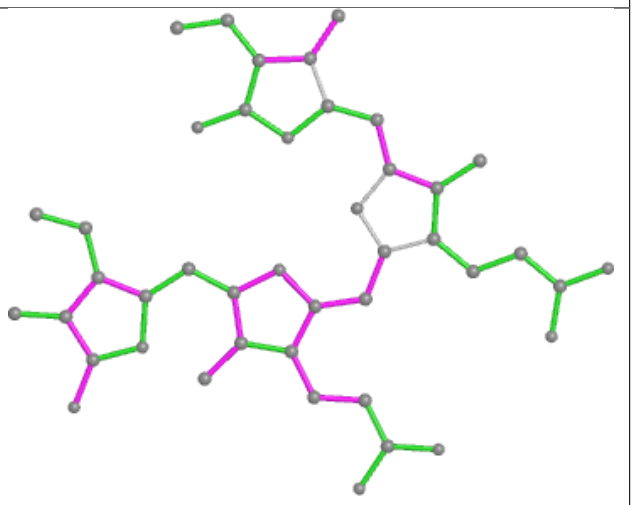

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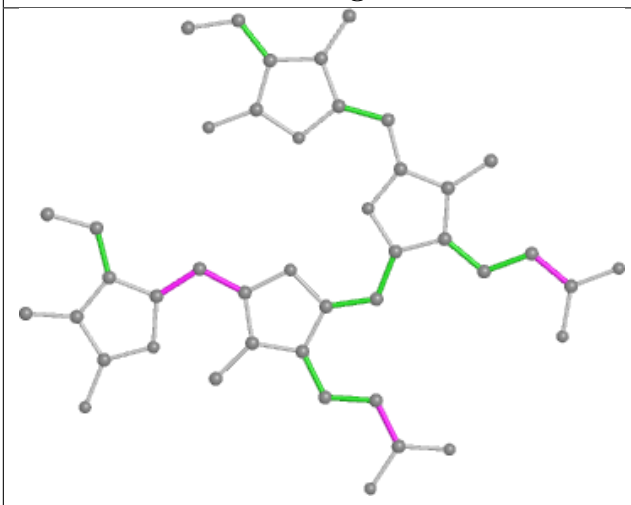

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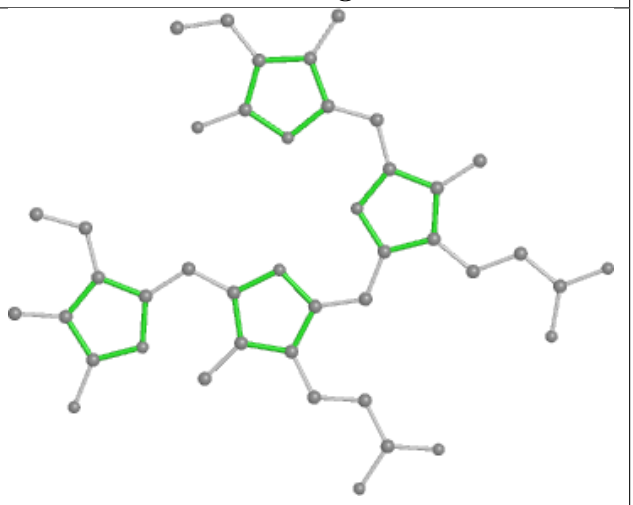
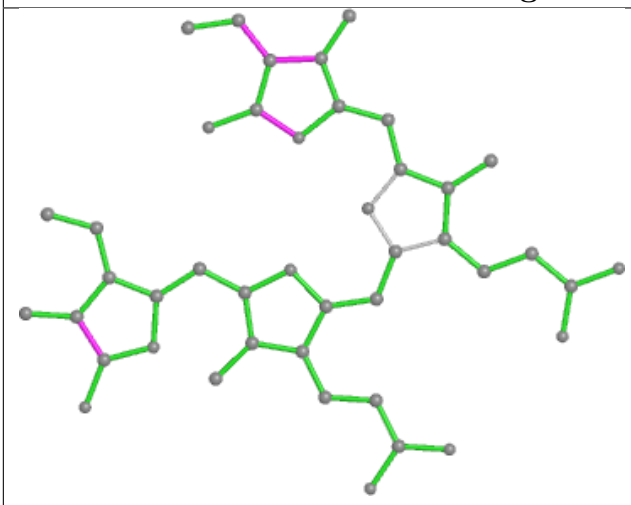


Rings

Ligand PEB ao 201



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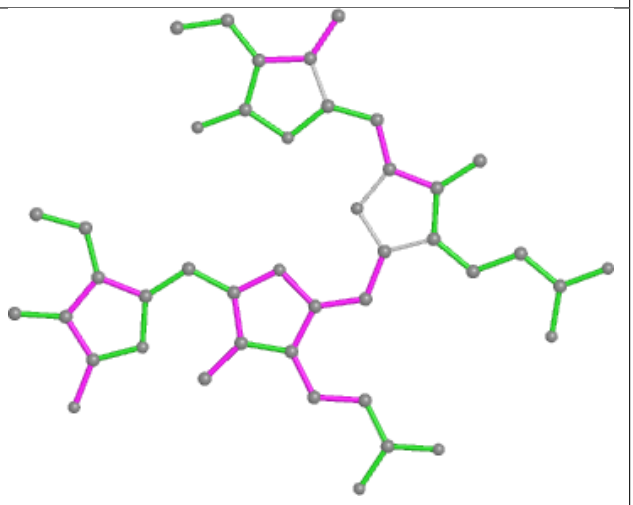

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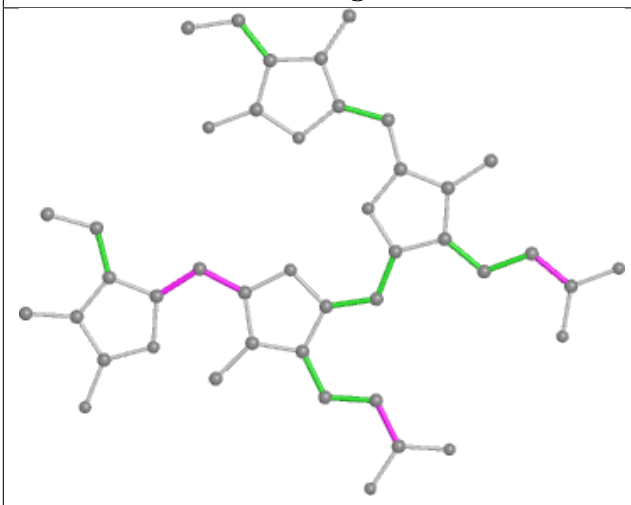

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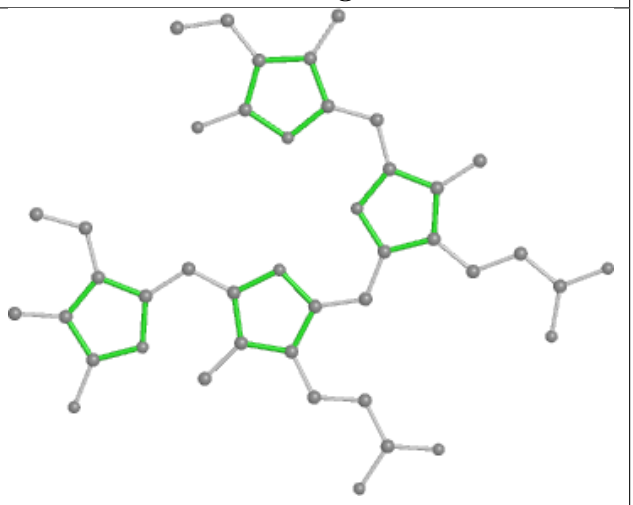
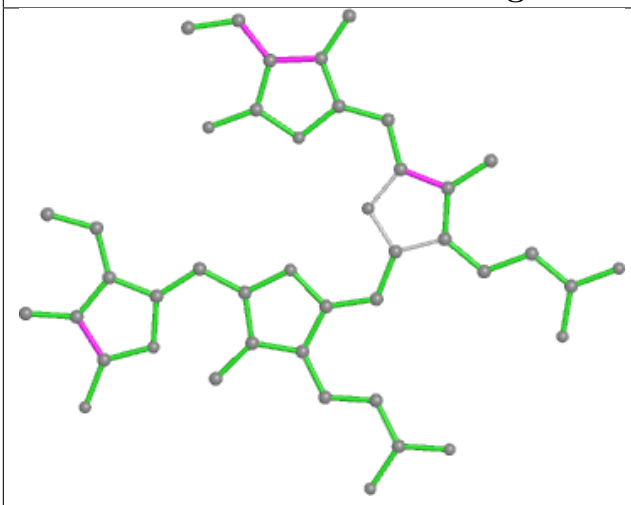


Rings

Ligand PEB eA 1002



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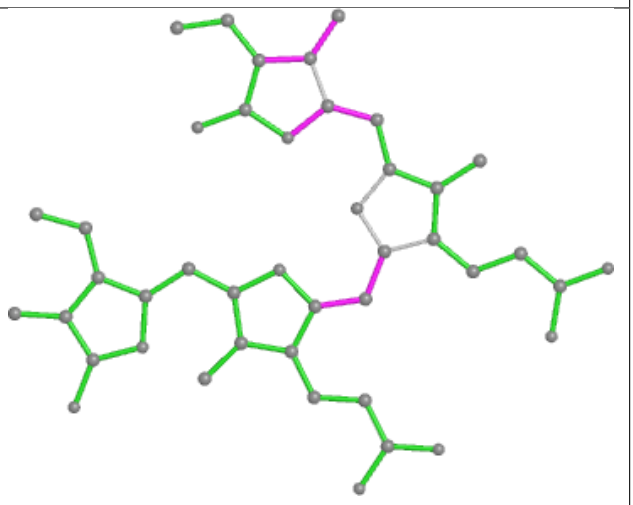

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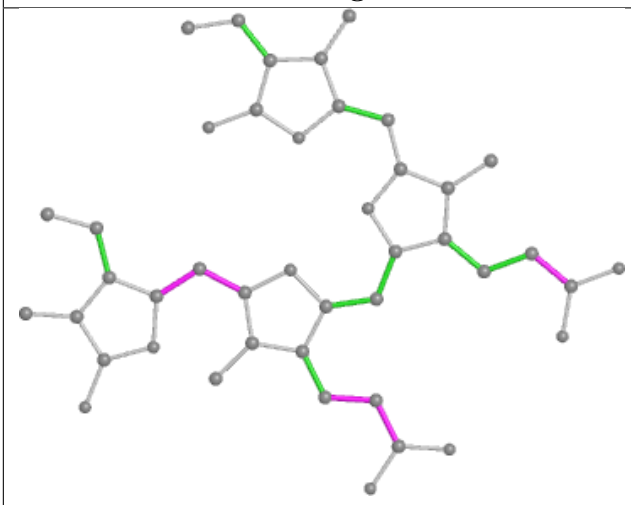

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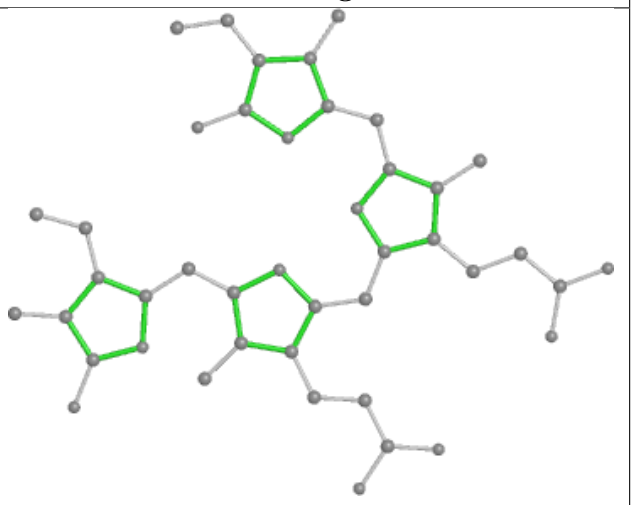
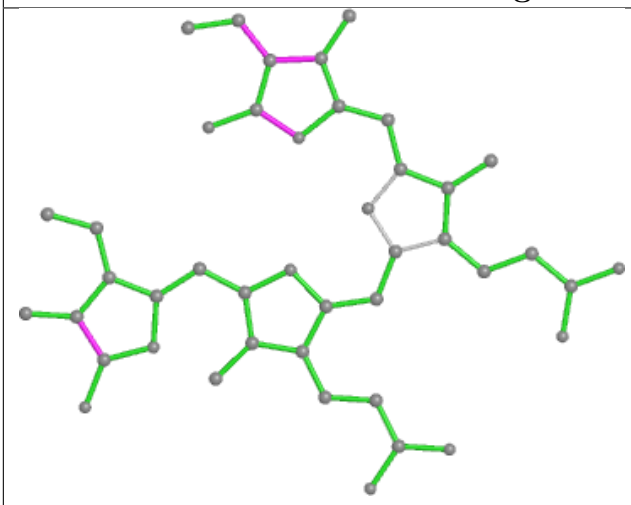


Rings

Ligand PEB m7 201



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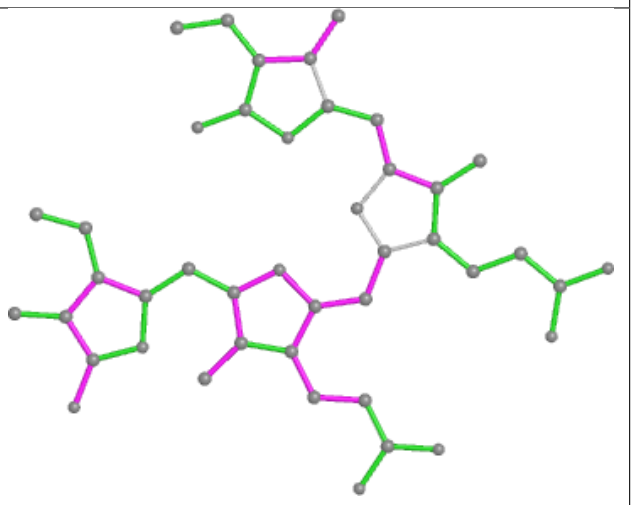

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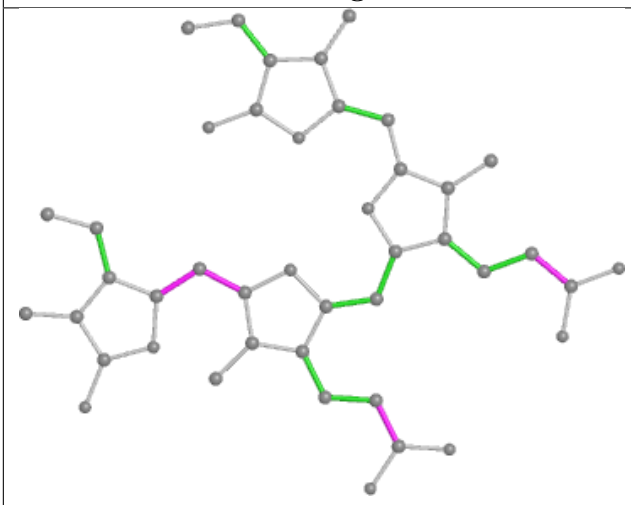

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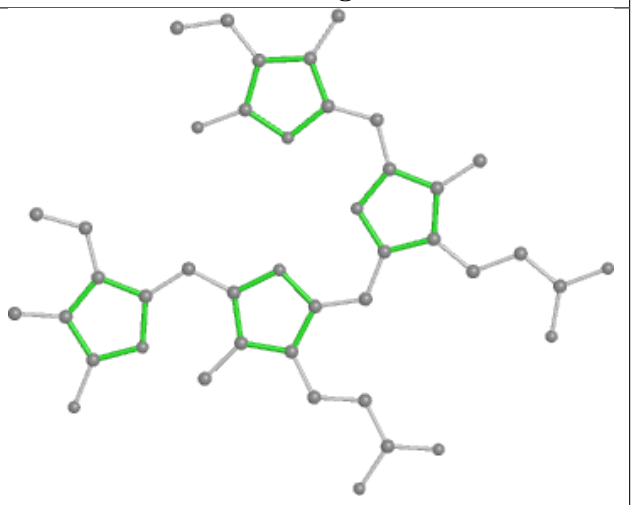
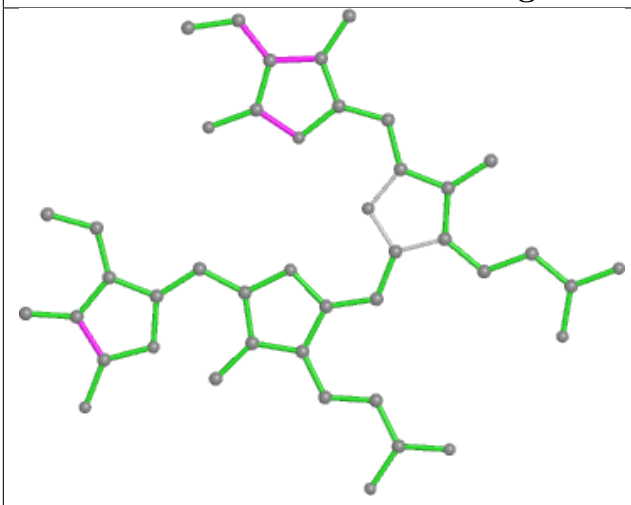


Rings

Ligand PEB L8 202



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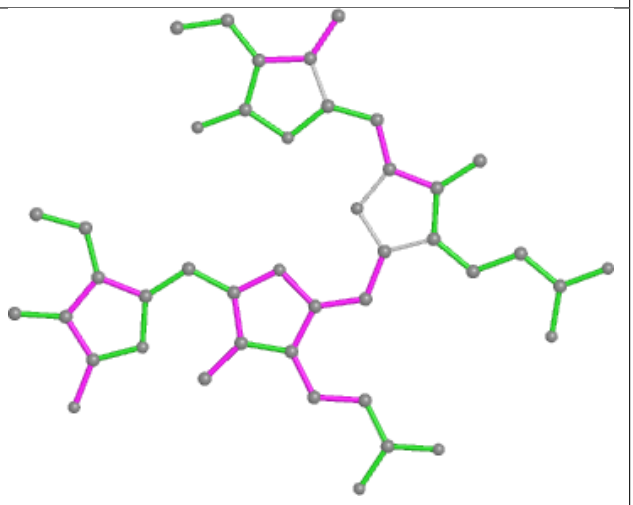
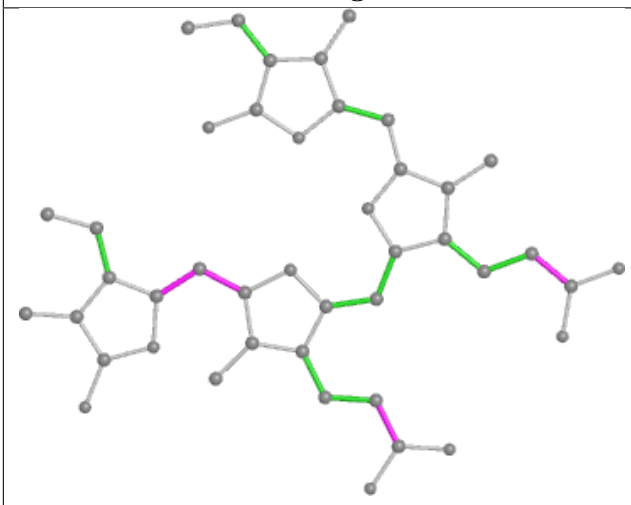
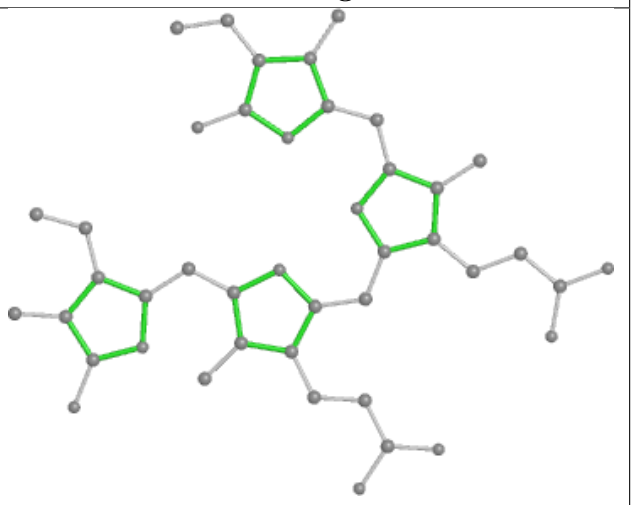


Bond angles

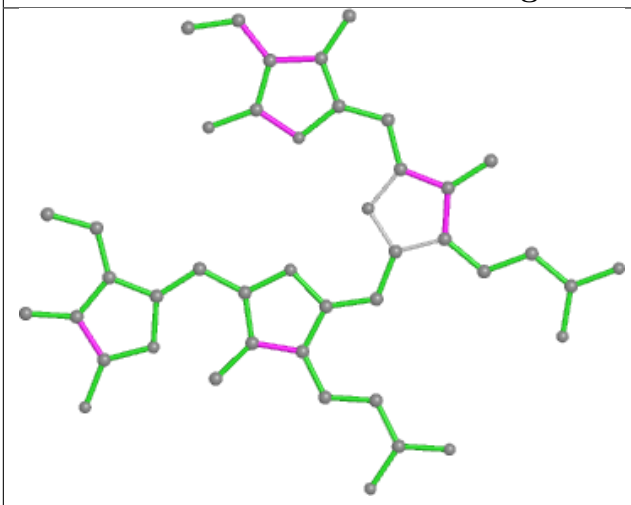


Torsions



Rings

Ligand PEB c7 202



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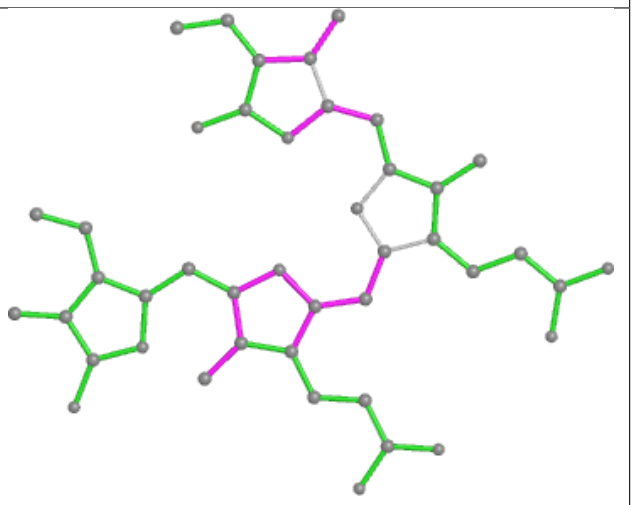

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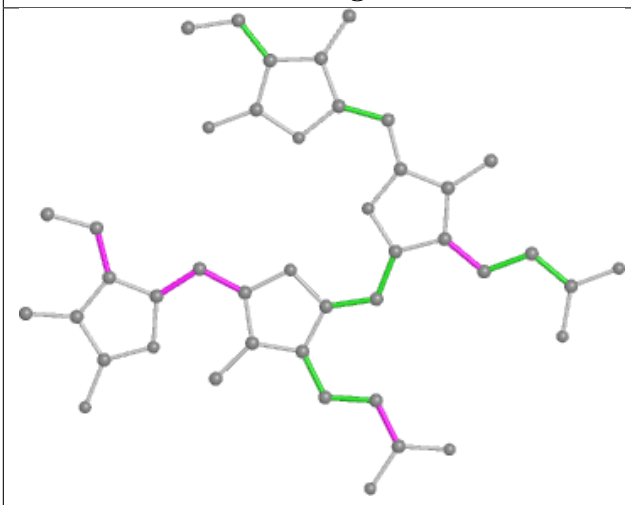

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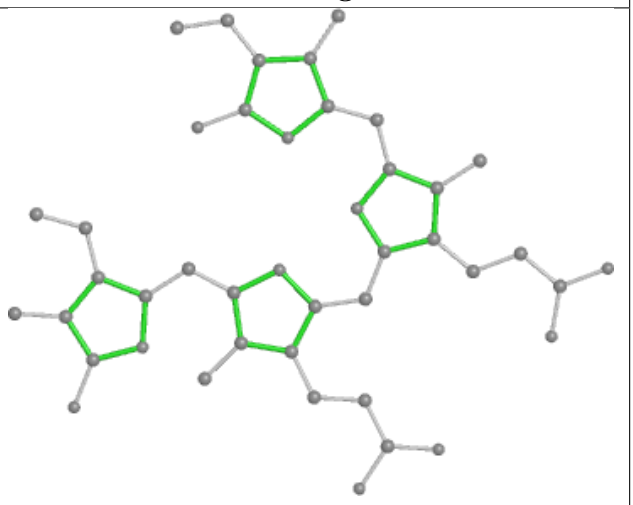
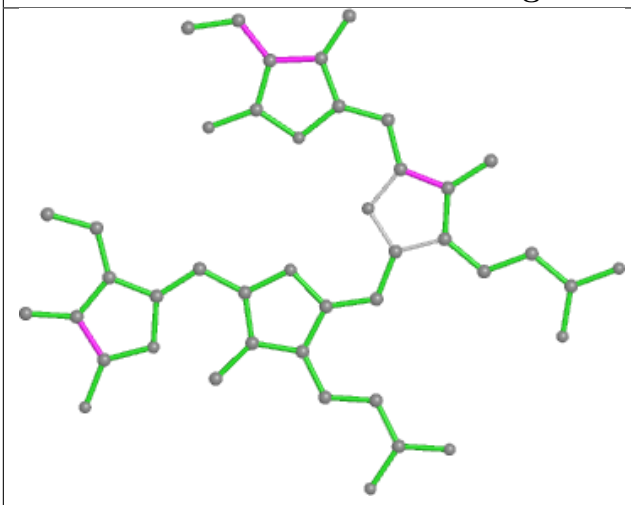


Rings

Ligand PEB et 201



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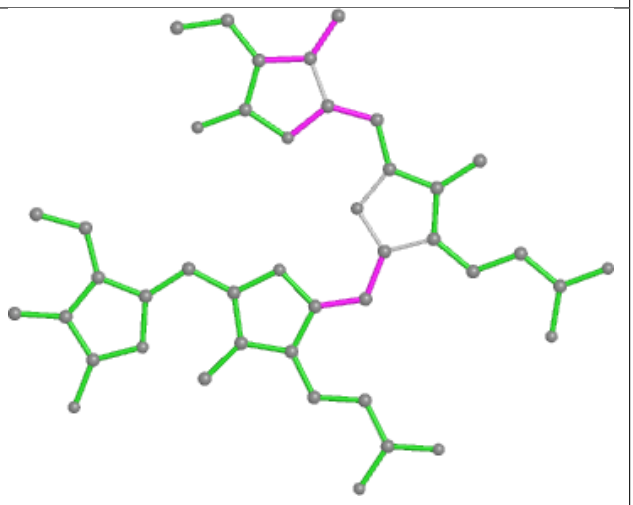

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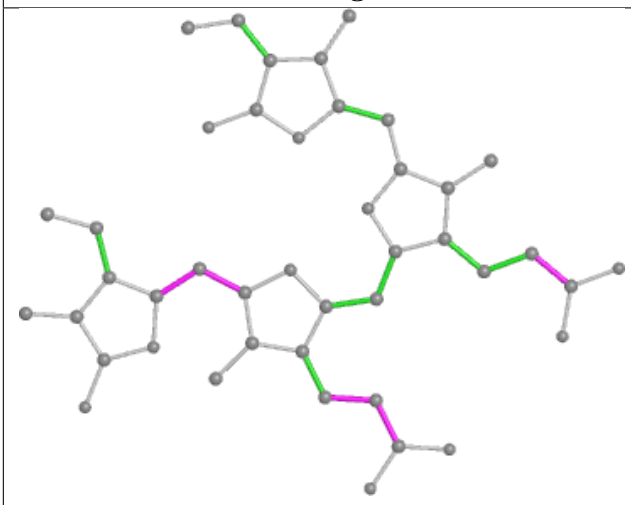

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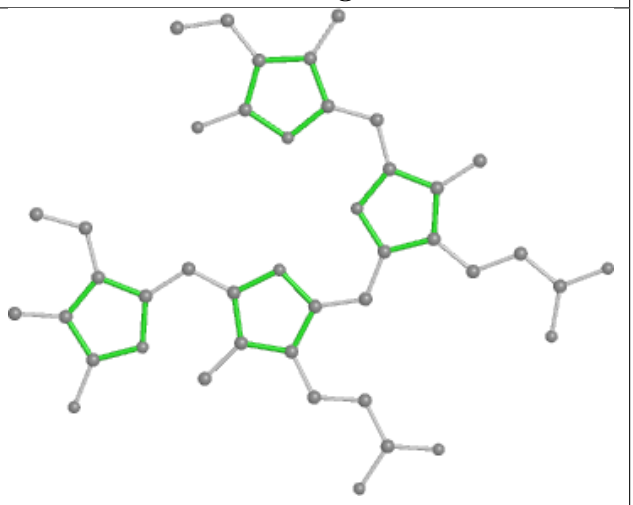

Rings

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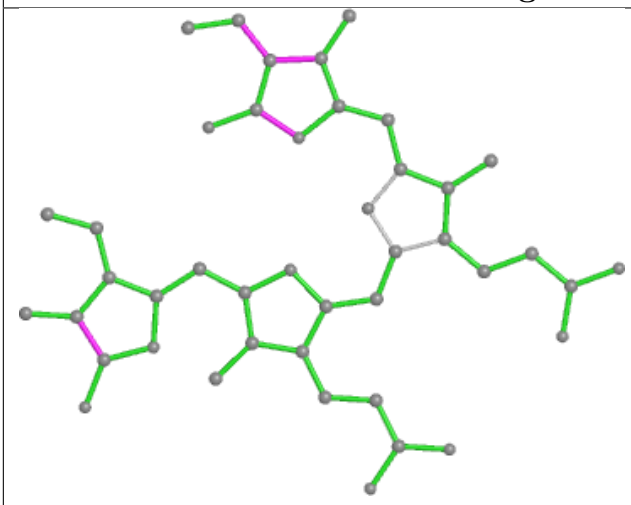

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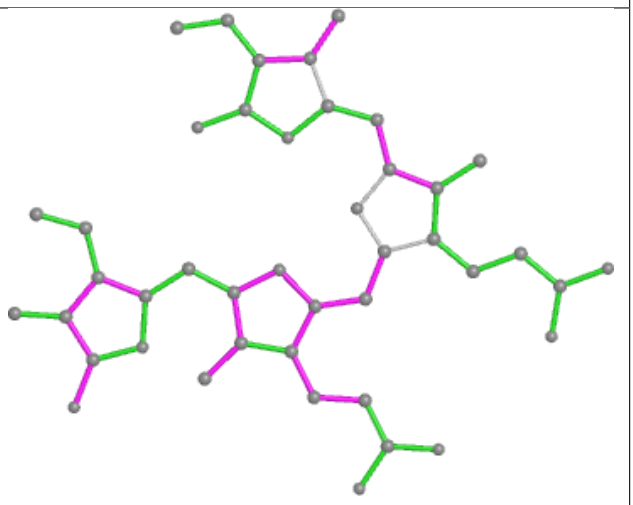

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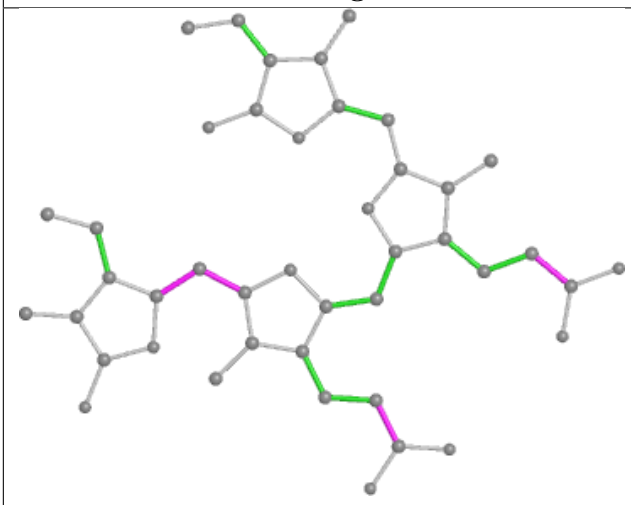

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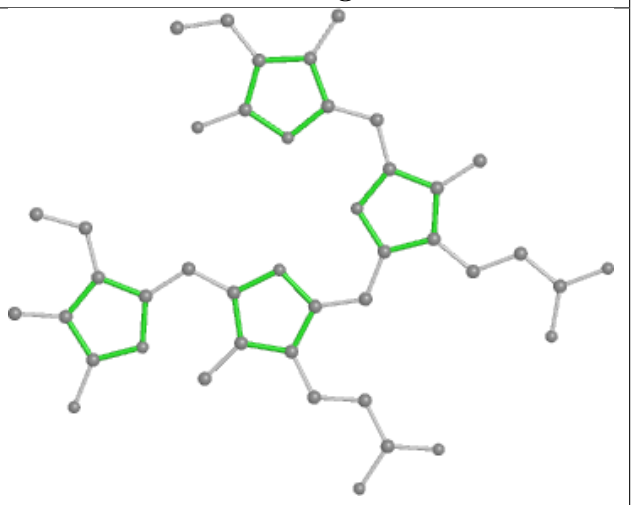
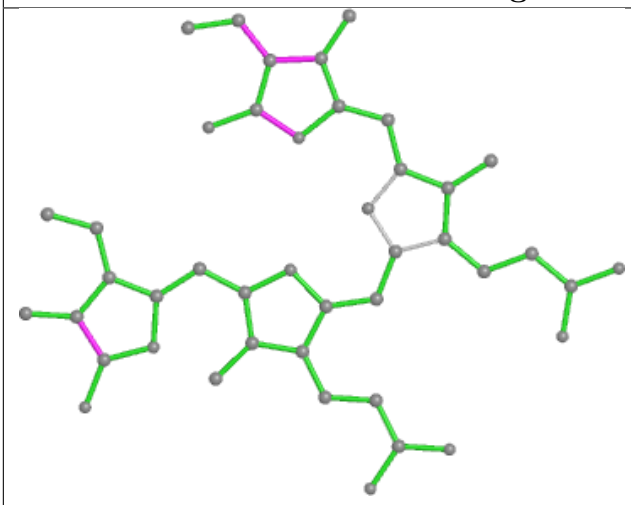


Rings

Ligand PEB by 1001



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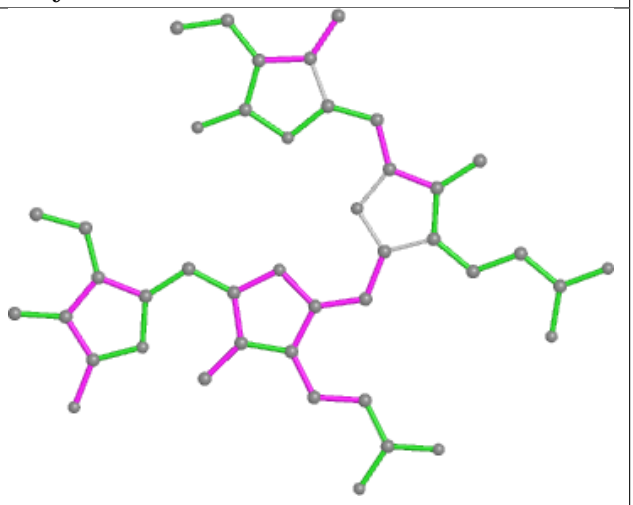

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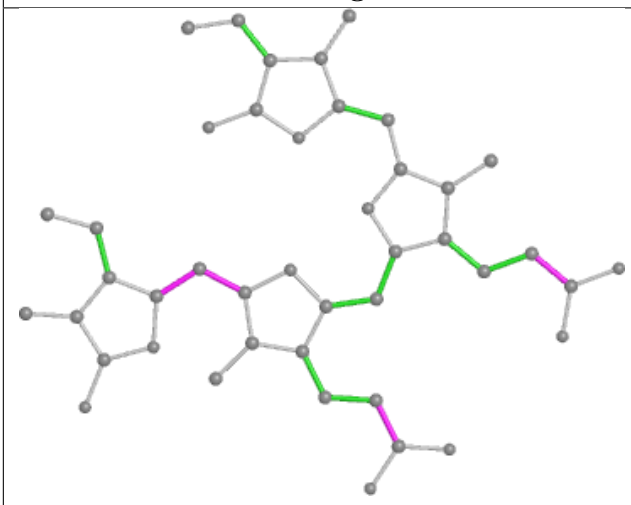

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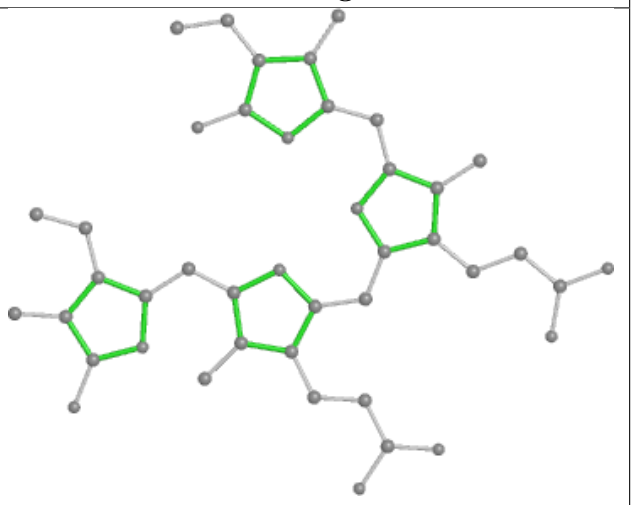

Rings

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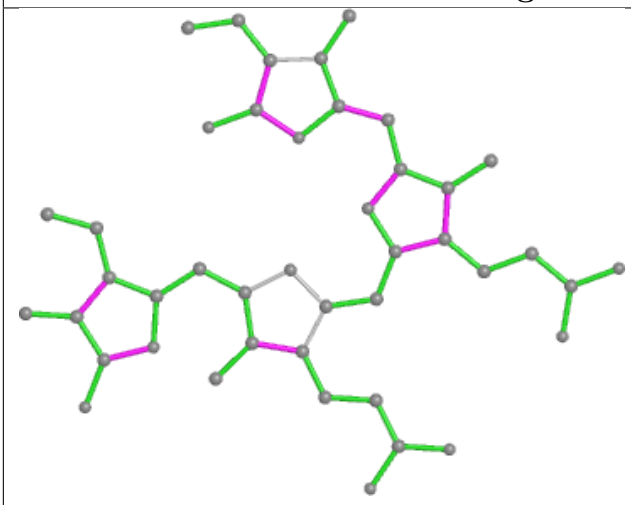

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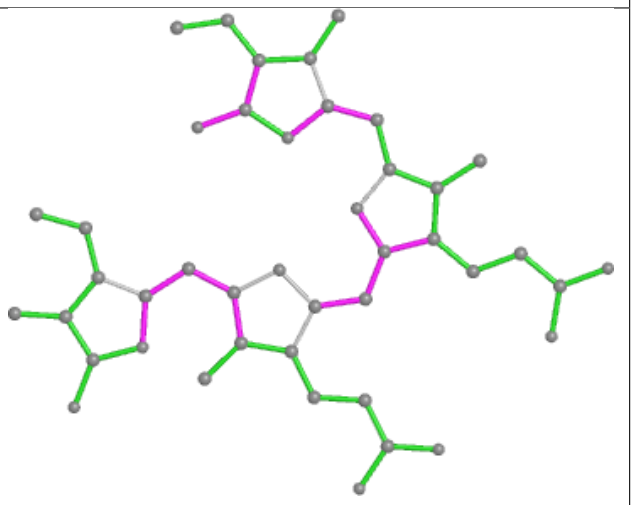

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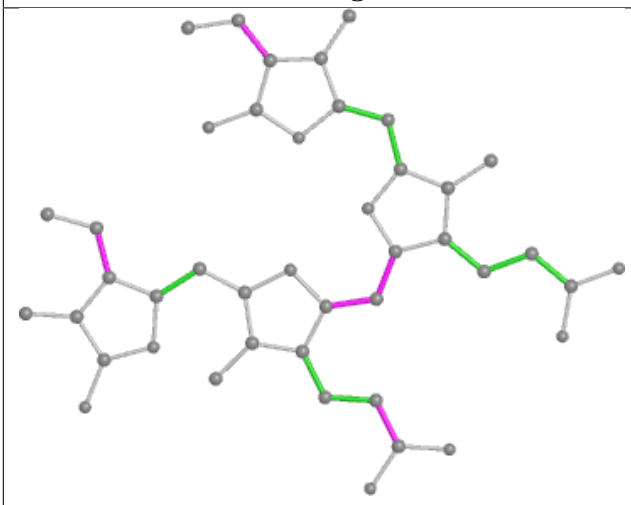

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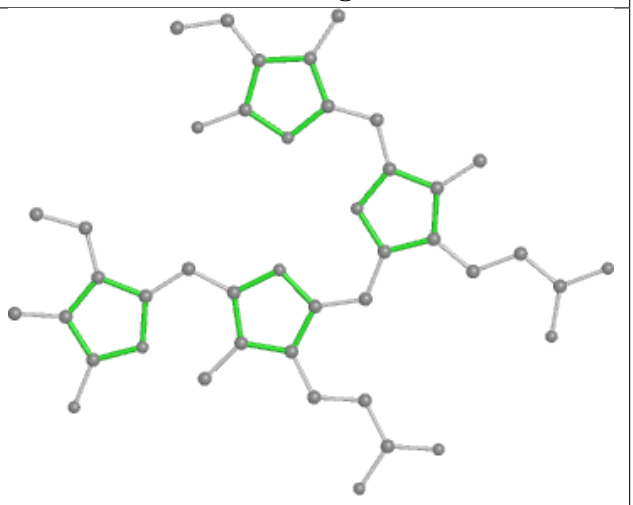

Rings

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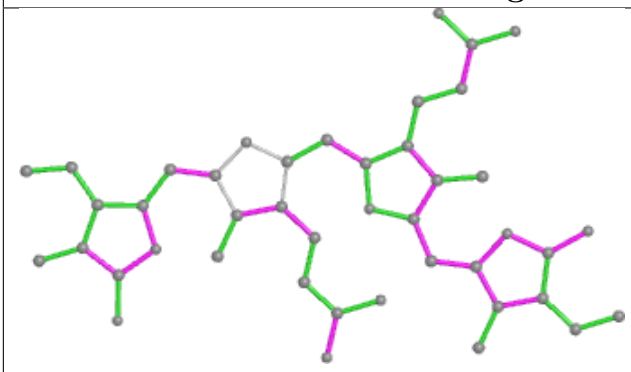

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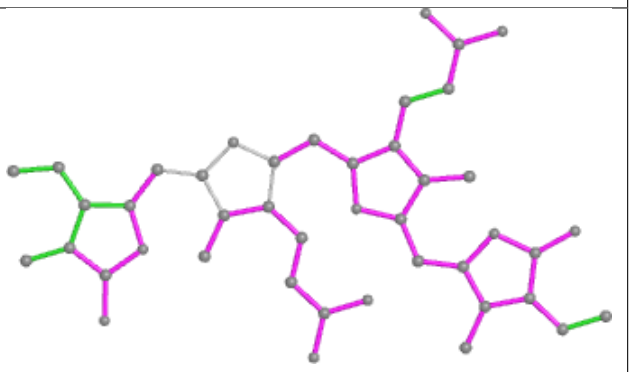

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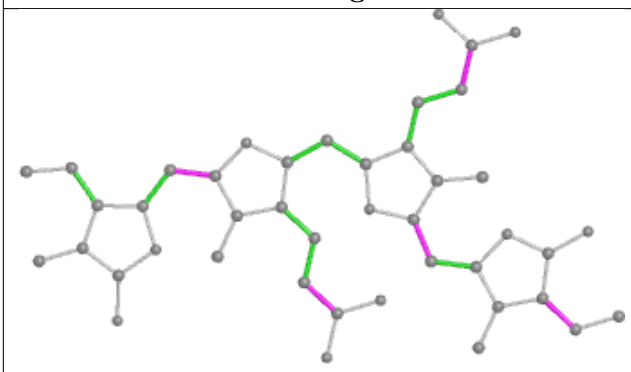

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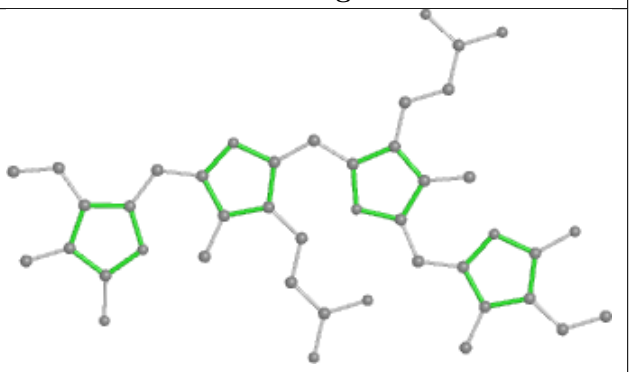
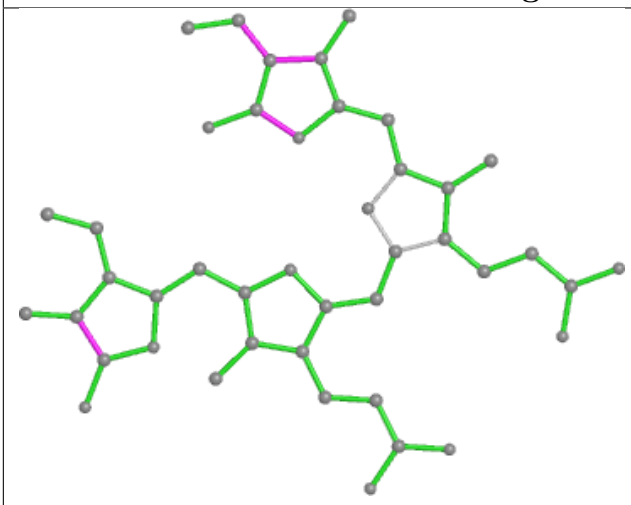


Rings

Ligand PEB I9 201



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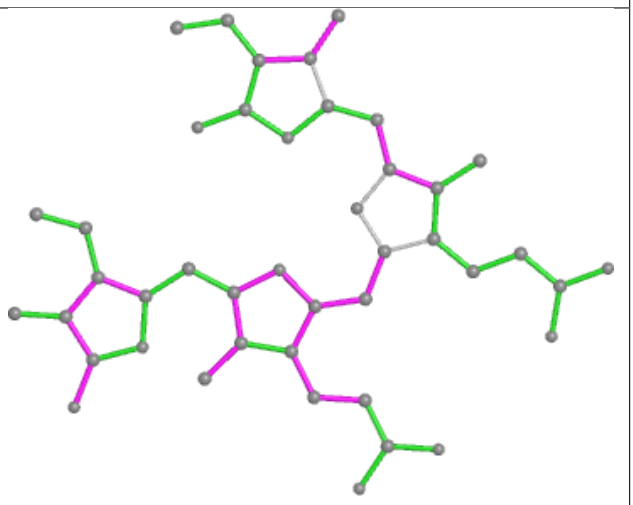

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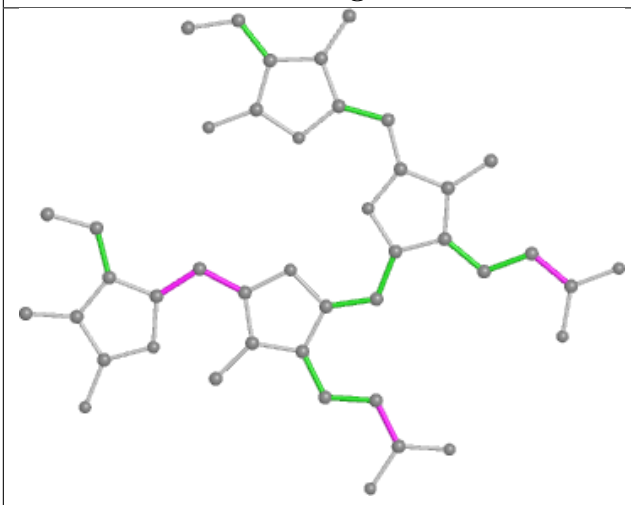

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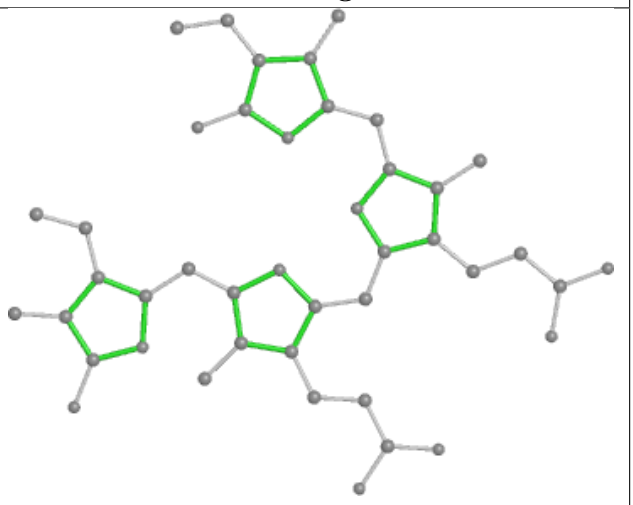
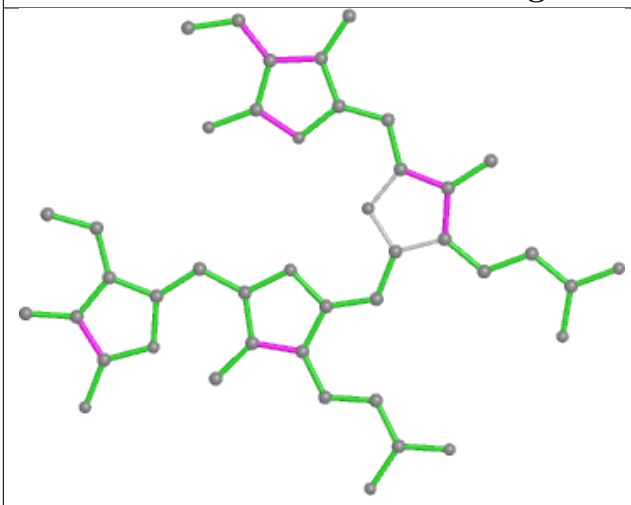


Rings

Ligand PEB ll 202



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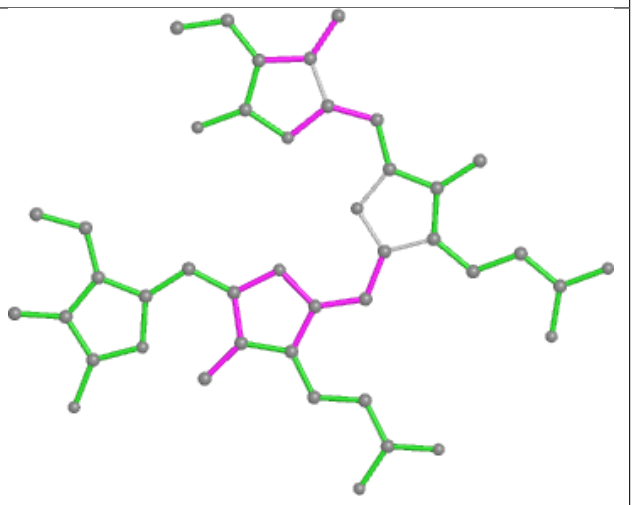

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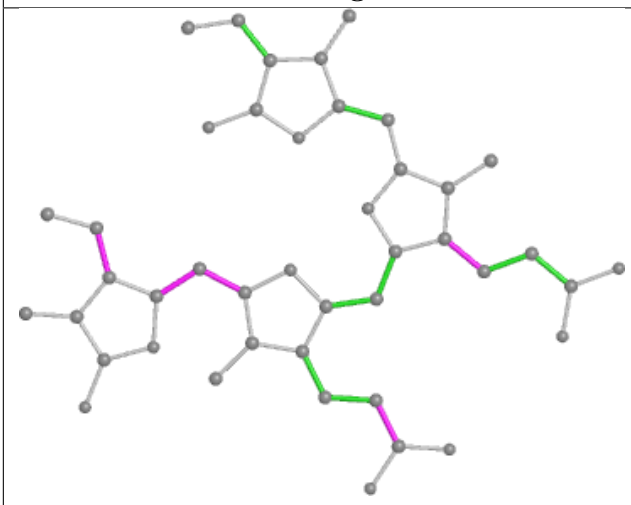

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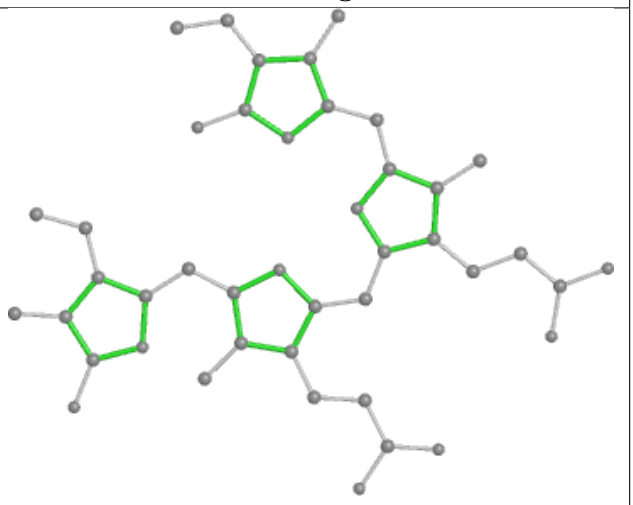

Rings

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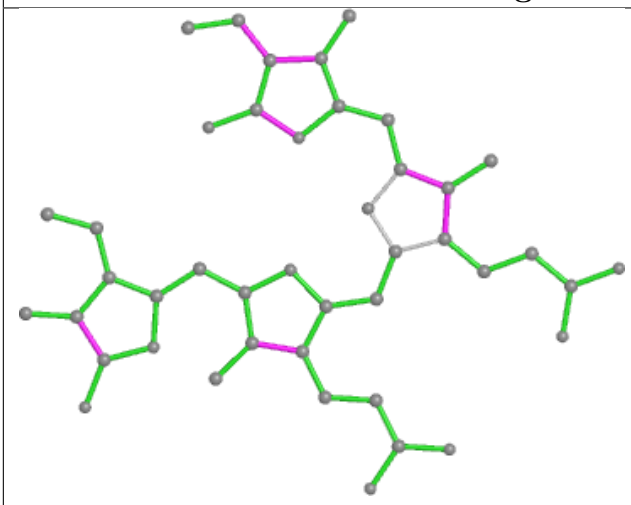

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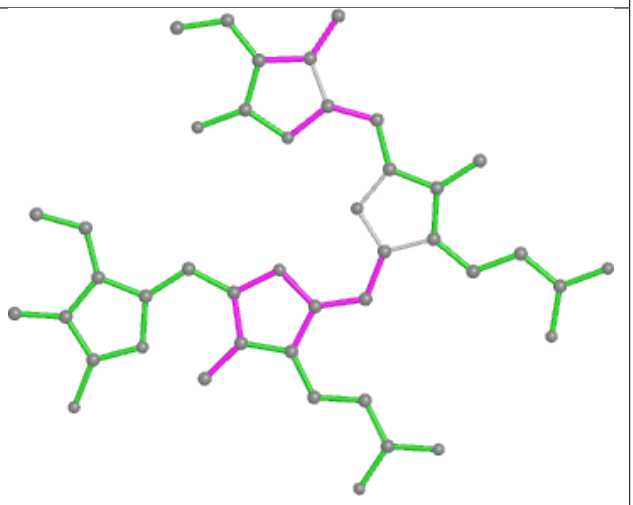

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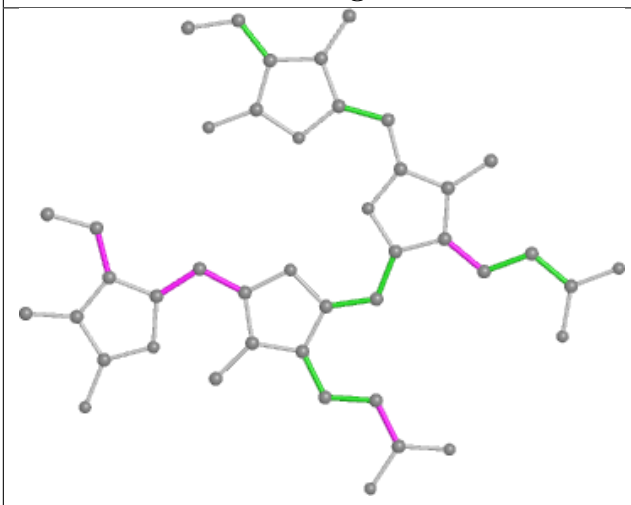

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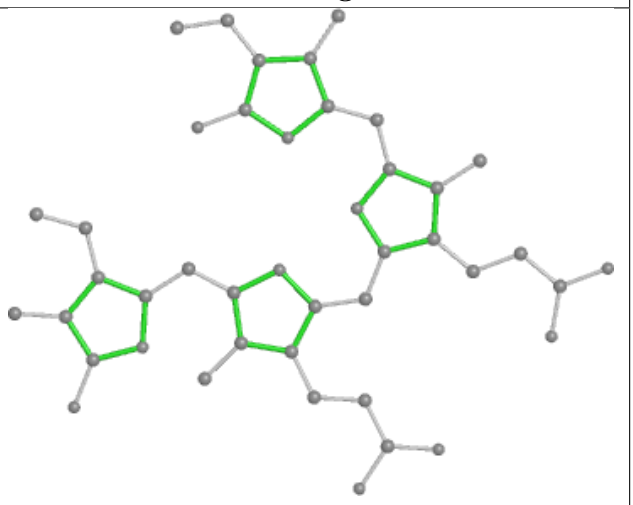

Rings

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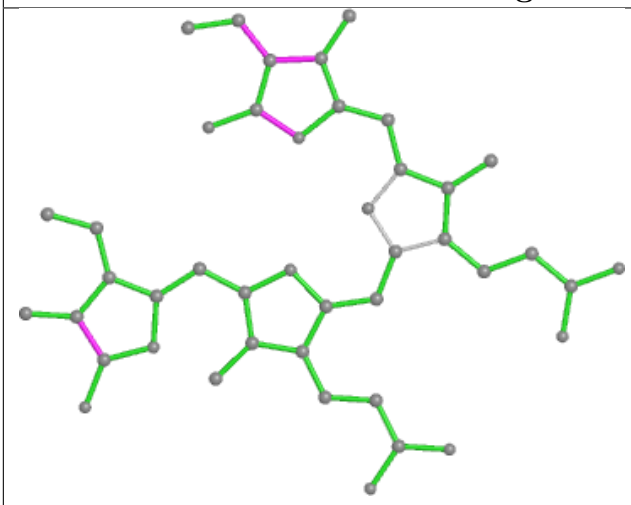

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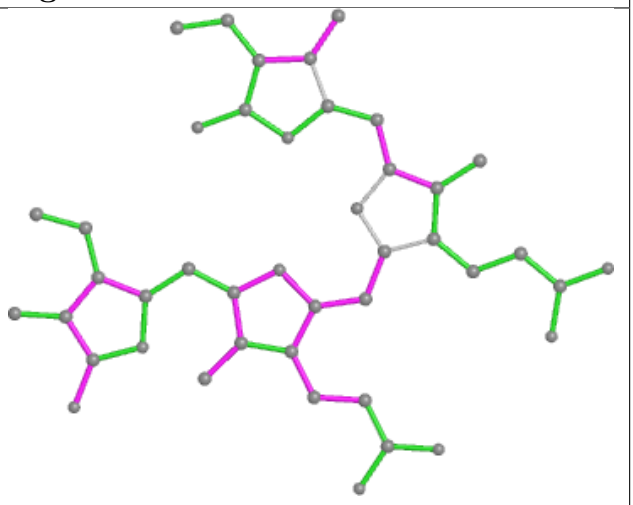

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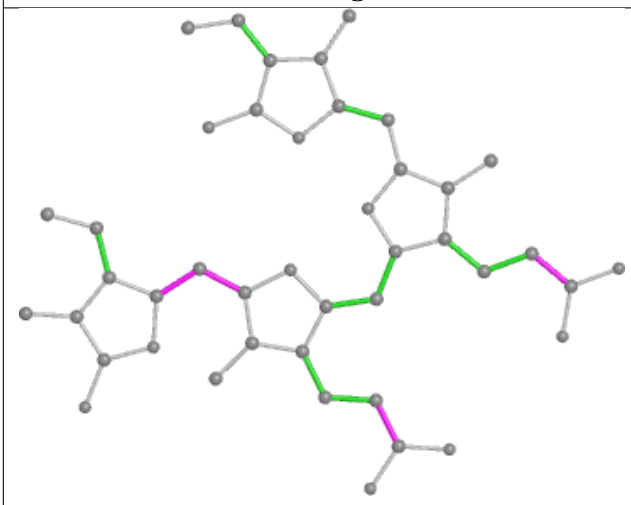

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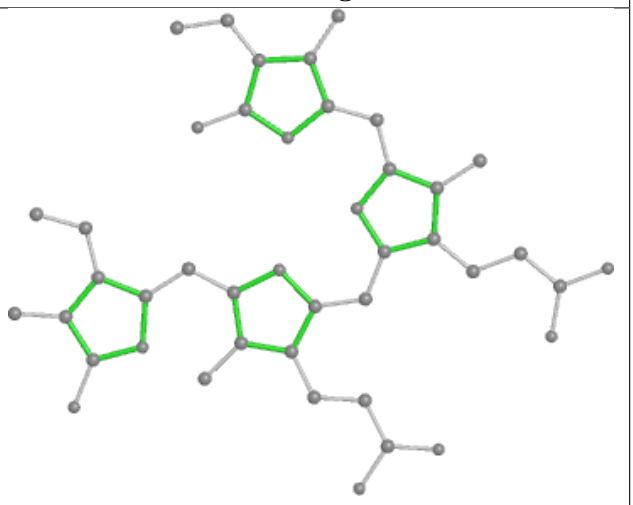

Rings

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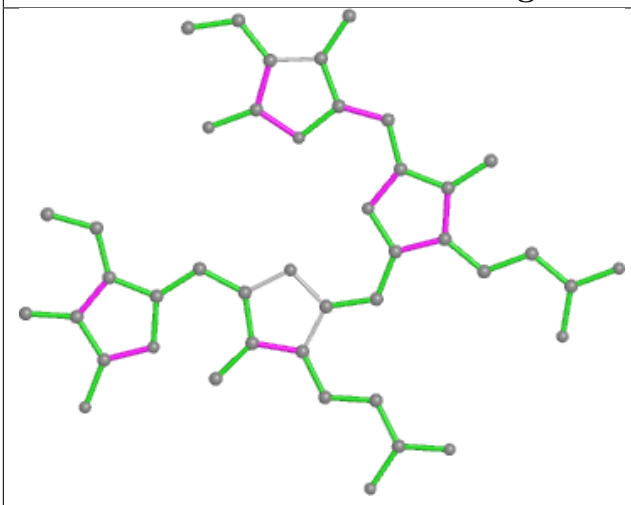

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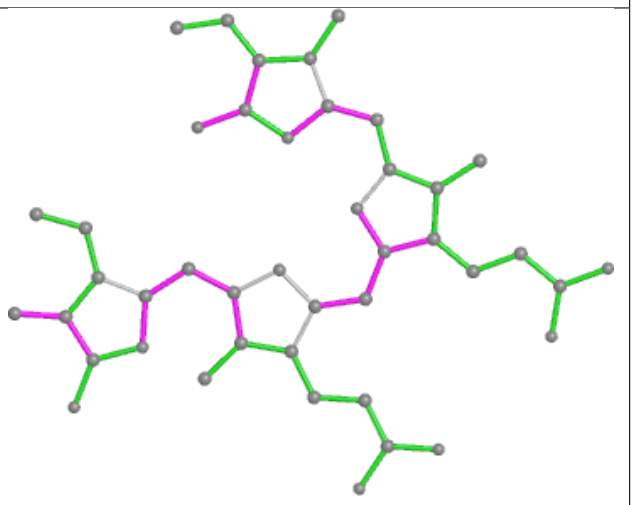

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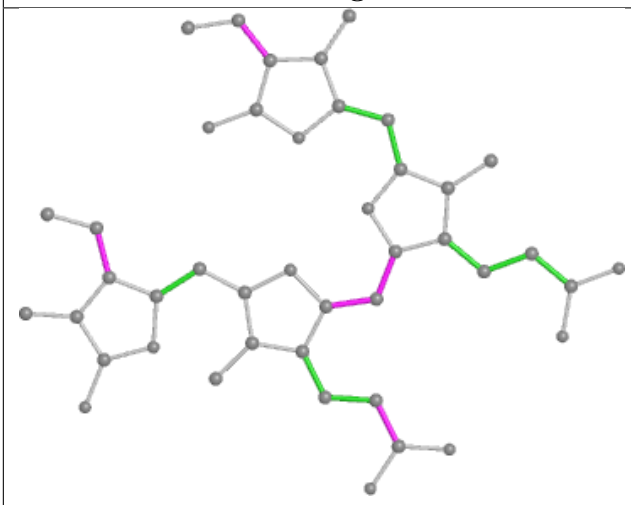

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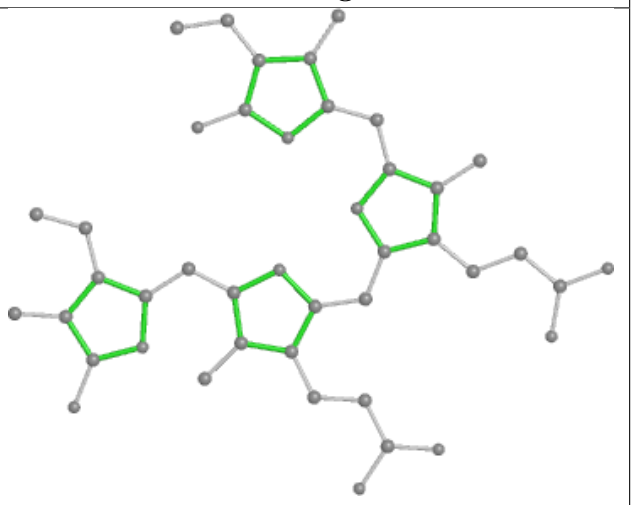

Rings

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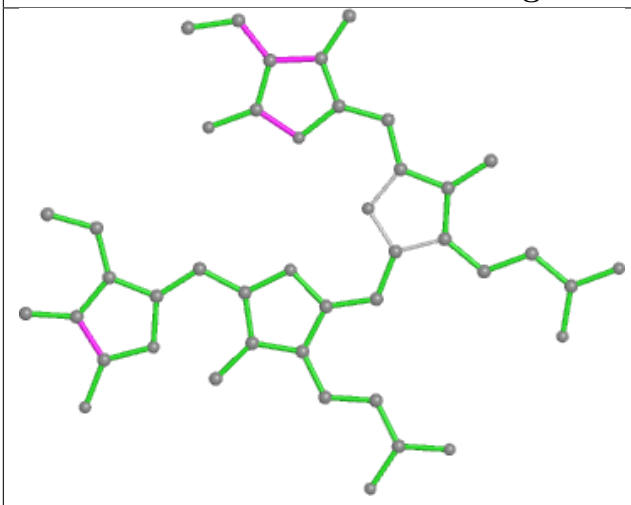

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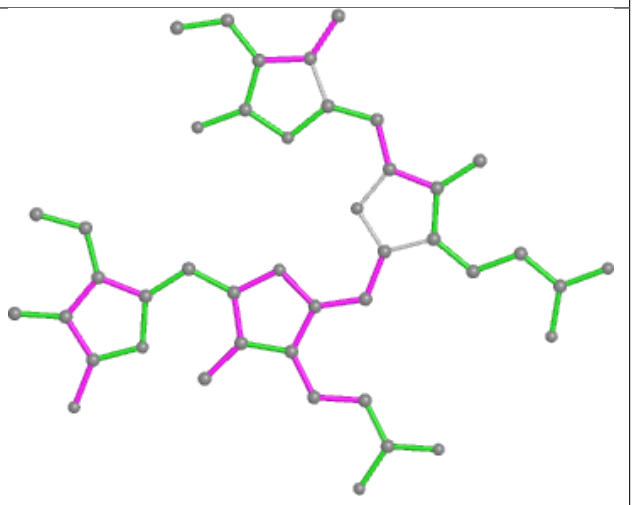

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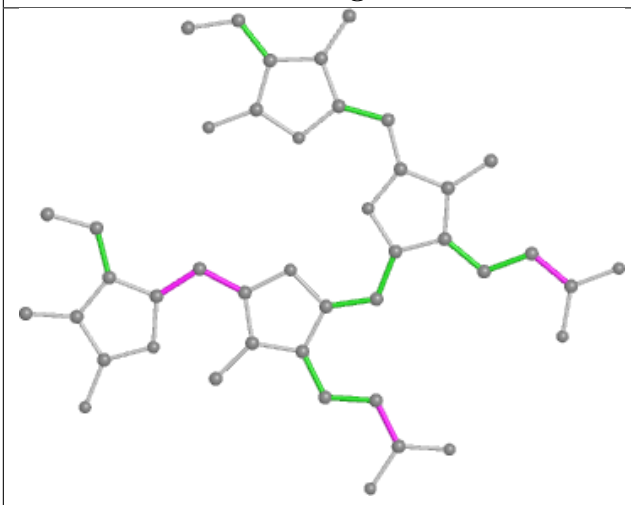

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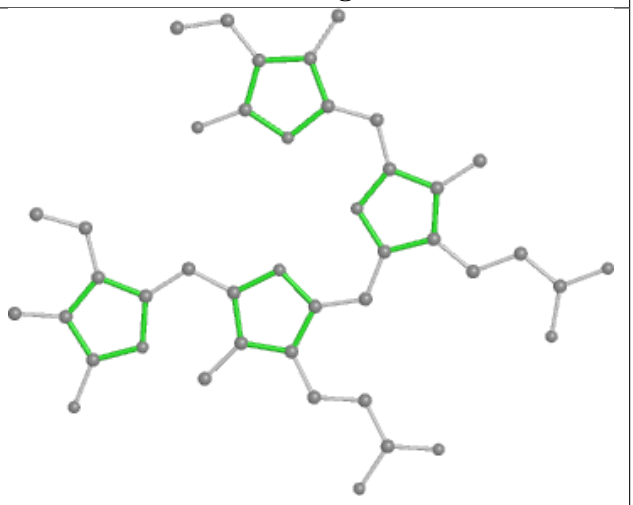
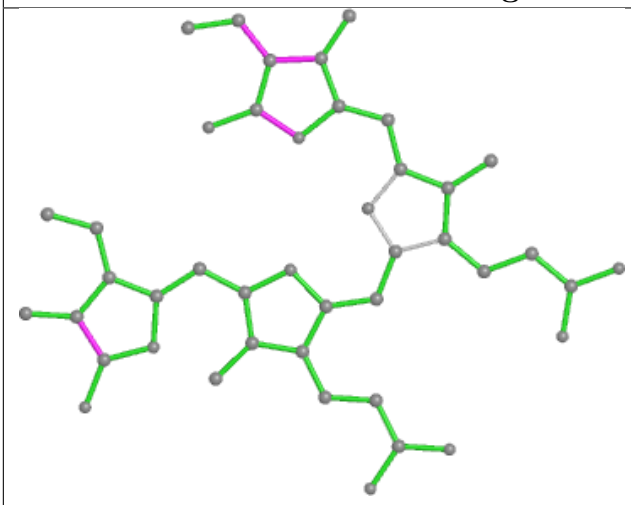


Rings

Ligand PEB dM 1001



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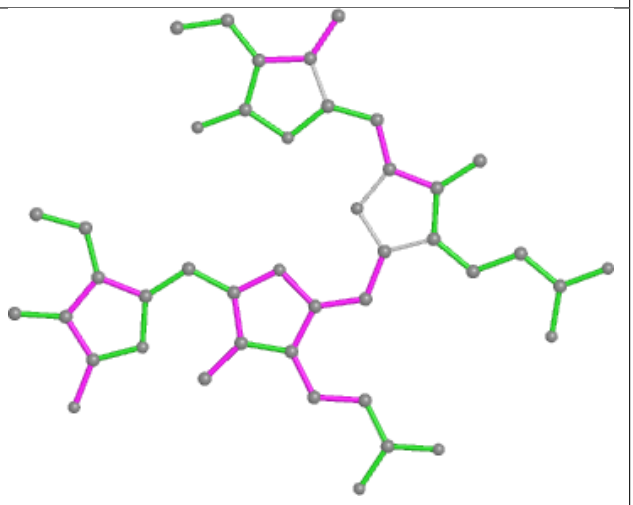

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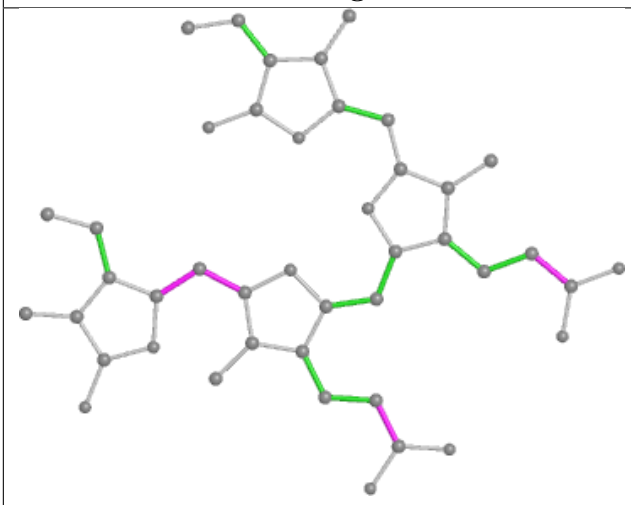
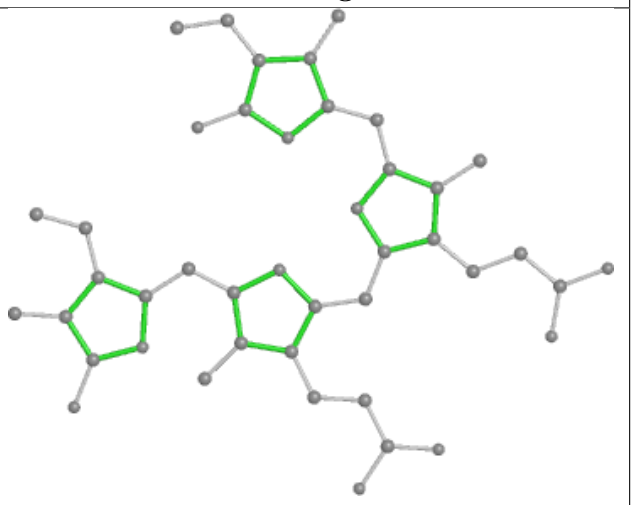
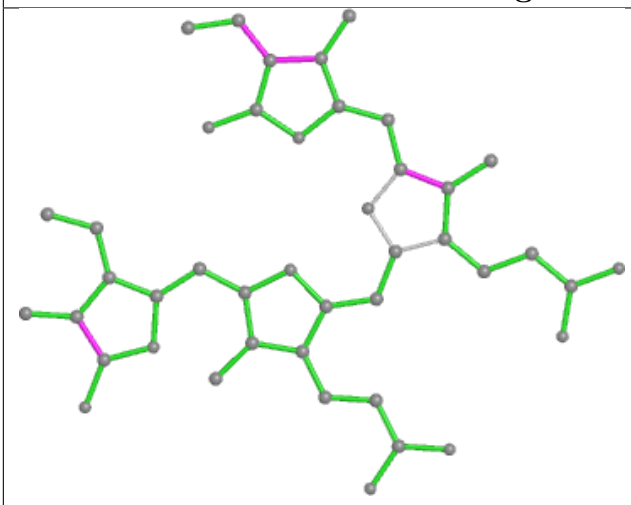


Torsions



Rings

Ligand PEB U5 202



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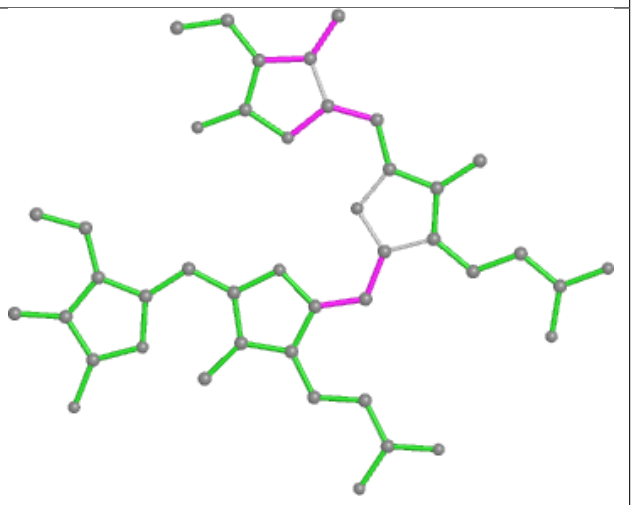

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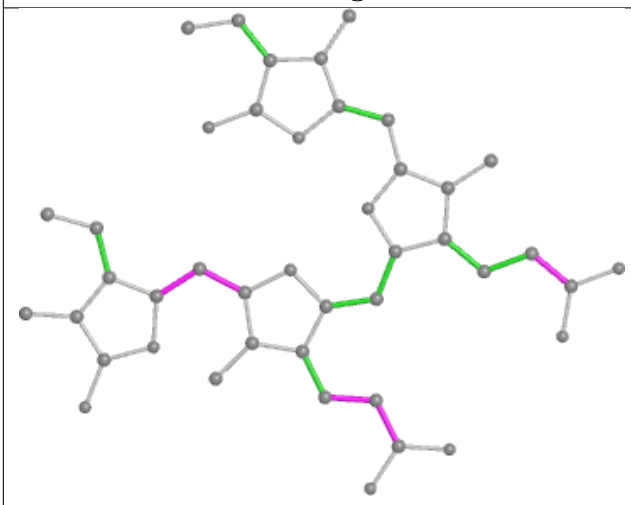

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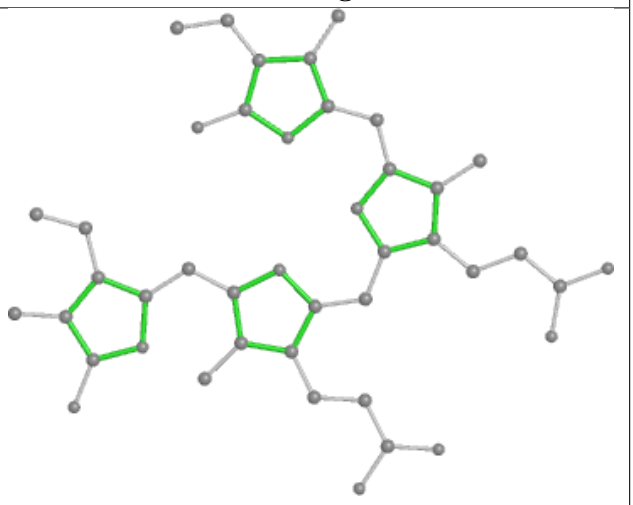
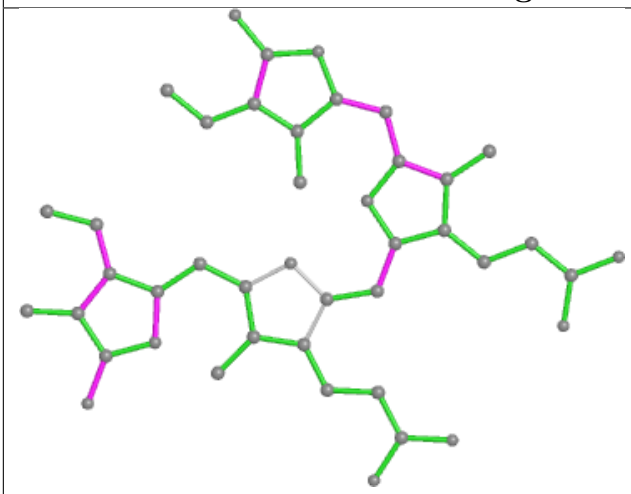


Rings

Ligand PVN aZ 303



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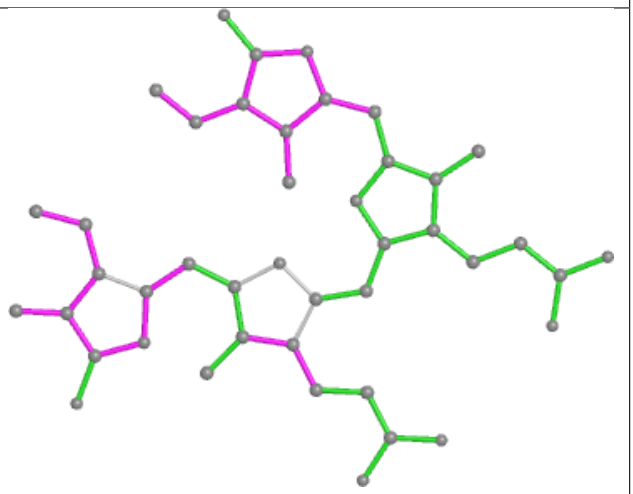

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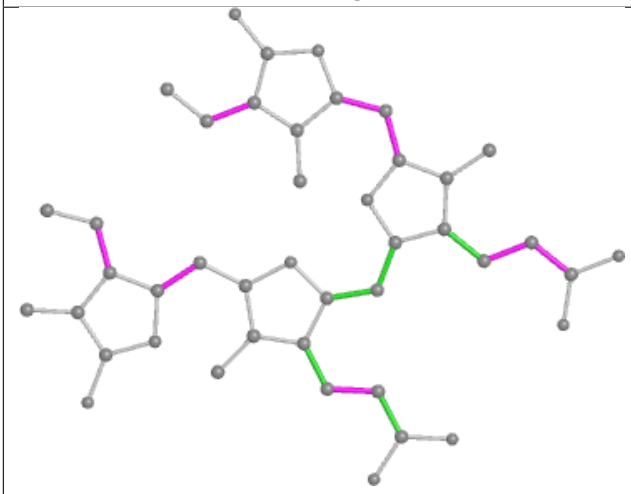

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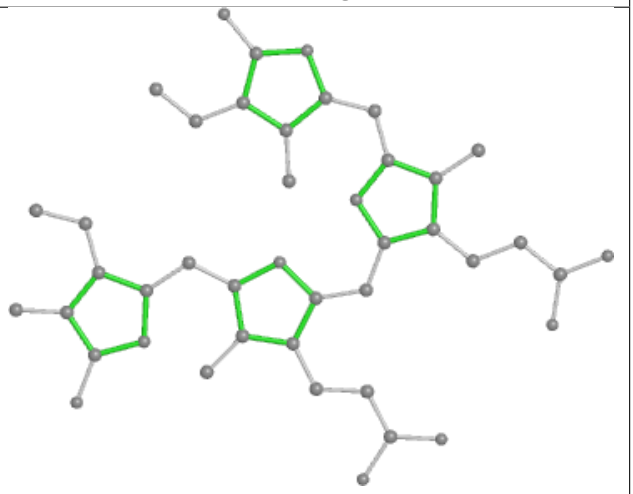
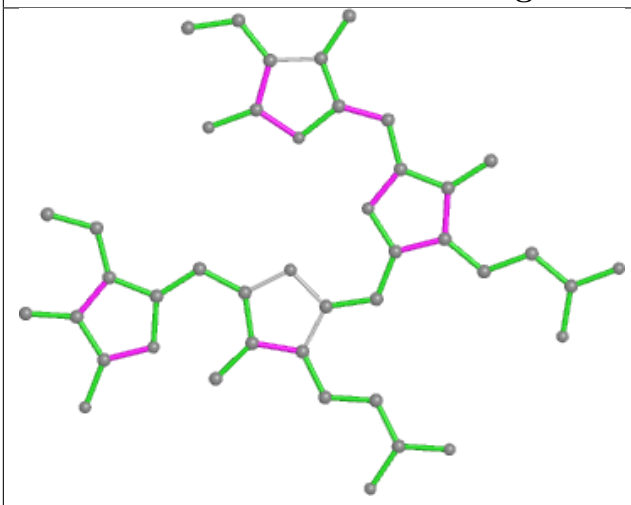


Rings

Ligand PUB F3 203



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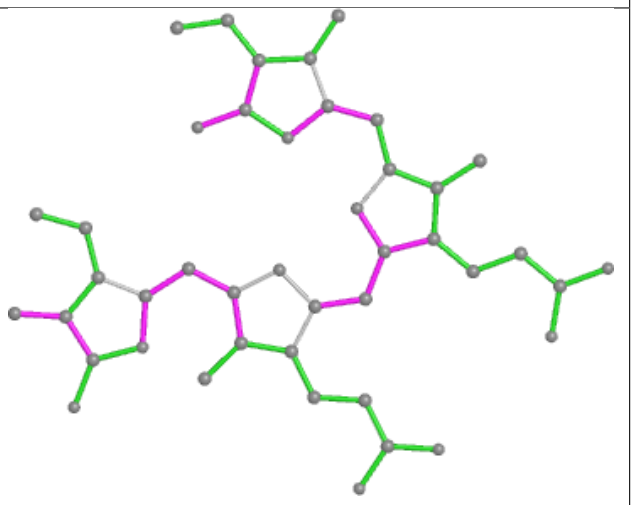

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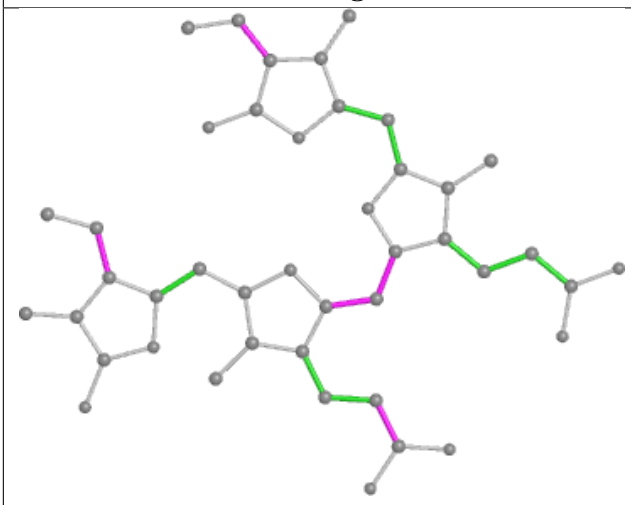

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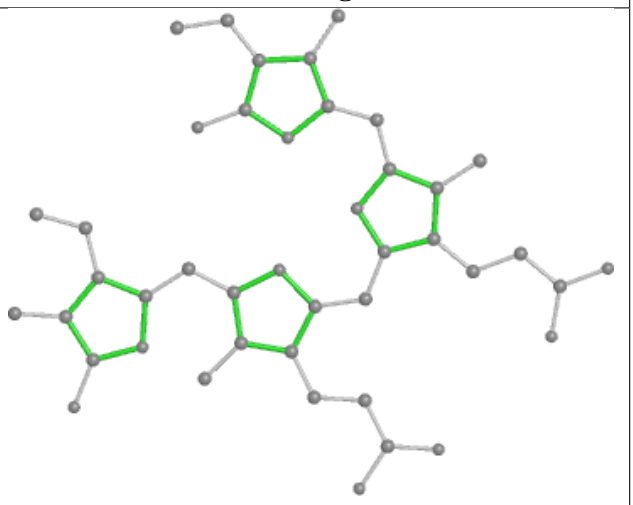
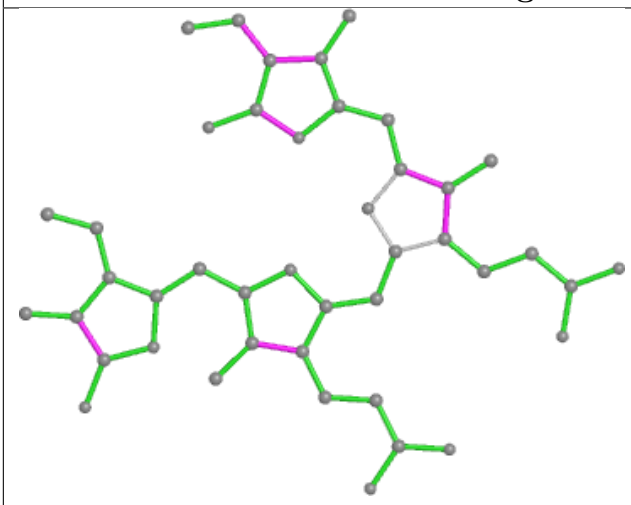


Rings

Ligand PEB eB 203



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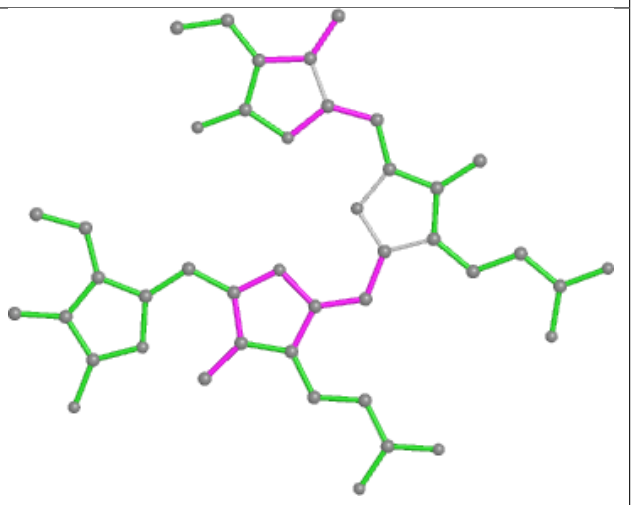

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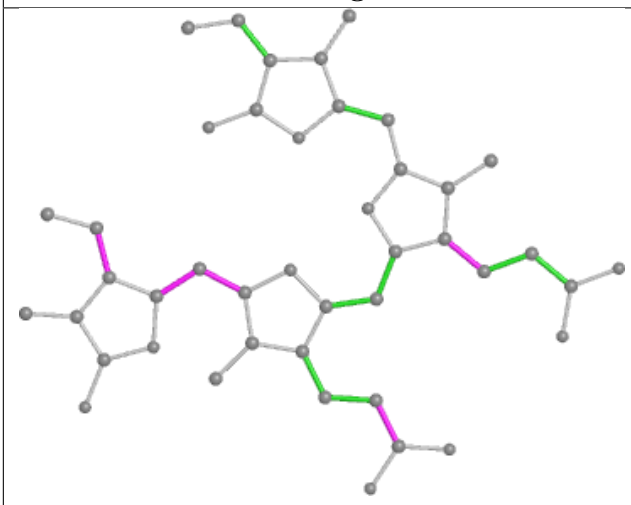

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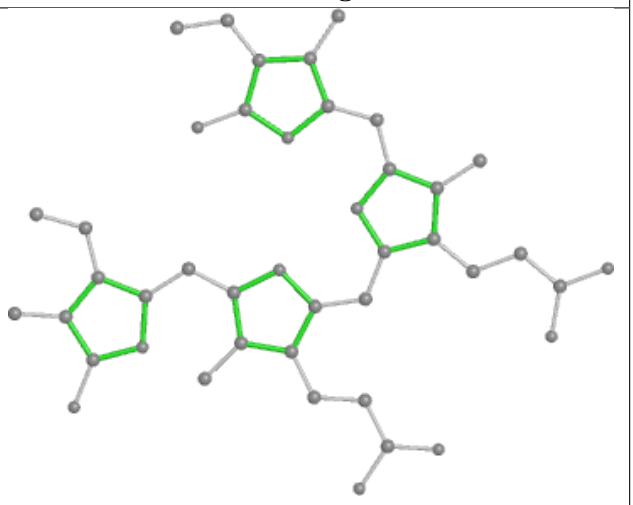
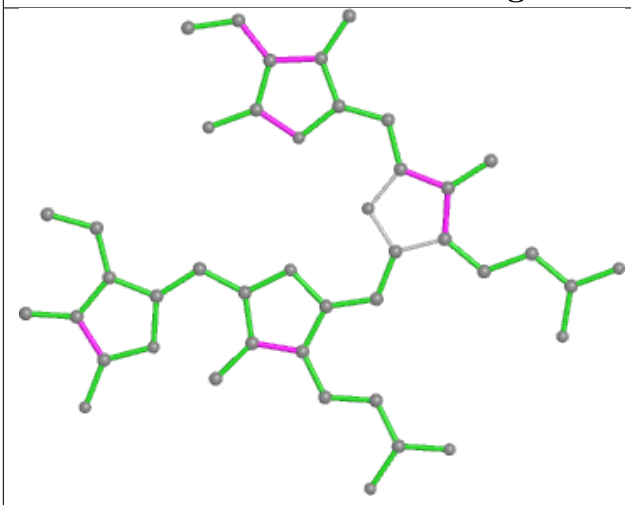


Rings

Ligand PEB kV 1002



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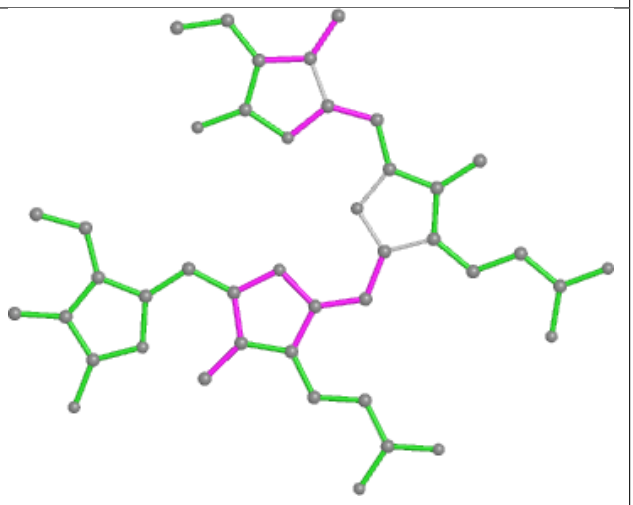

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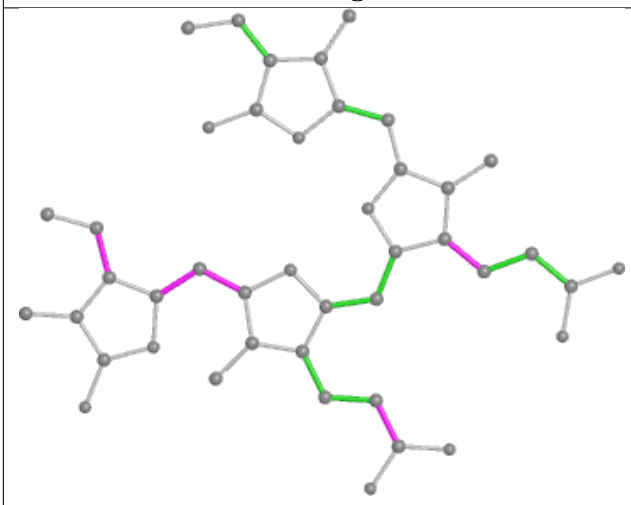

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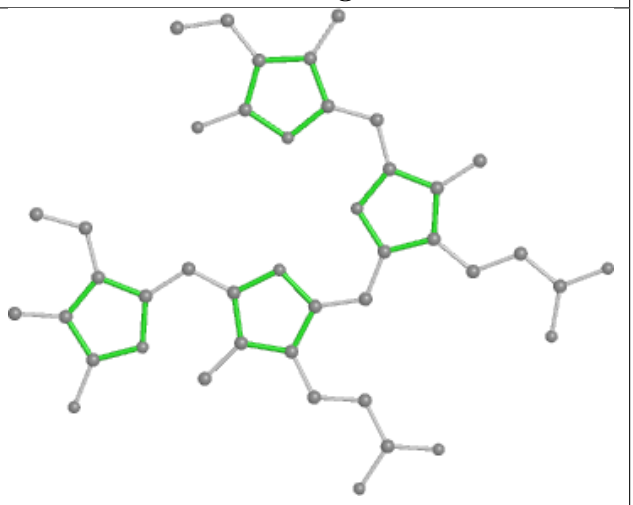

Rings

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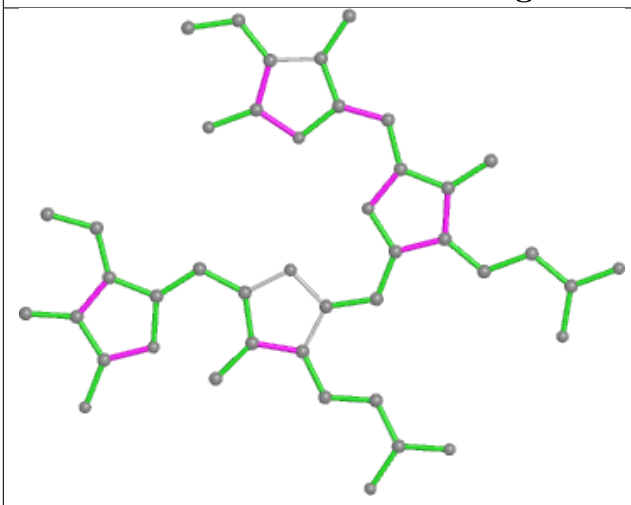

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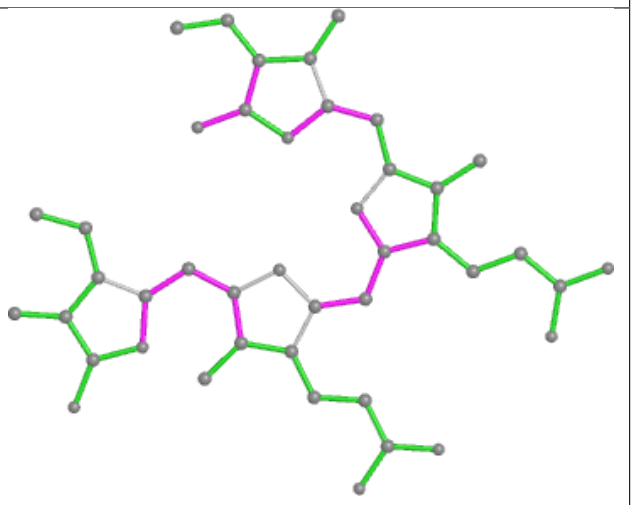

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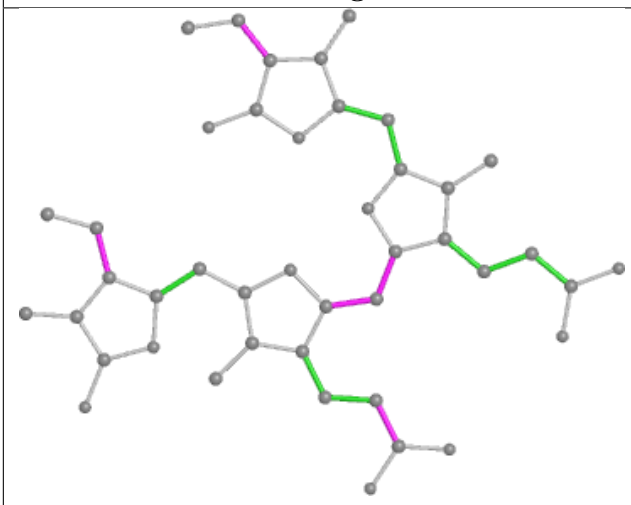

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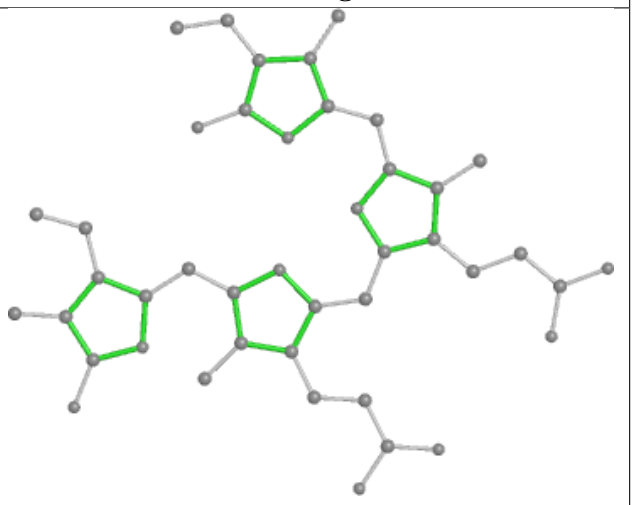
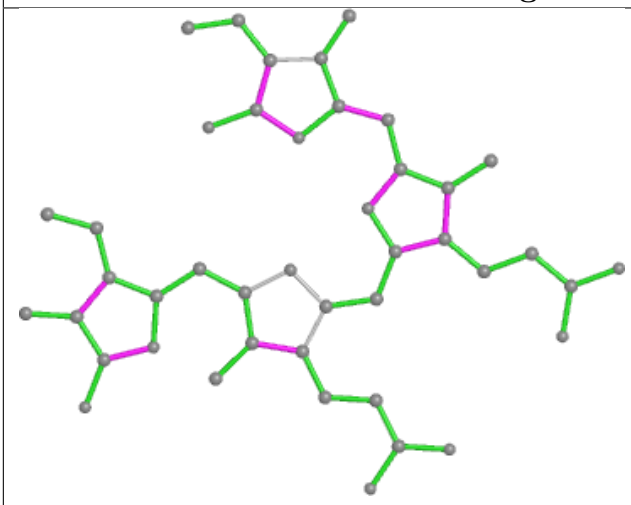


Rings

Ligand PUB t2 203



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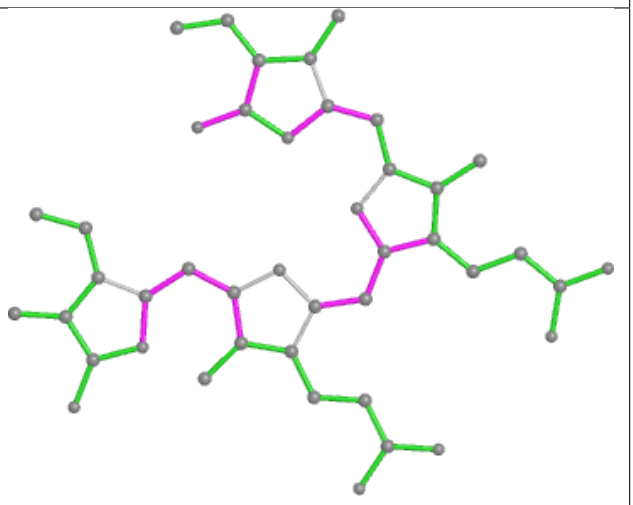

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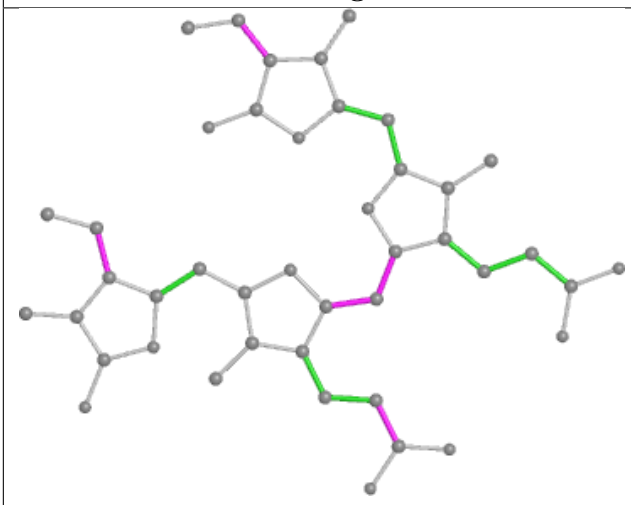

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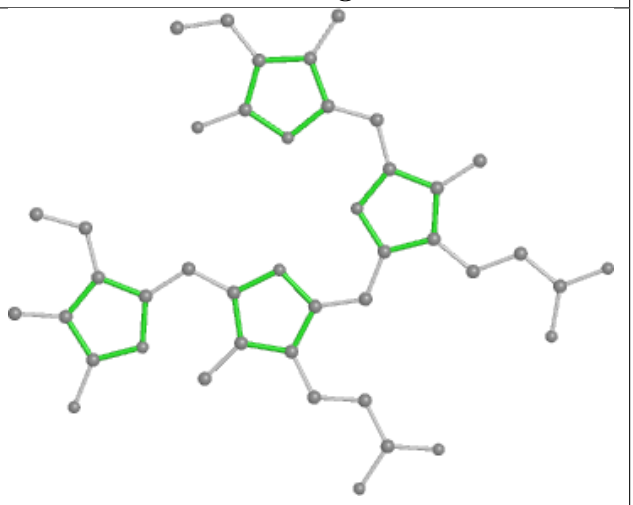
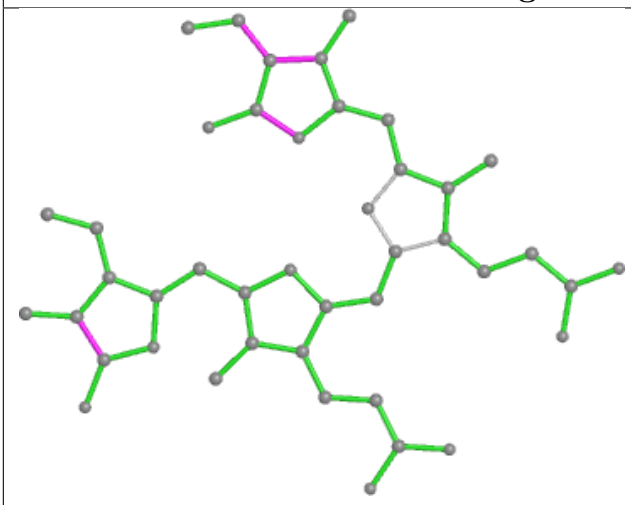


Rings

Ligand PEB b6 202



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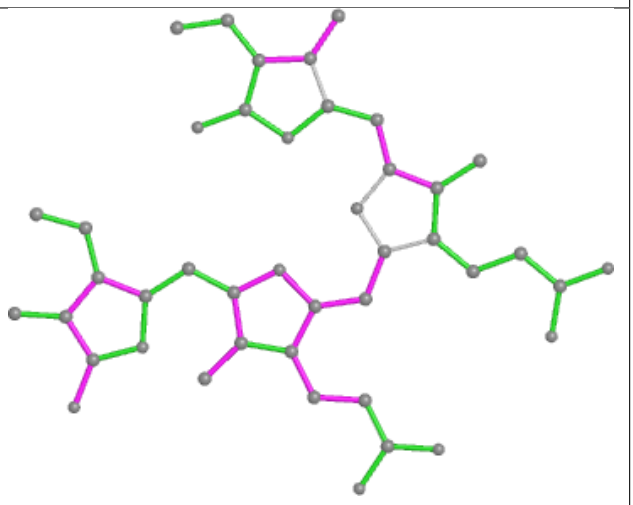

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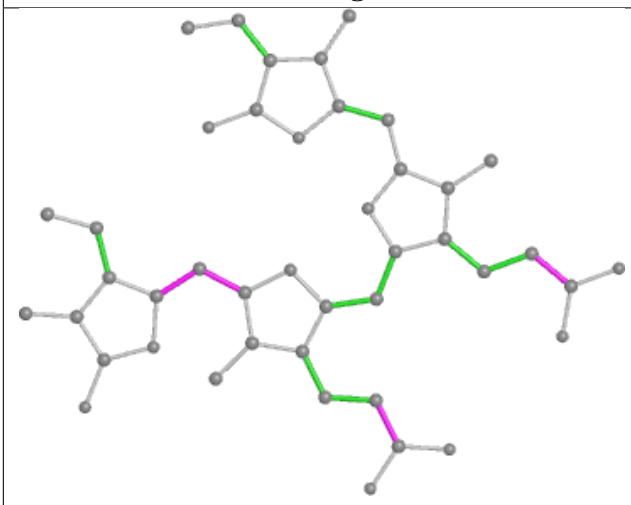

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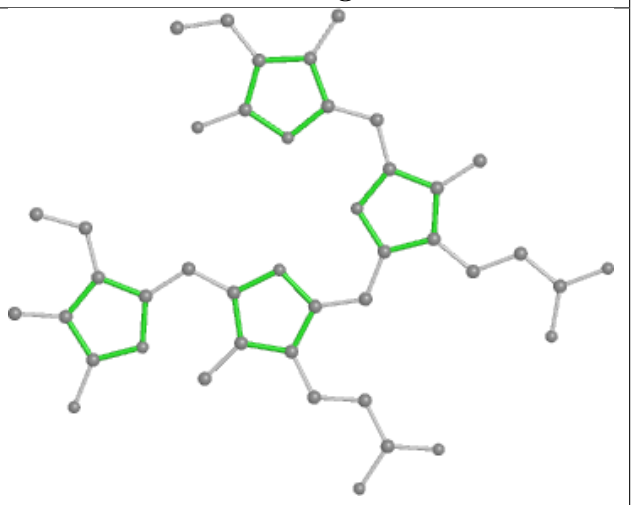
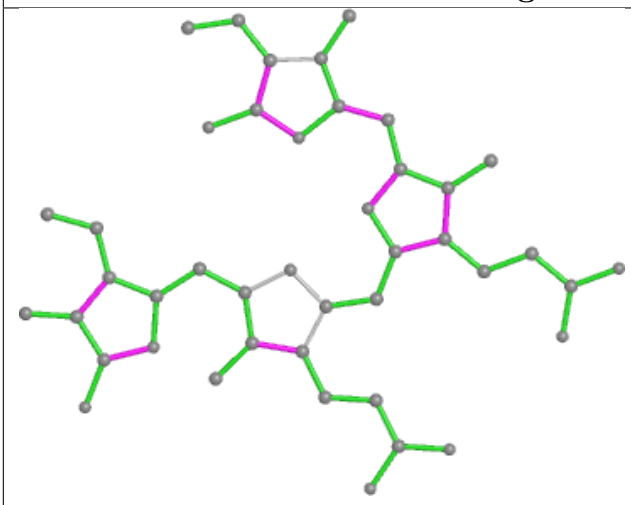


Rings

Ligand PUB ax 202



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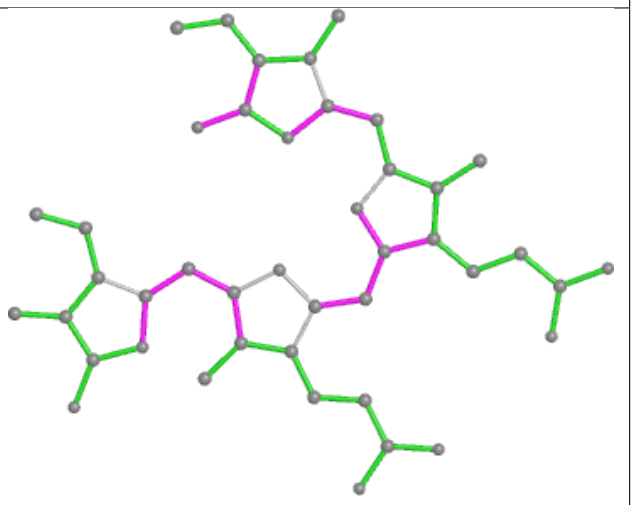

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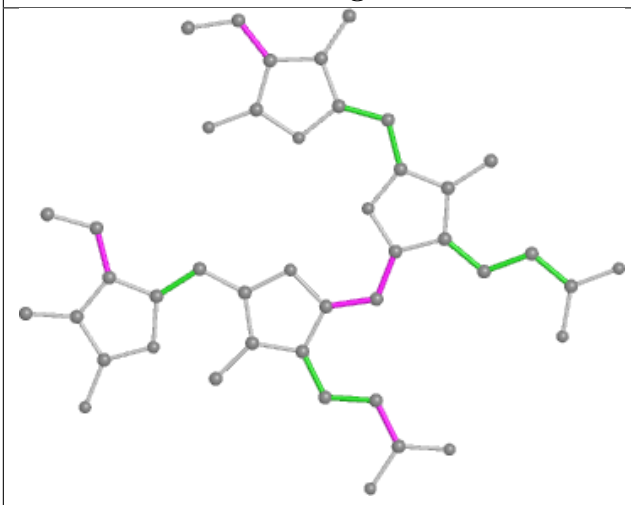

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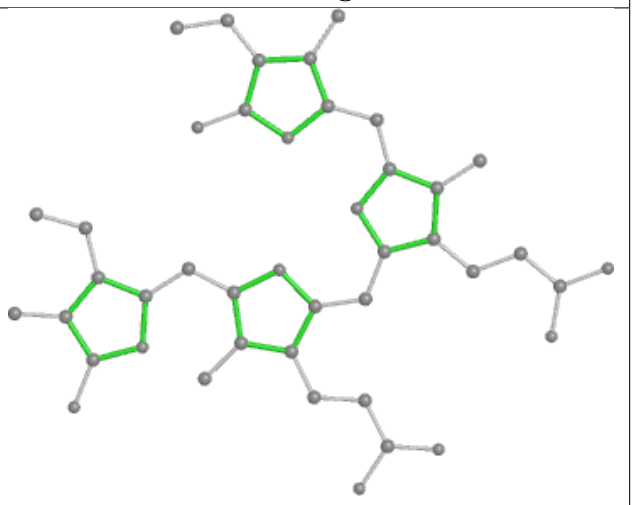
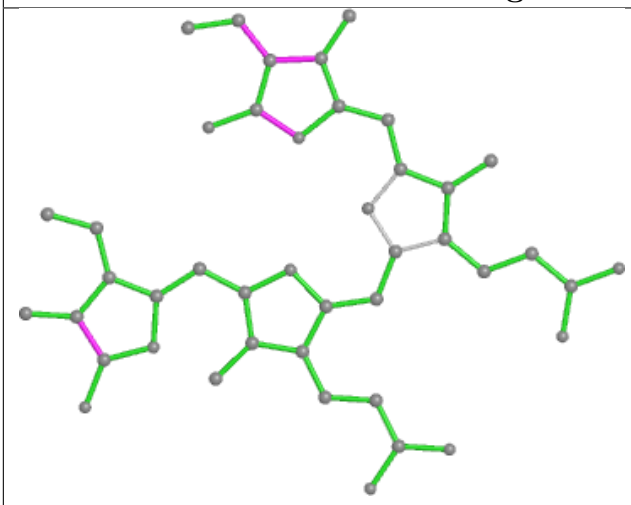


Rings

Ligand PEB O4 1001



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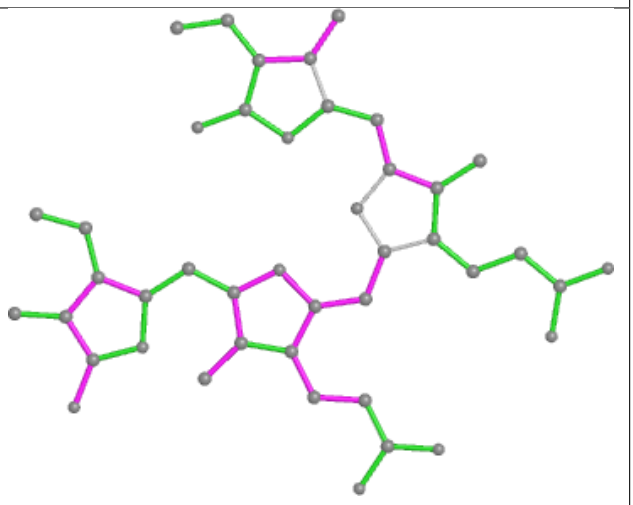

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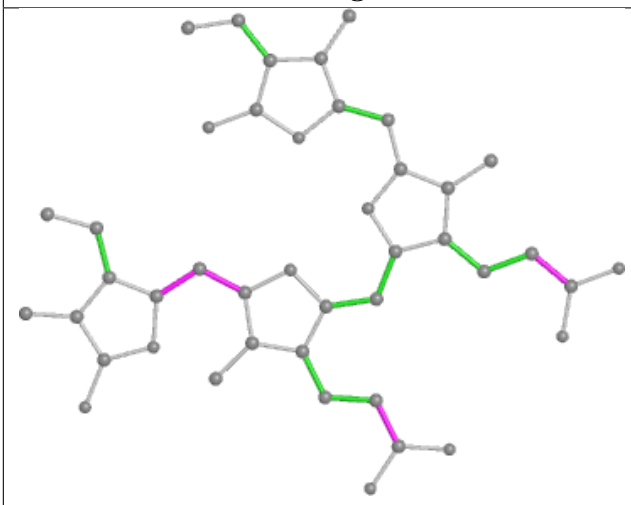

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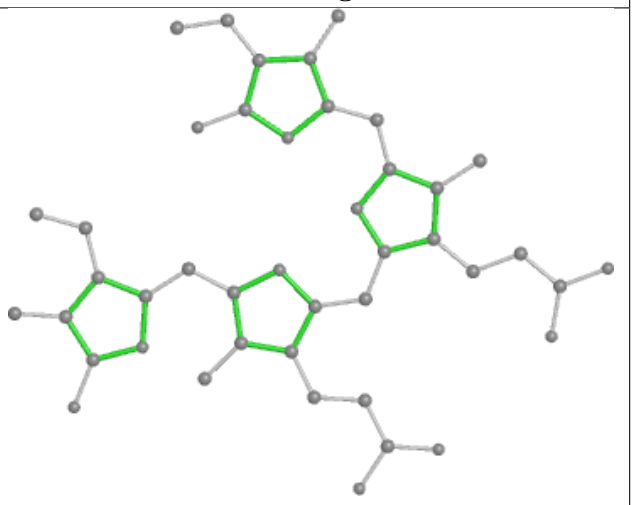
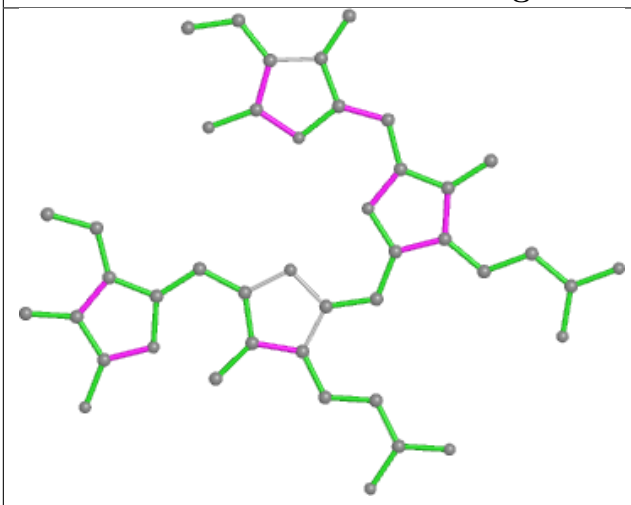


Rings

Ligand PUB K8 203



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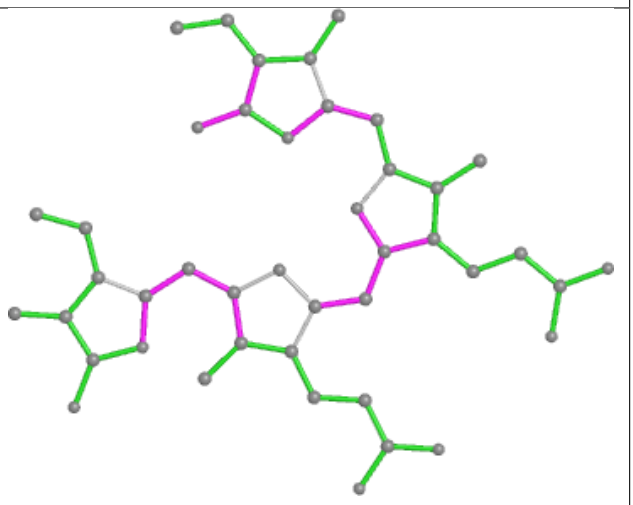

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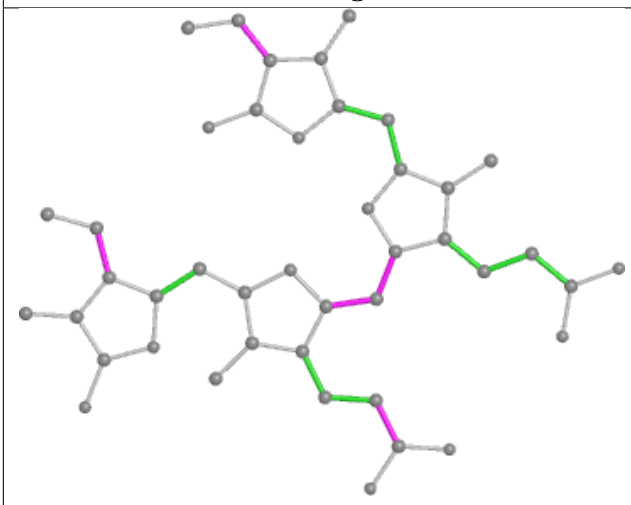

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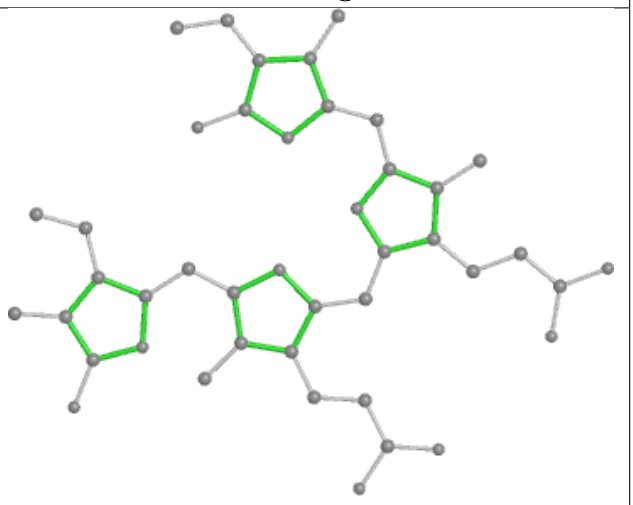
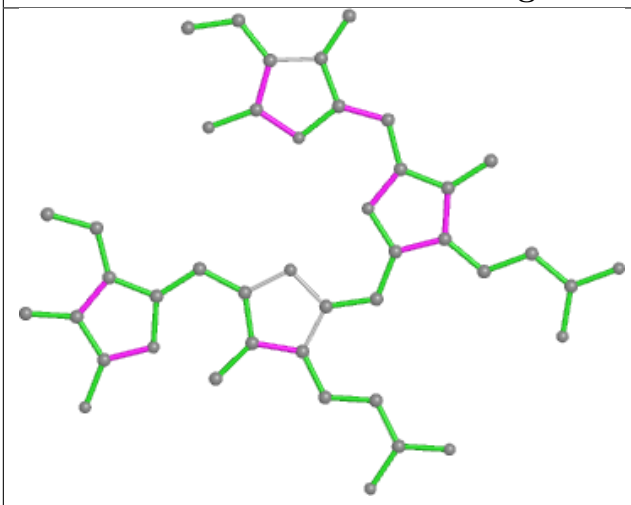


Rings

Ligand PUB ev 203



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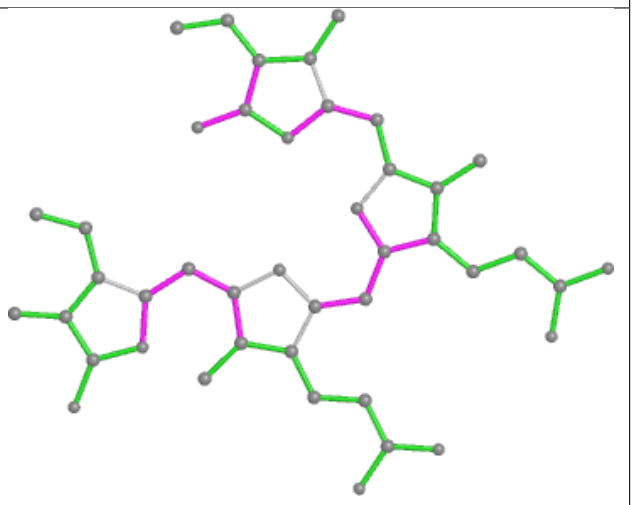

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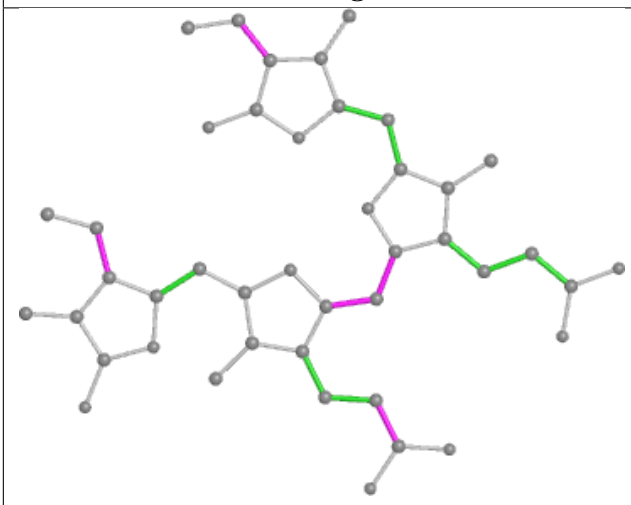

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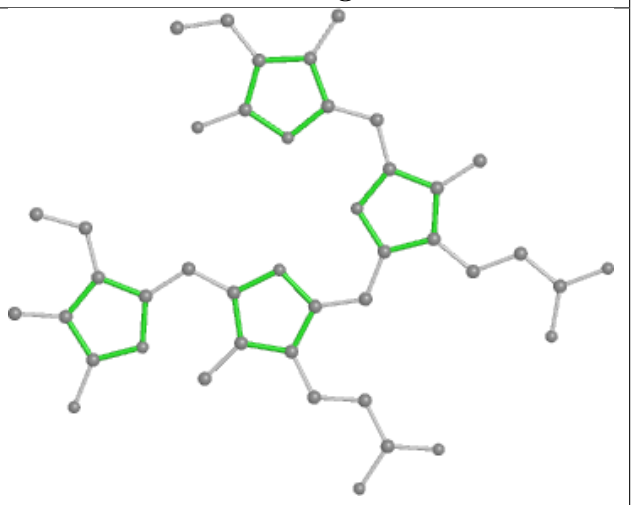
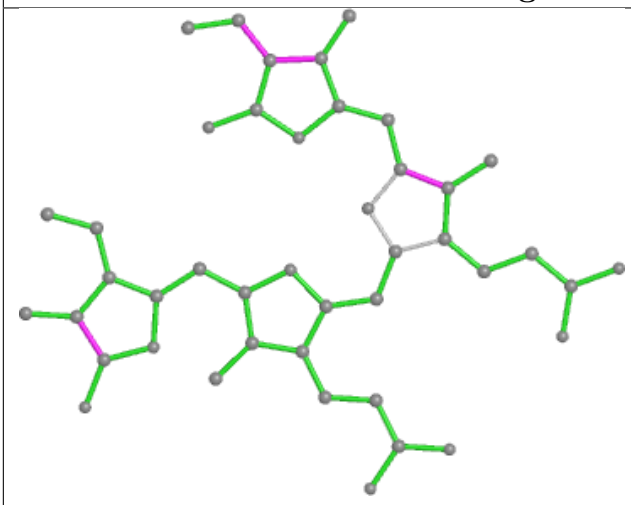


Rings

Ligand PEB u3 202



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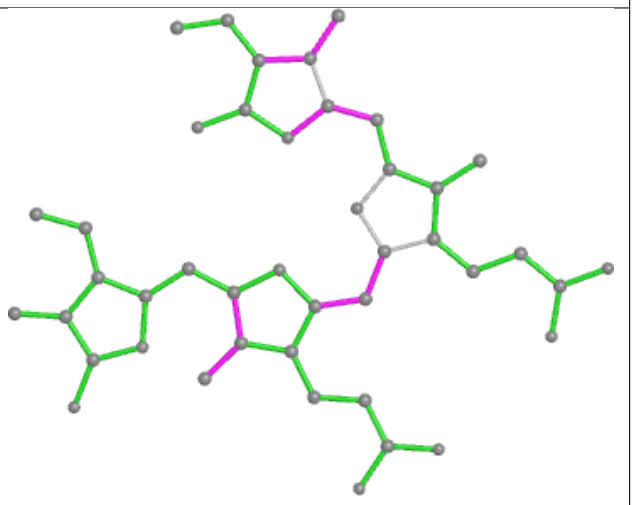
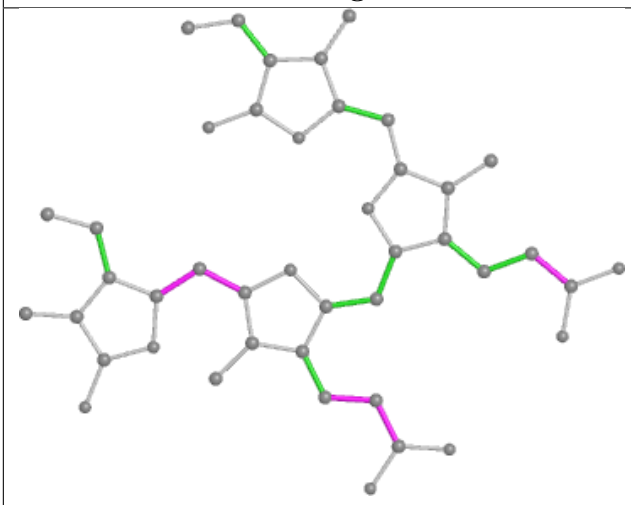


Bond angles



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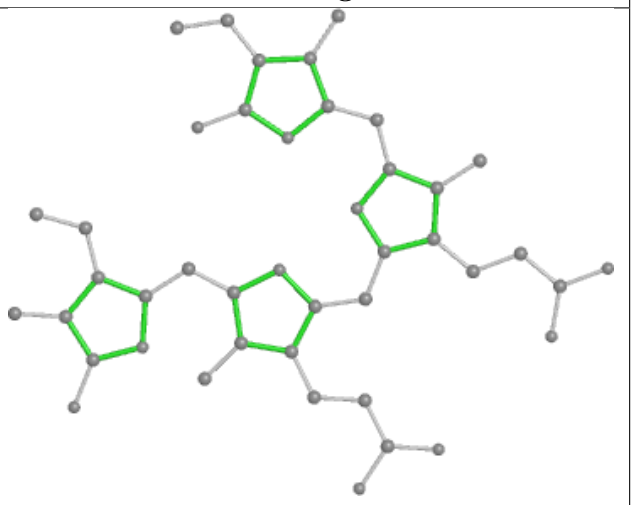
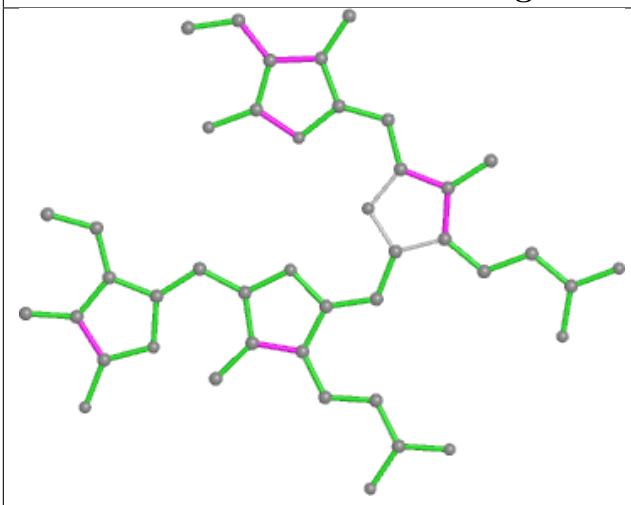
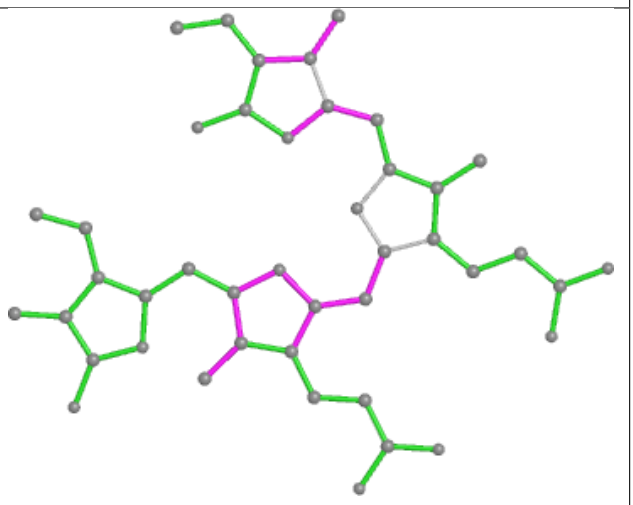


Rings

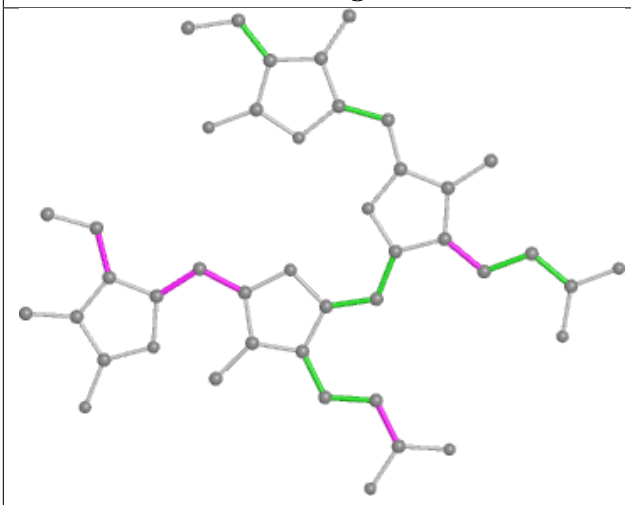
Ligand PEB D3 202



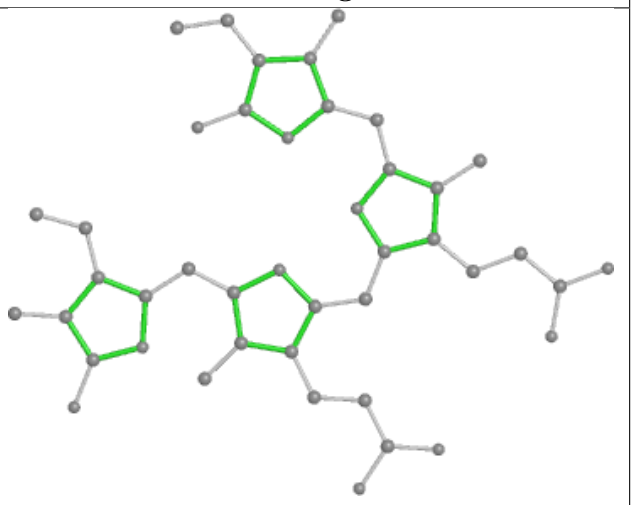
Bond lengths



Bond angles

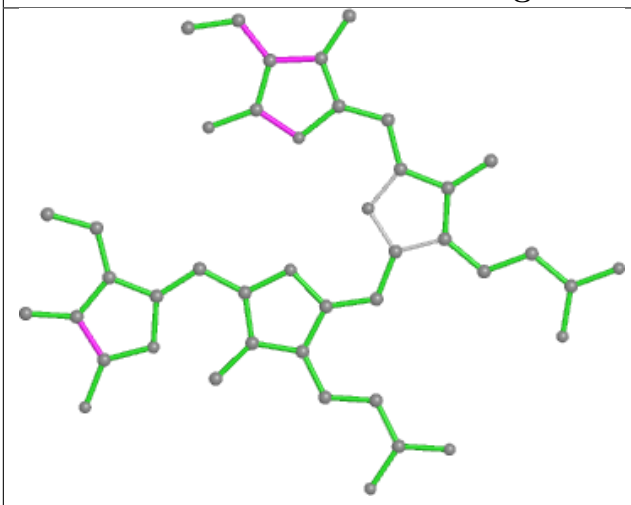


Torsions



Rings

Ligand PEB bH 201



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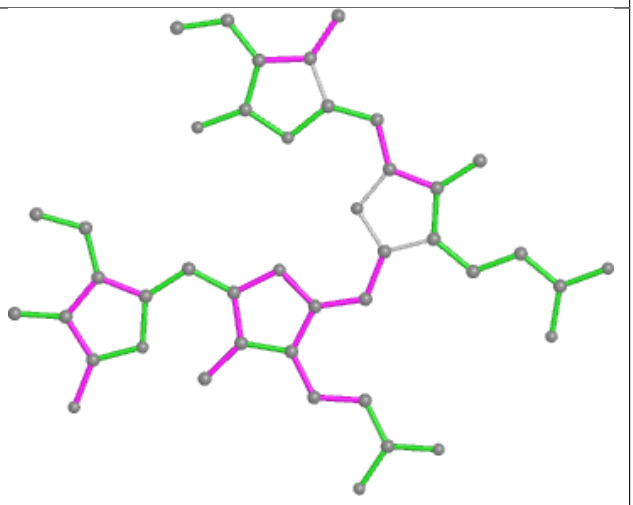

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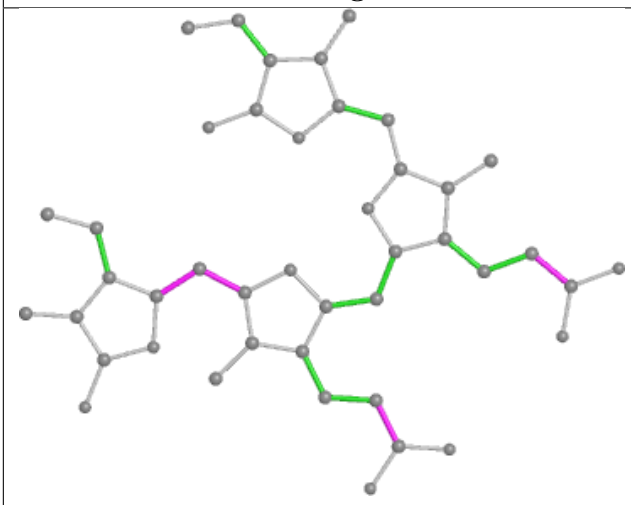

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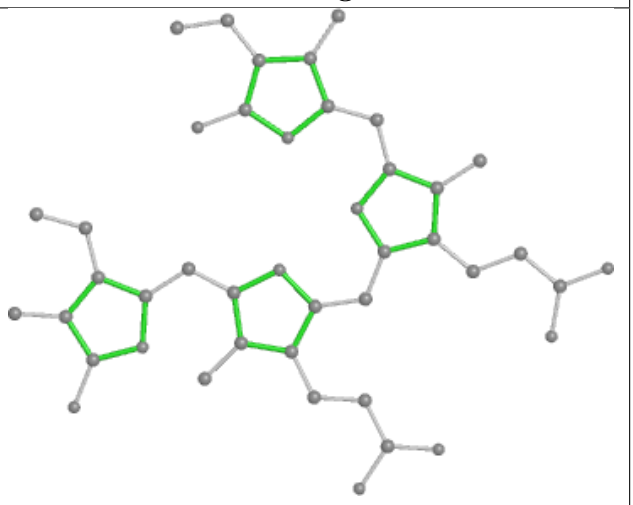
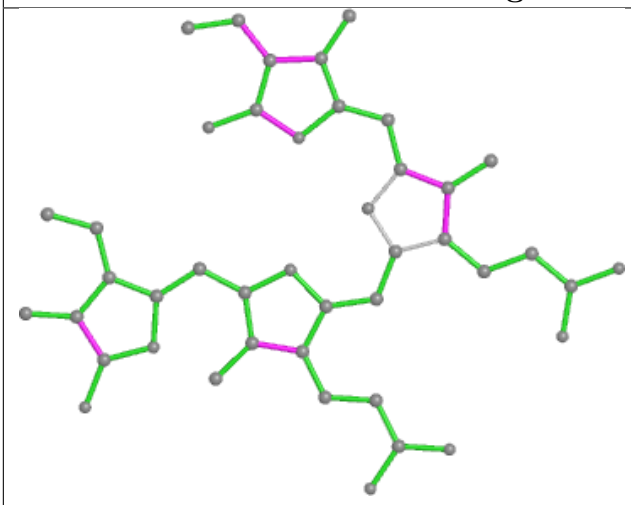


Rings

Ligand PEB Y7 1003



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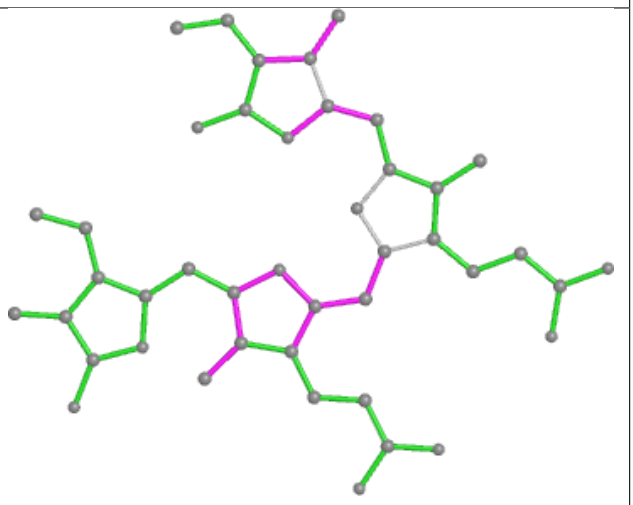

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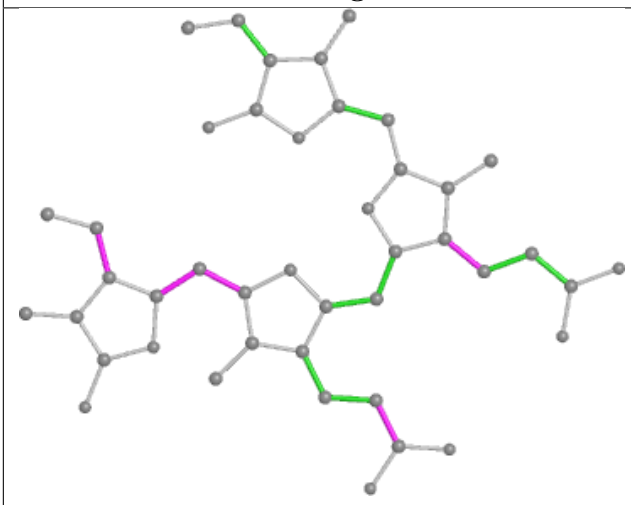

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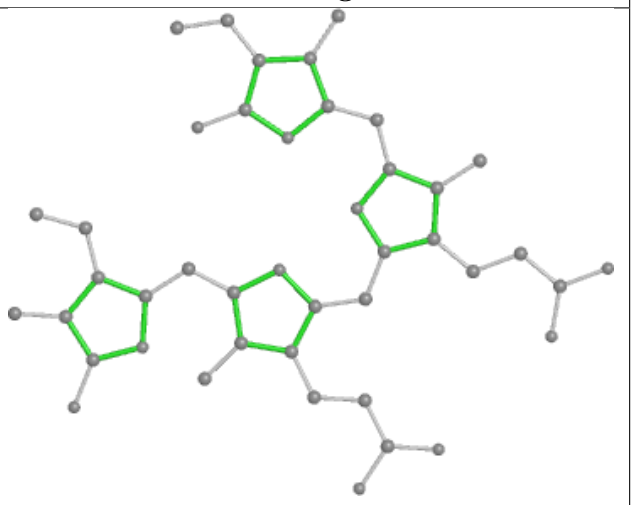

Rings

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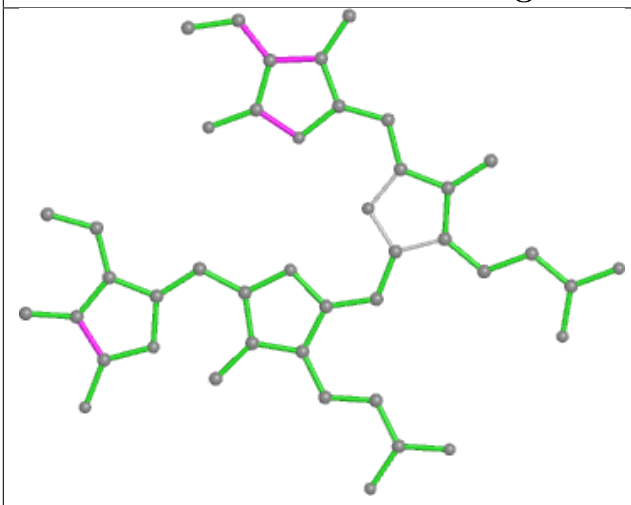

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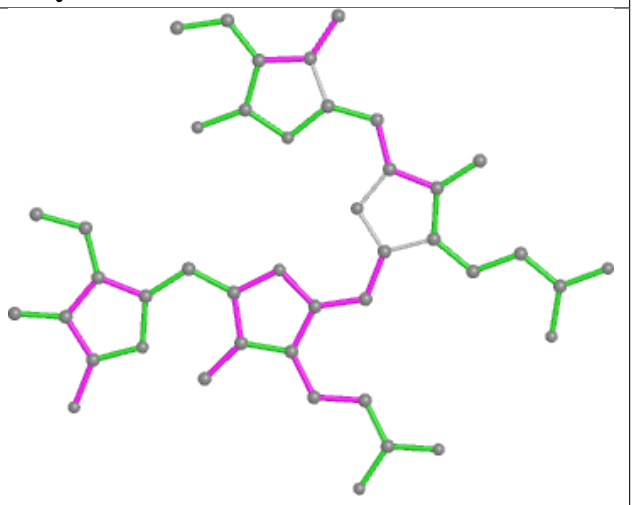

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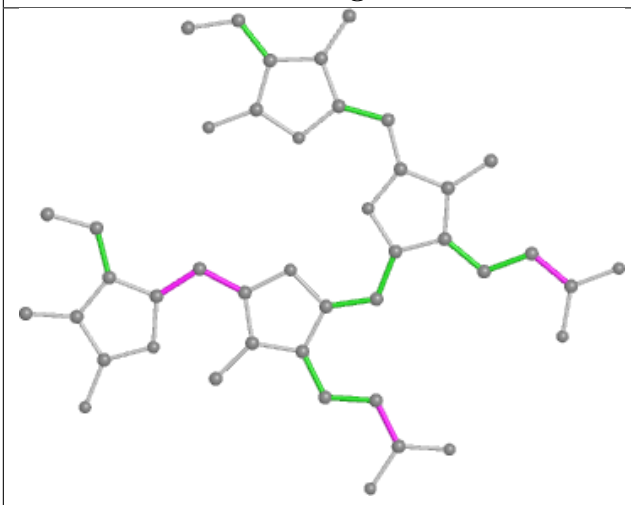

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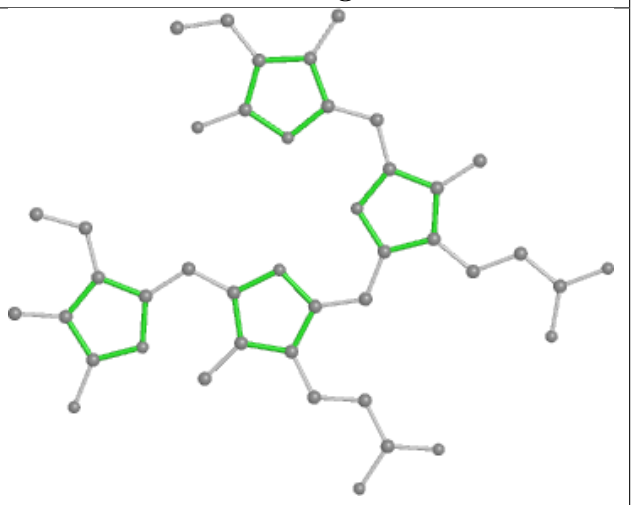
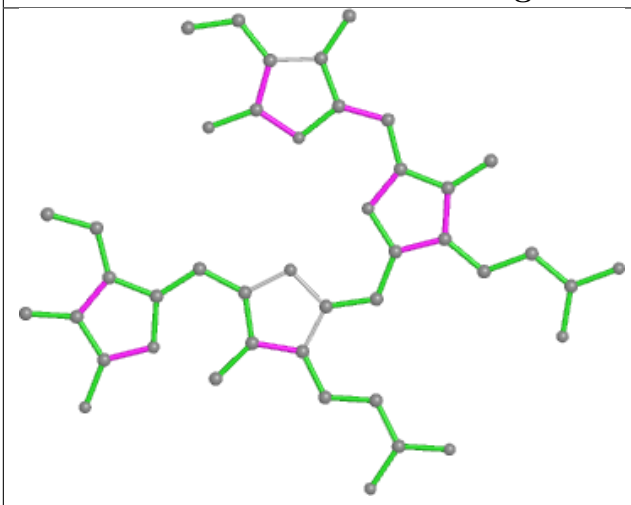


Rings

Ligand PUB P4 203



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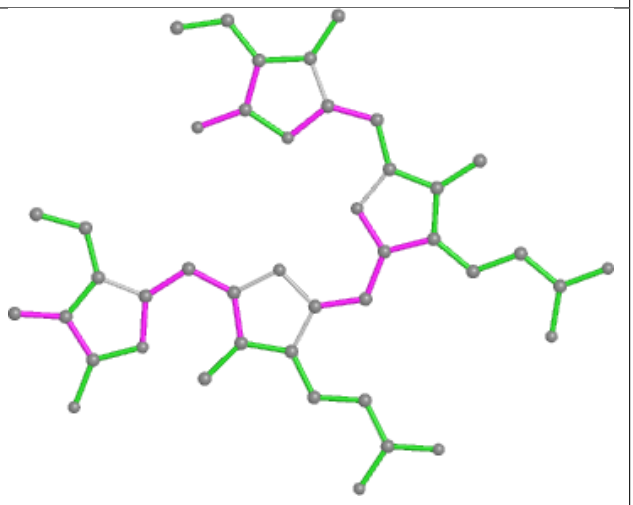

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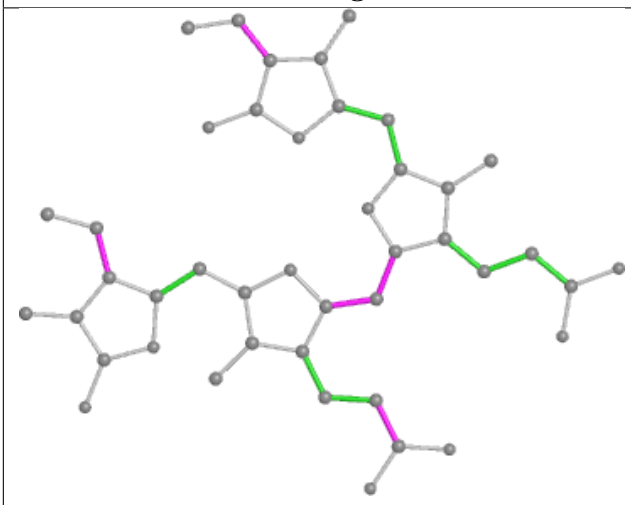

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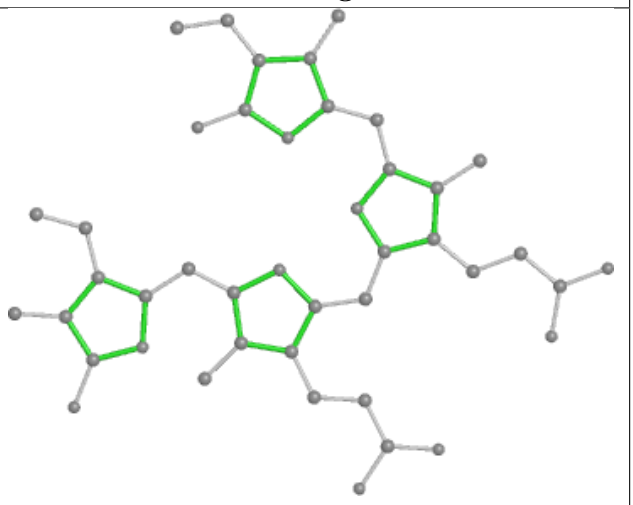

Rings

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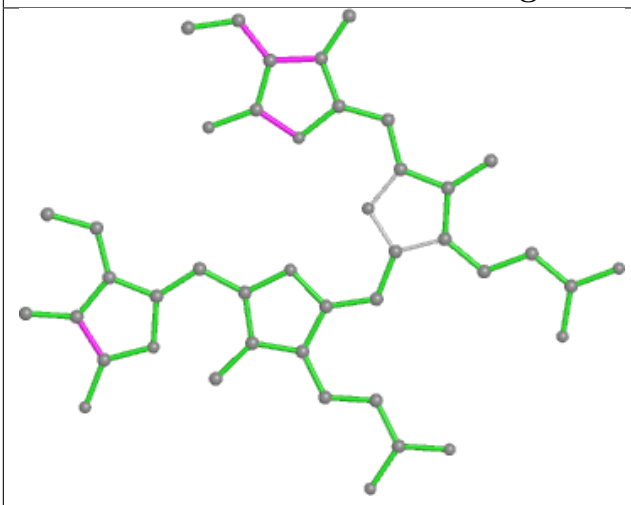

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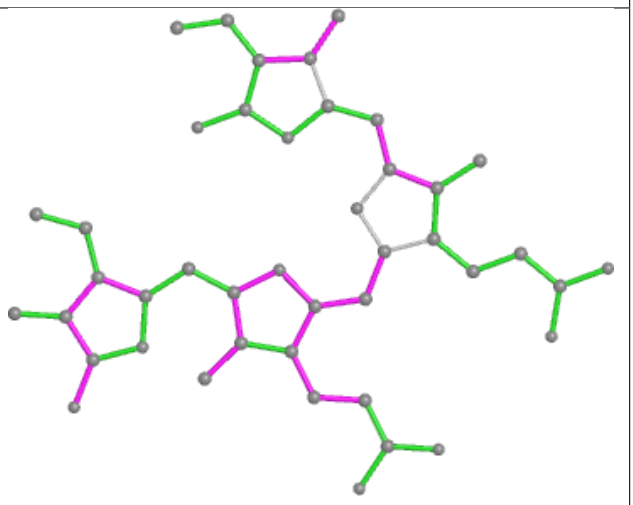

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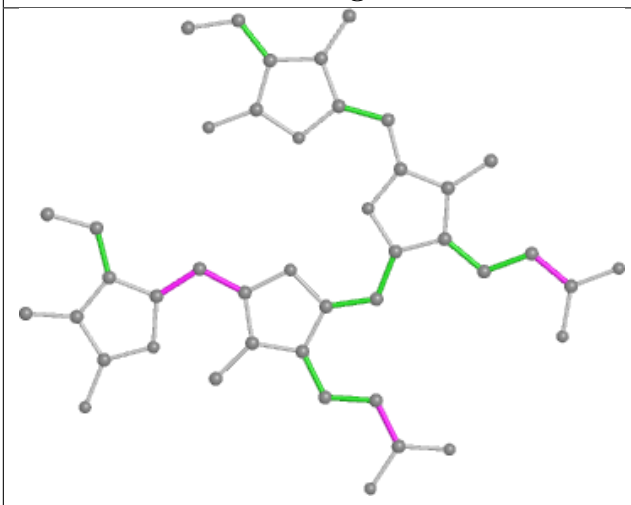

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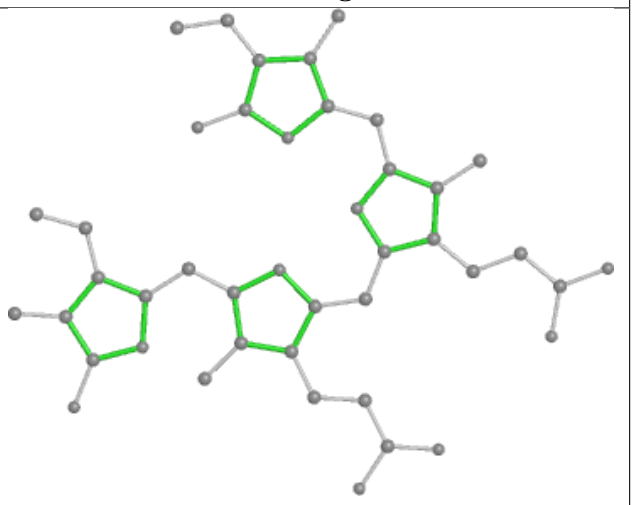

Rings

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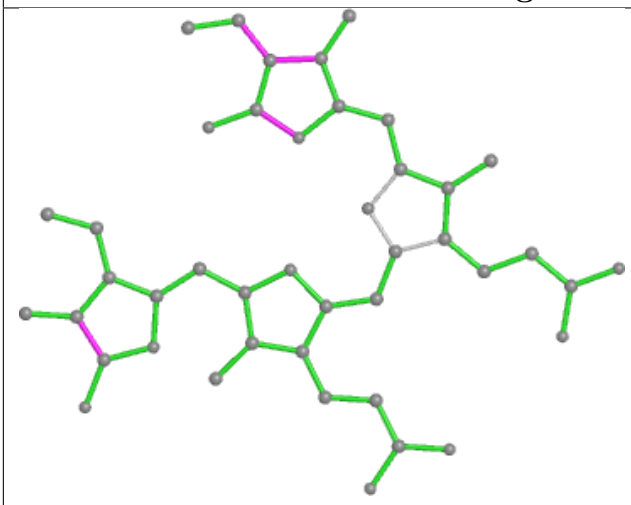

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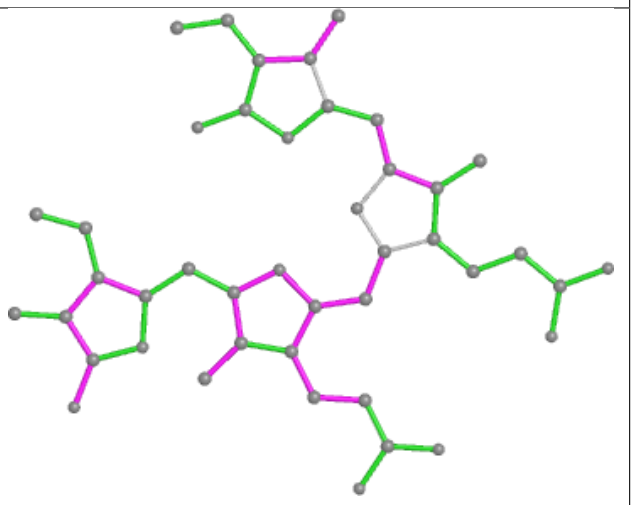

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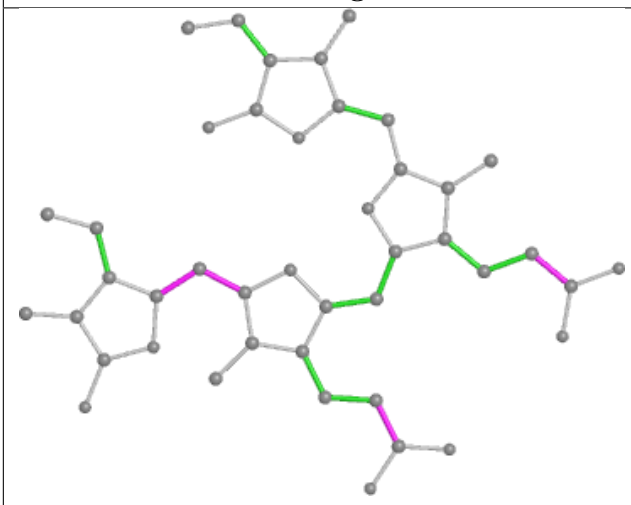

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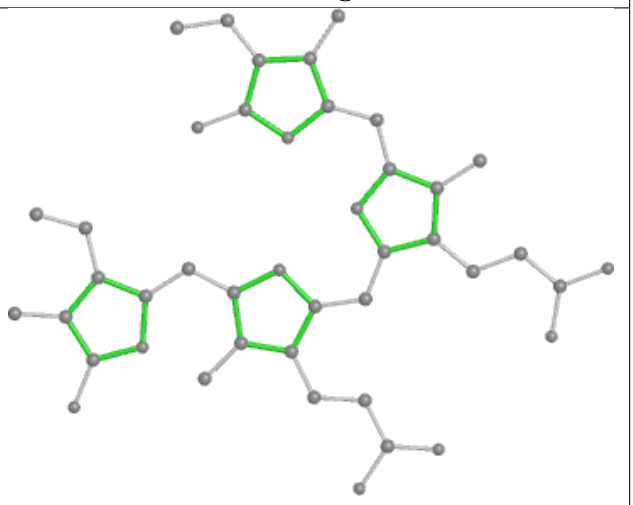

Rings

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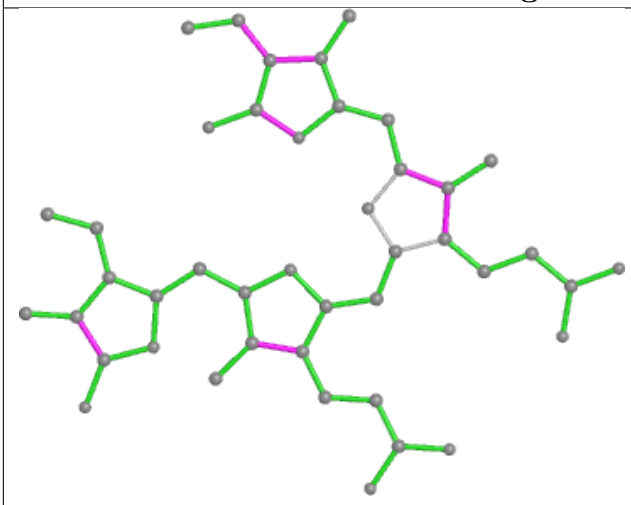

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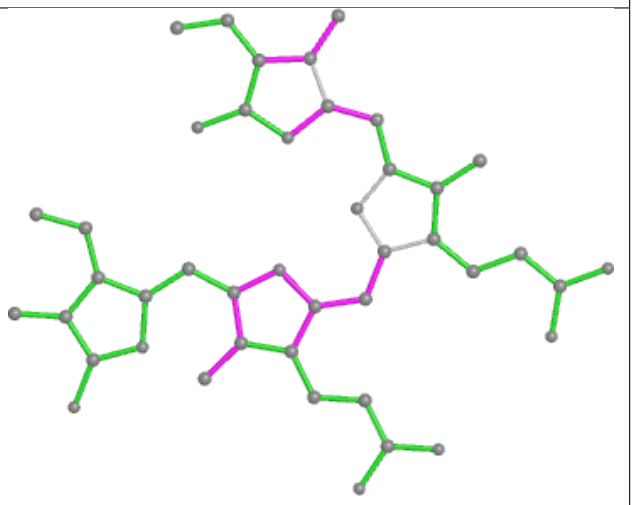

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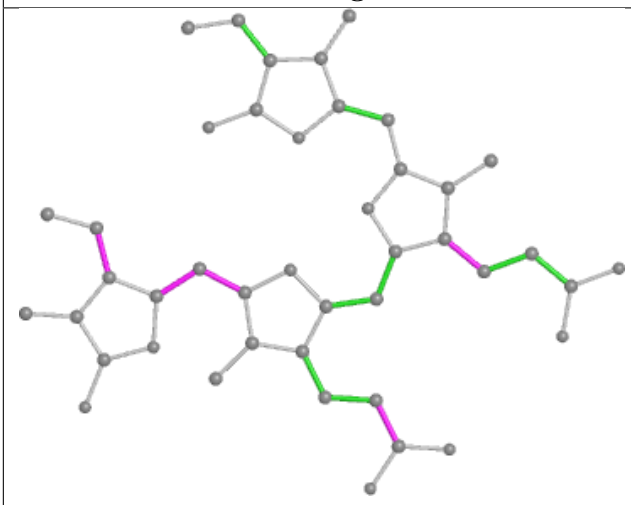

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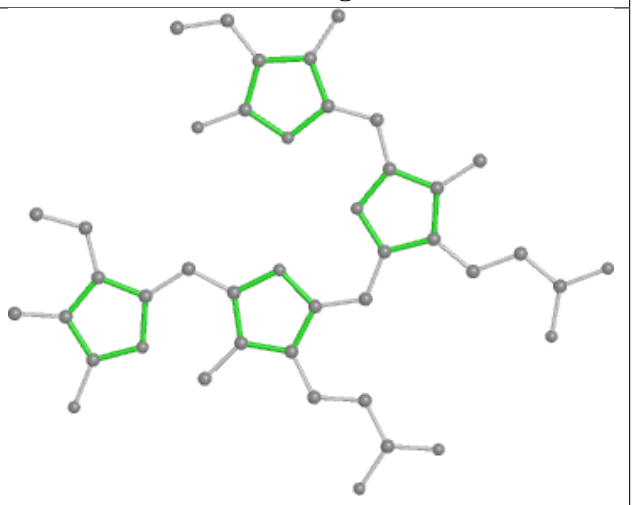

Rings

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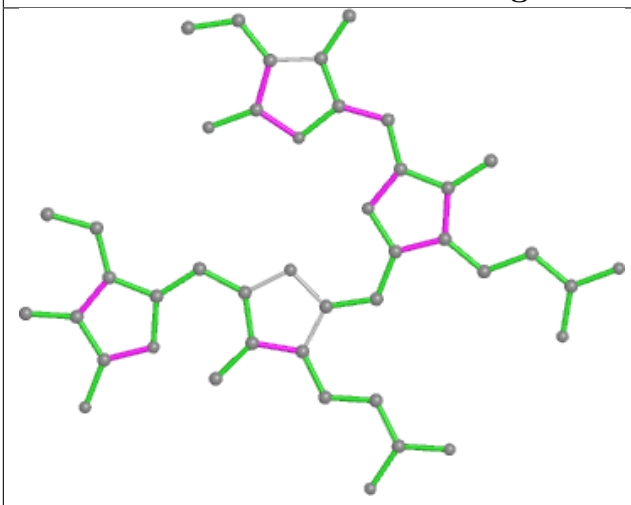

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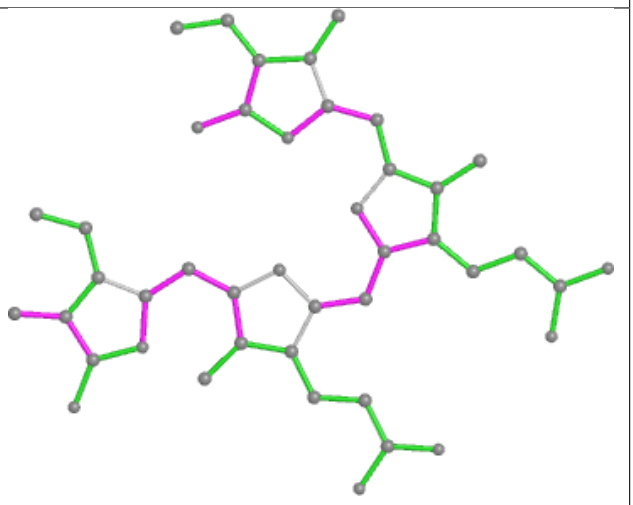

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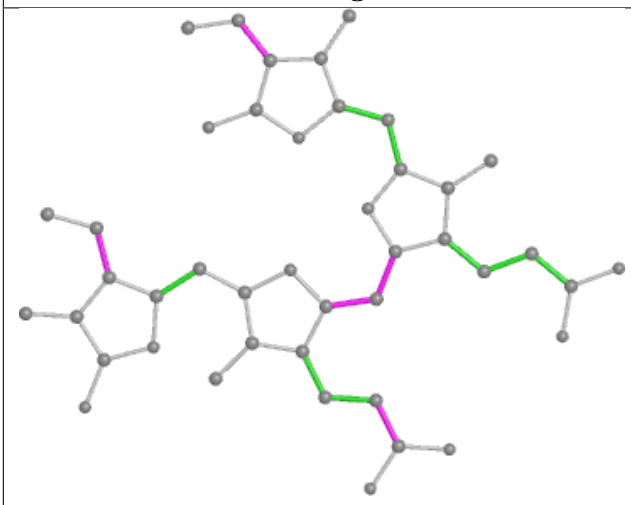

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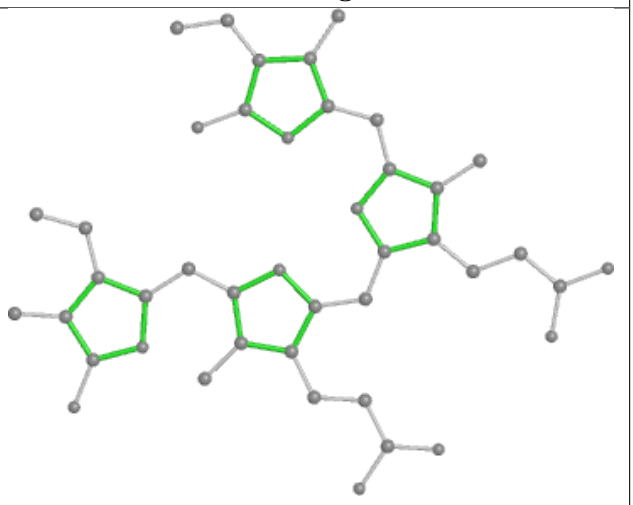

Rings

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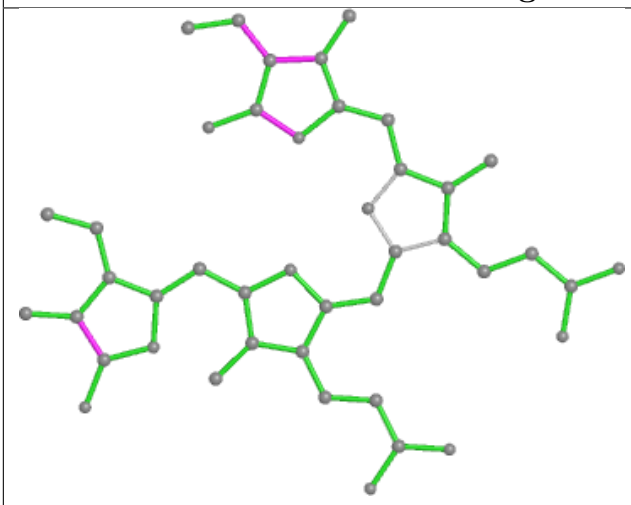

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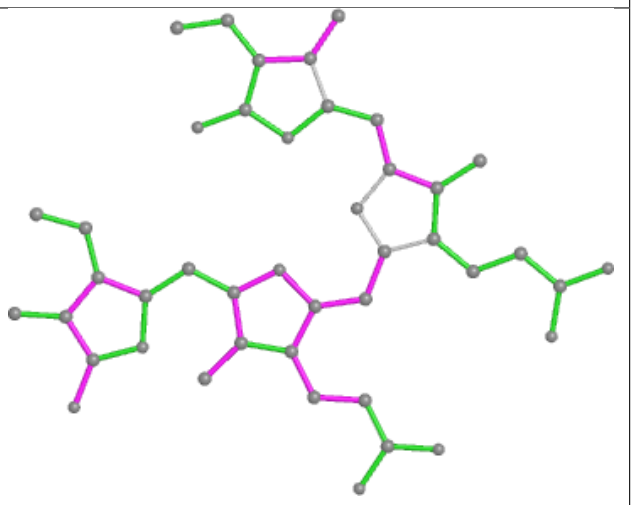

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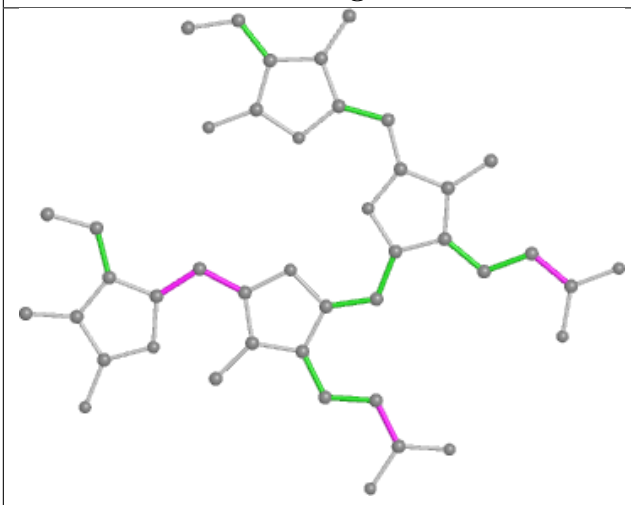

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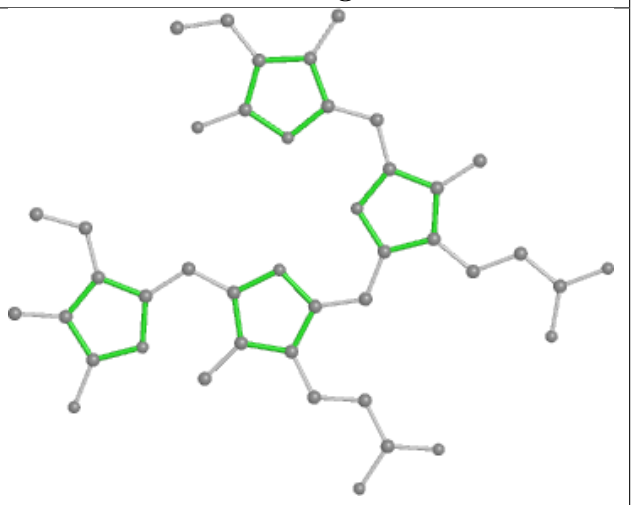
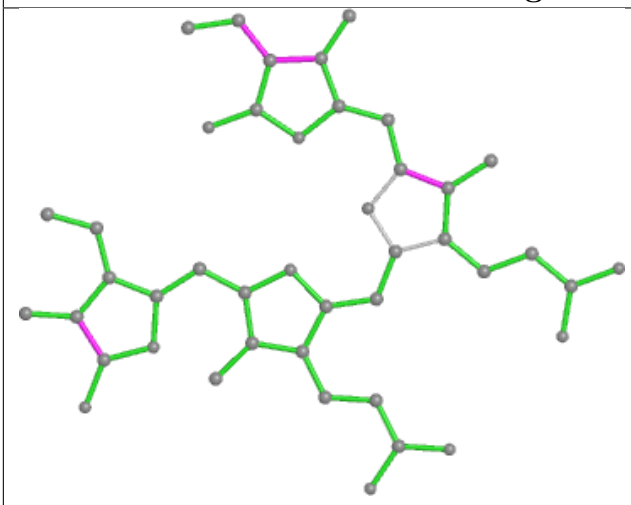


Rings

Ligand PEB fr 202



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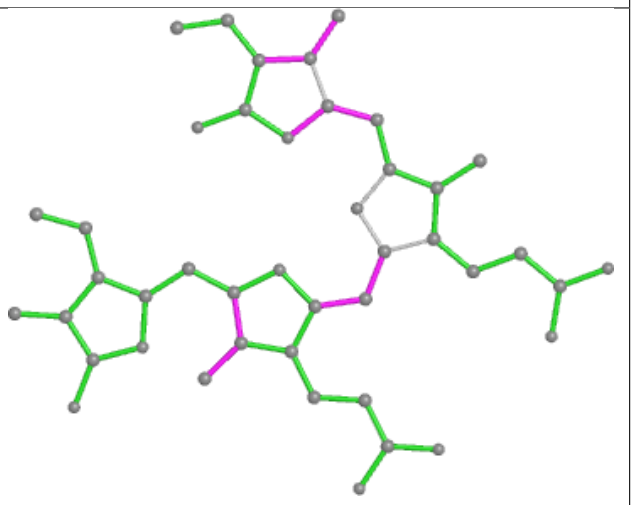

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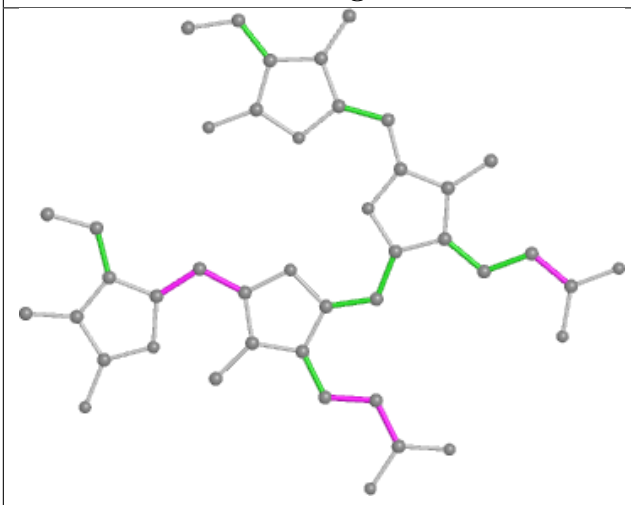

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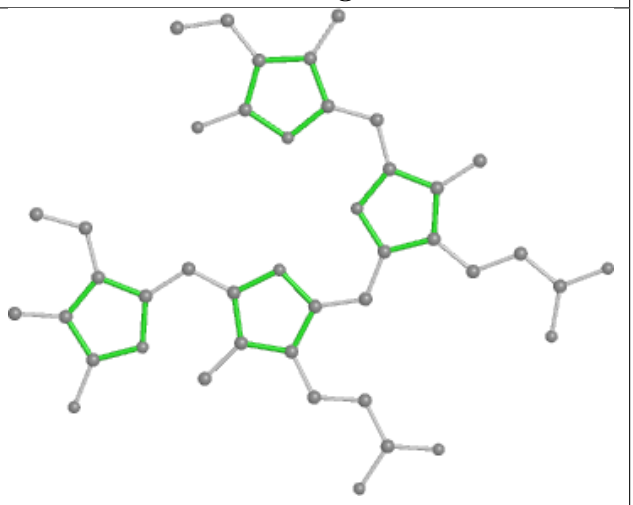
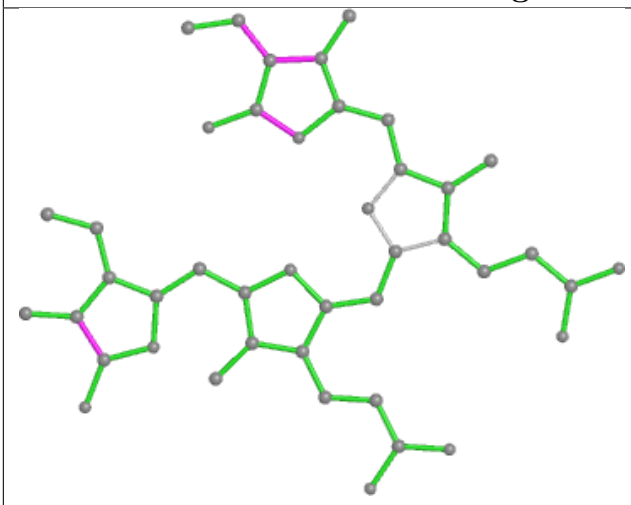


Rings

Ligand PEB bs 1002



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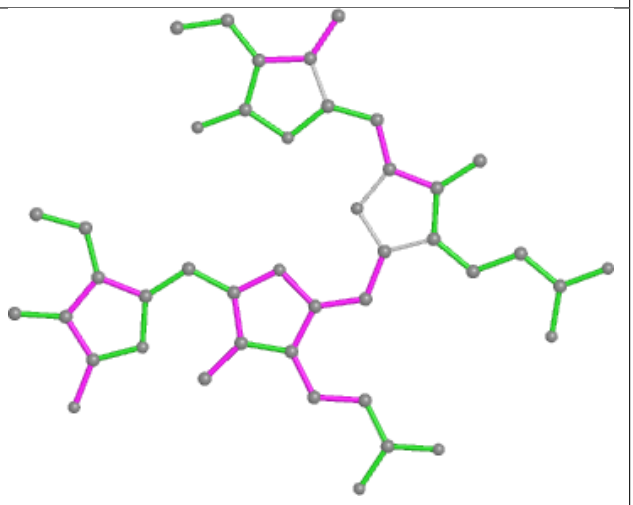
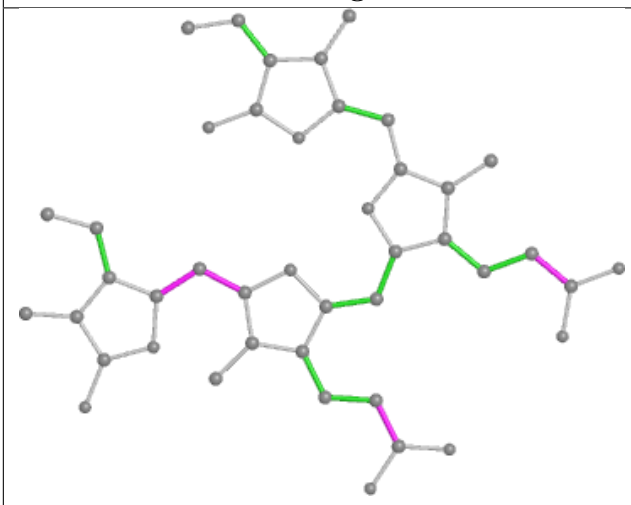


Bond angles



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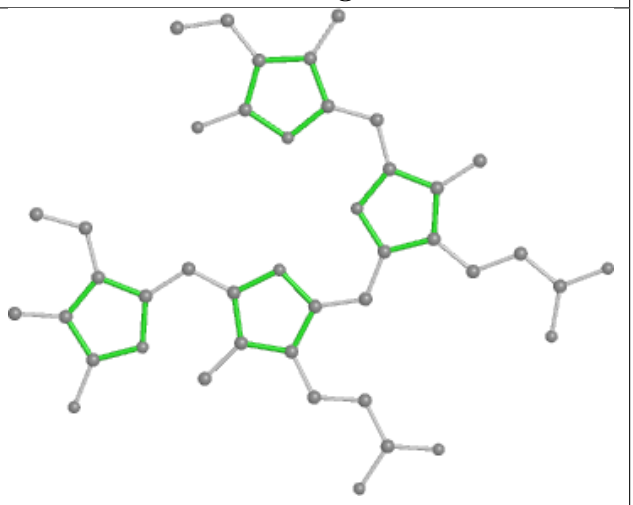
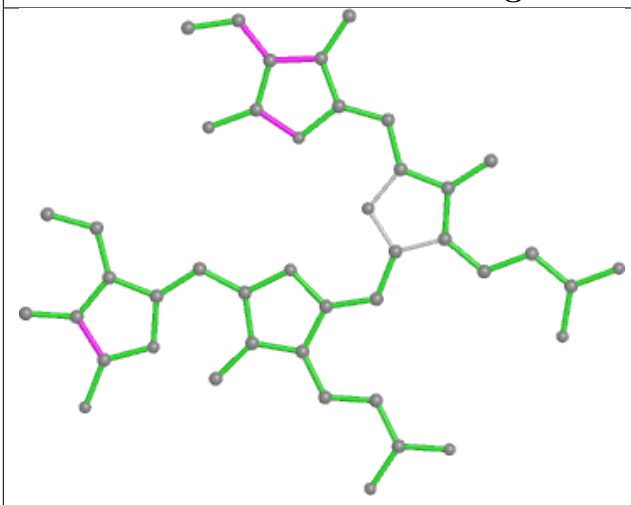


Rings

Ligand PEB gm 1001



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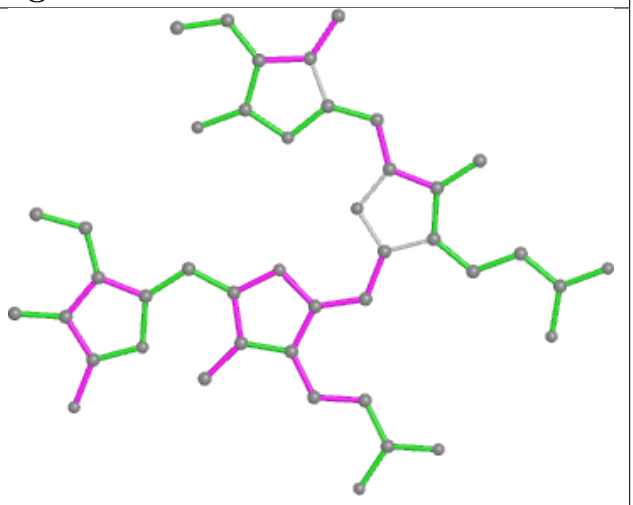

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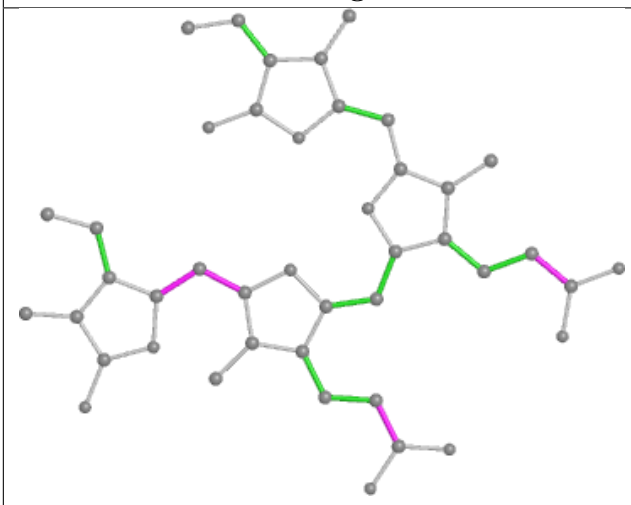

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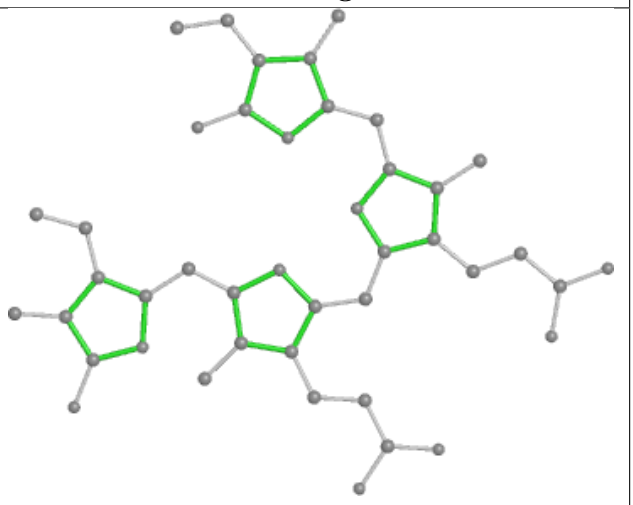
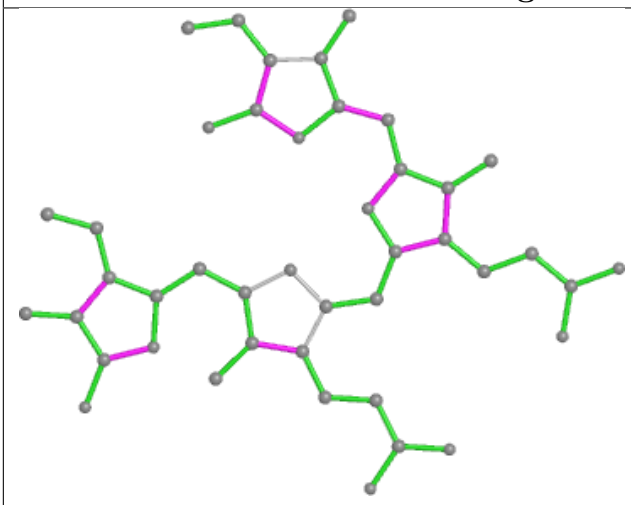


Rings

Ligand PUB x2 202



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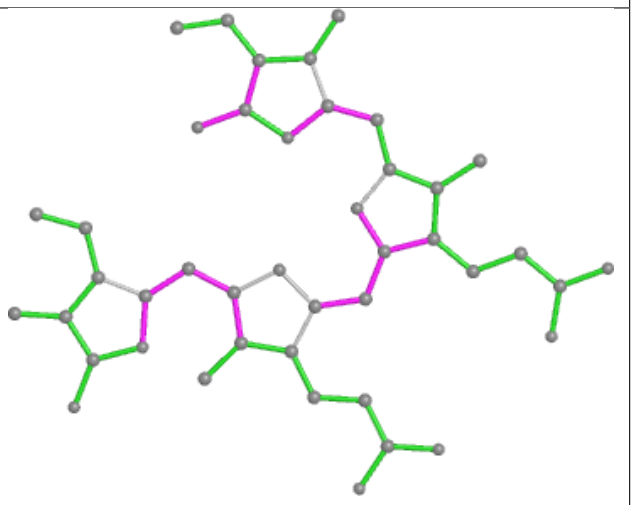
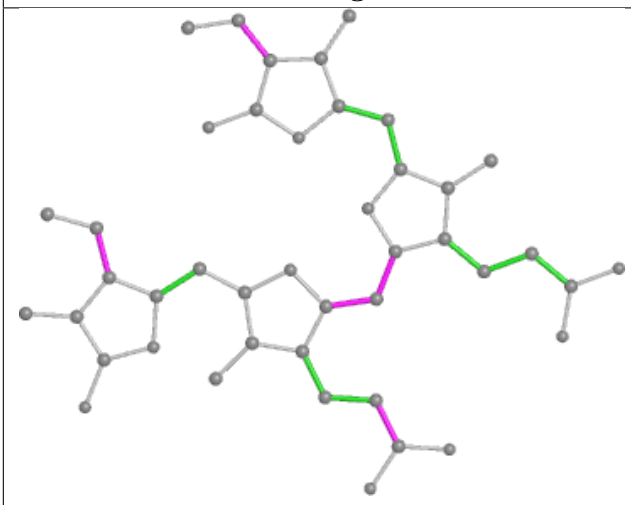
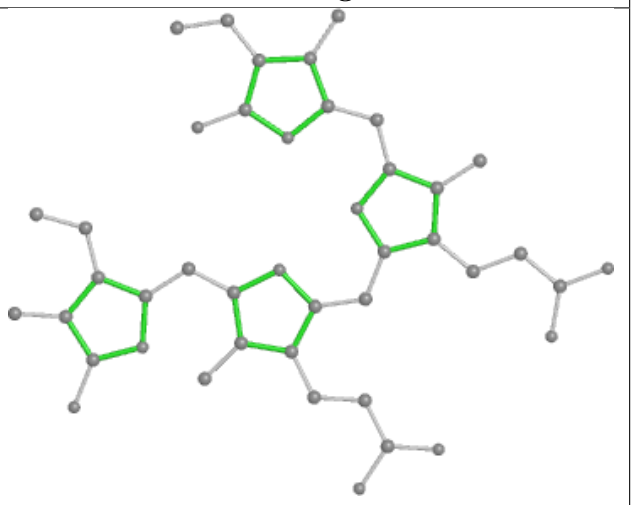


Bond angles

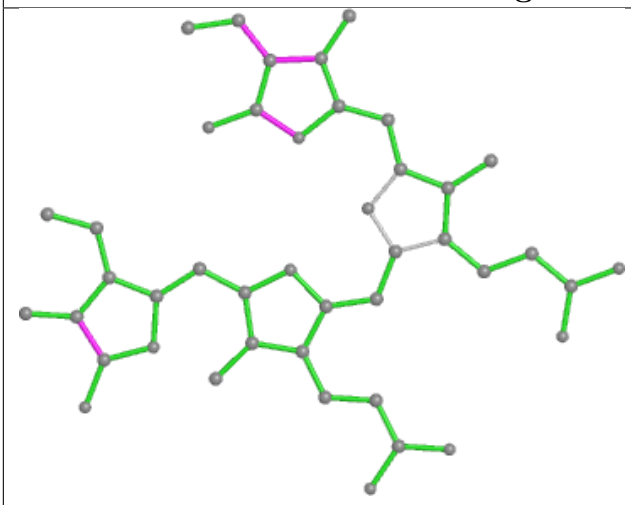


Torsions



Rings

Ligand PEB U4 202



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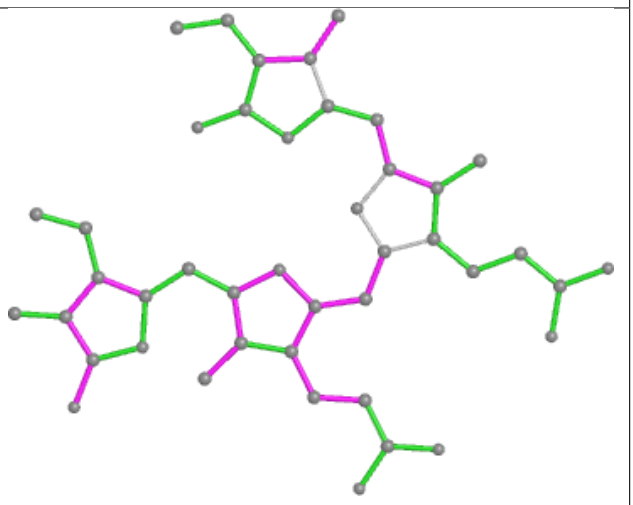

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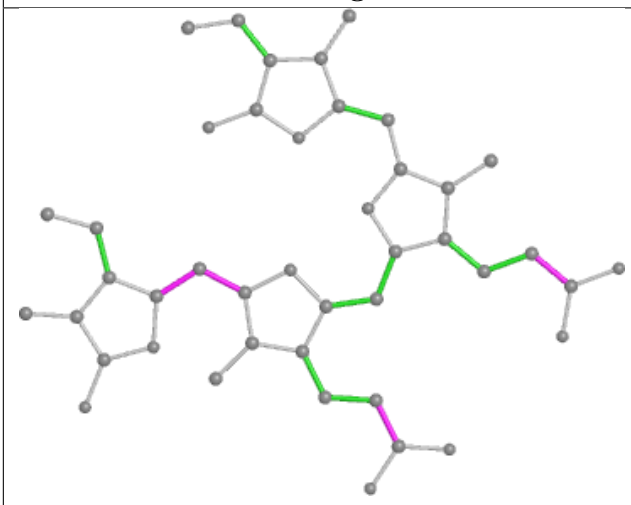

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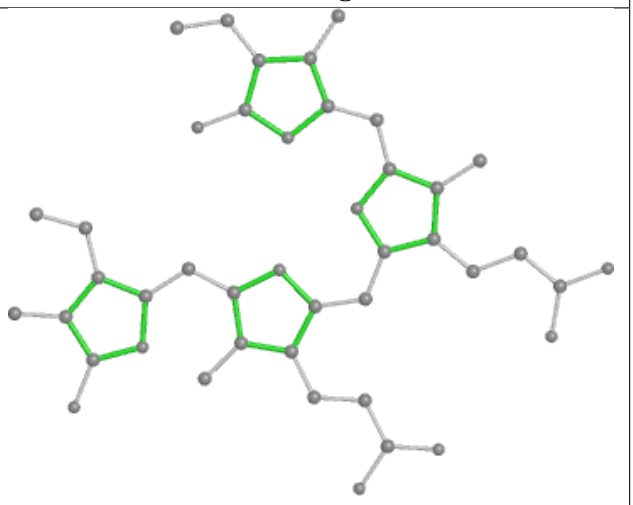
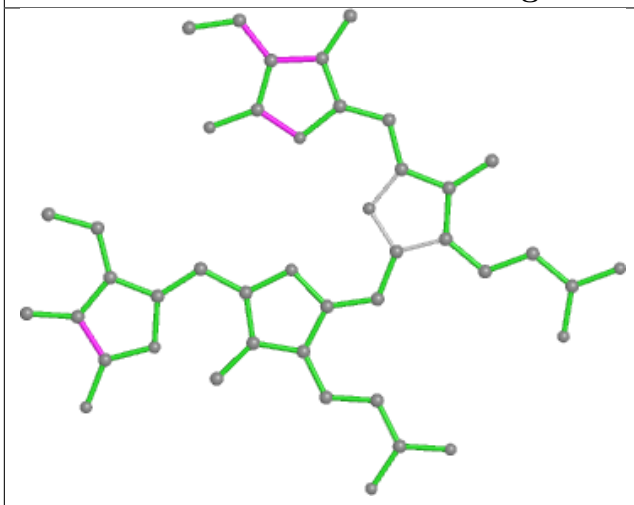


Rings

Ligand PEB dr 201



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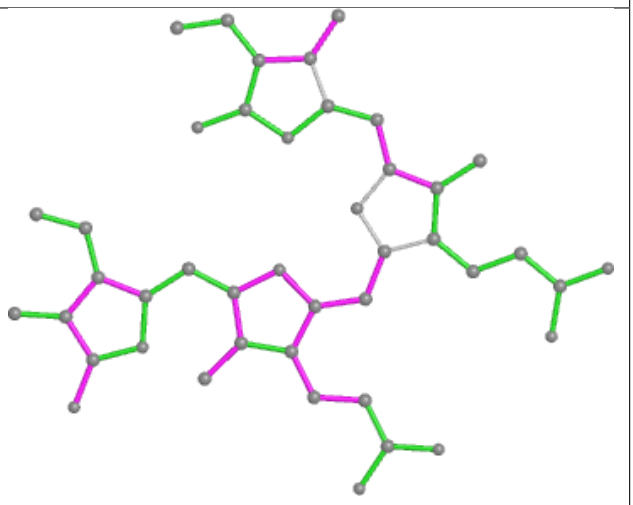

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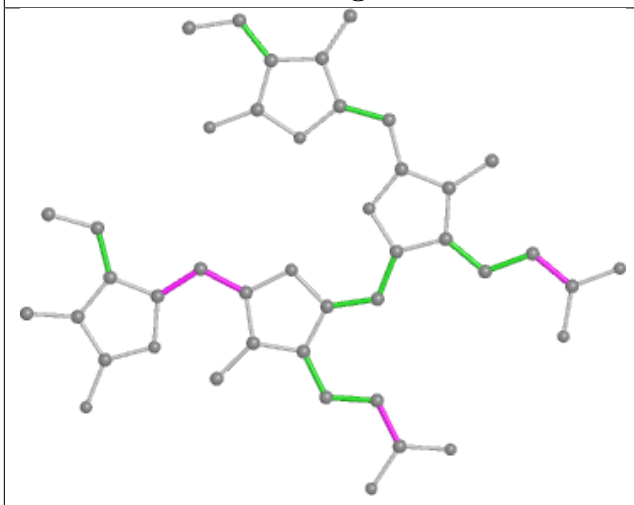

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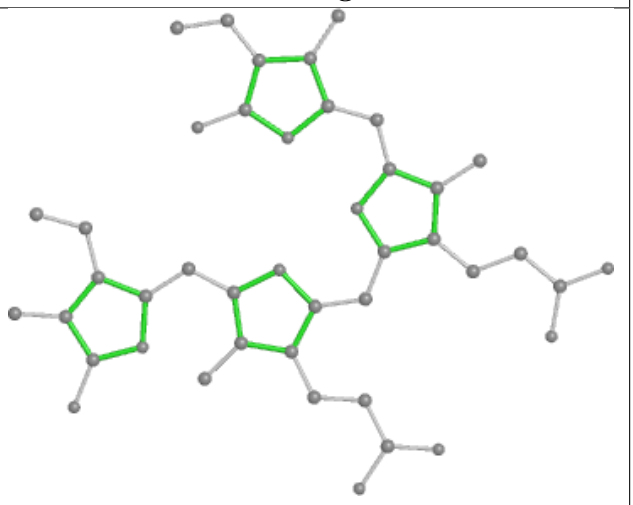

Rings

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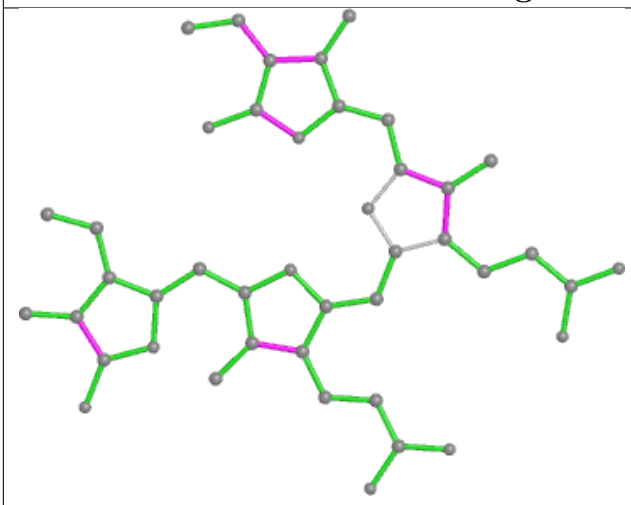

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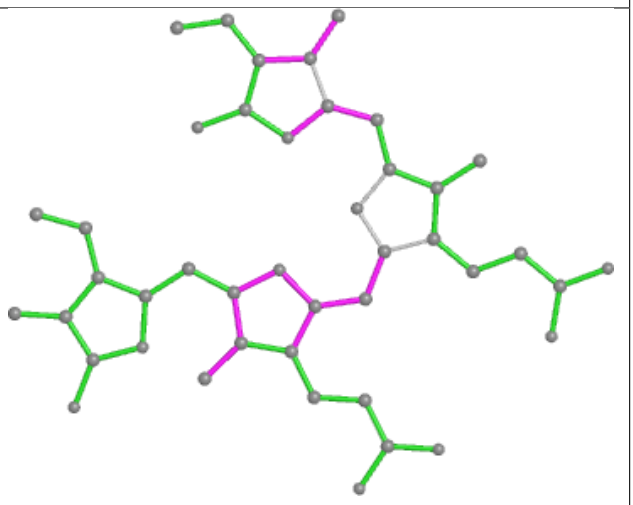

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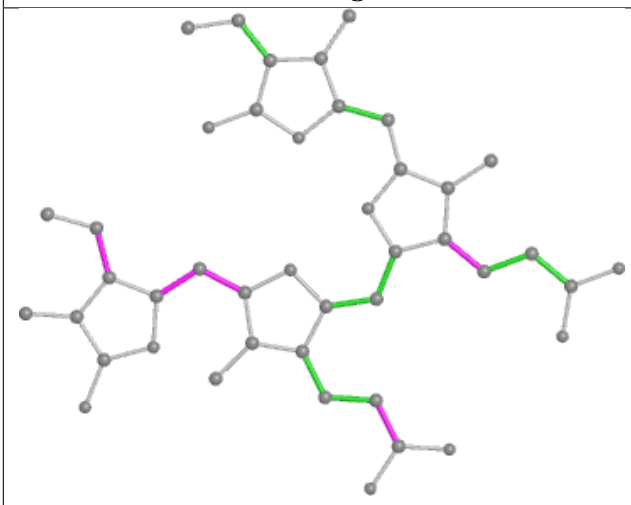

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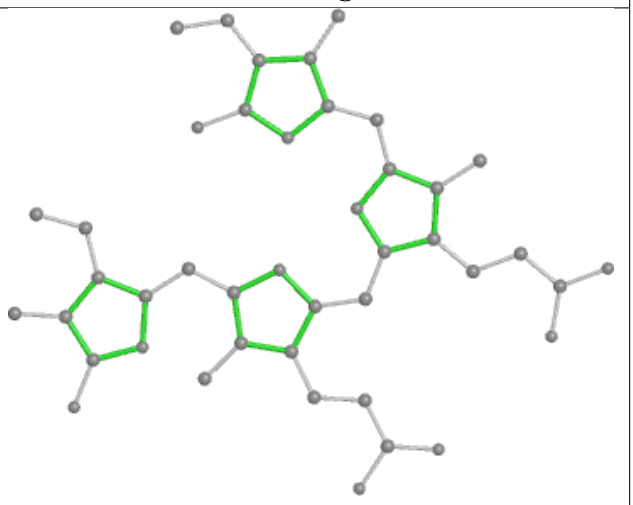
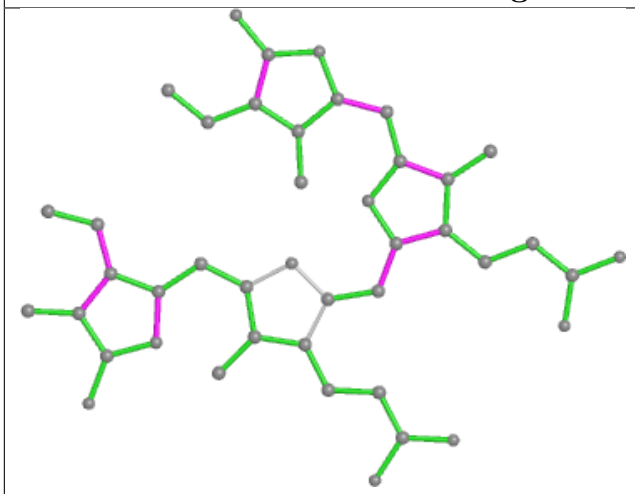


Rings

Ligand PVN ez 1004



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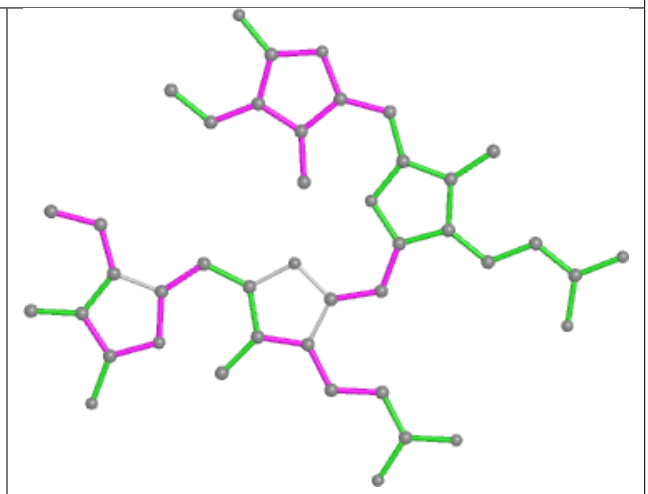

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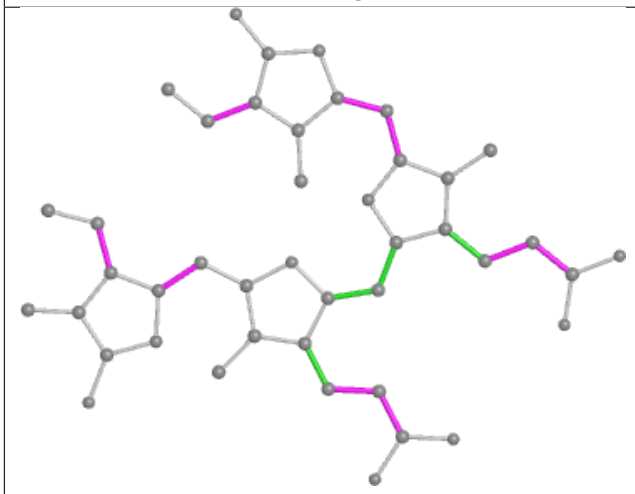

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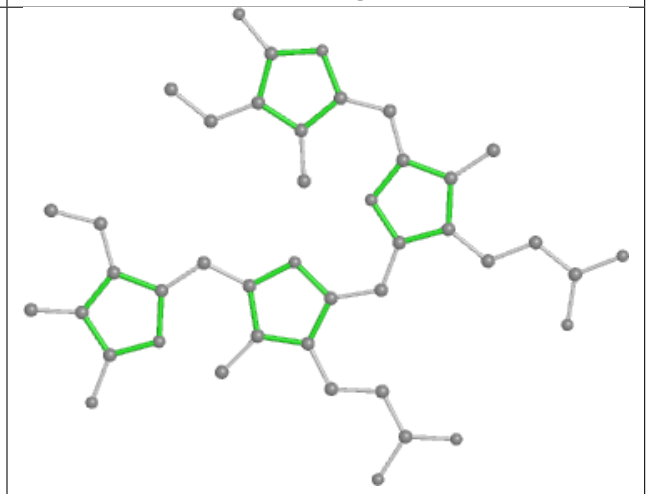

Rings

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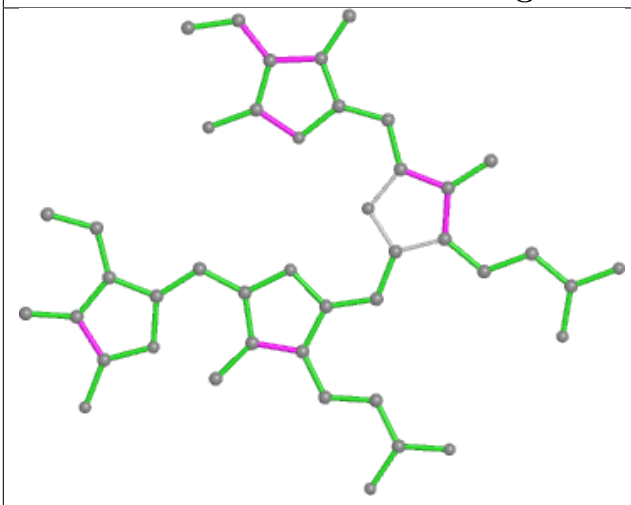

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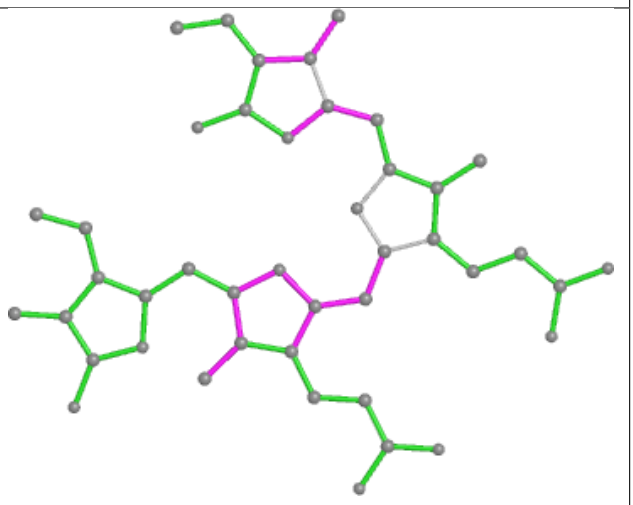

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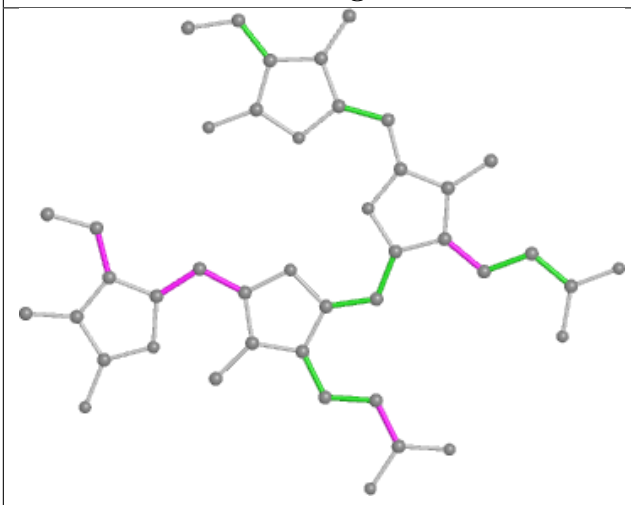

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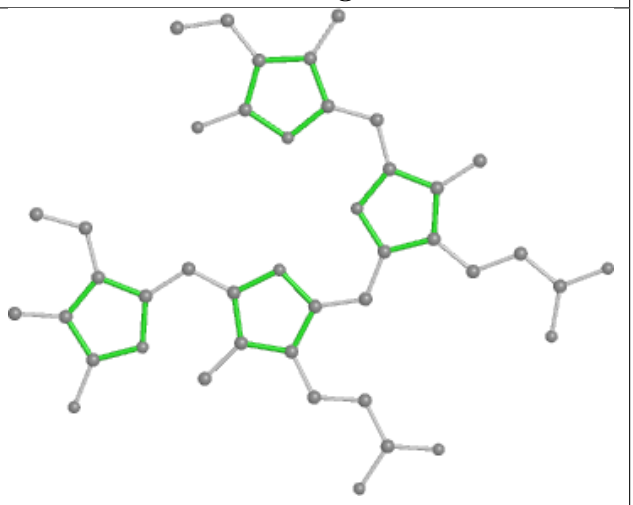

Rings

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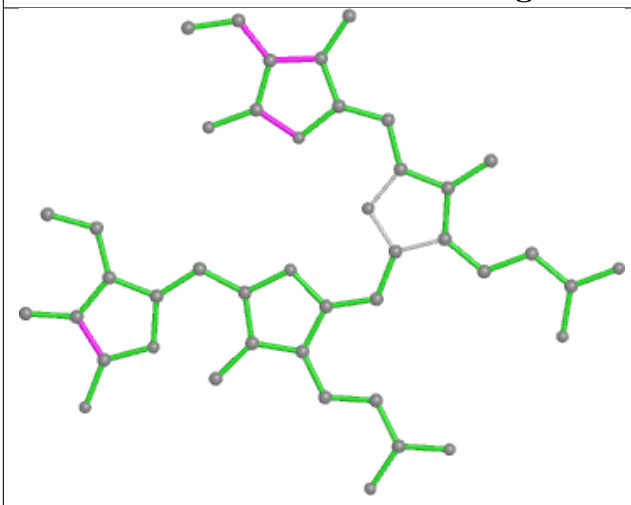

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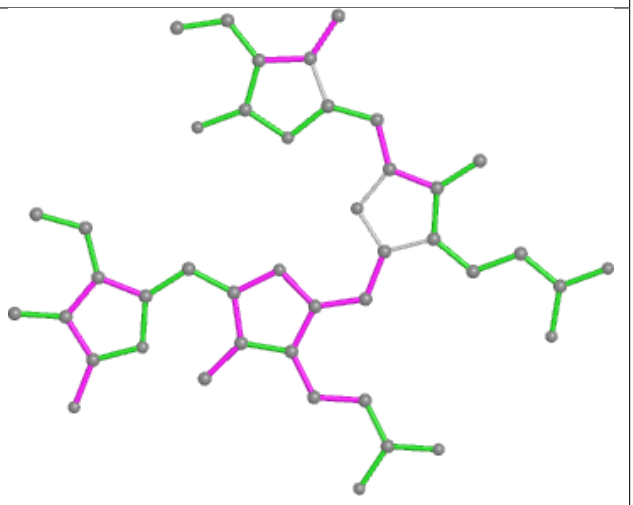

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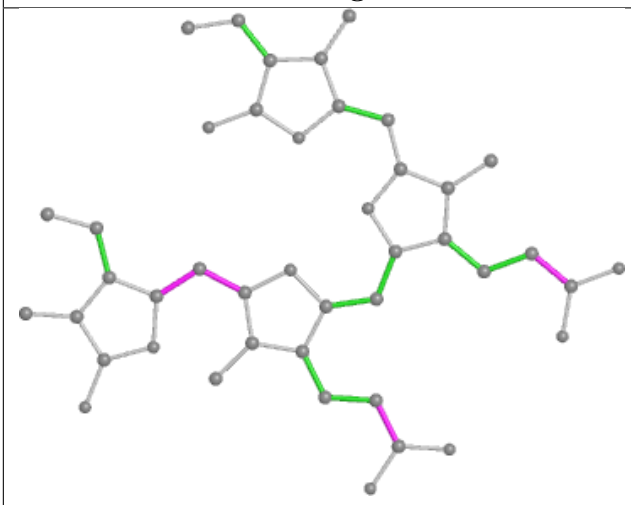

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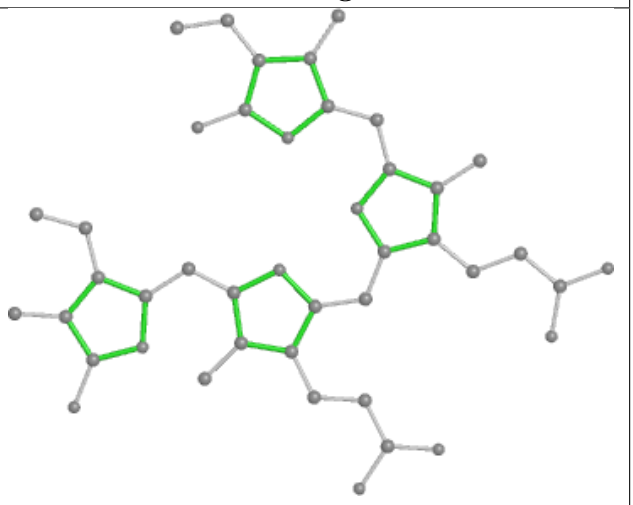

Rings

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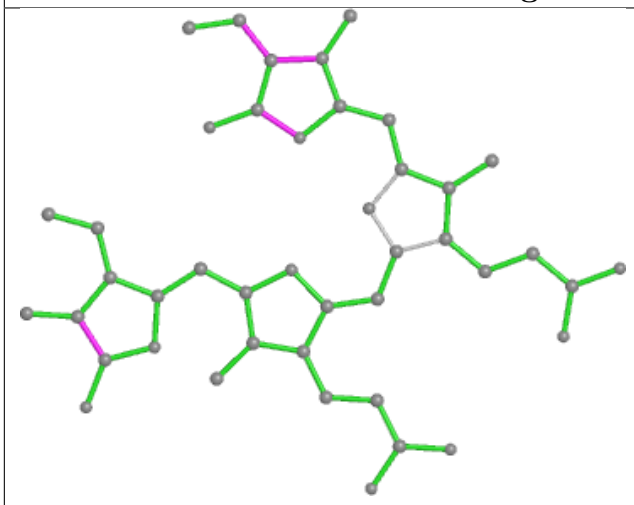

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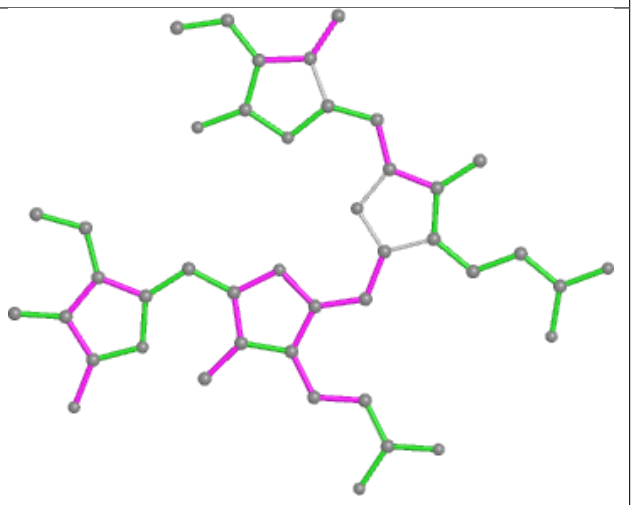

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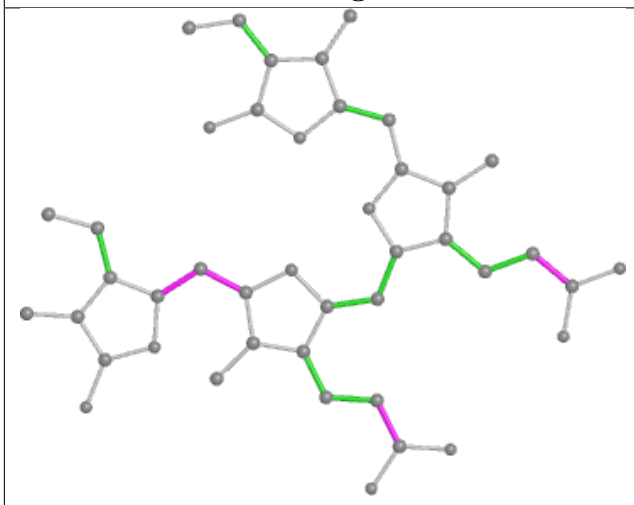

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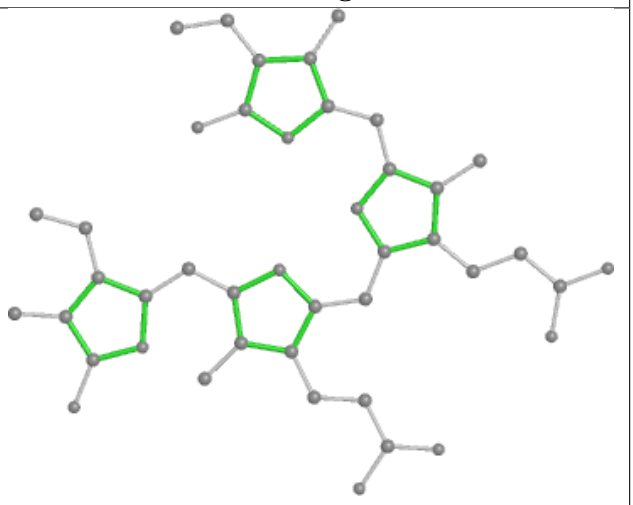

Rings

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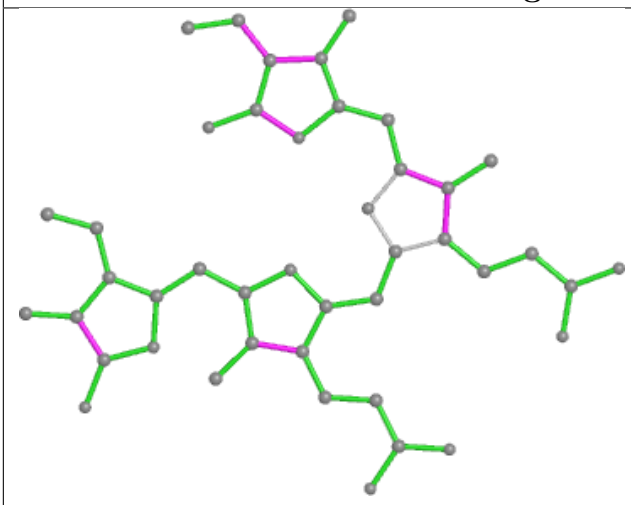

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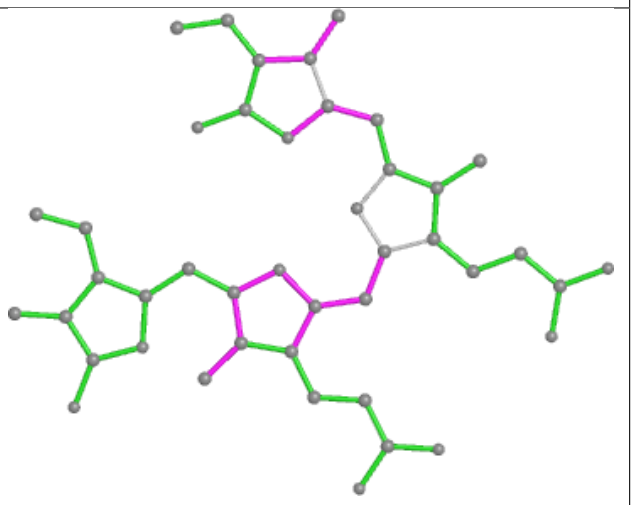

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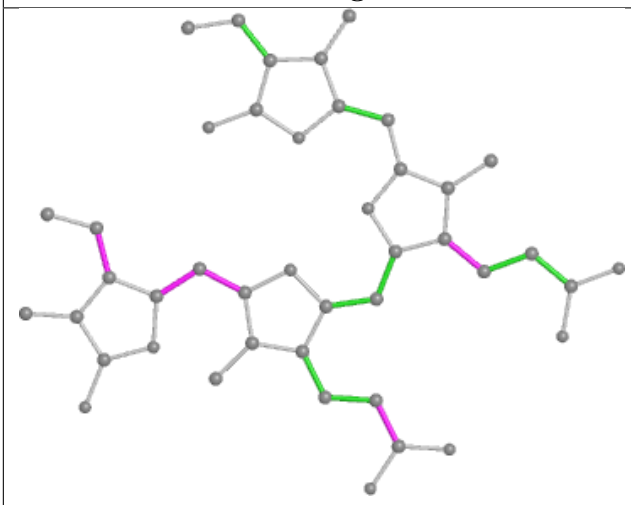

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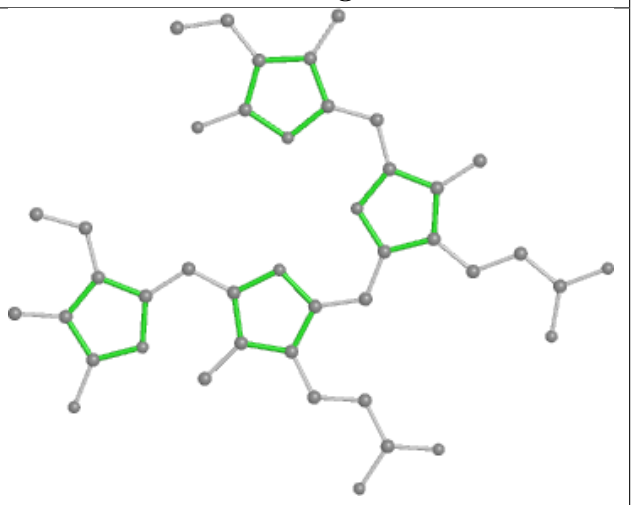

Rings

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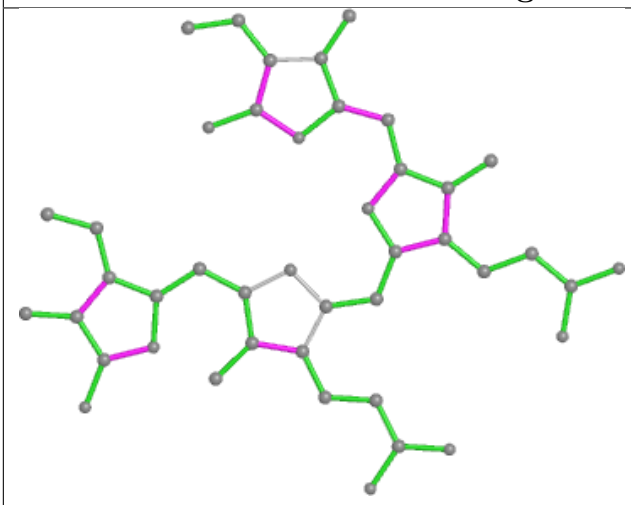

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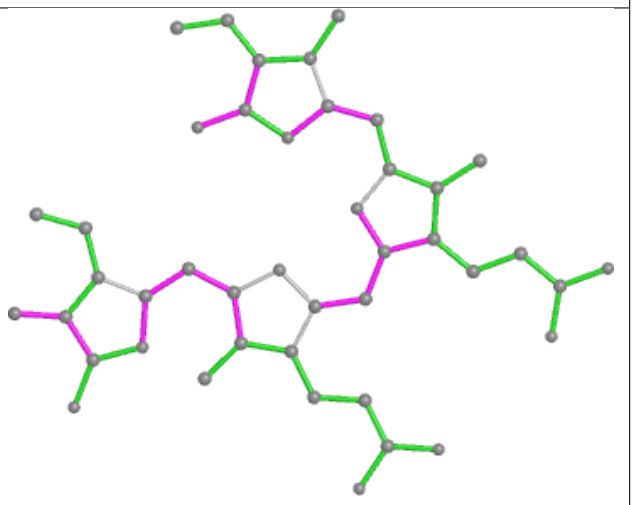

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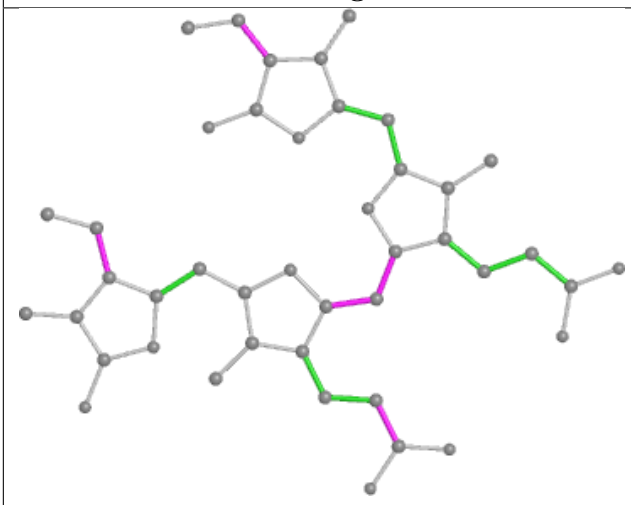

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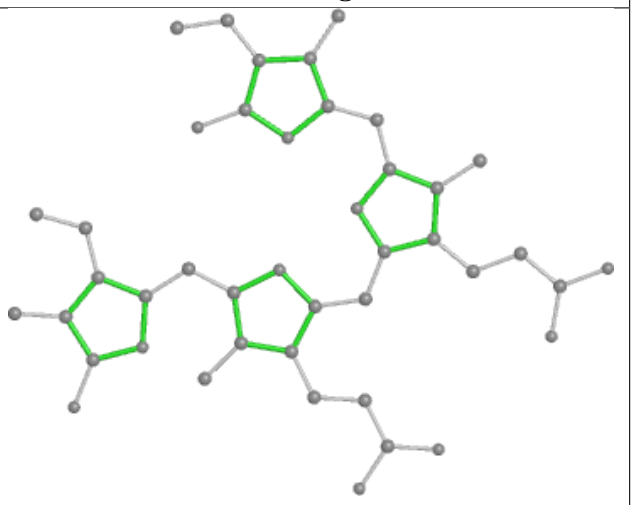

Rings

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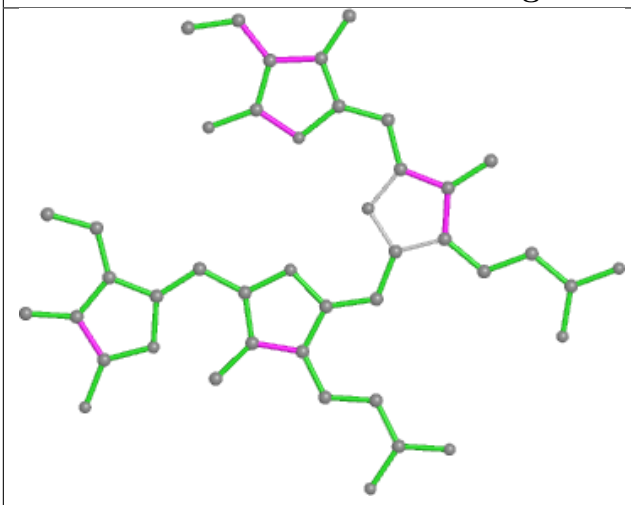

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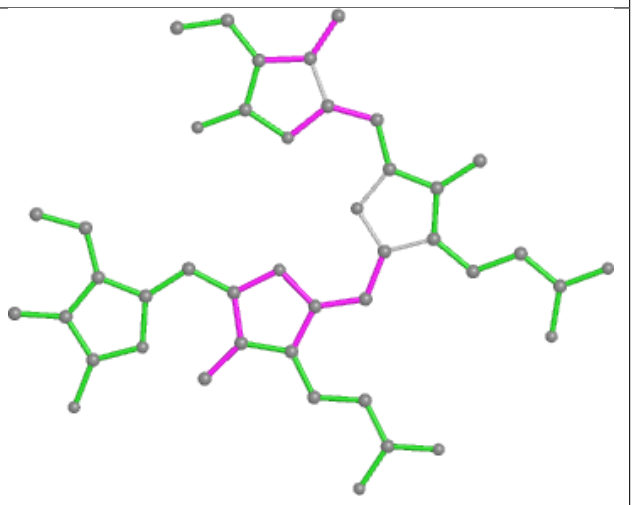

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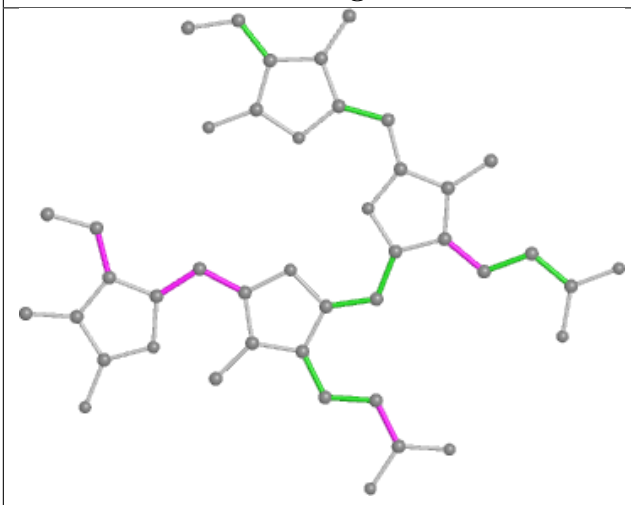

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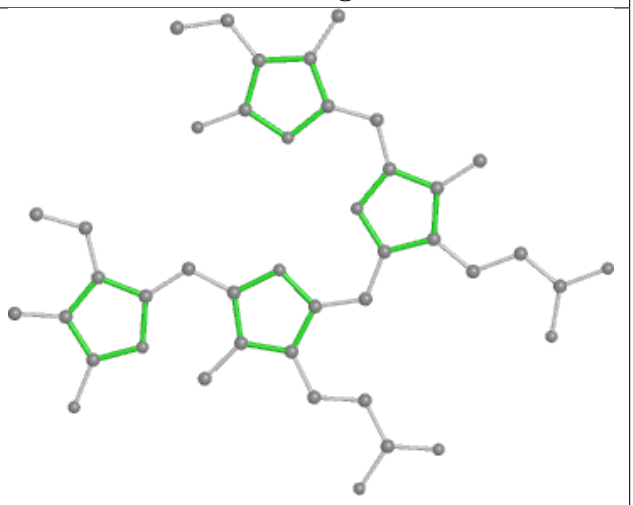
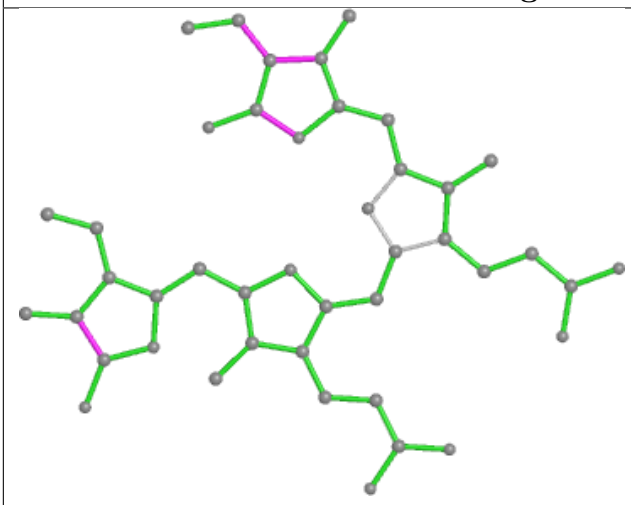


Rings

Ligand PEB ch 201



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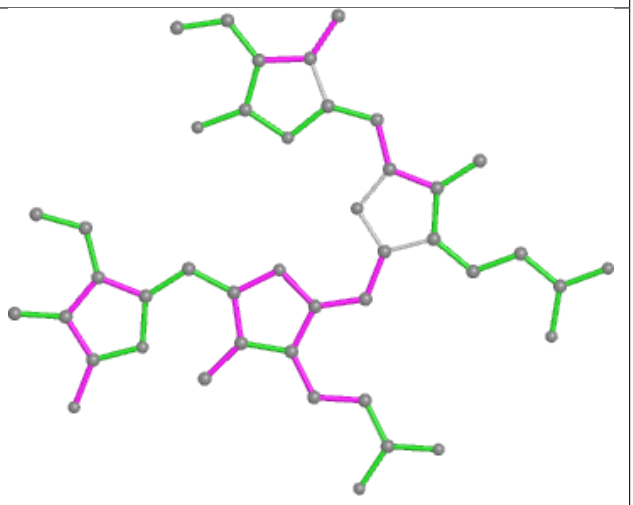

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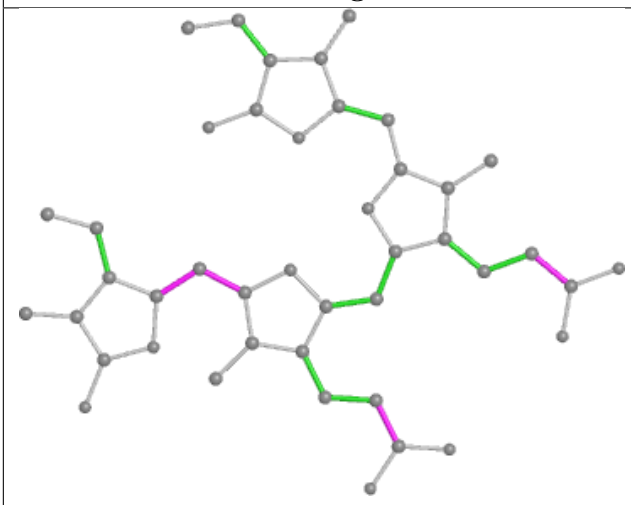

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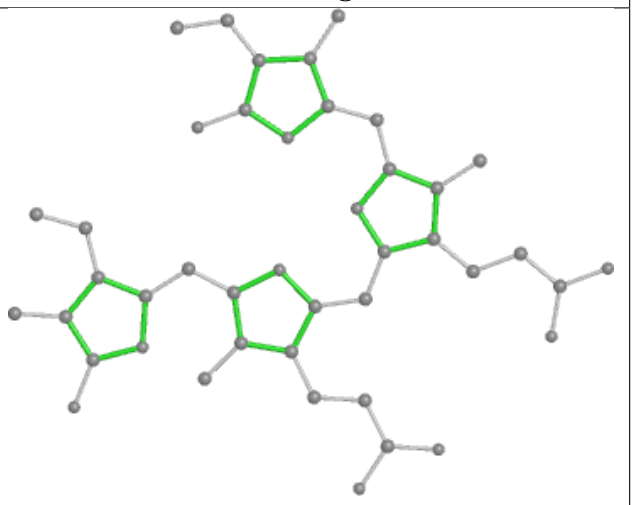
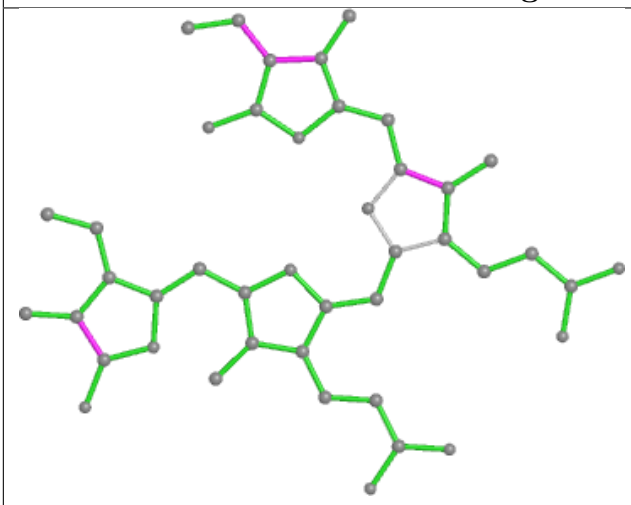


Rings

Ligand PEB bI 202



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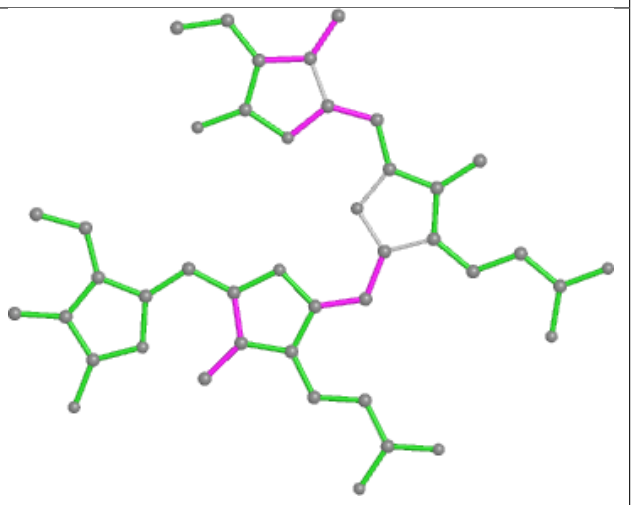

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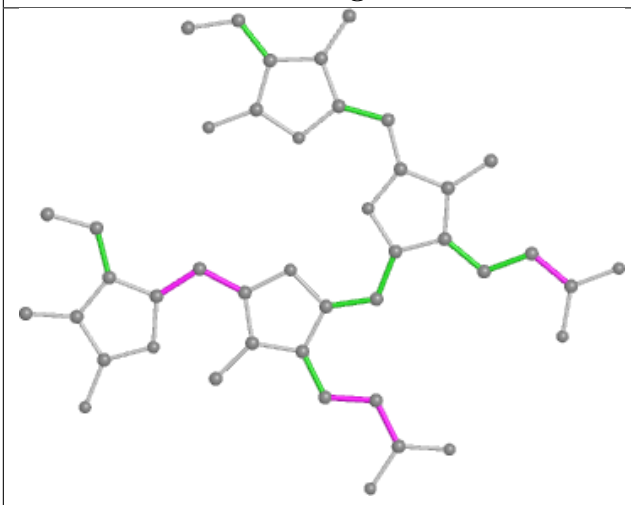

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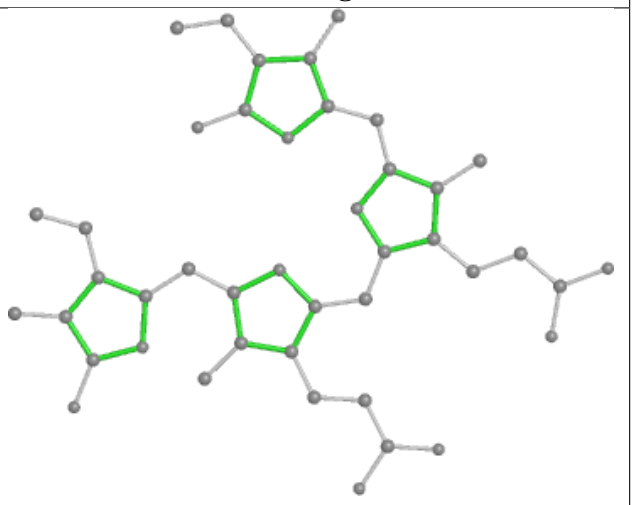
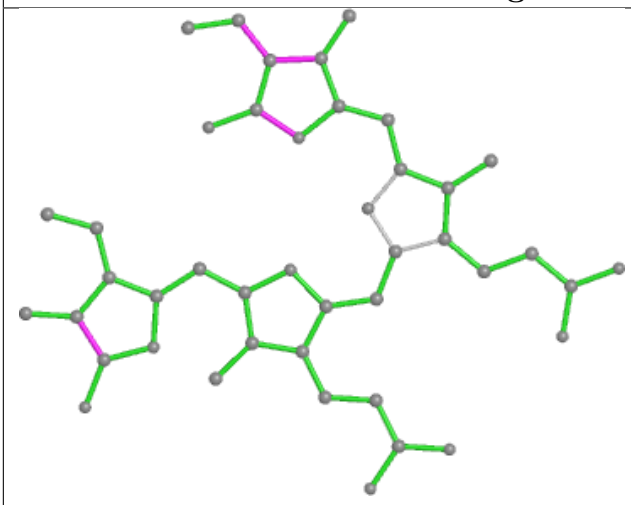


Rings

Ligand PEB kV 1001



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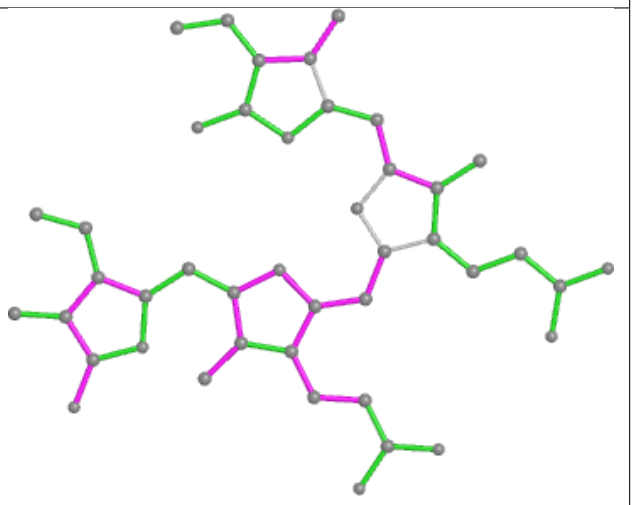

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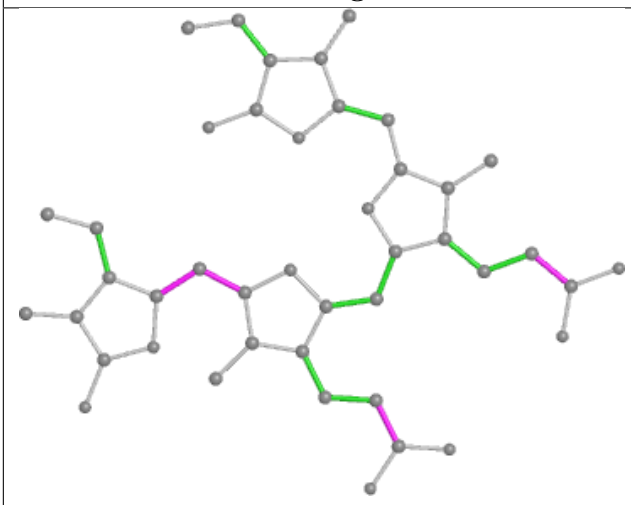
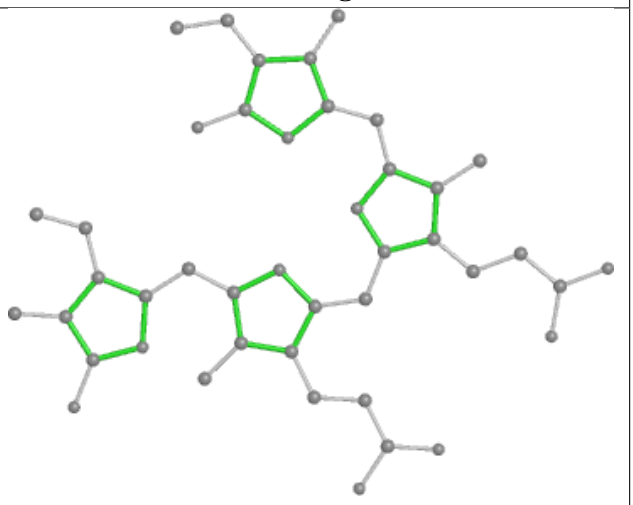
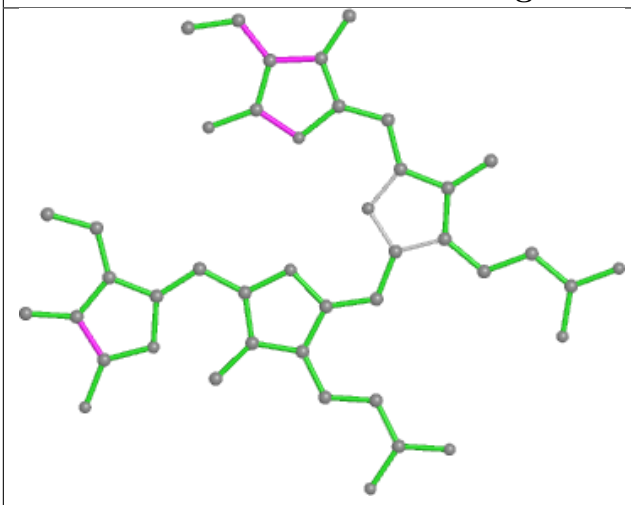


Torsions



Rings

Ligand PEB R6 201



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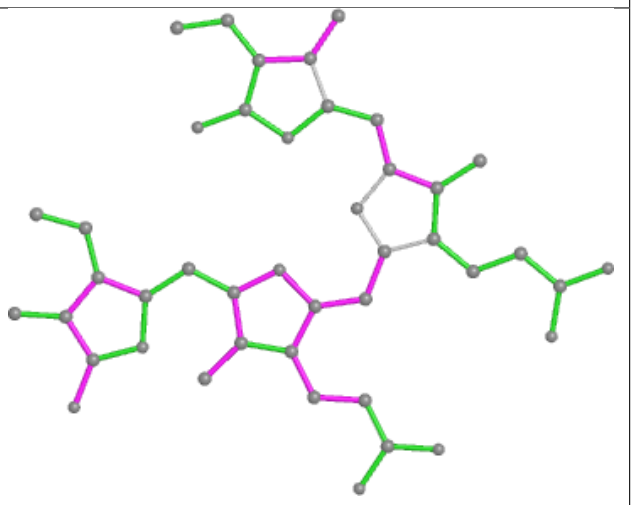

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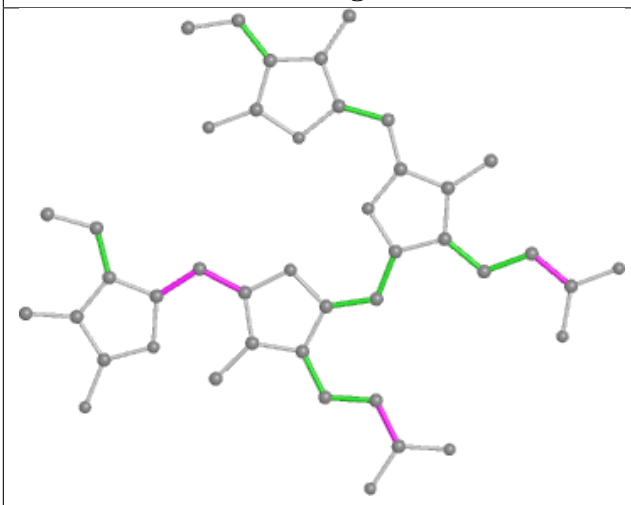

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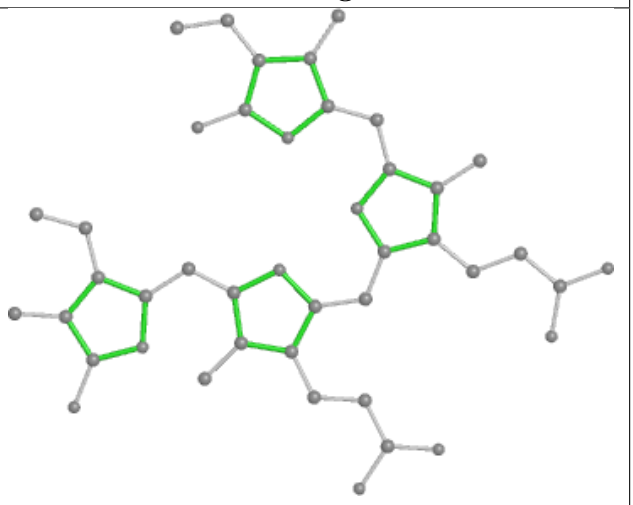
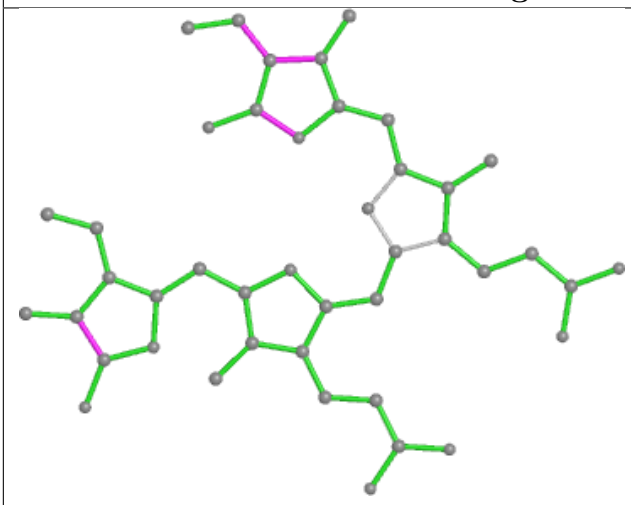


Rings

Ligand PEB ey 1003



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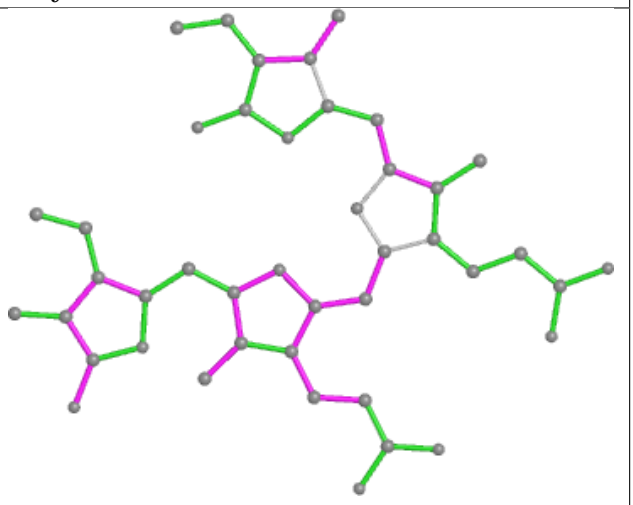

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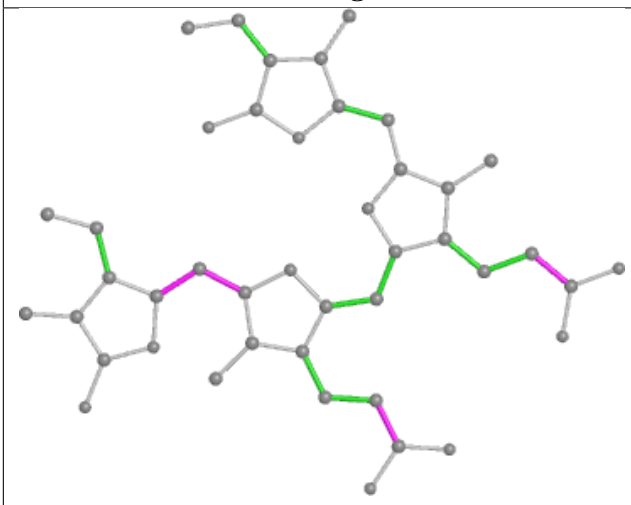

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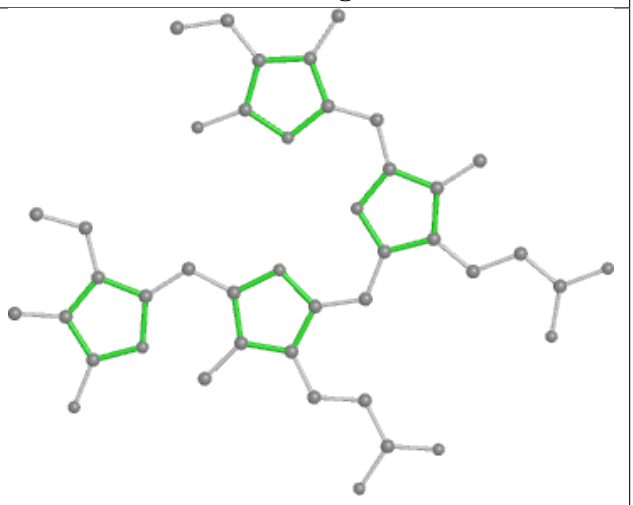
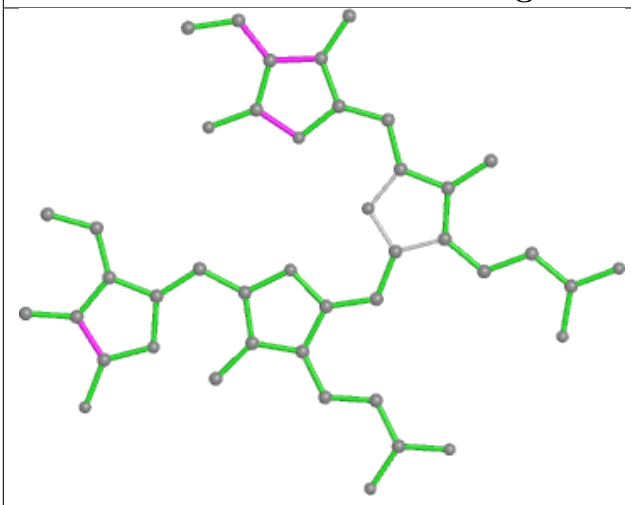


Rings

Ligand PEB w8 202



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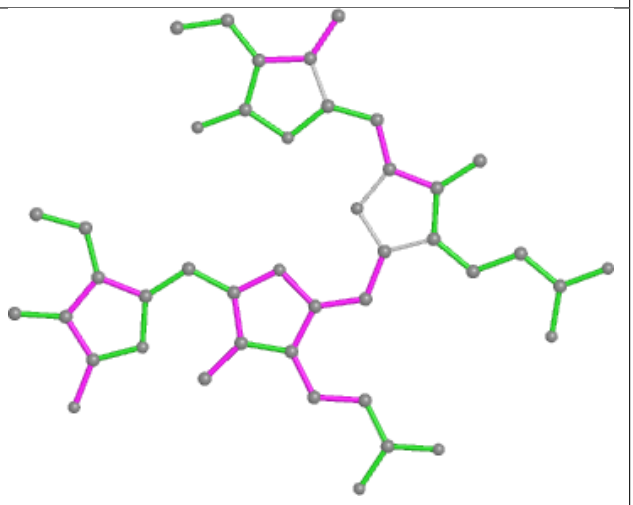

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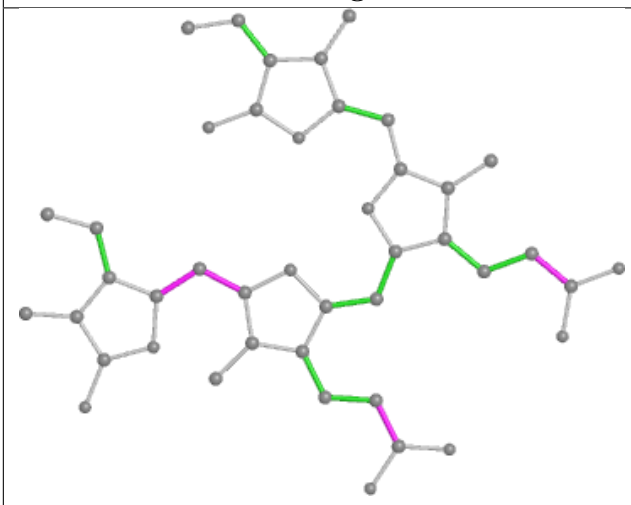

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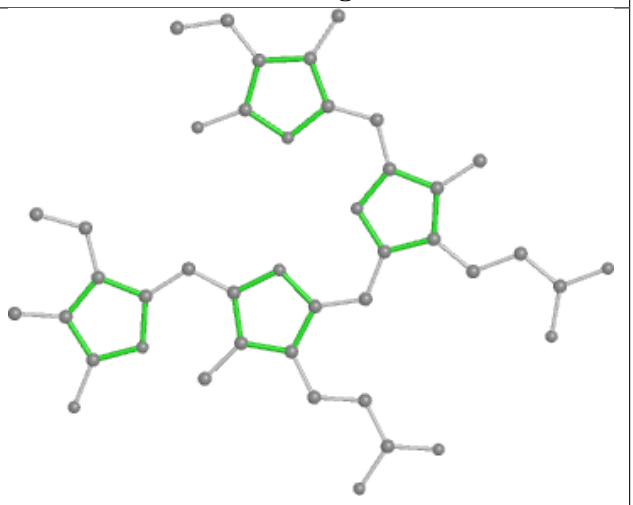
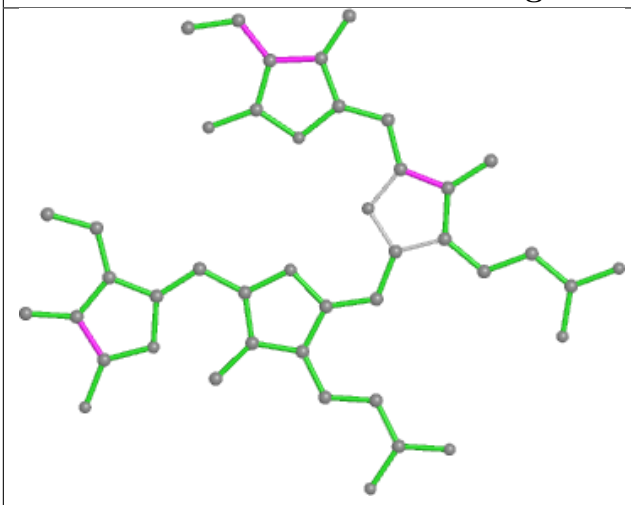


Rings

Ligand PEB ft 202



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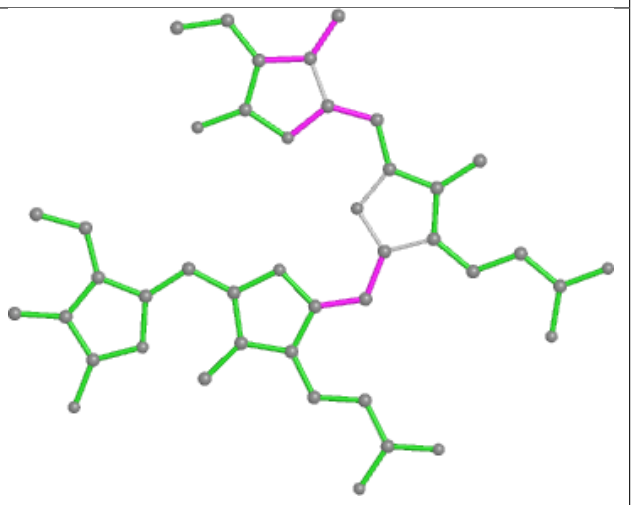

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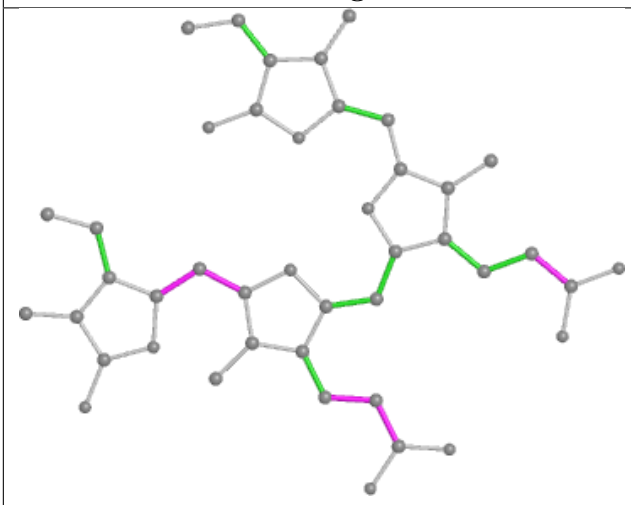

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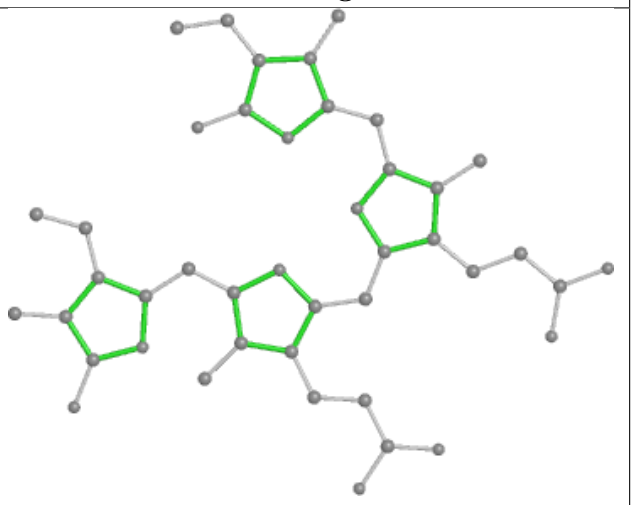
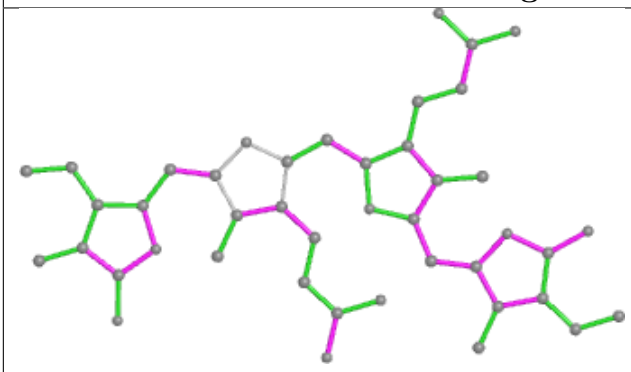


Rings

Ligand CYC j1 201



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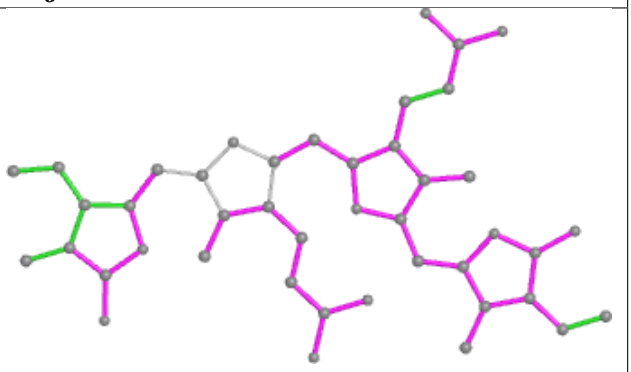

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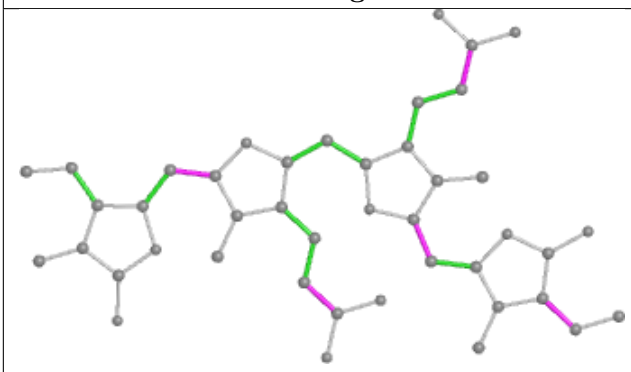

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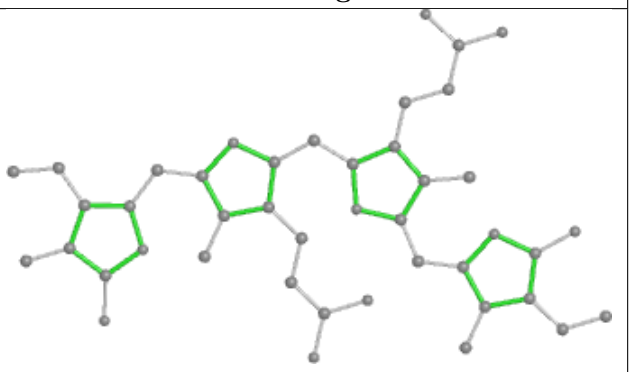
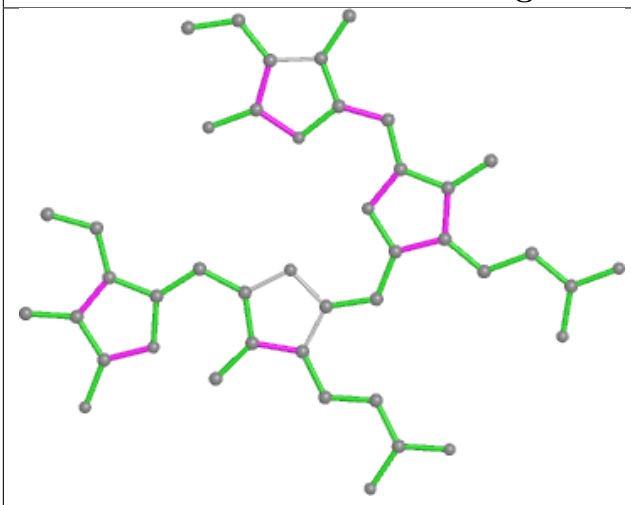


Rings

Ligand PUB bq 203



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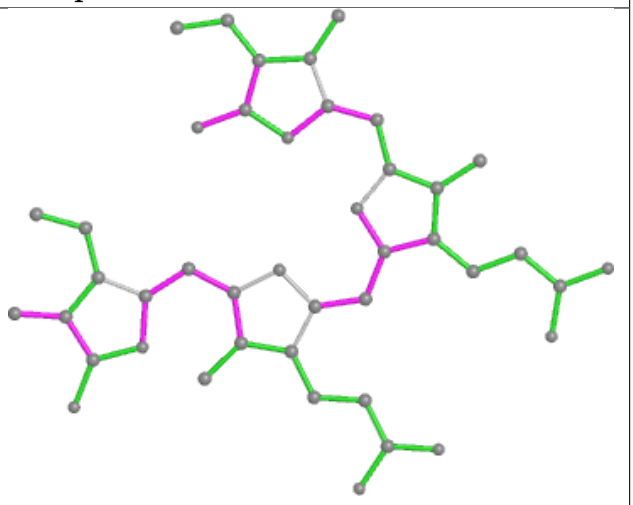

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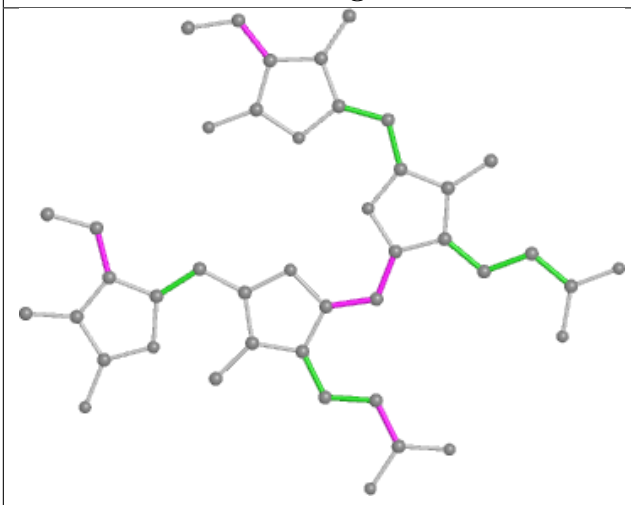

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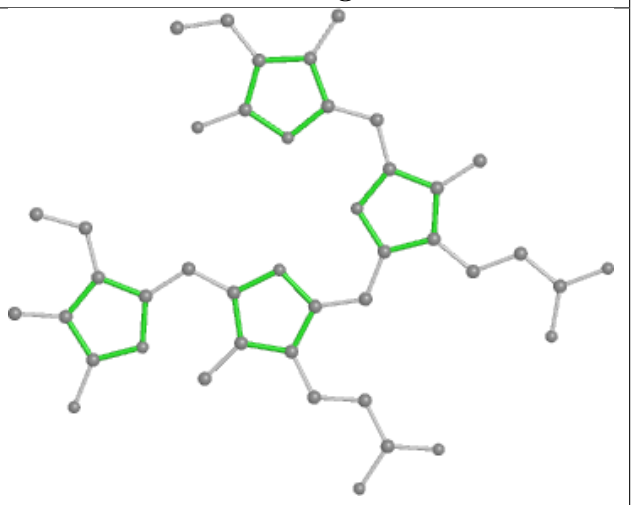

Rings

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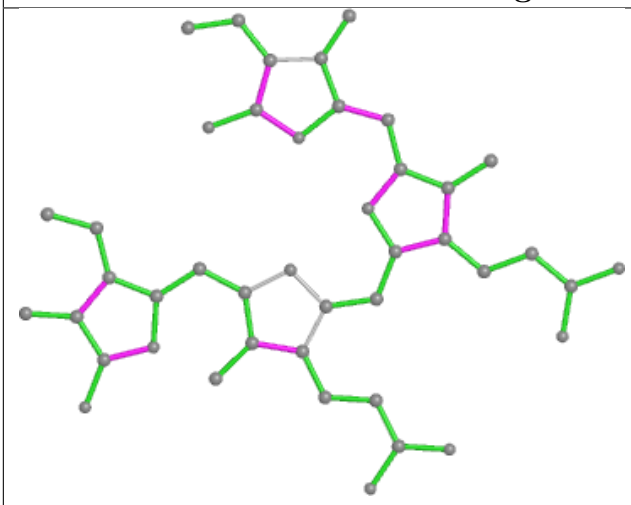

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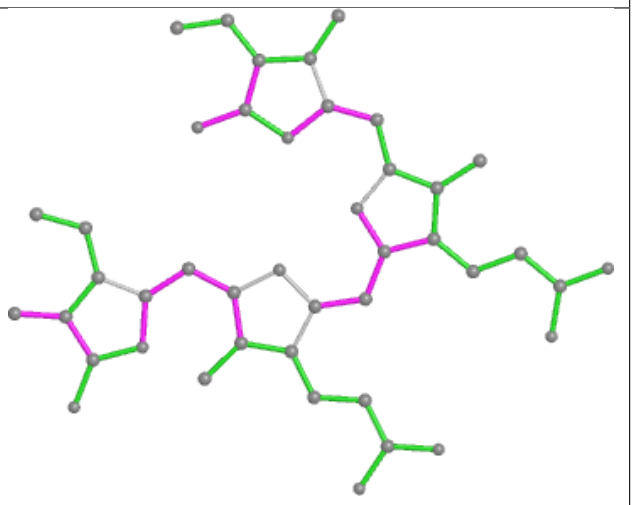

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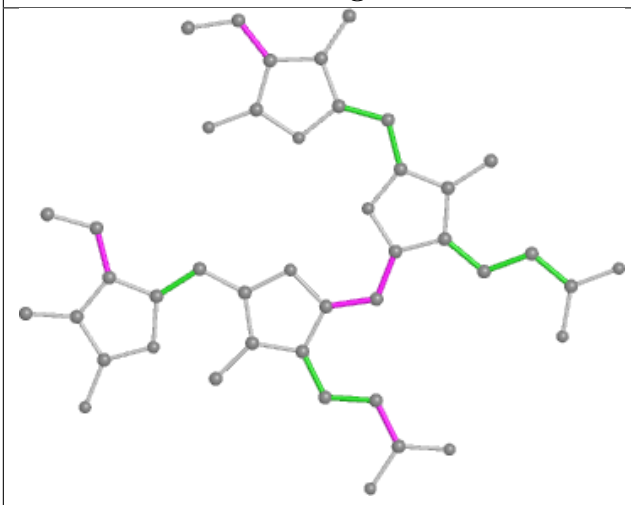

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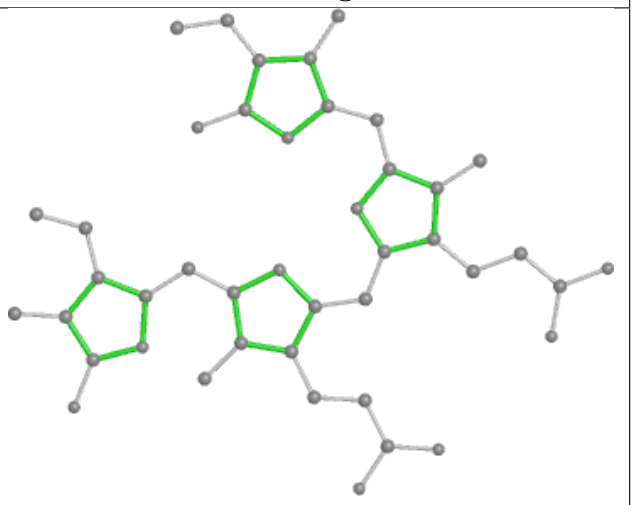
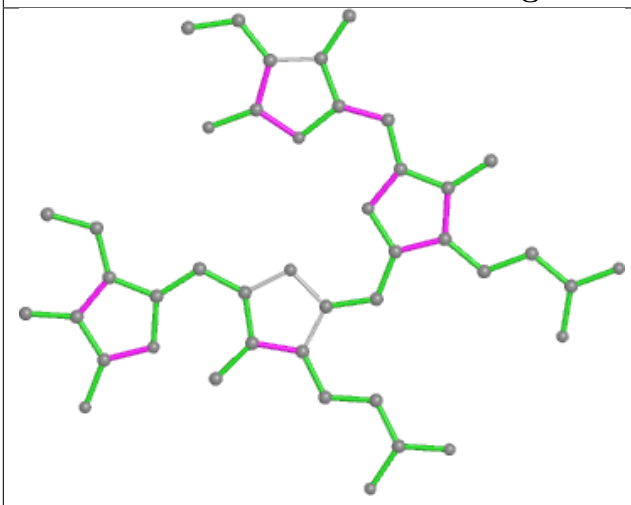


Rings

Ligand PUB l6 203



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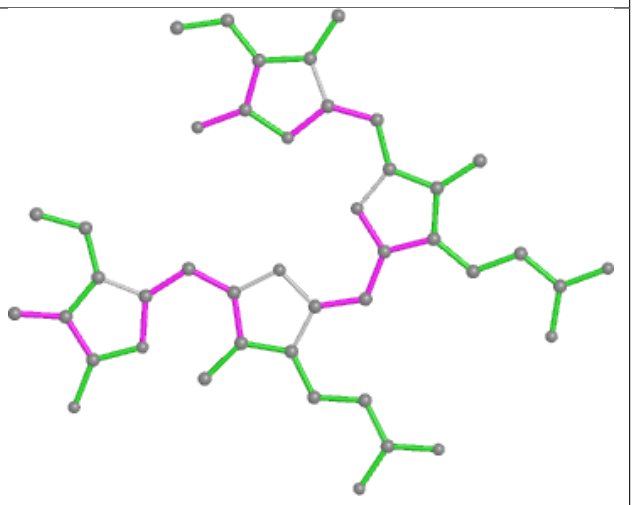

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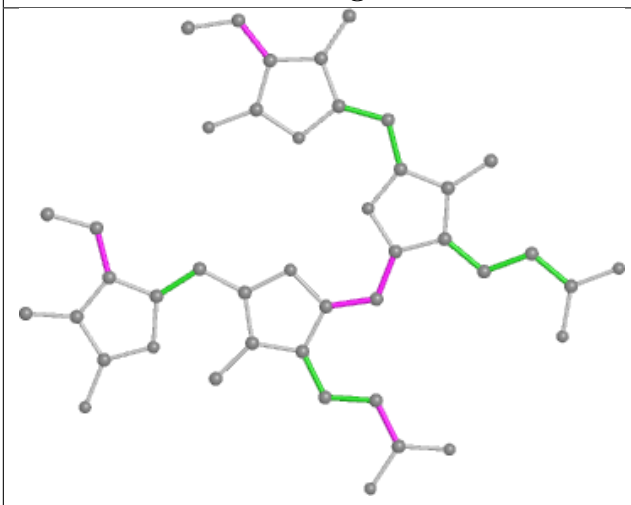

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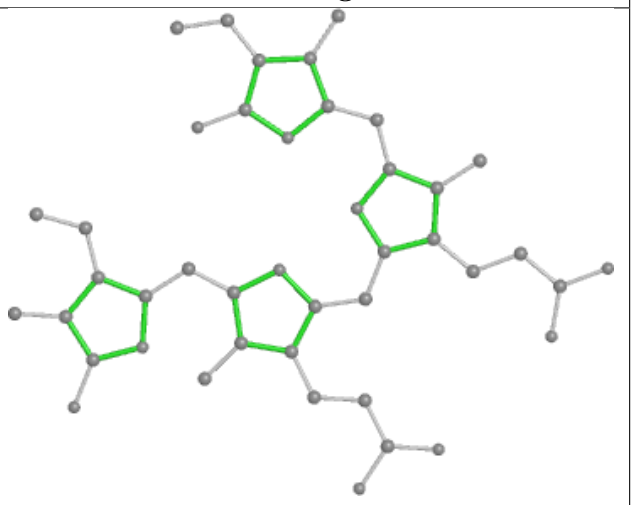

Rings

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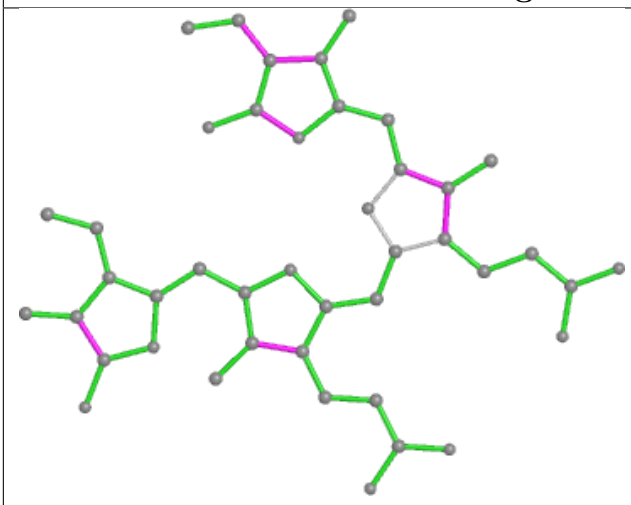

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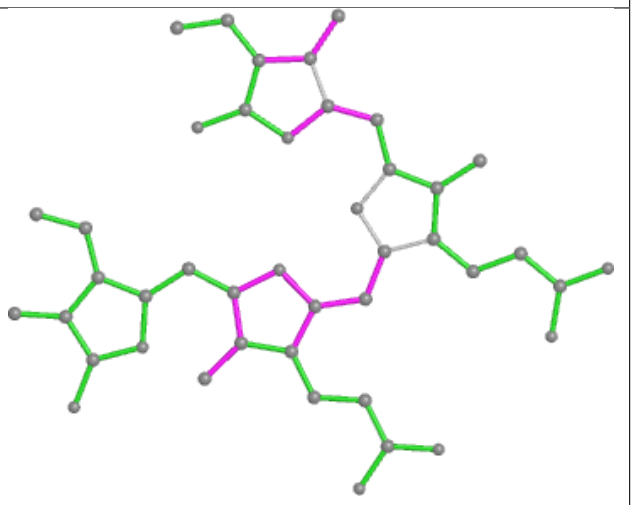

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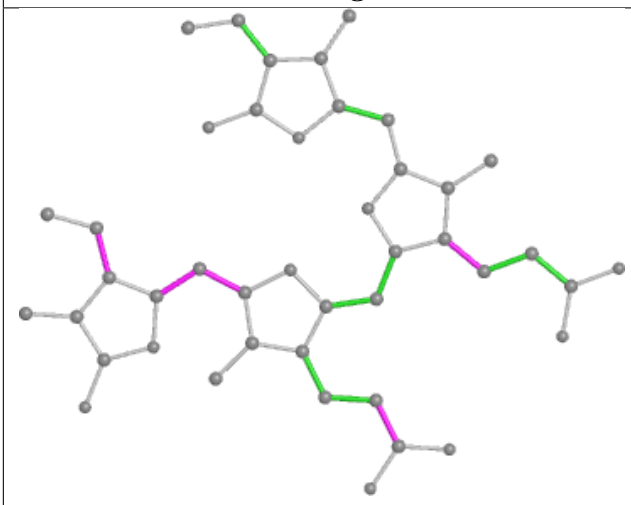

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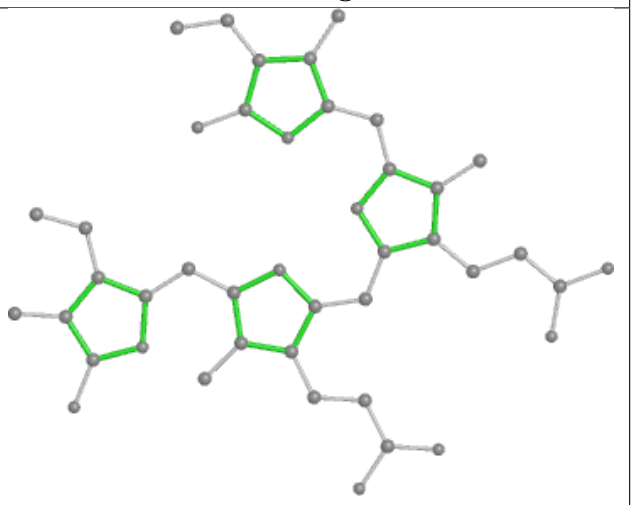

Rings

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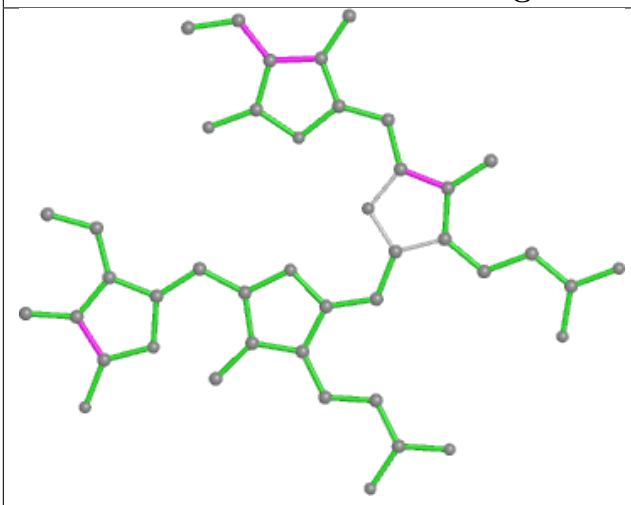

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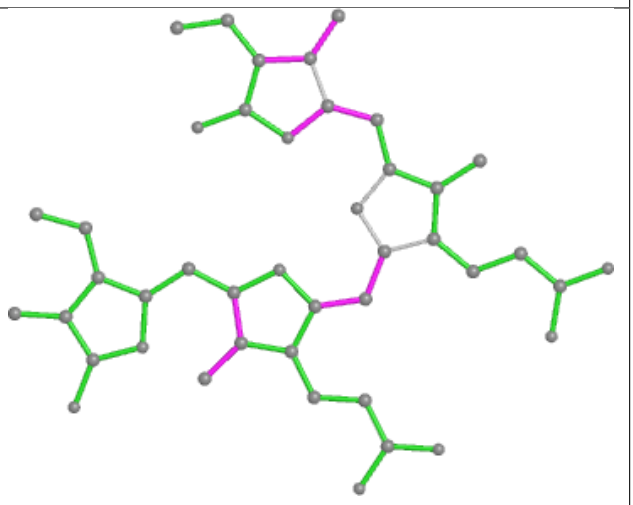

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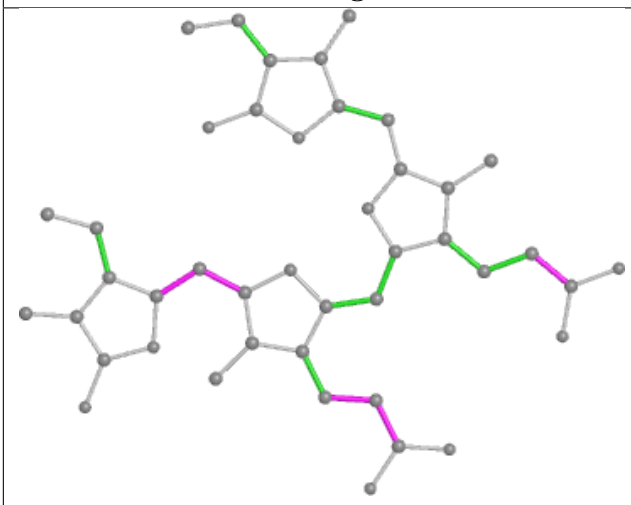

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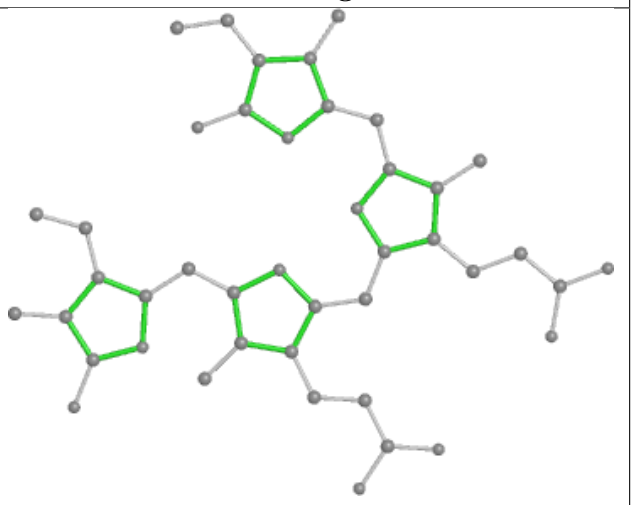
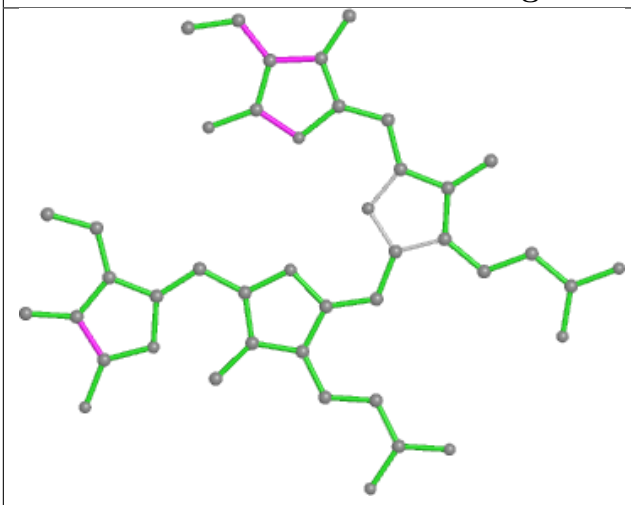


Rings

Ligand PEB cz 201



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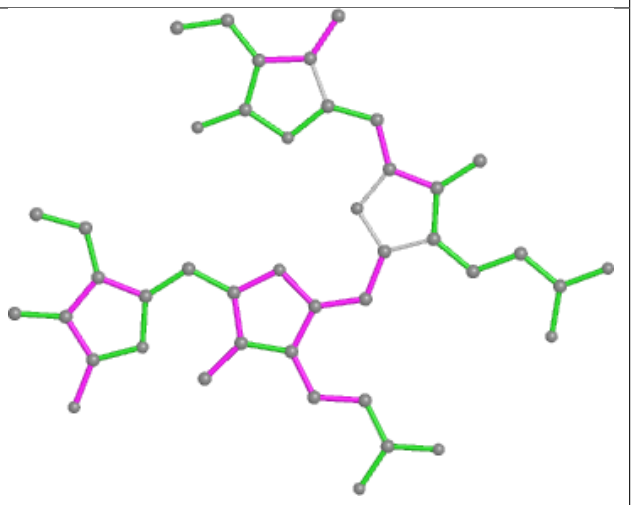

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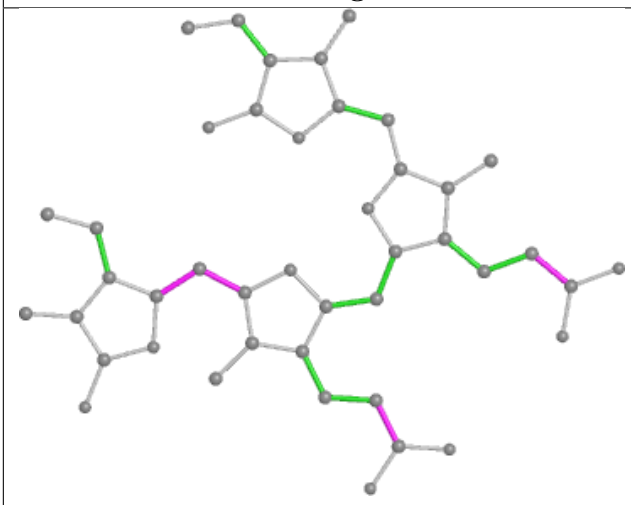

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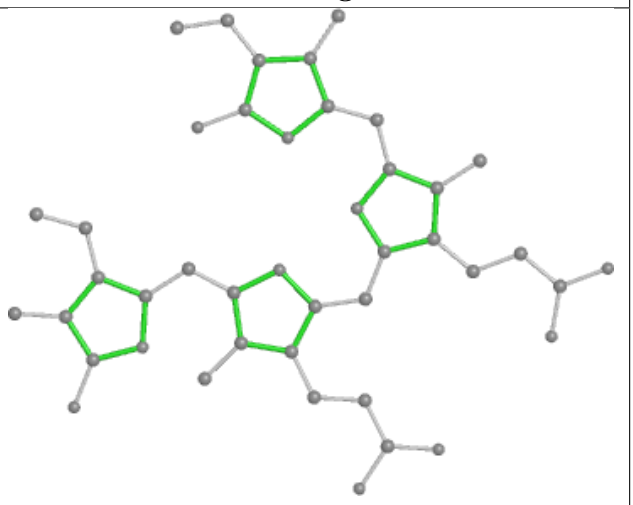

Rings

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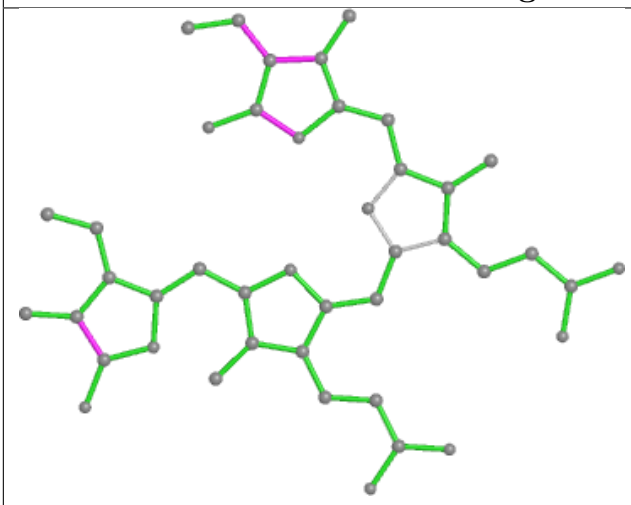

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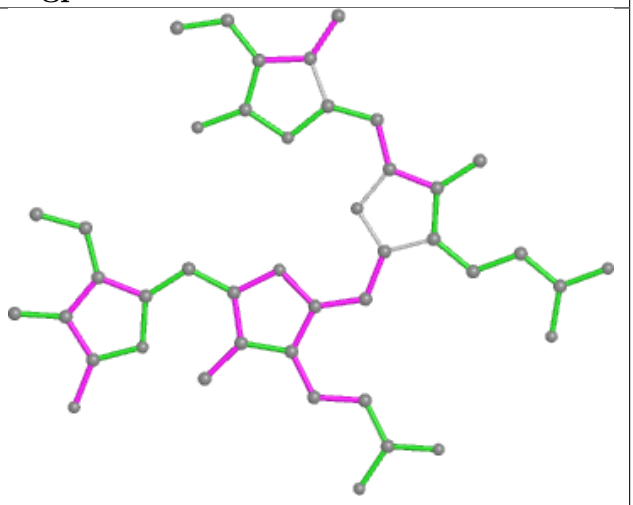

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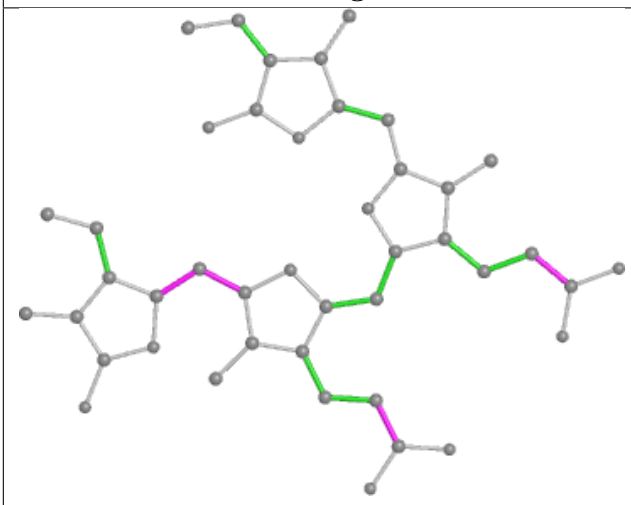

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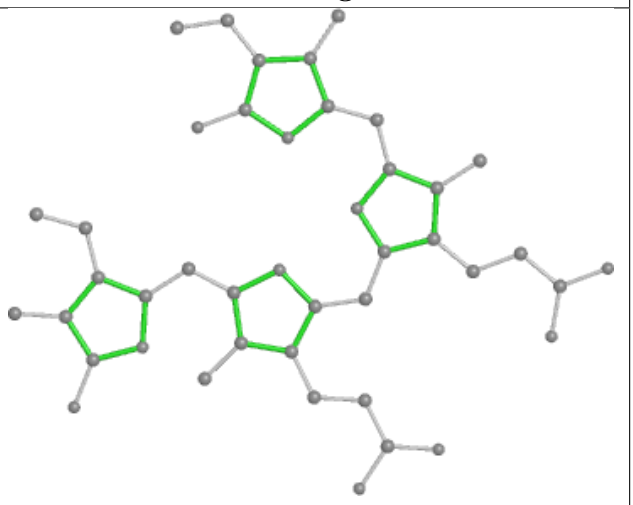
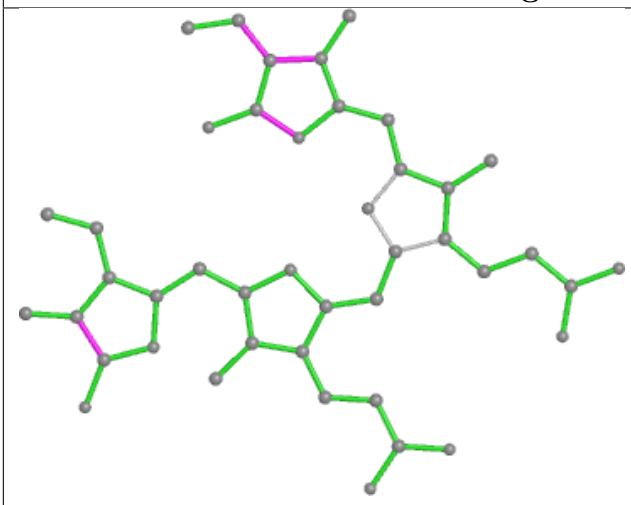


Rings

Ligand PEB ce 201



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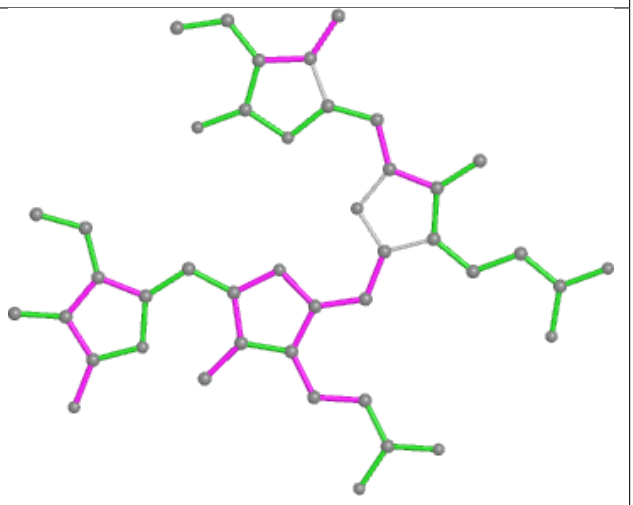

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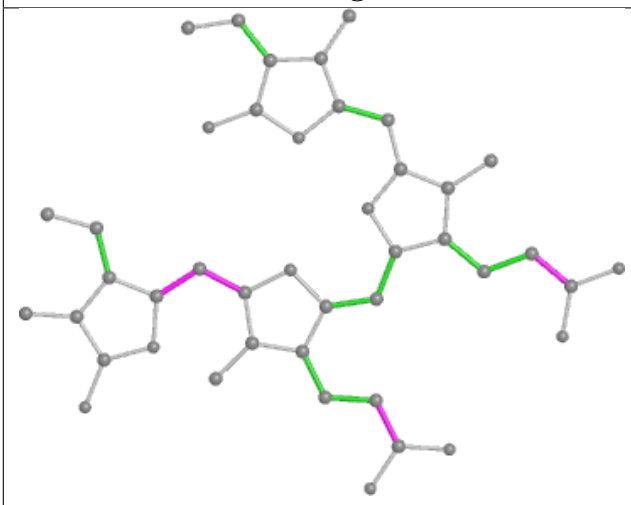

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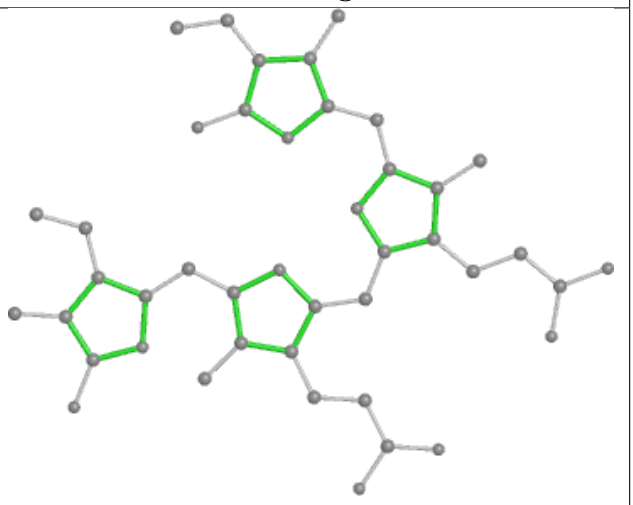
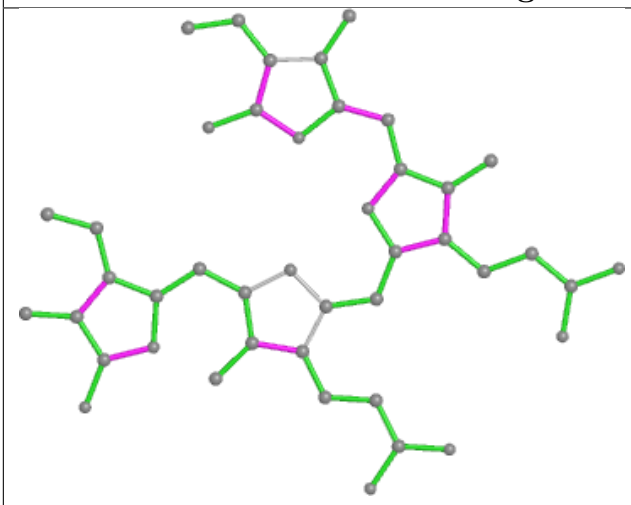
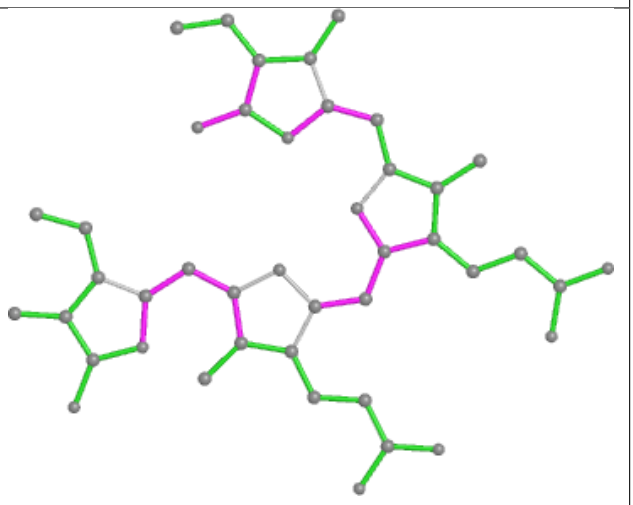


Rings

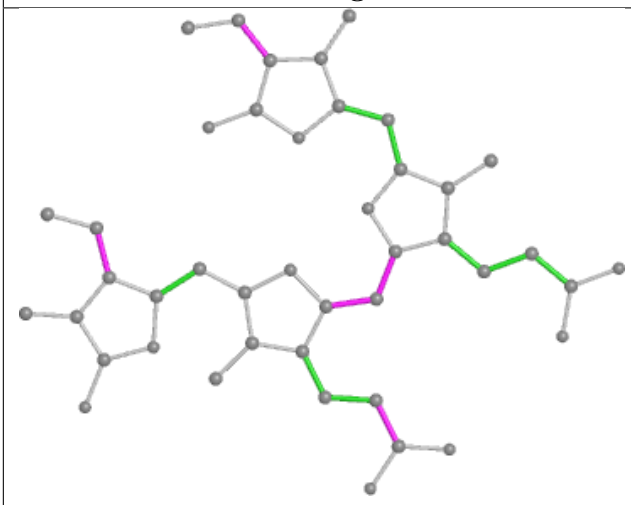
Ligand PUB x9 203



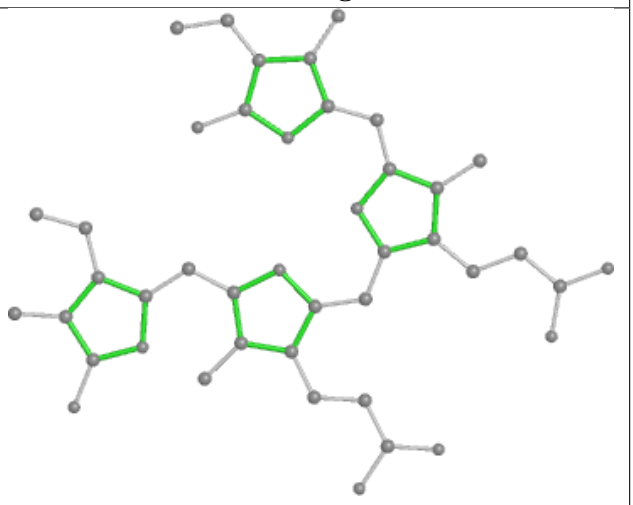
Bond lengths



Bond angles

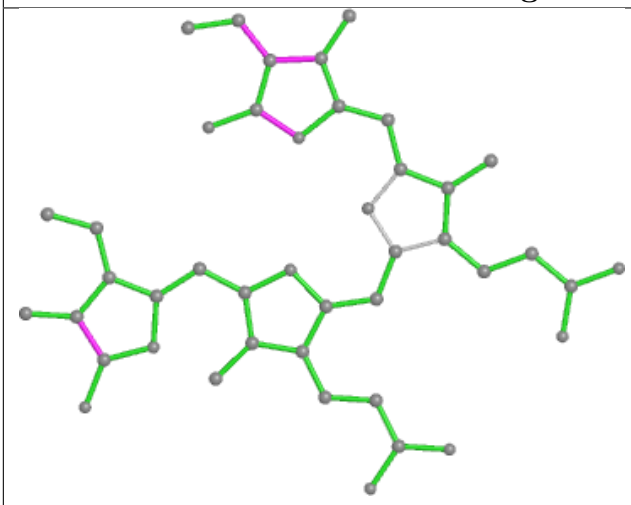


Torsions



Rings

Ligand PEB e4 201



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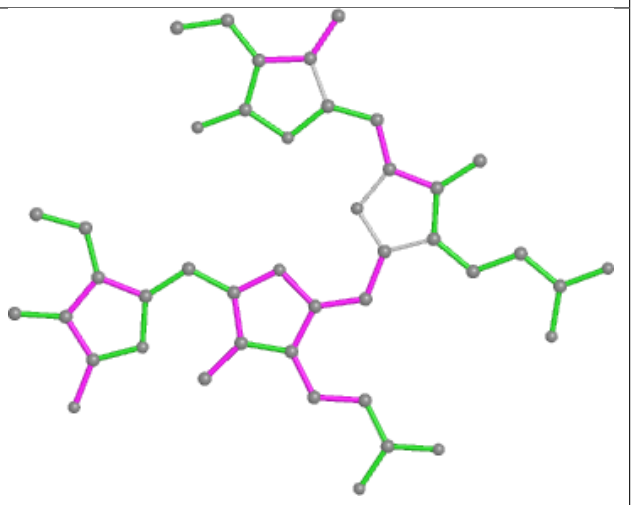

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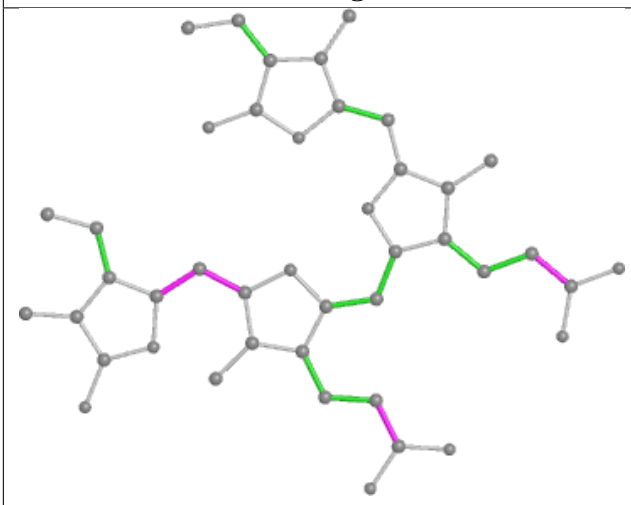

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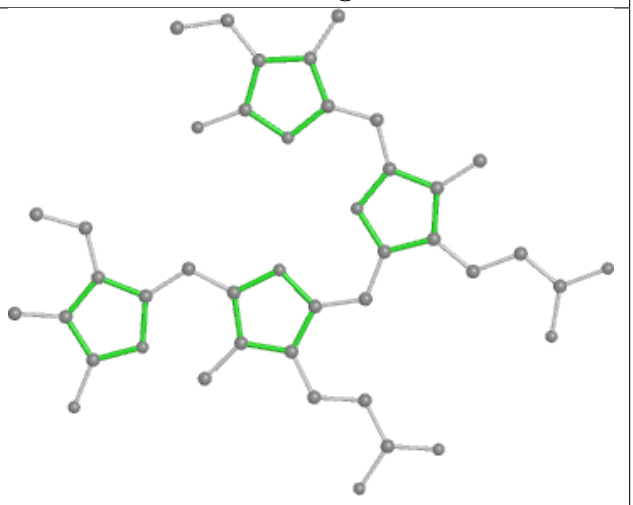
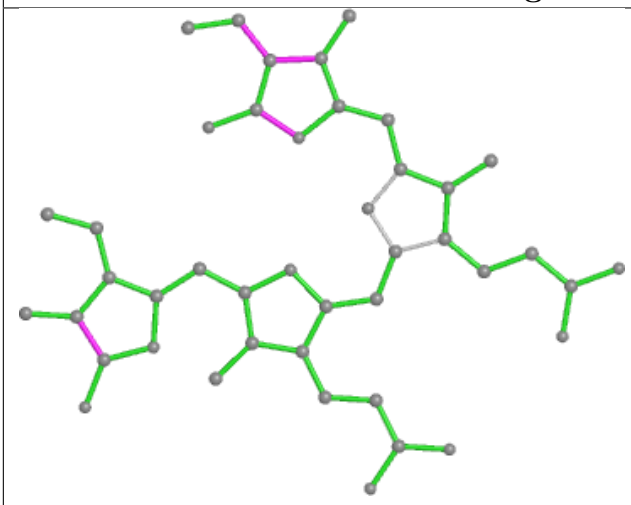


Rings

Ligand PEB lz 401



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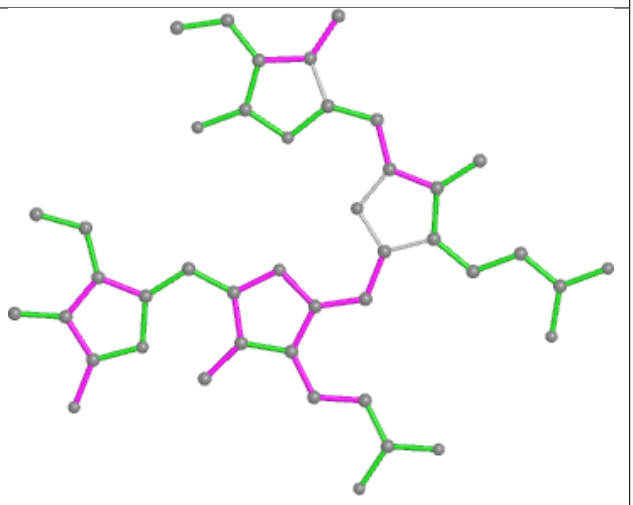

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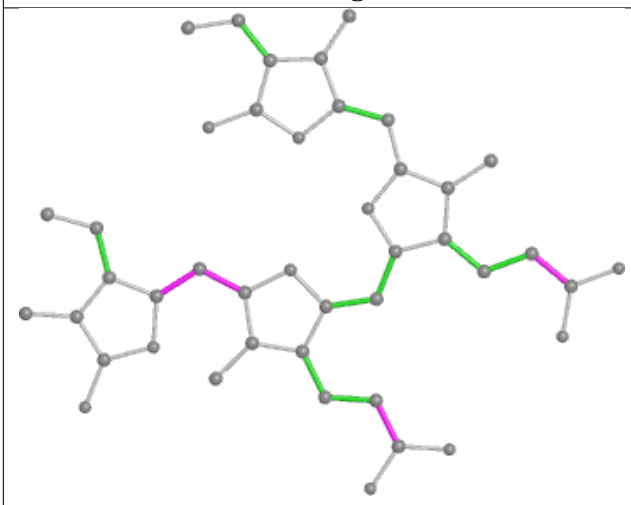

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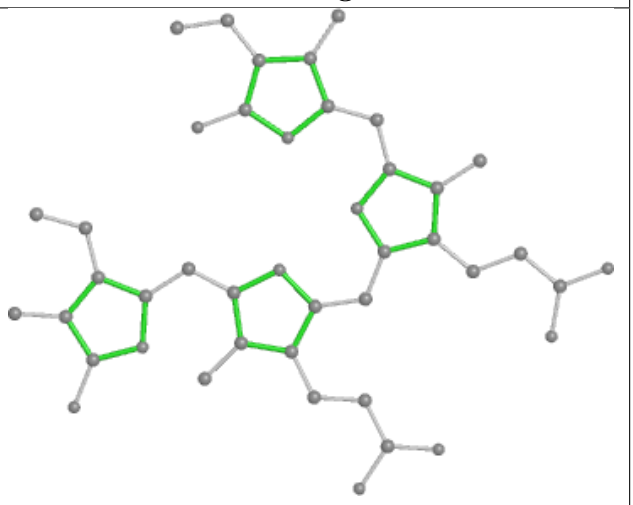
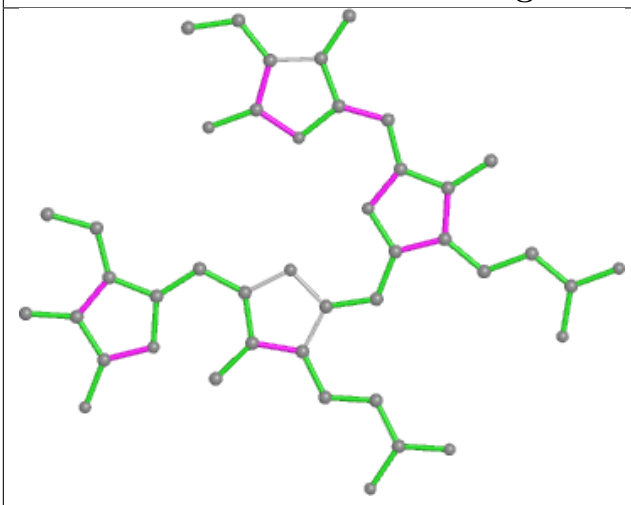


Rings

Ligand PUB L6 202



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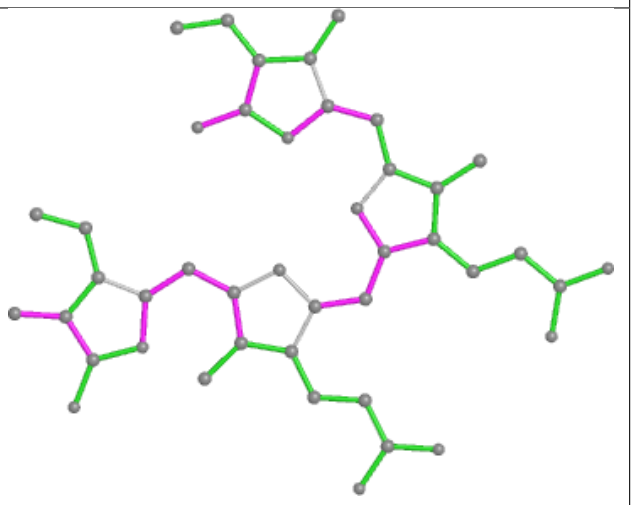

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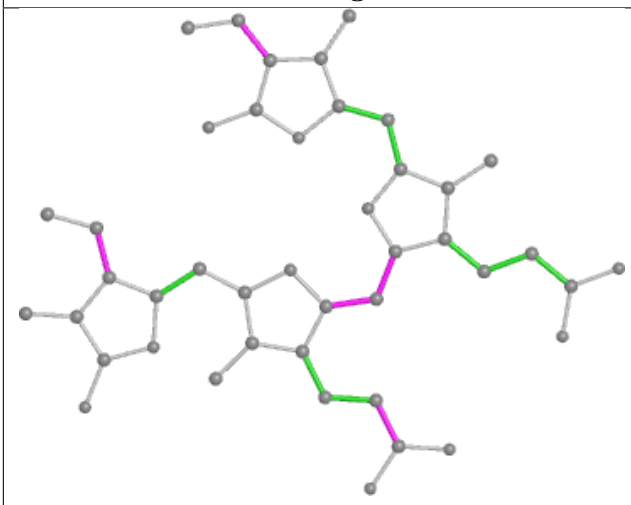

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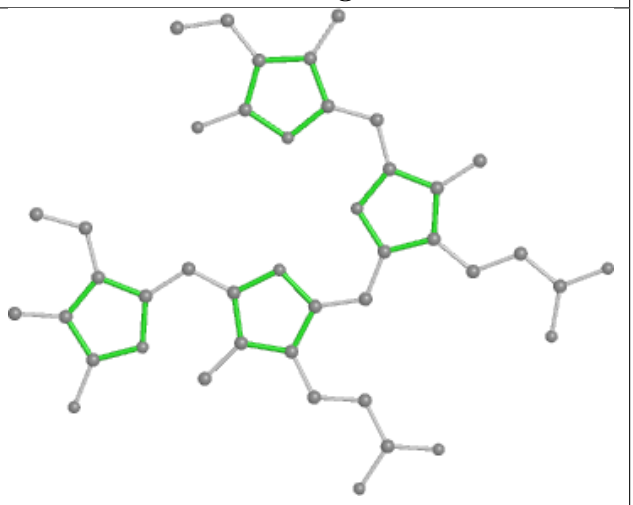
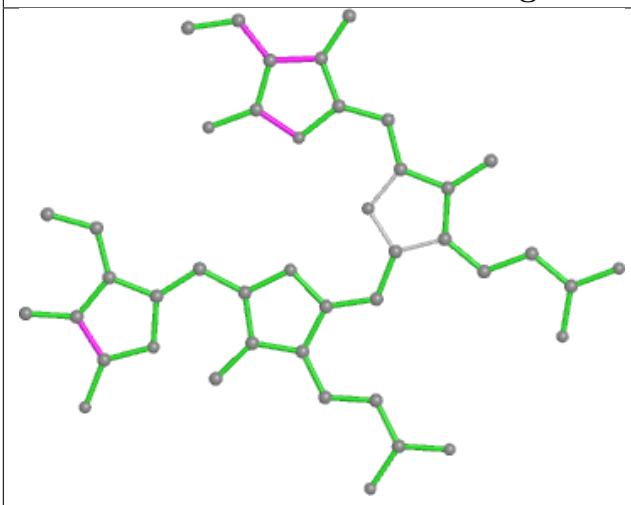


Rings

Ligand PEB q7 201



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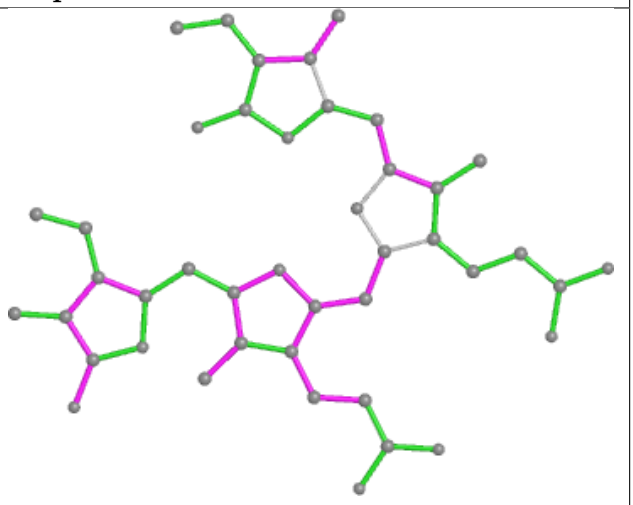

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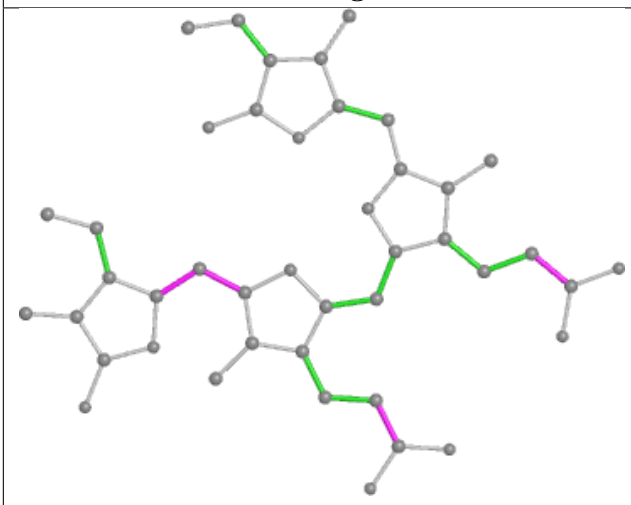

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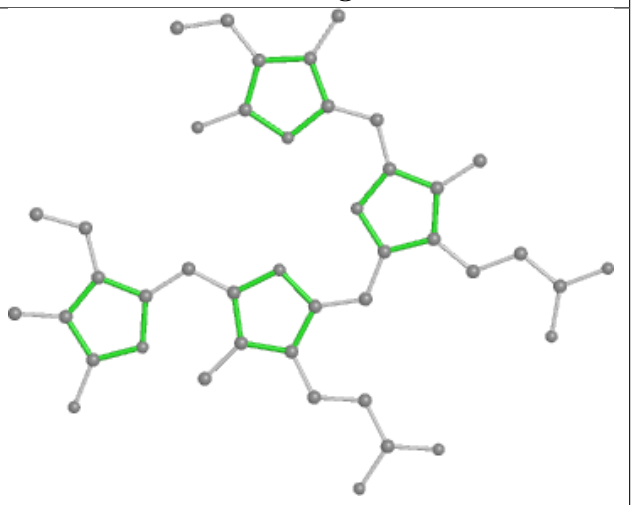

Rings

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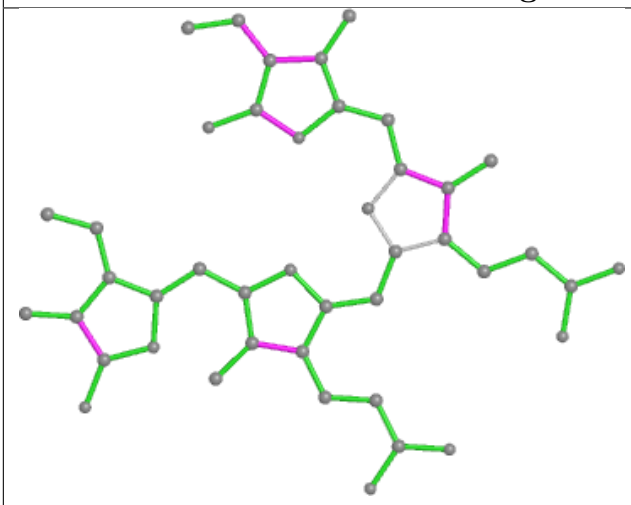

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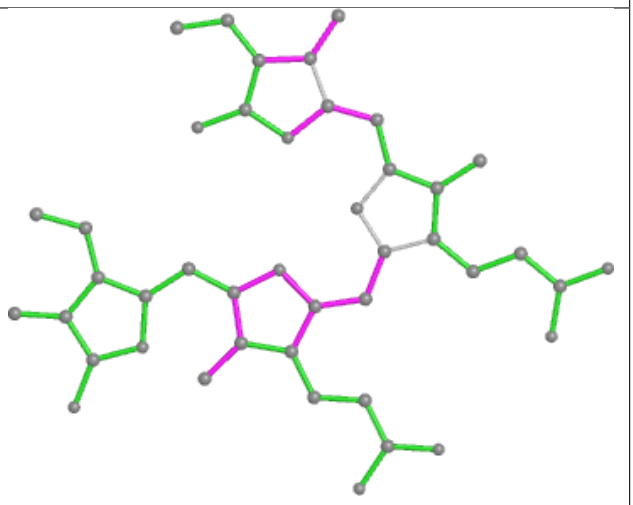

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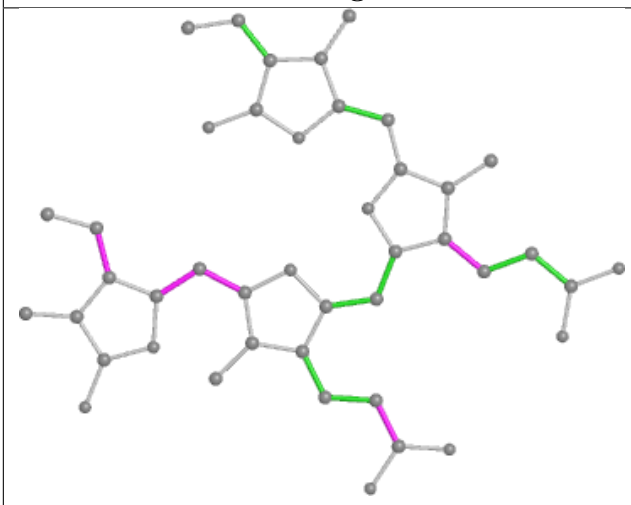

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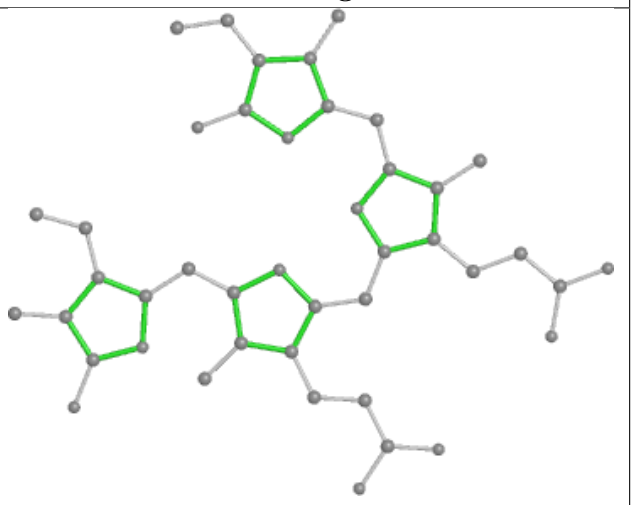

Rings

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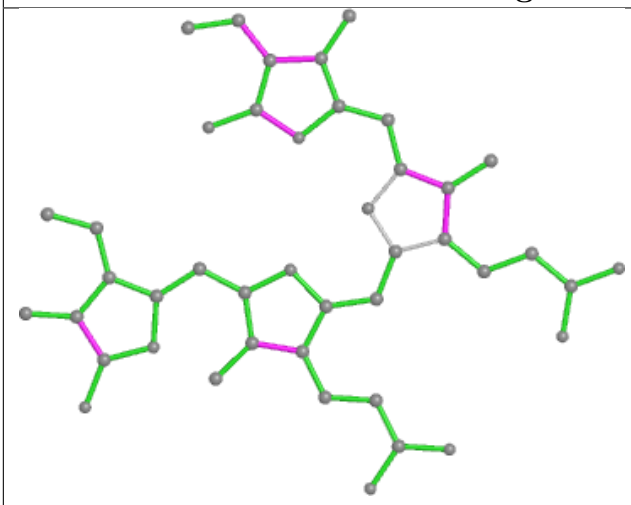

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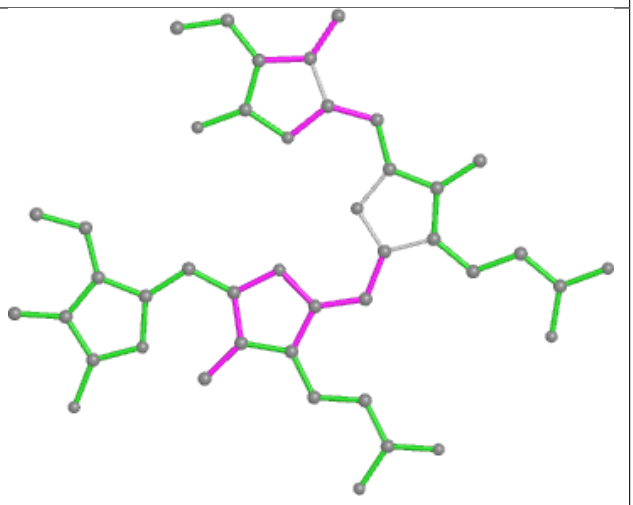

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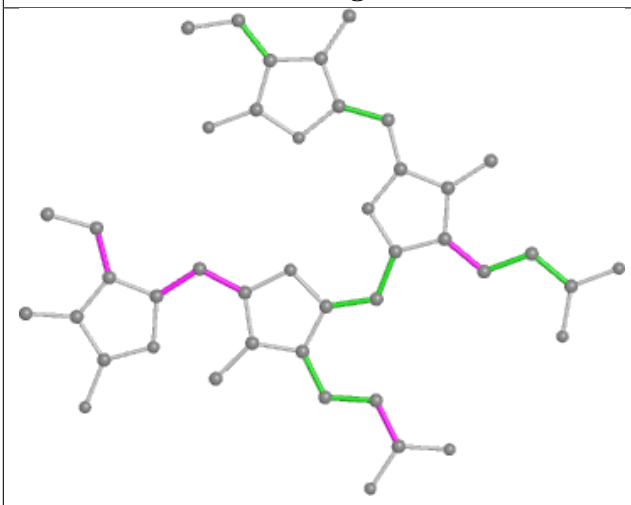

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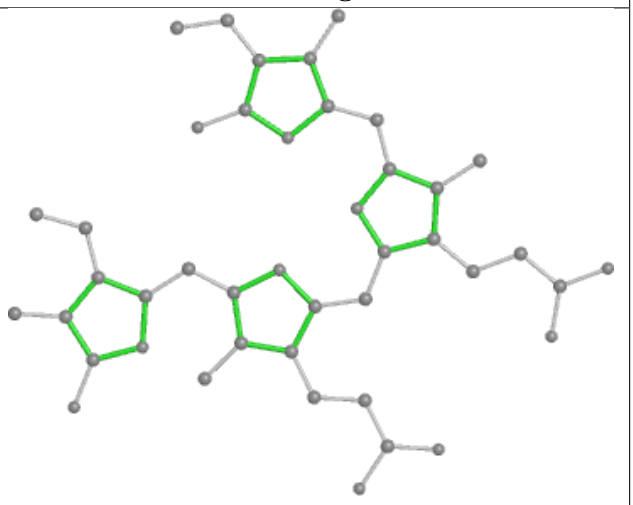
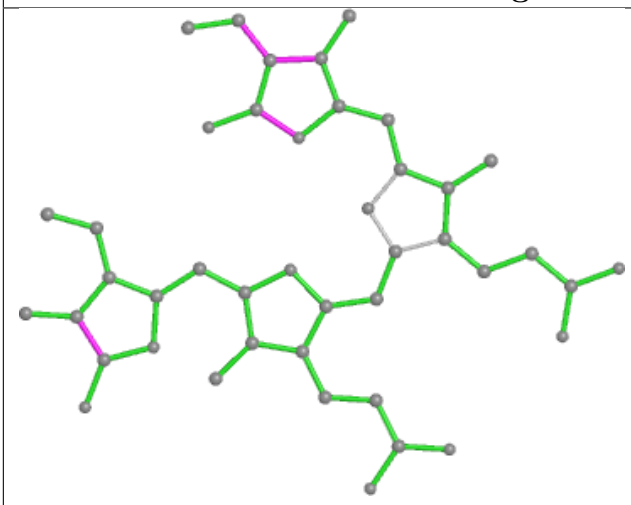


Rings

Ligand PEB bs 1001



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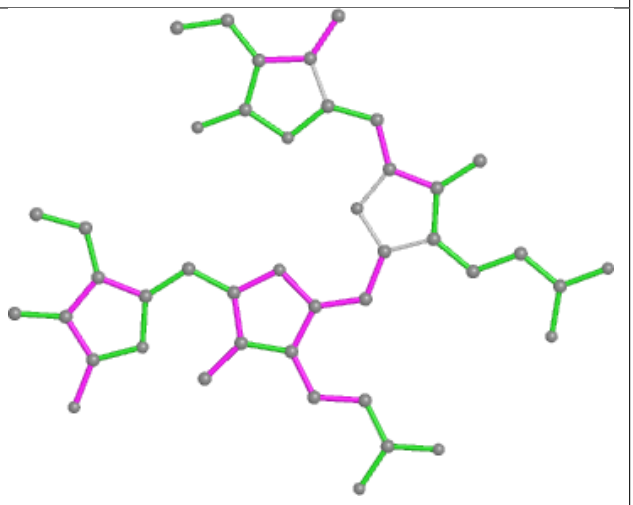

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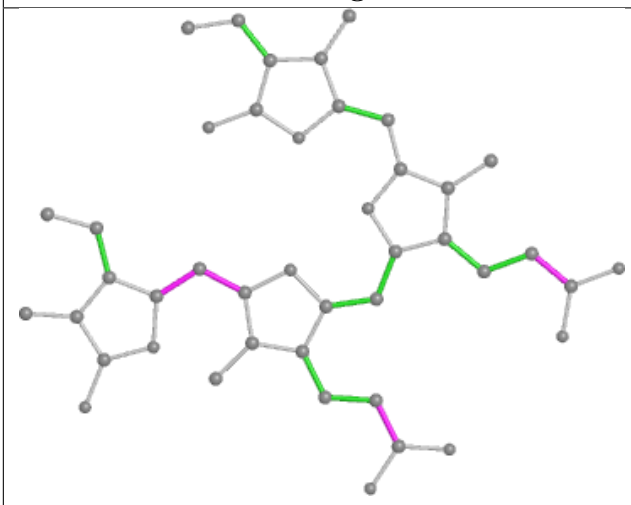

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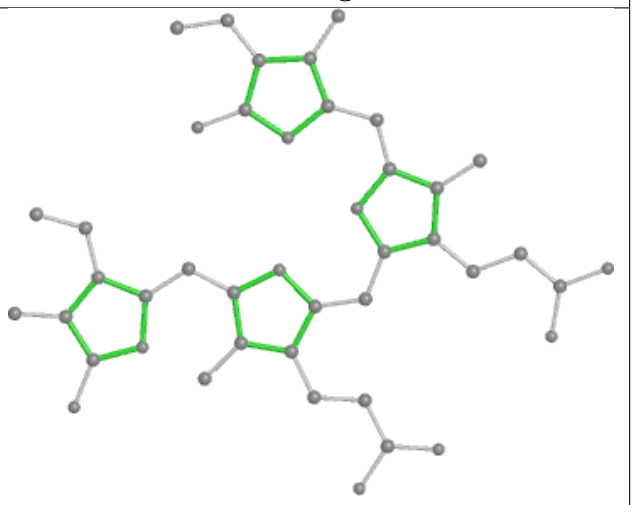

Rings

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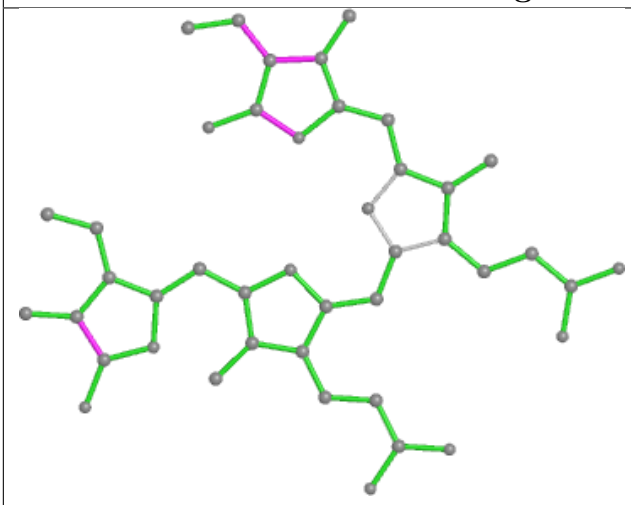

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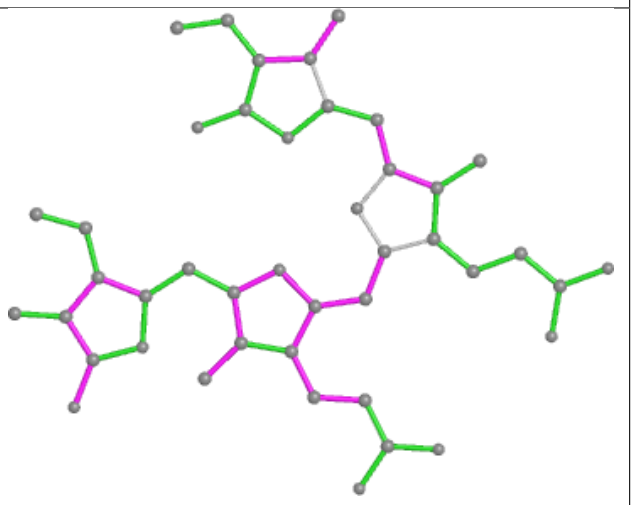

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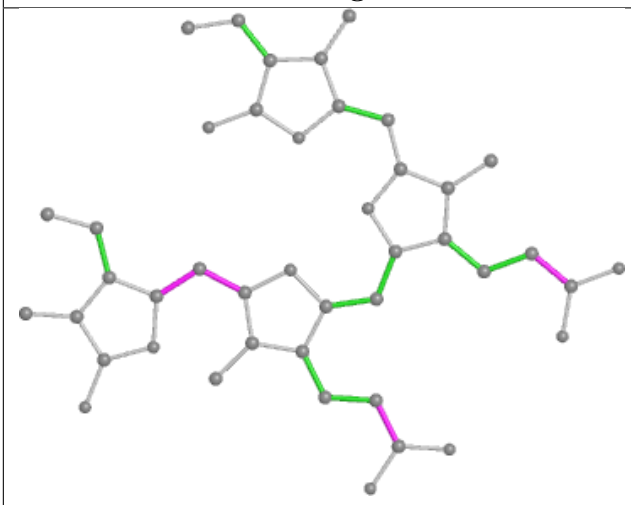

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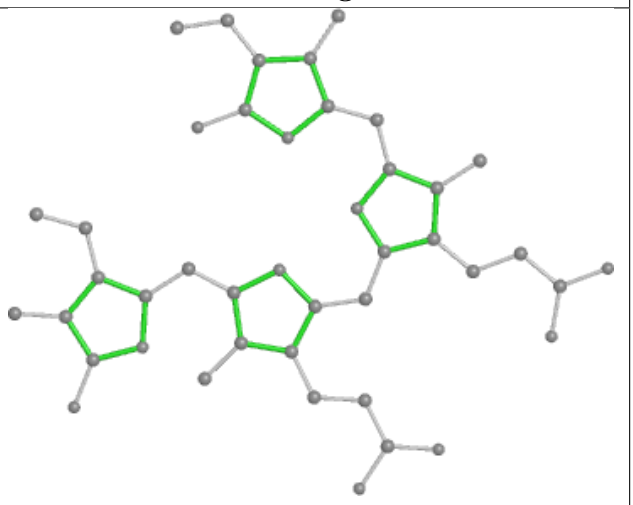

Rings

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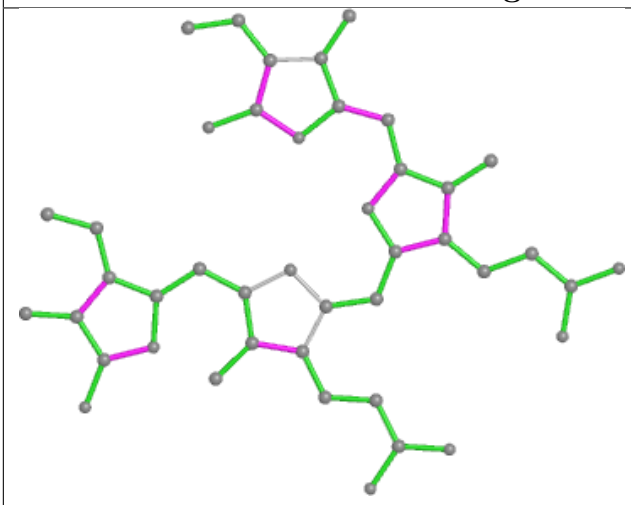

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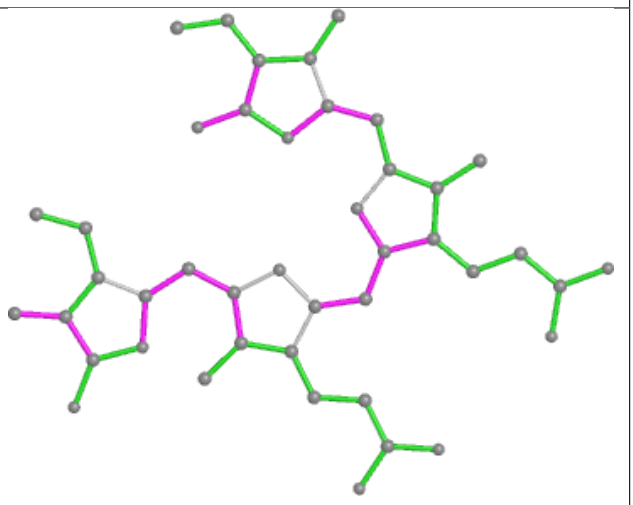

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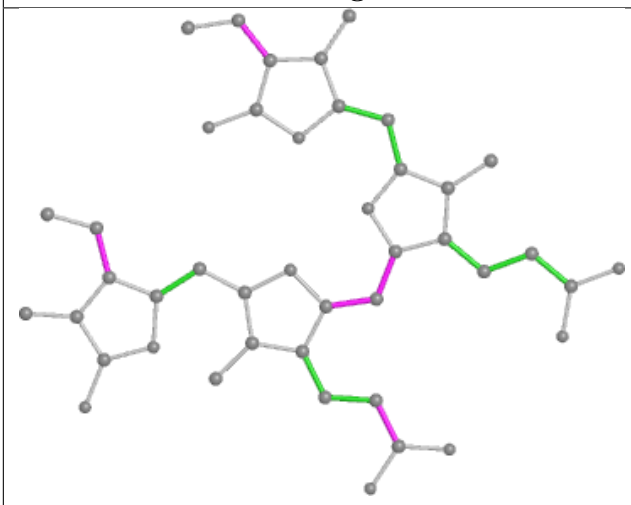

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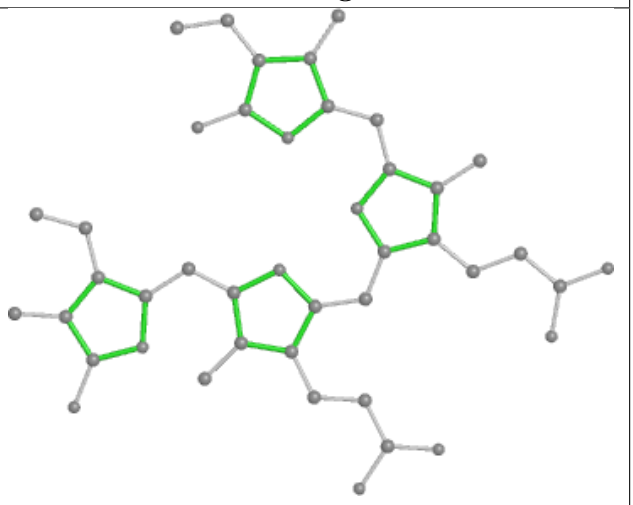
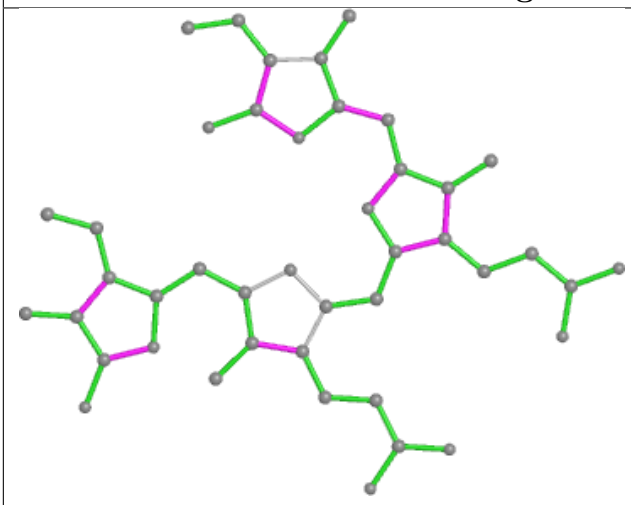


Rings

Ligand PUB L7 202



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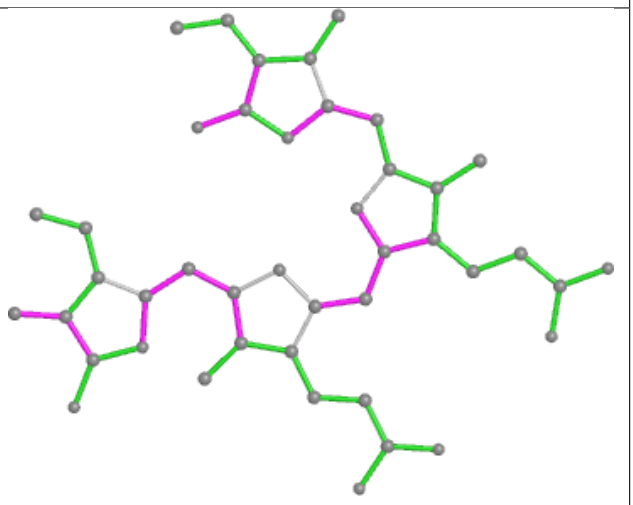

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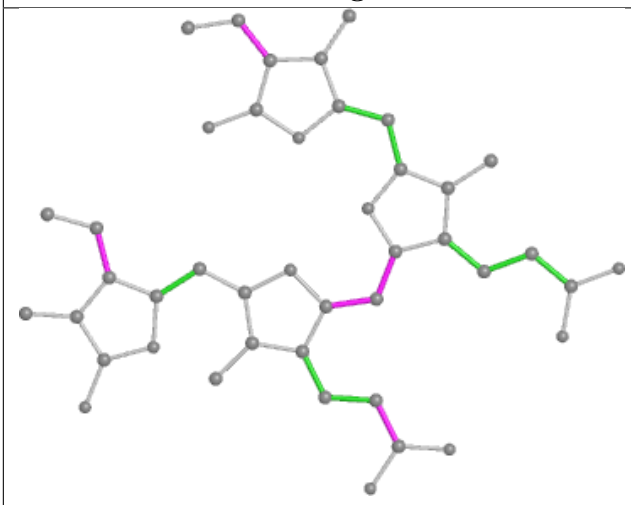

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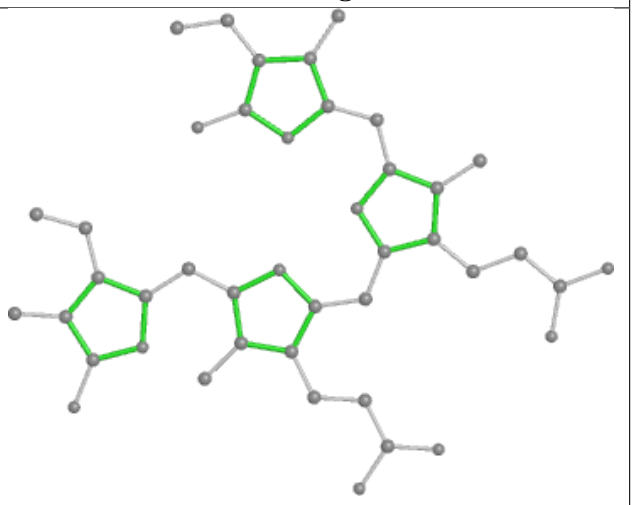
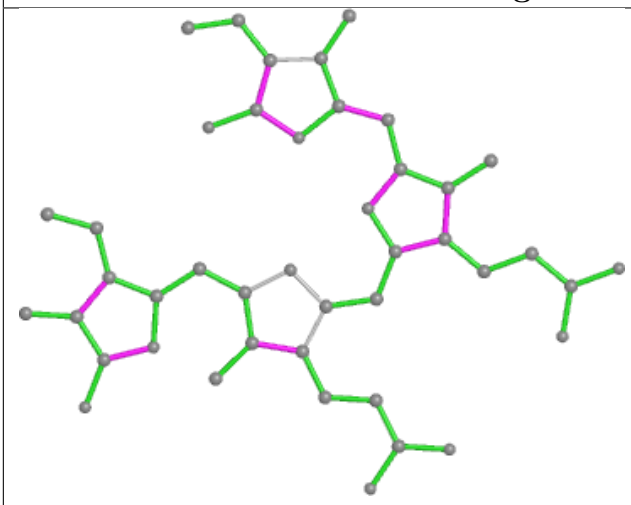


Rings

Ligand PUB V3 203



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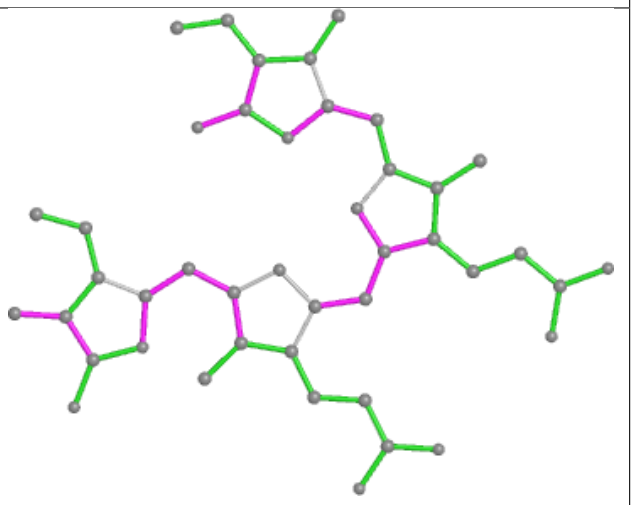

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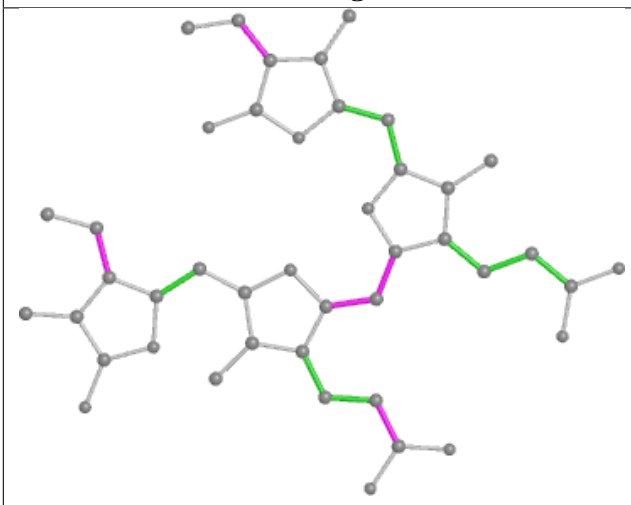

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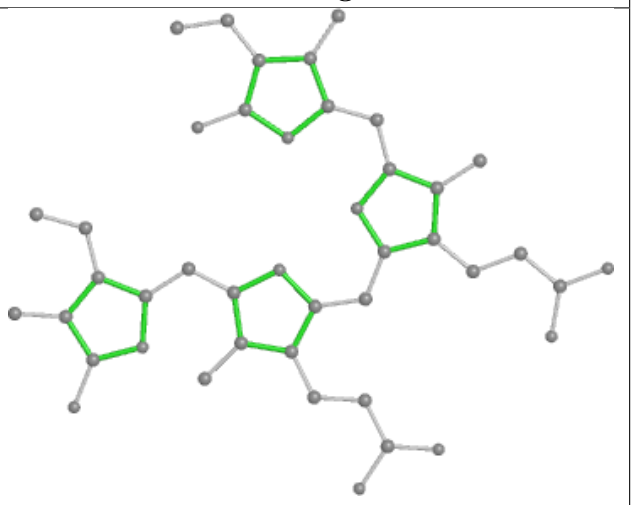

Rings

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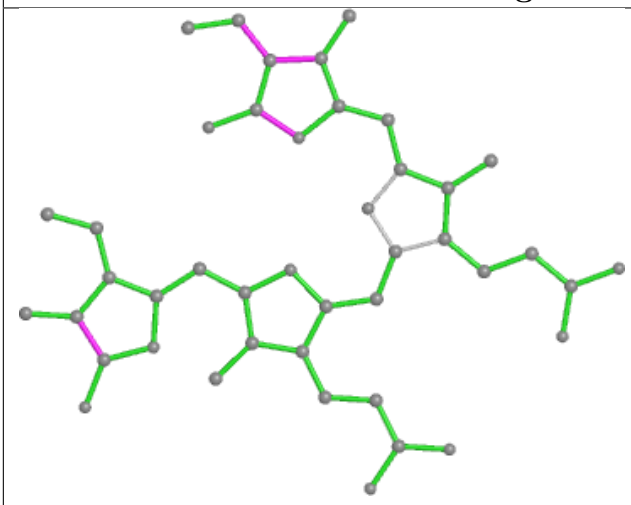

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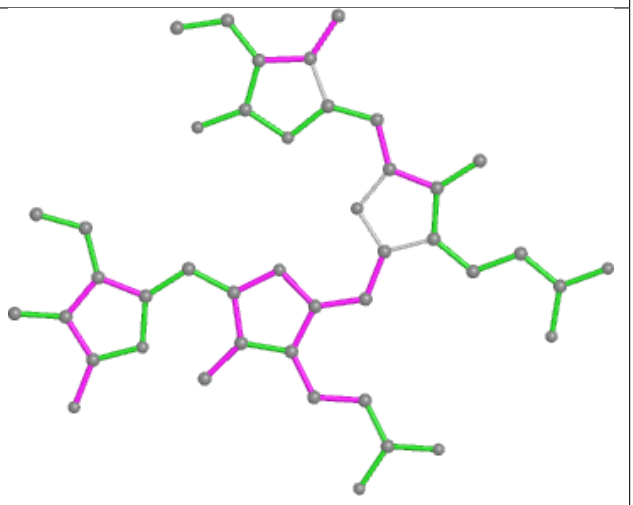

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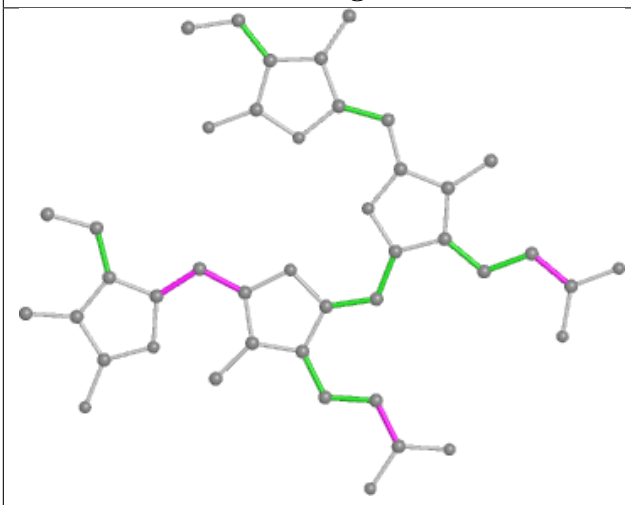

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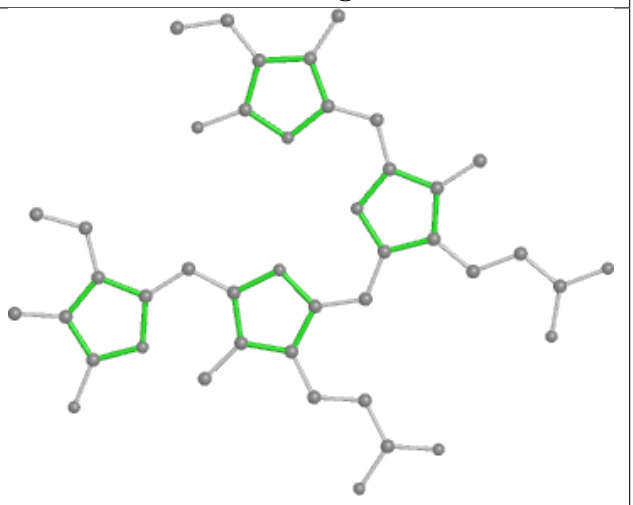

Rings

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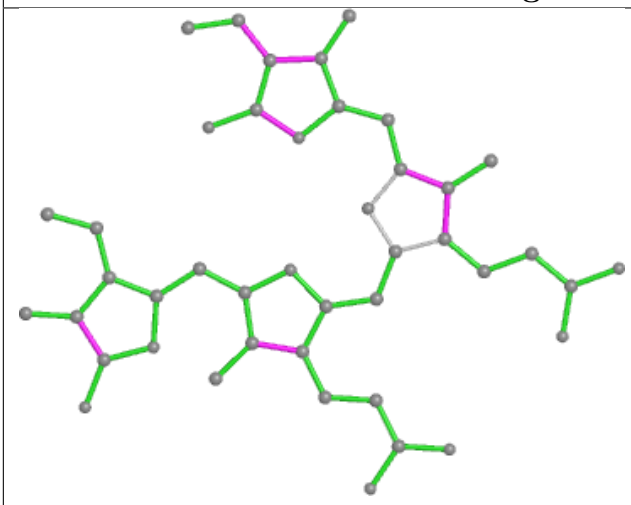

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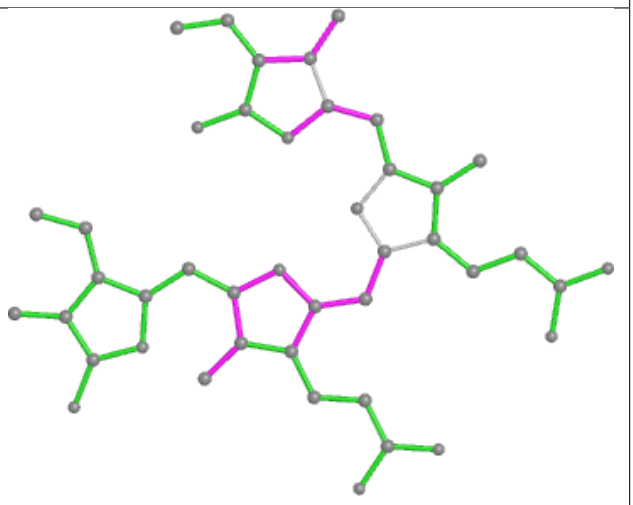
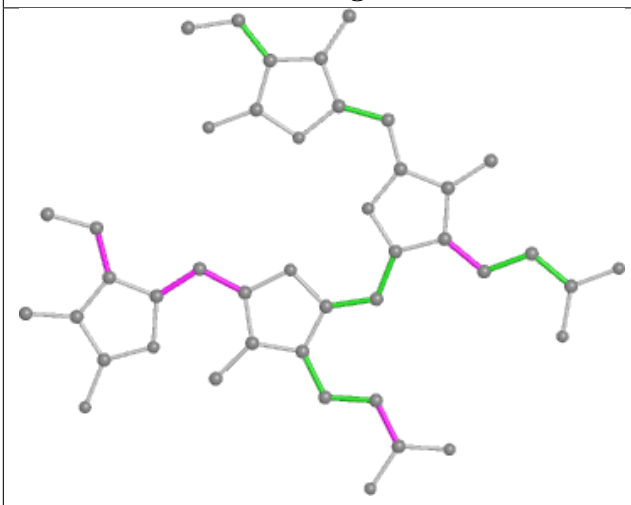
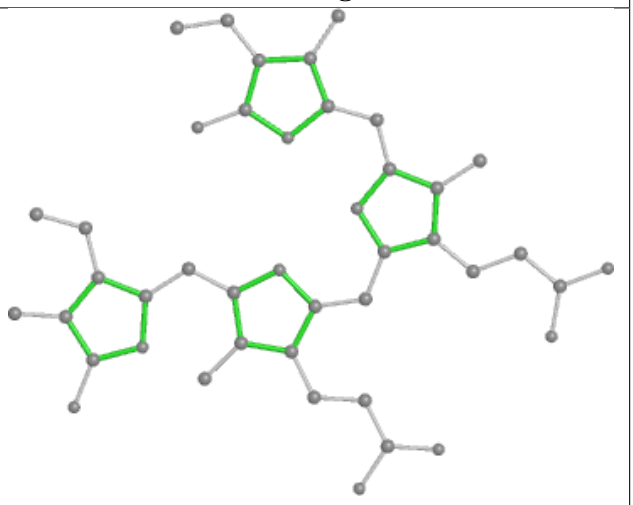


Bond angles

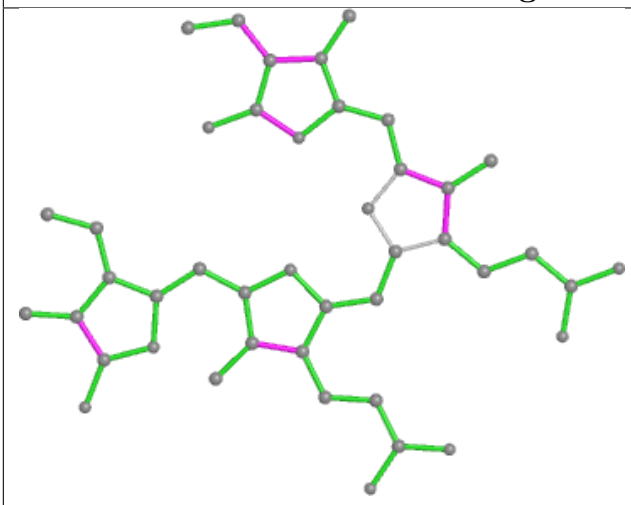


Torsions



Rings

Ligand PEB ap 202



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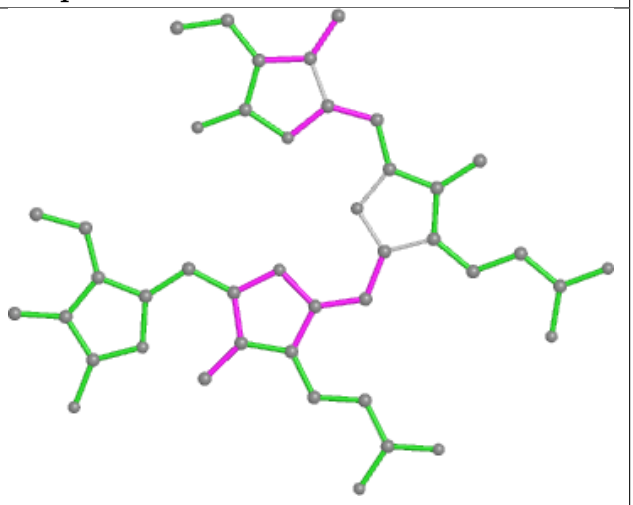

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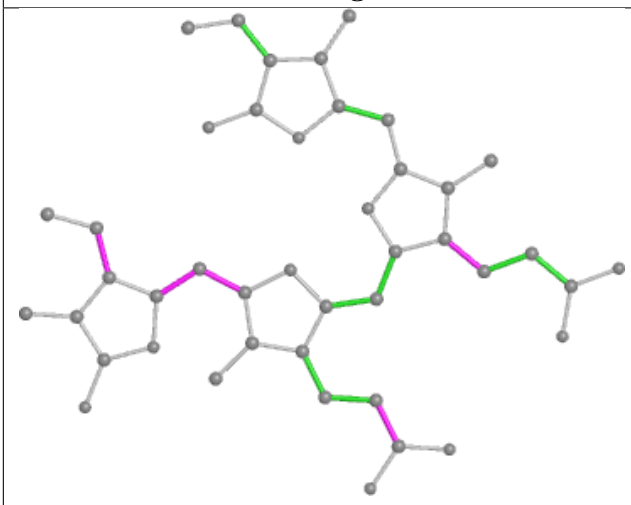

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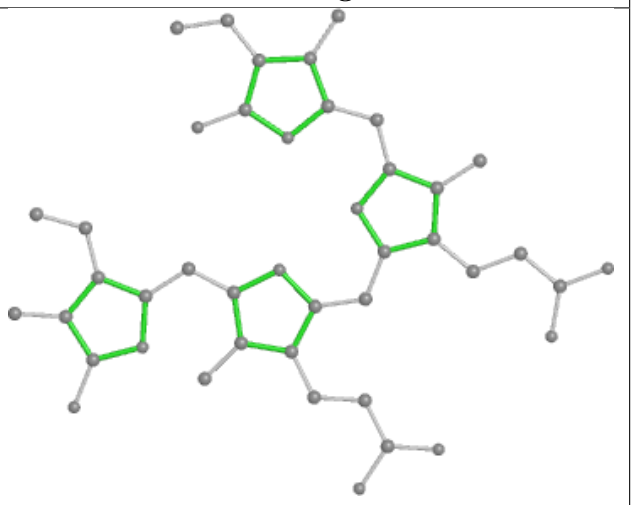
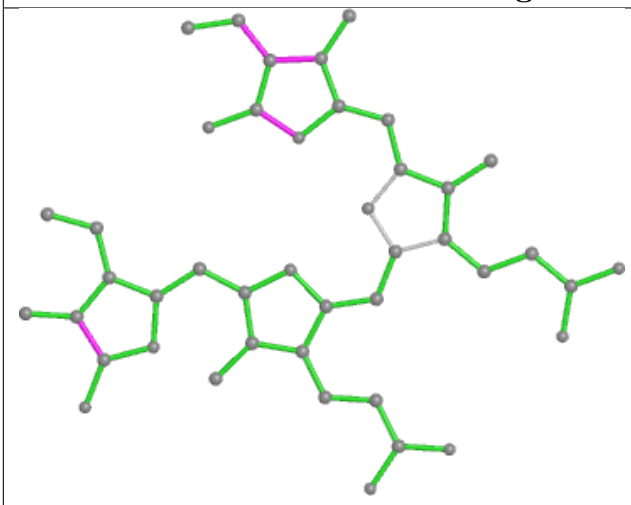


Rings

Ligand PEB O2 202



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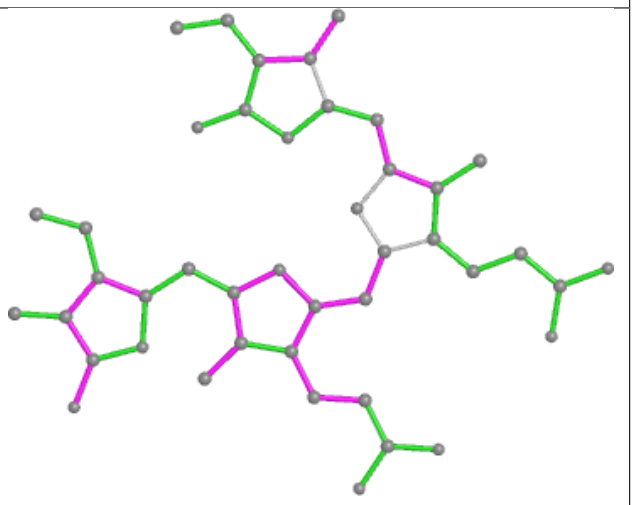

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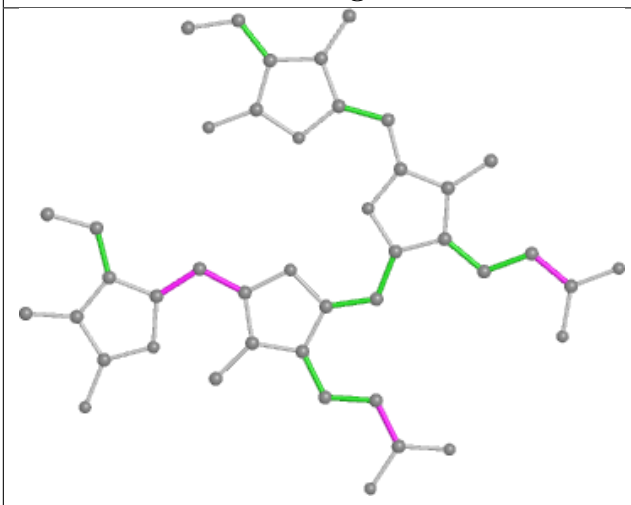

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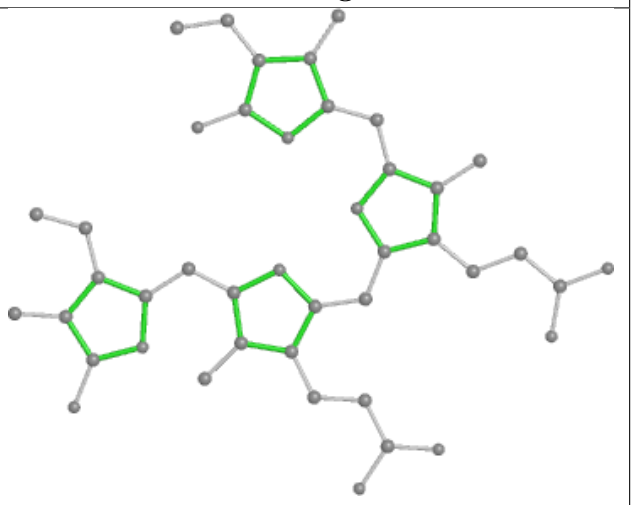
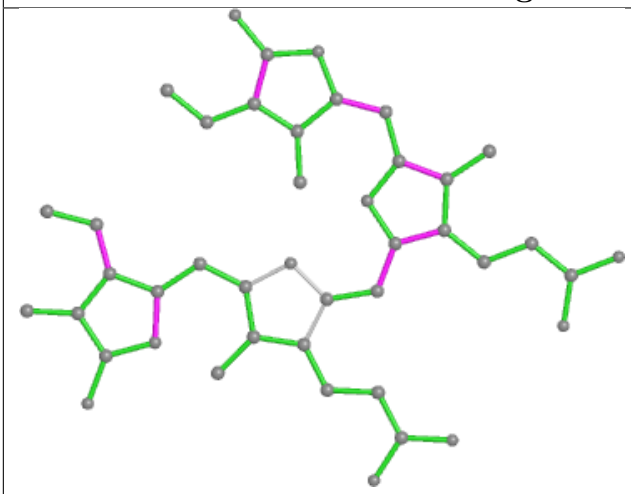


Rings

Ligand PVN b9 405



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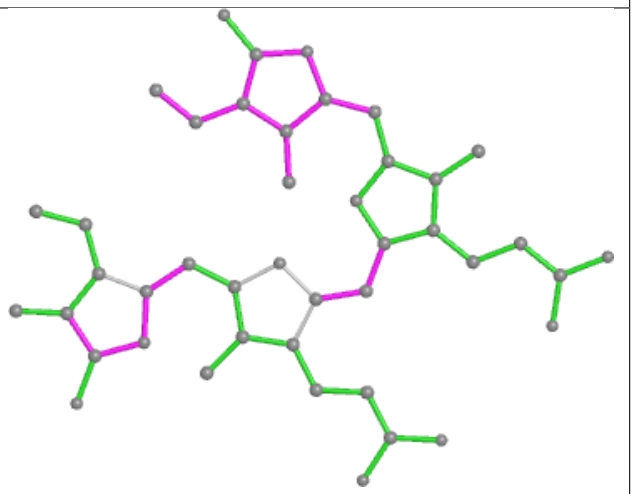

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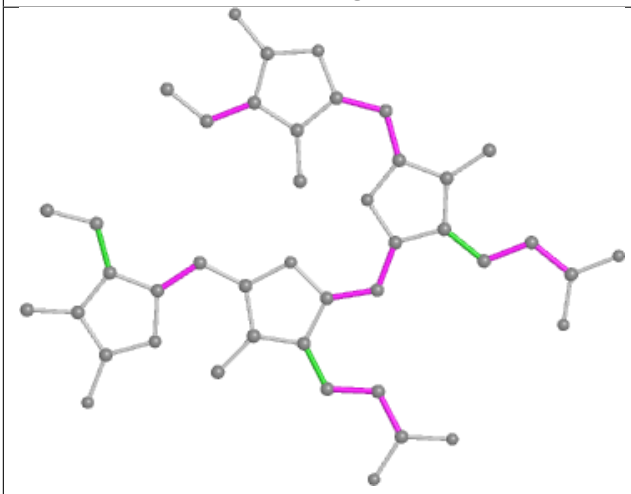

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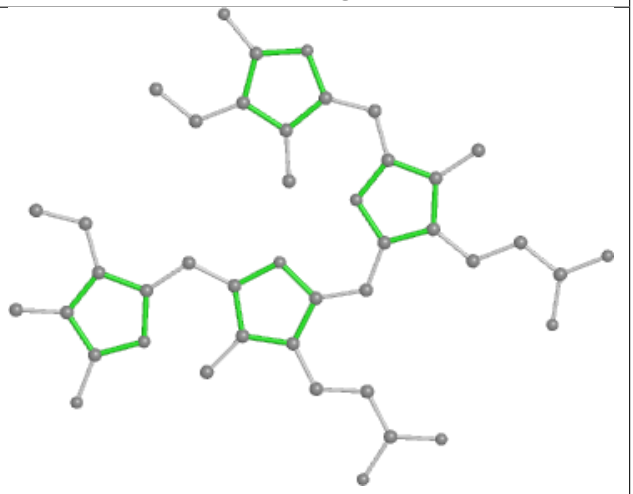
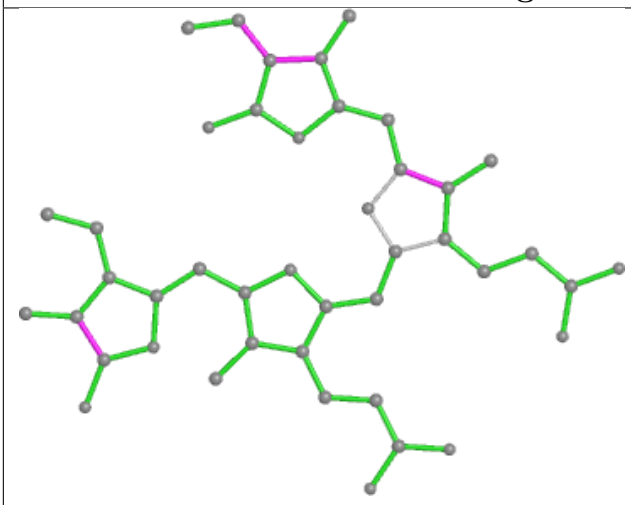


Rings

Ligand PEB hZ 401



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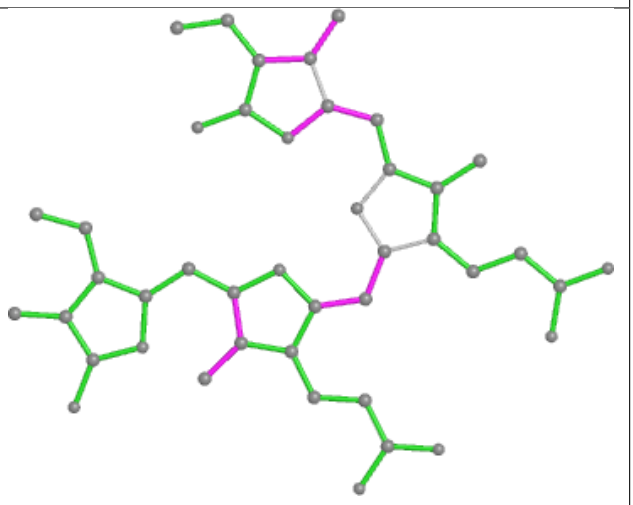

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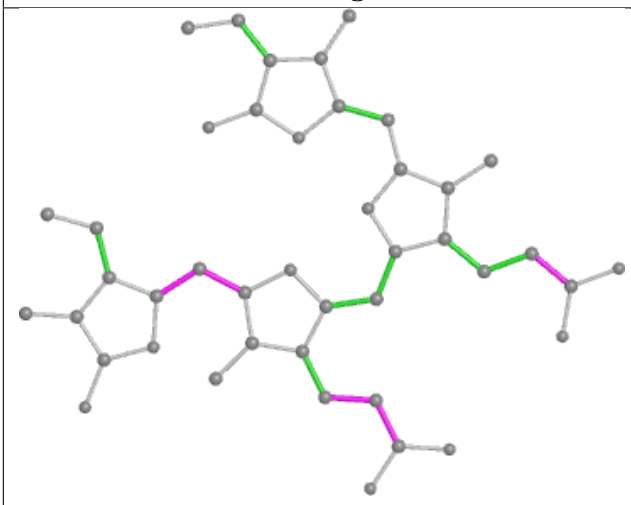

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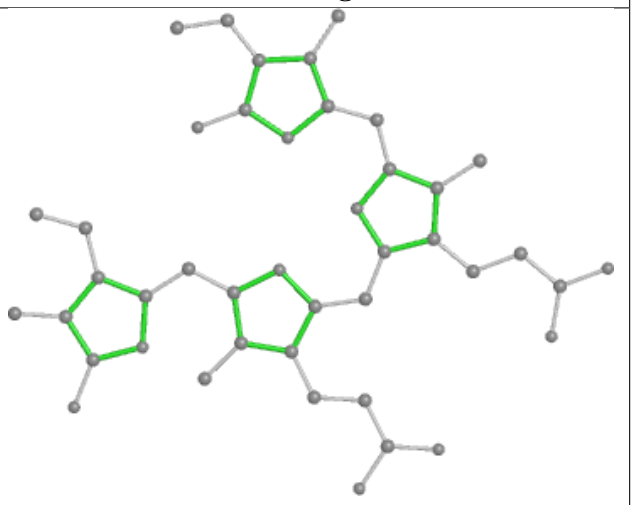
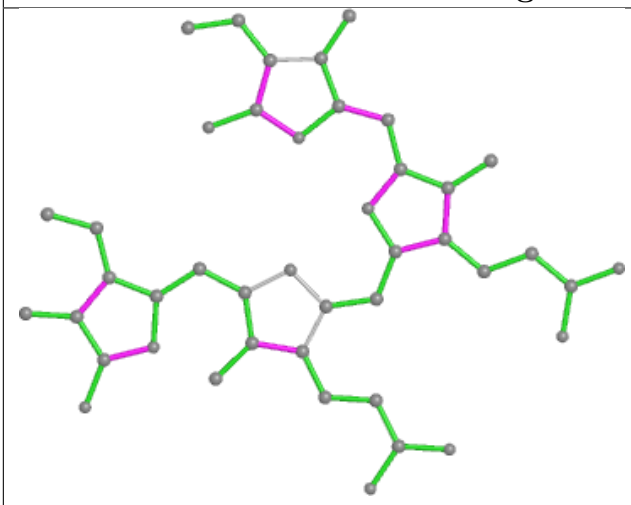


Rings

Ligand PUB n2 203



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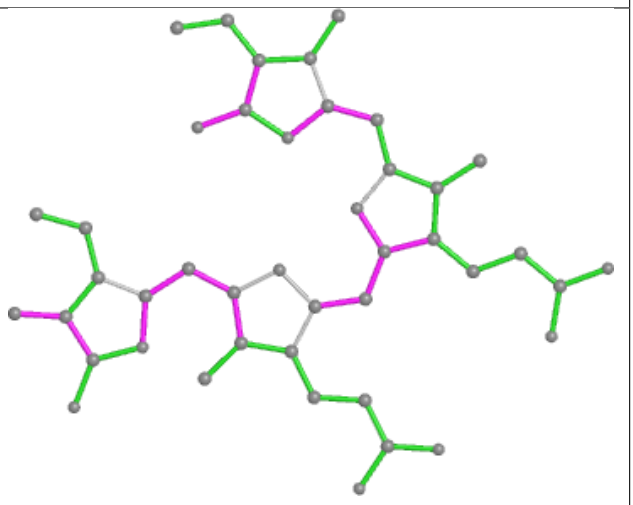

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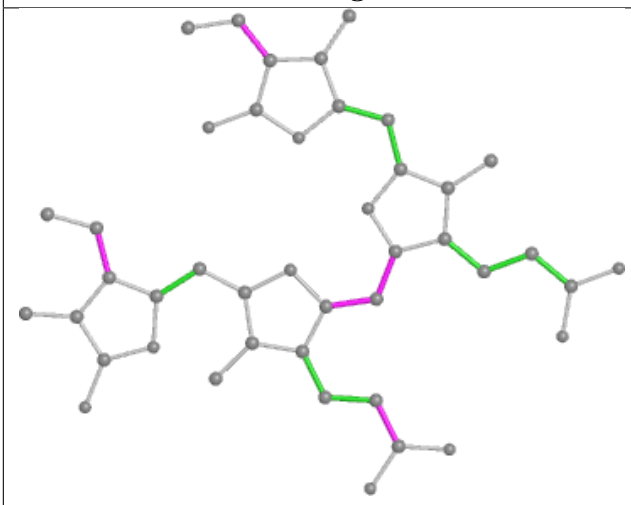

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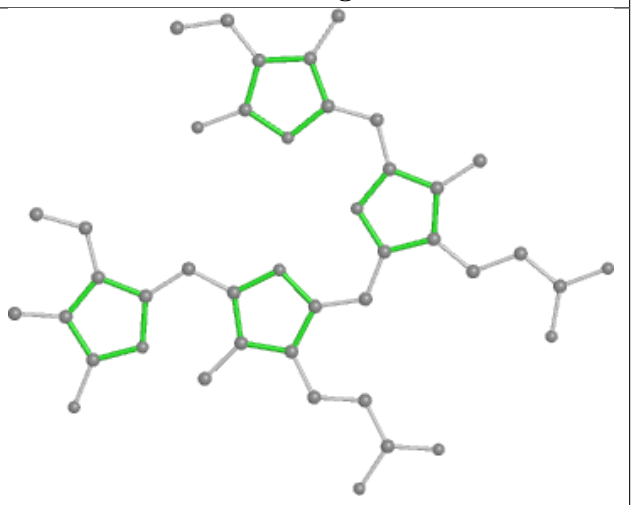

Rings

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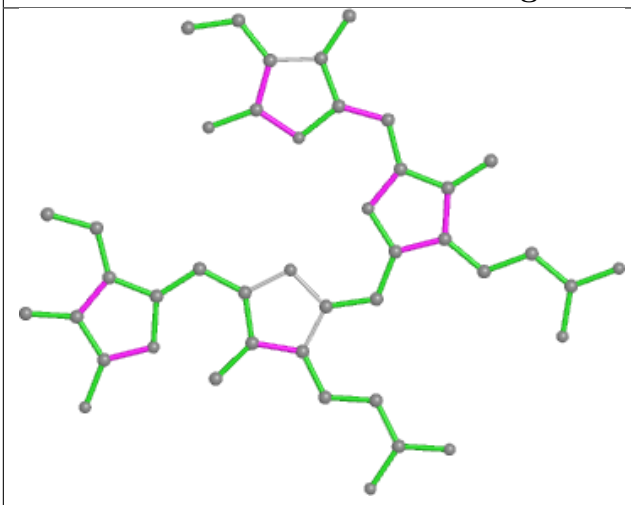

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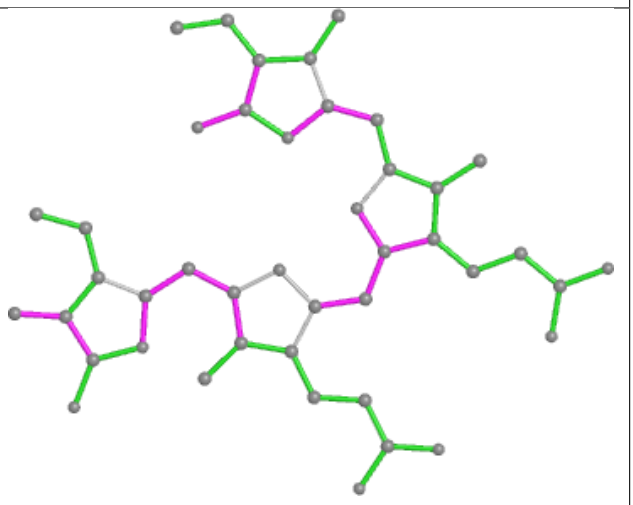

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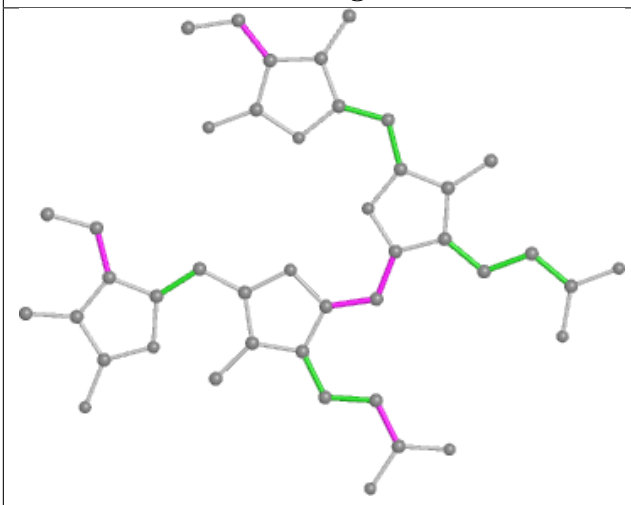

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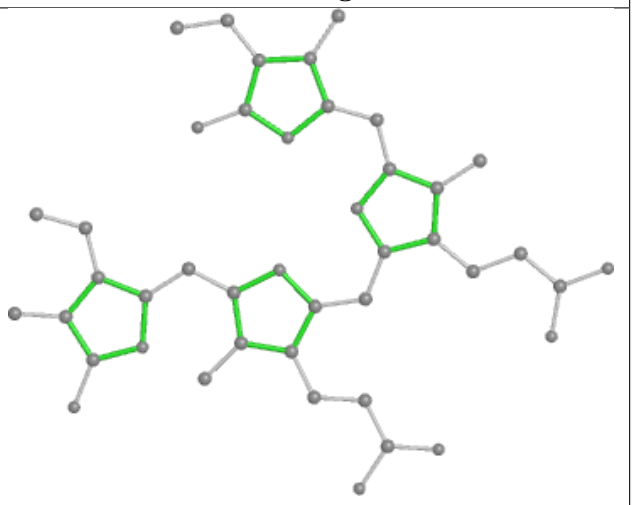
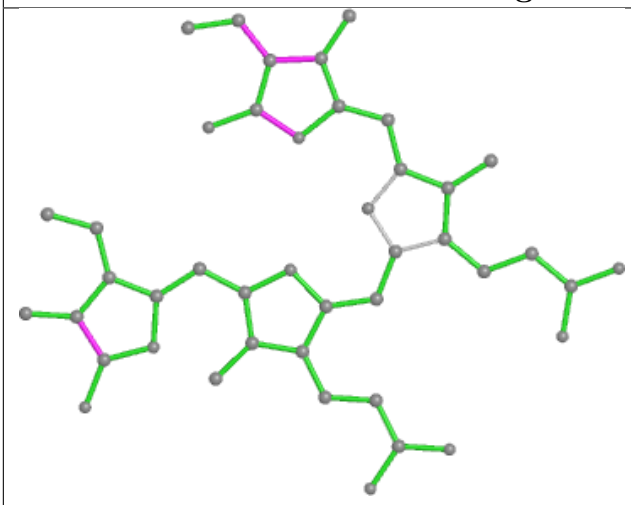


Rings

Ligand PEB Y8 201



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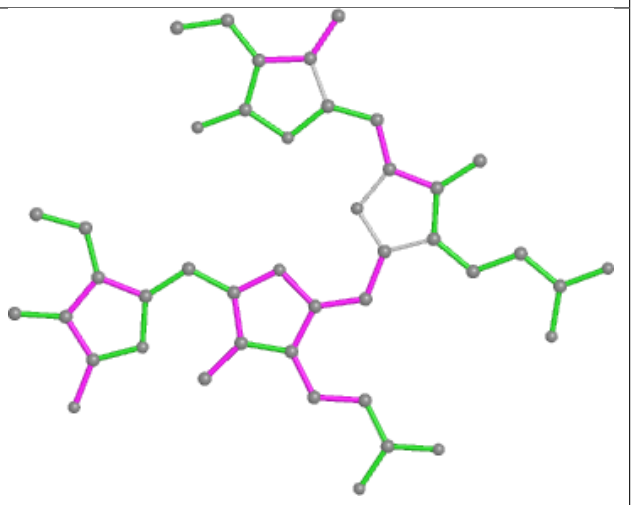

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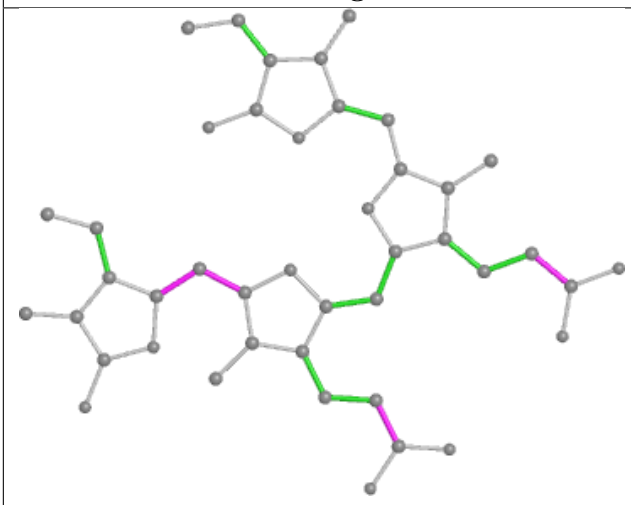

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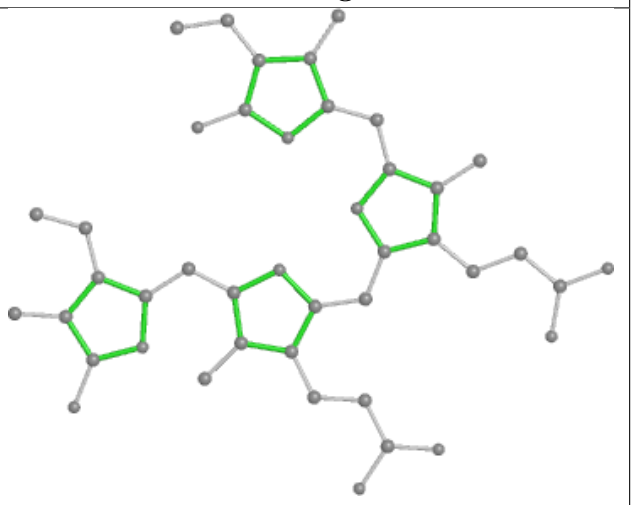
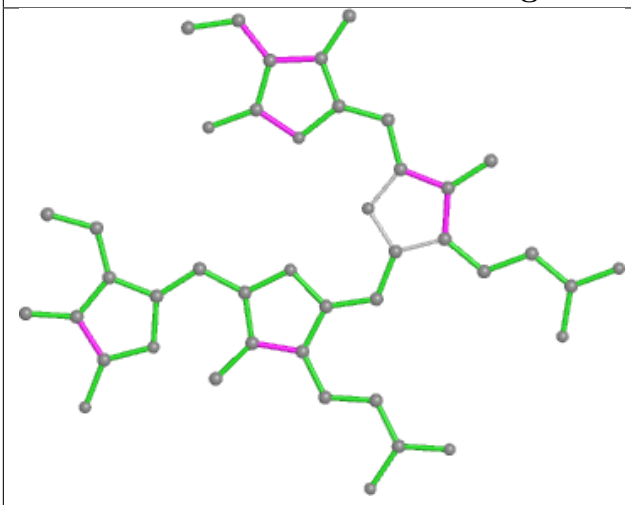


Rings

Ligand PEB z3 202



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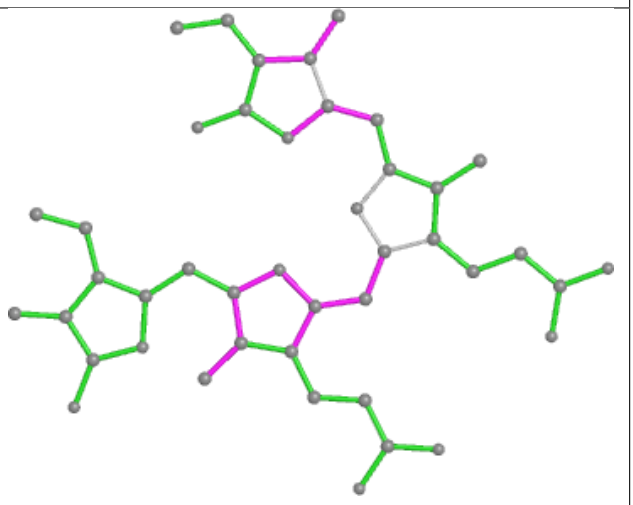
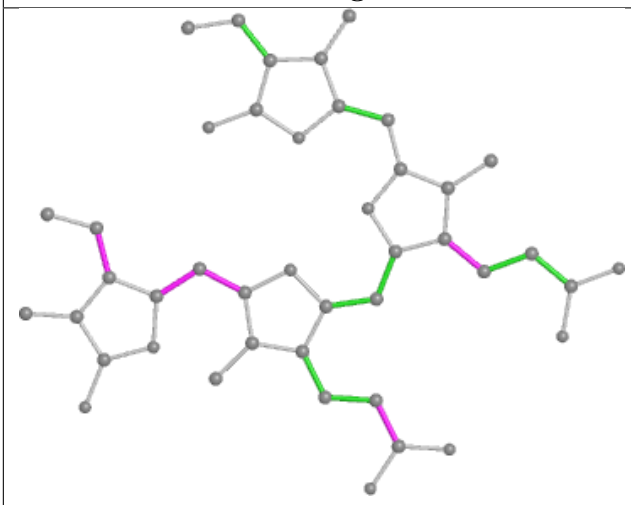


Bond angles



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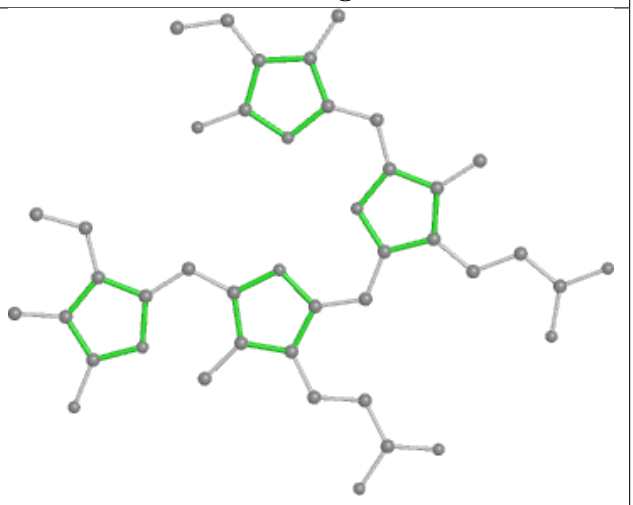

Rings

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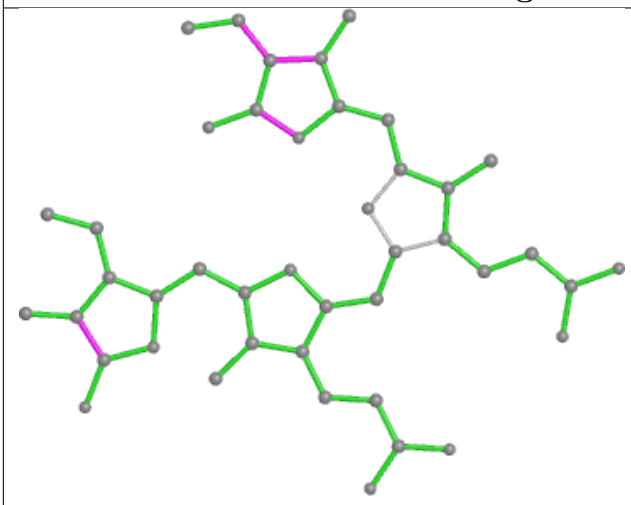

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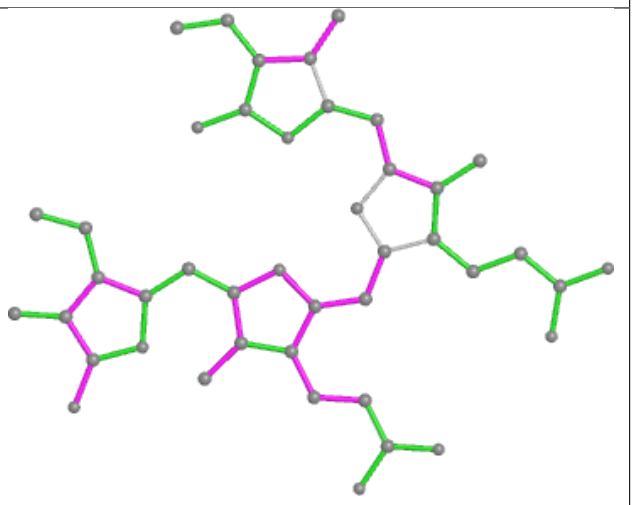

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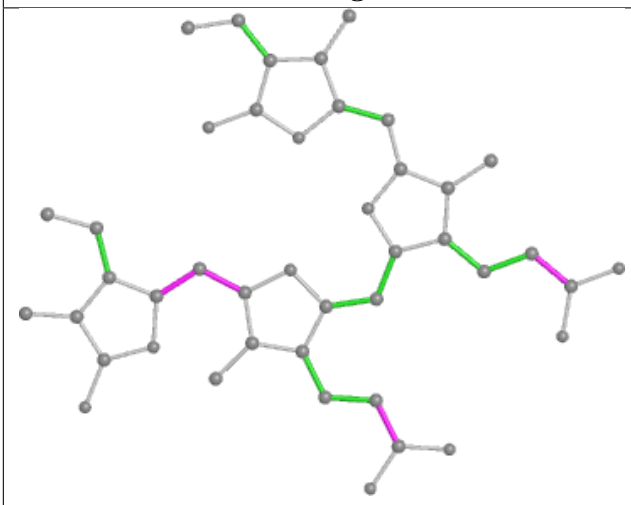

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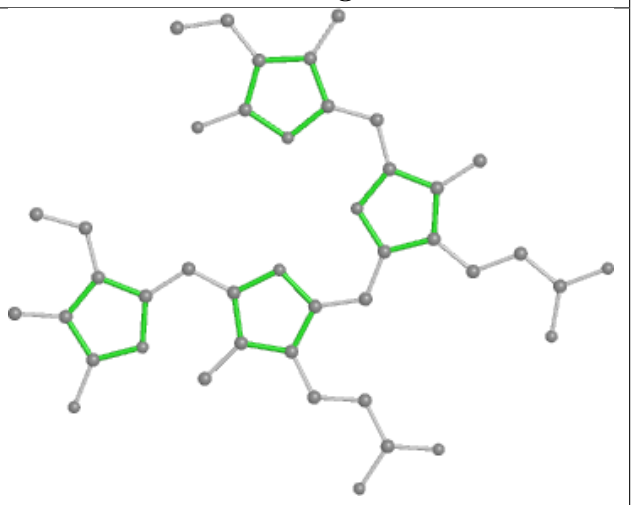
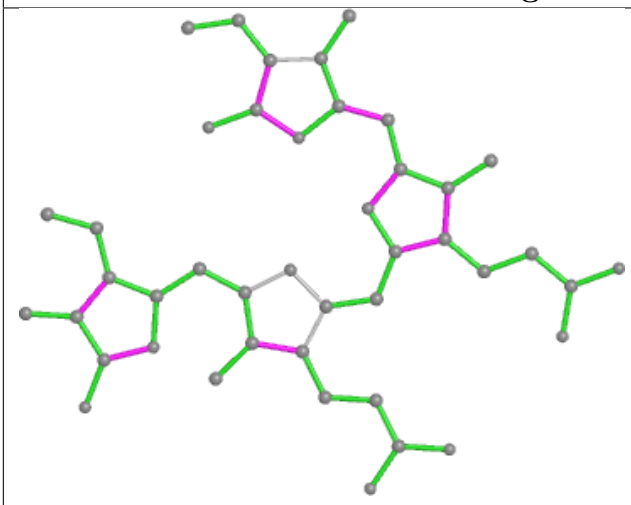


Rings

Ligand PUB l3 202



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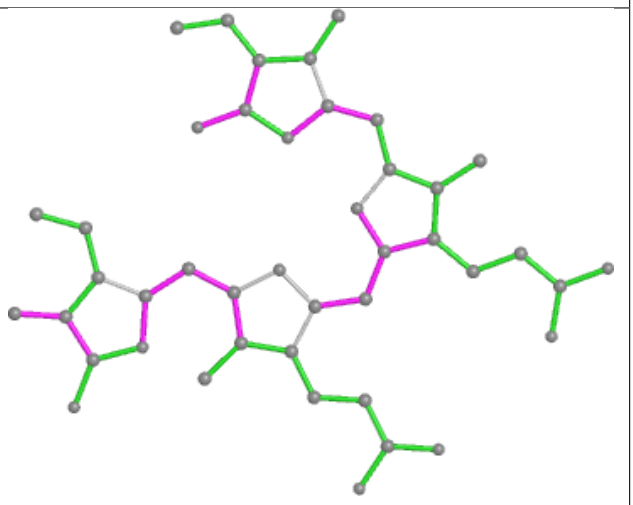

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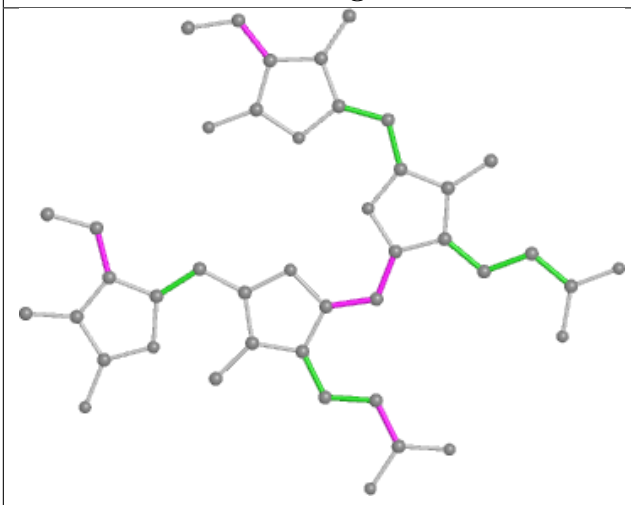

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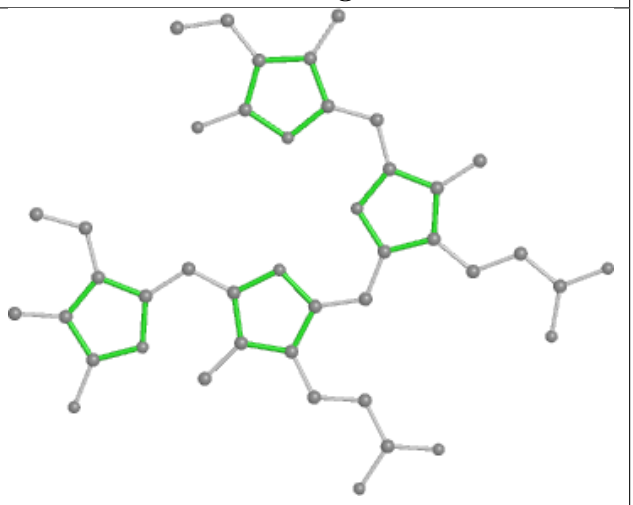
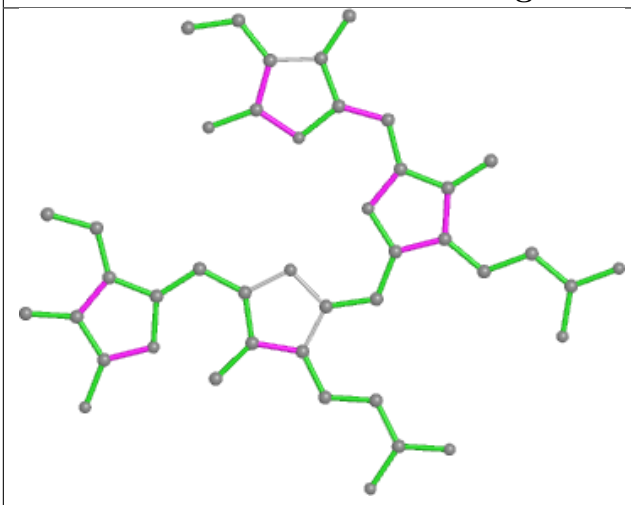


Rings

Ligand PUB F2 203



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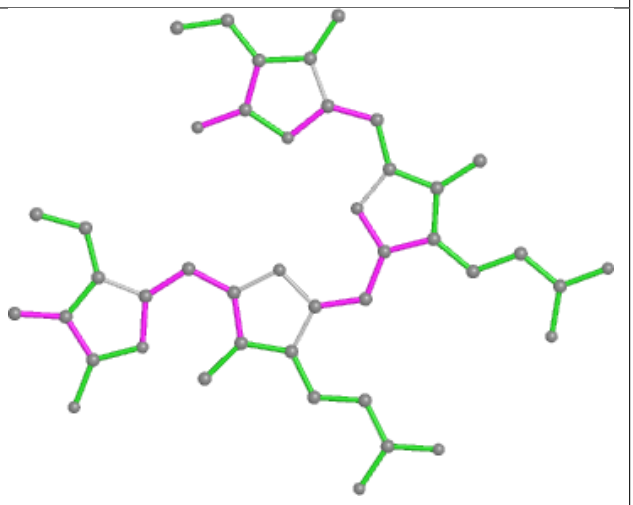

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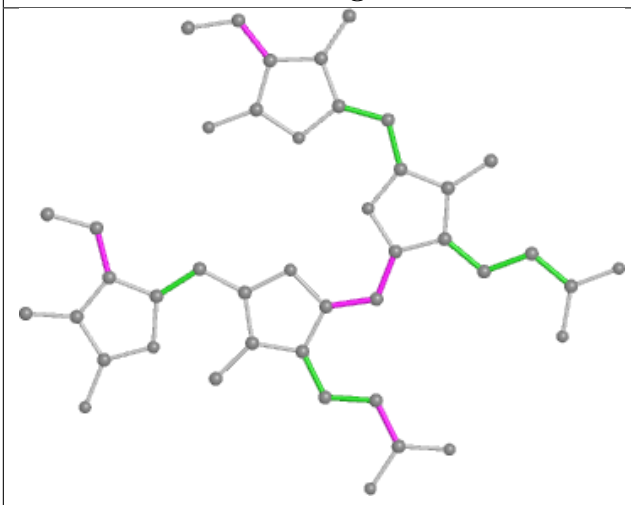

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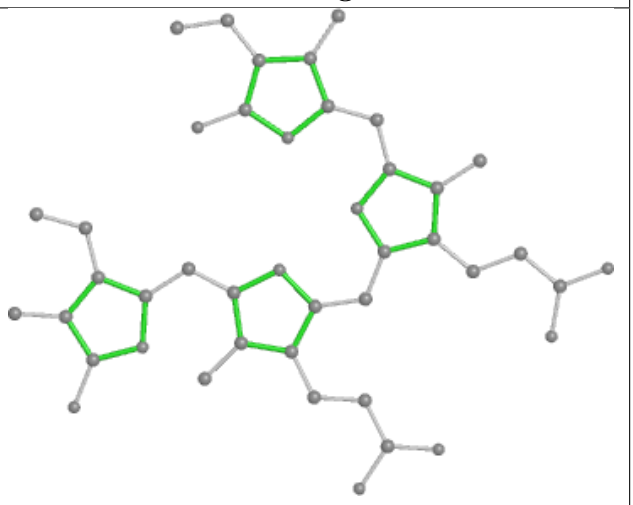
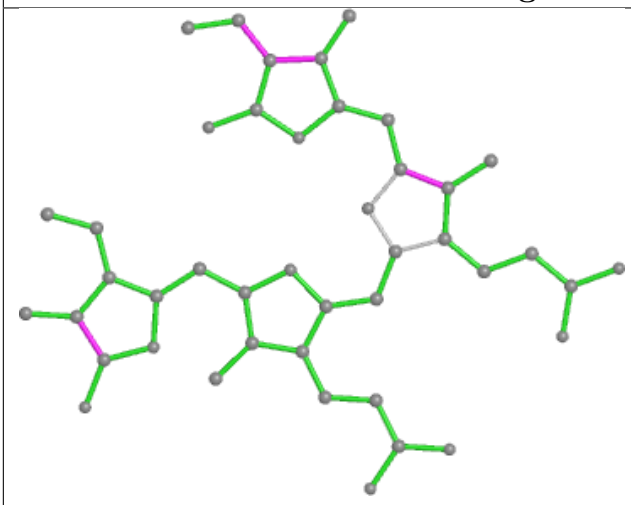


Rings

Ligand PEB d6 202



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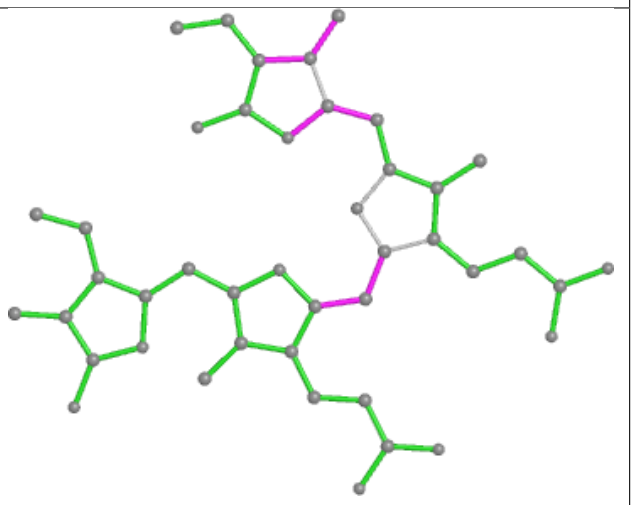

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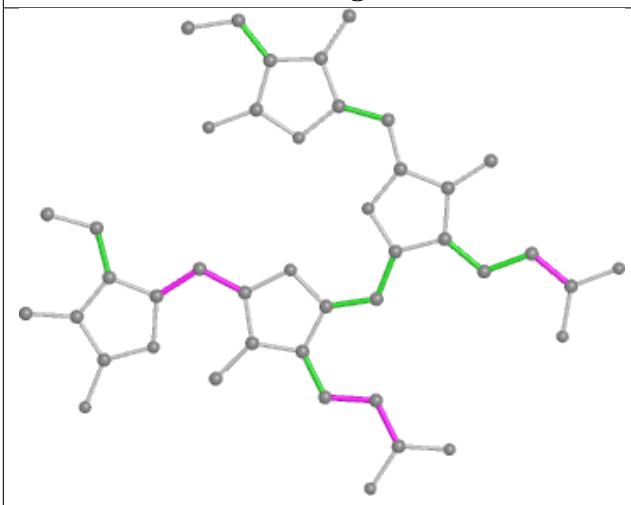

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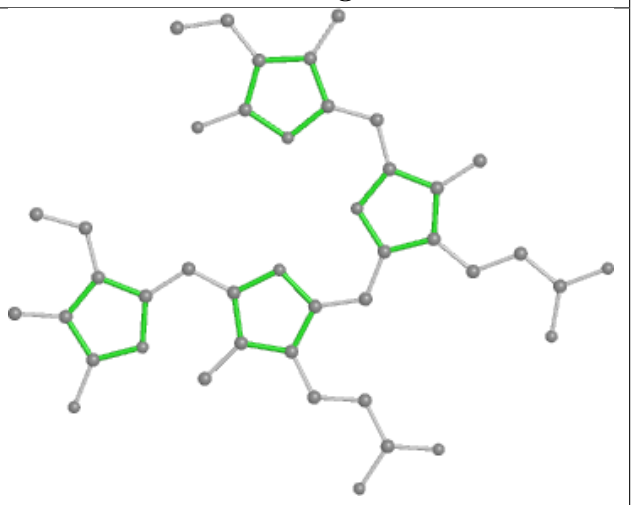
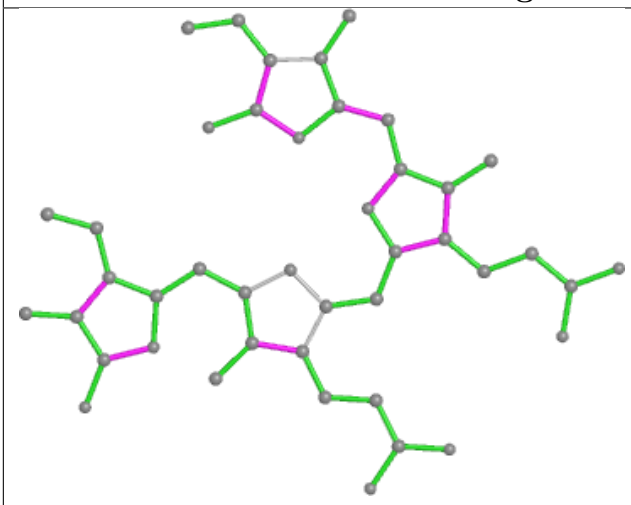


Rings

Ligand PUB L4 203



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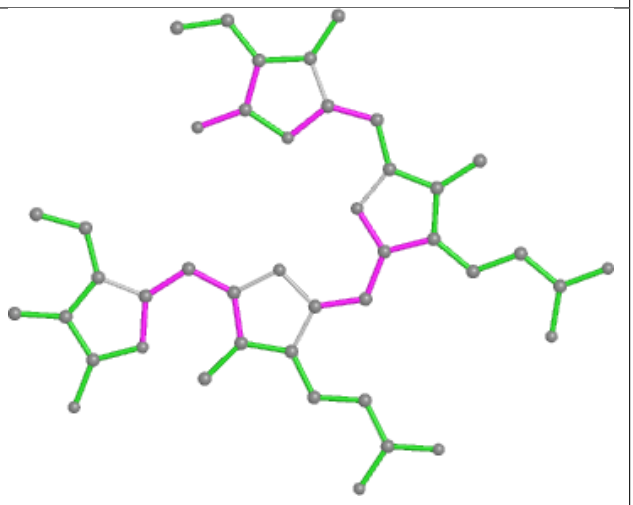
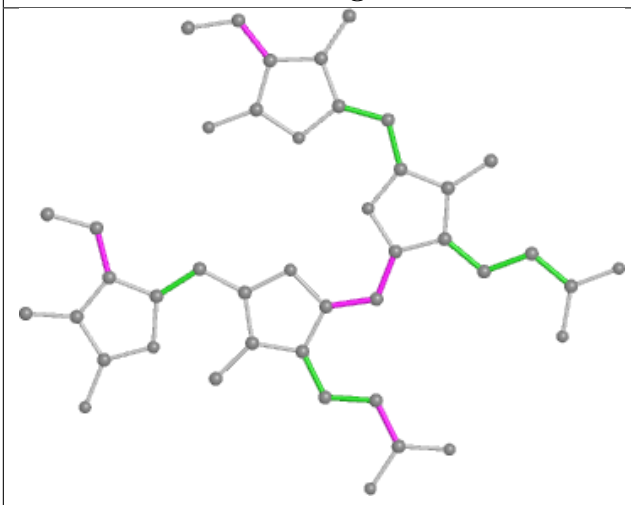
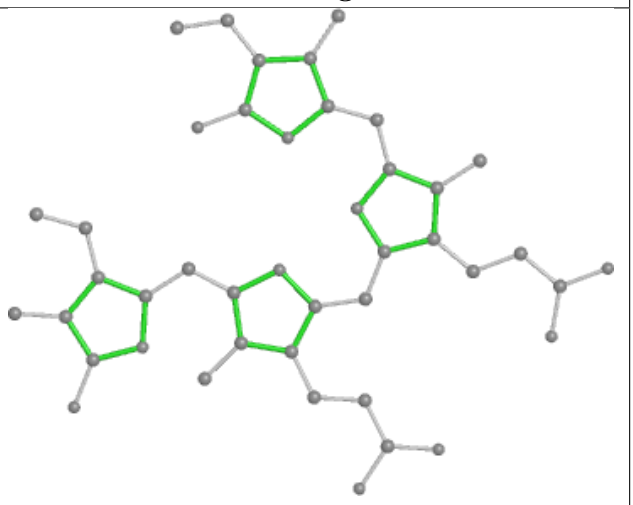


Bond angles

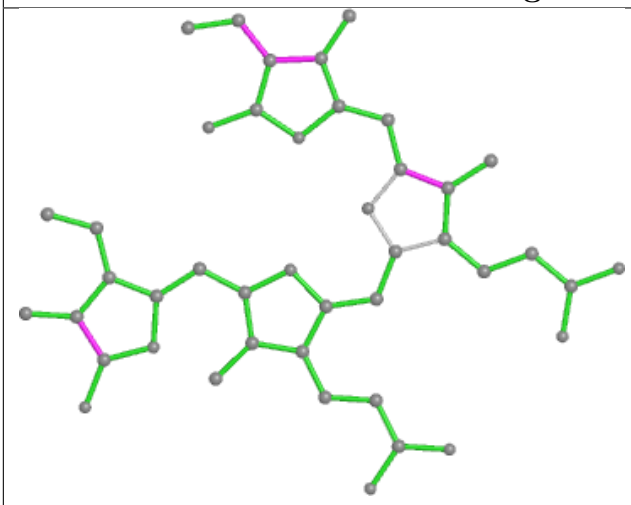


Torsions



Rings

Ligand PEB lg 202



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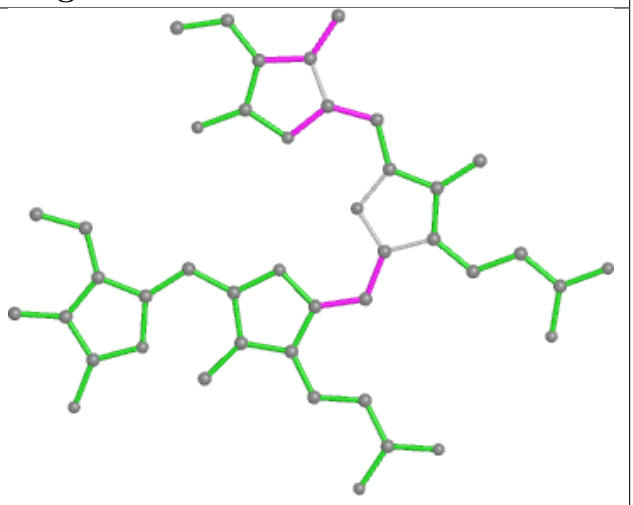

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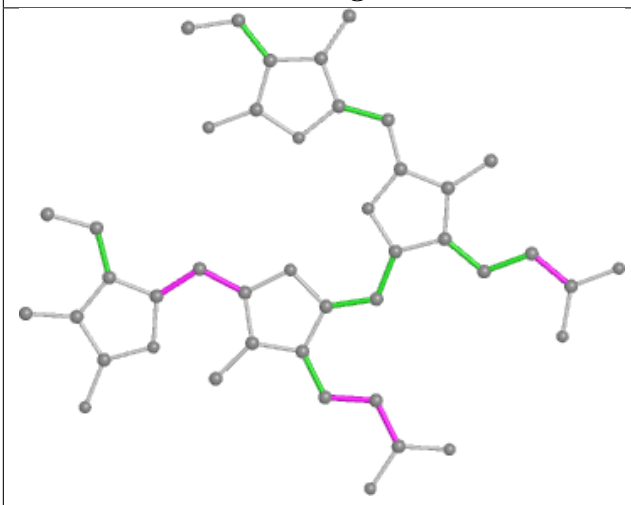

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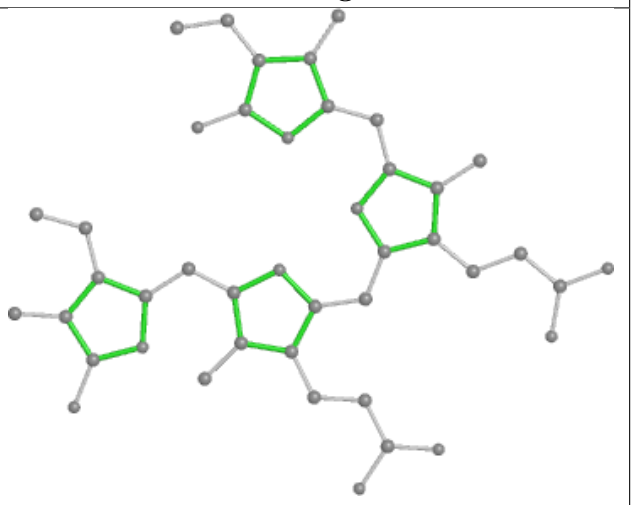
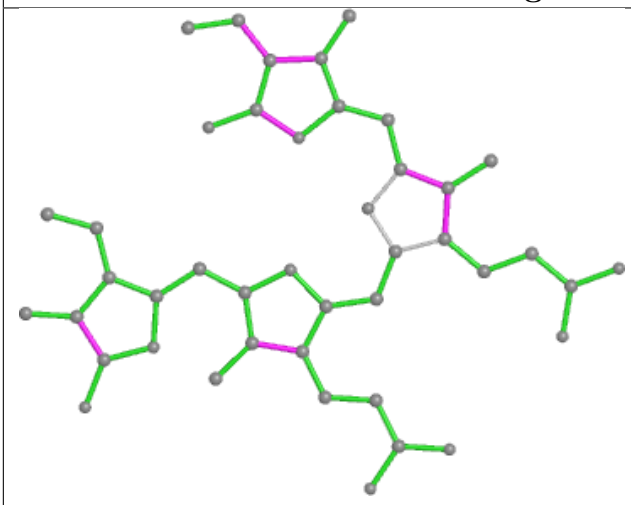


Rings

Ligand PEB ei 202



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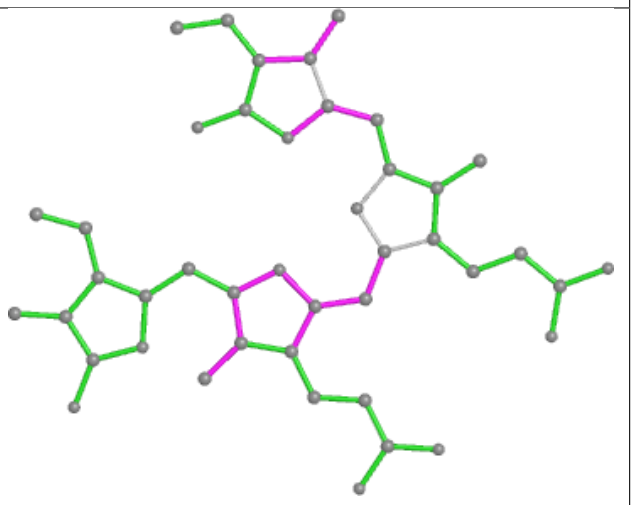

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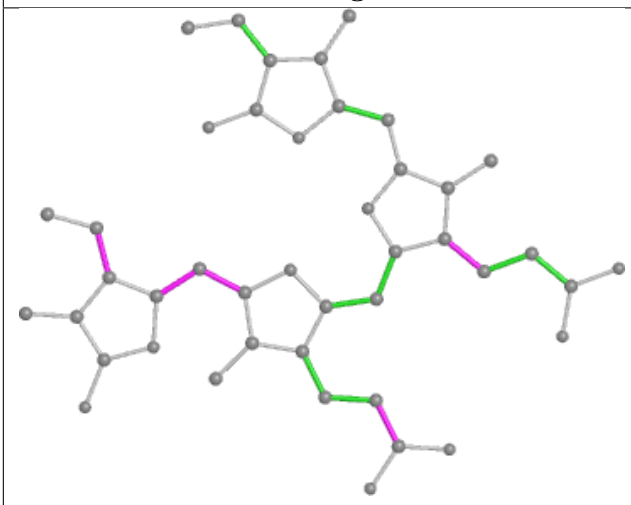

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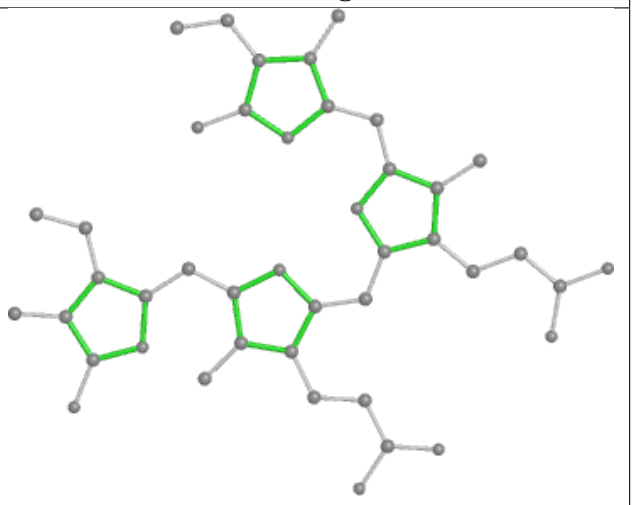
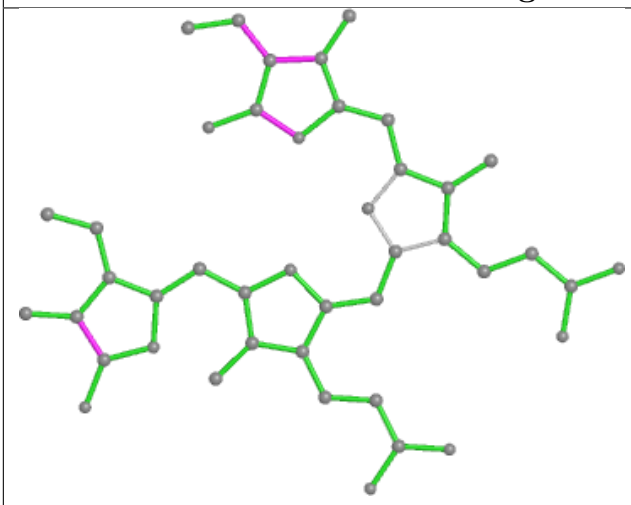


Rings

Ligand PEB bo 201



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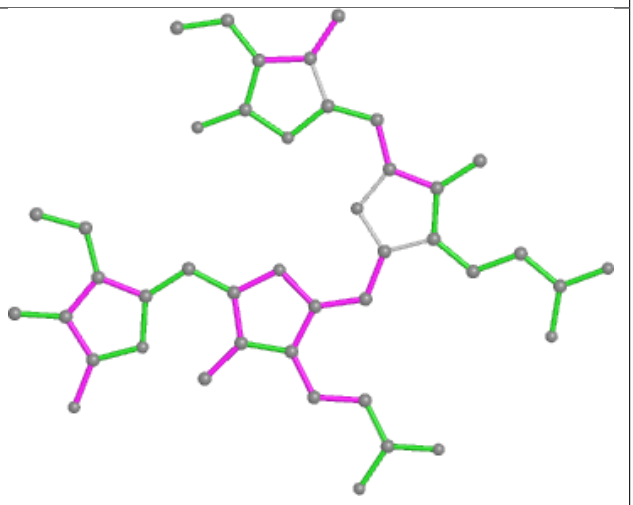

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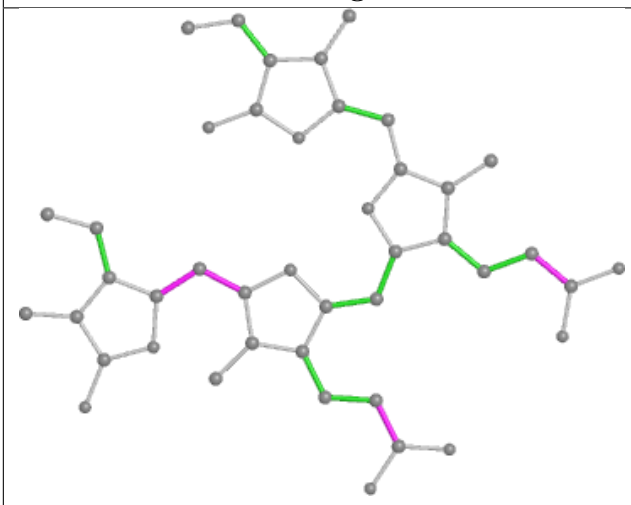

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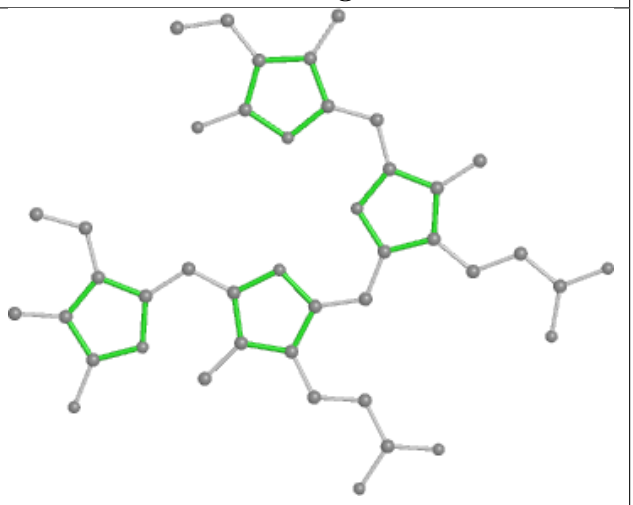
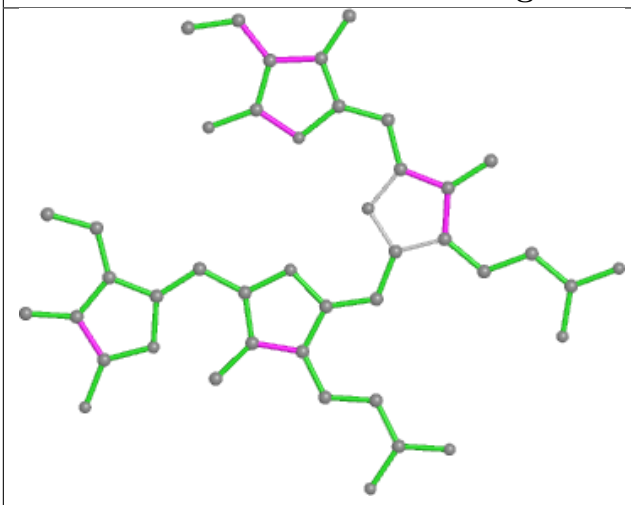


Rings

Ligand PEB P9 202



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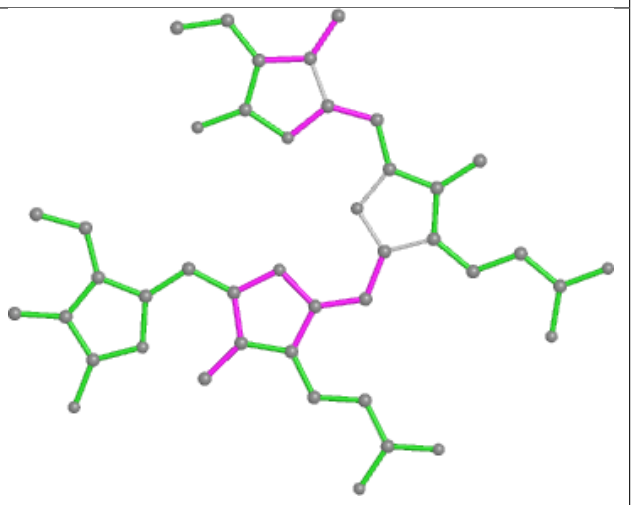

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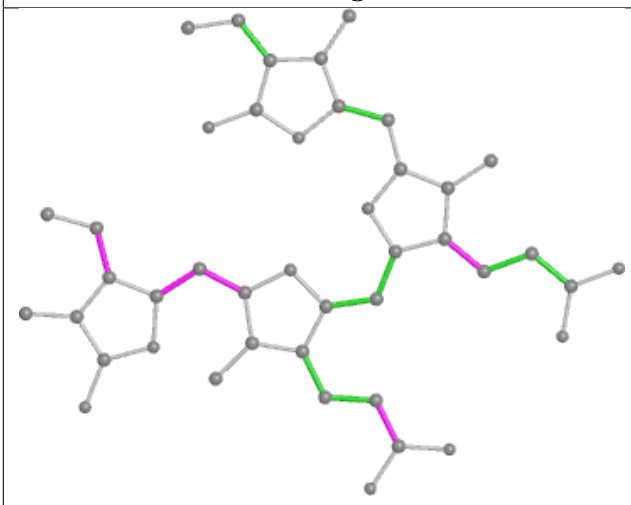

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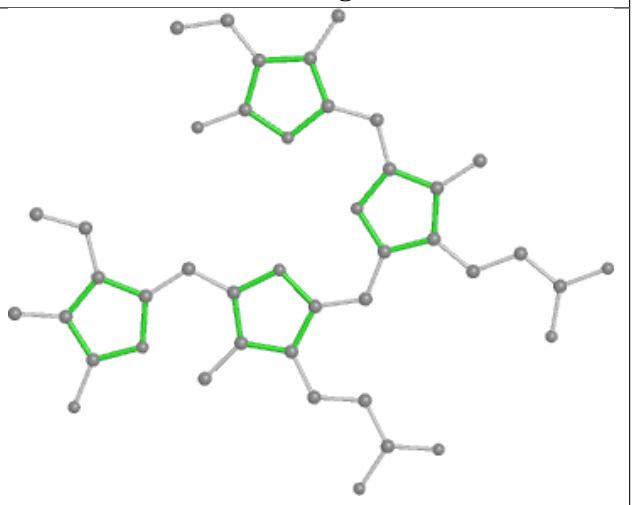
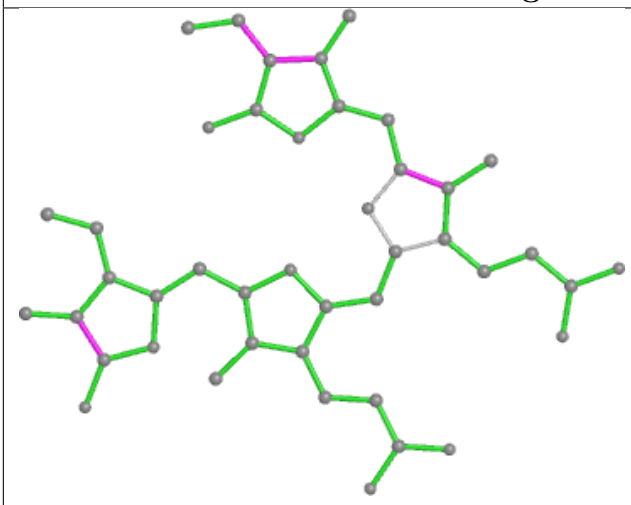


Rings

Ligand PEB fb 202



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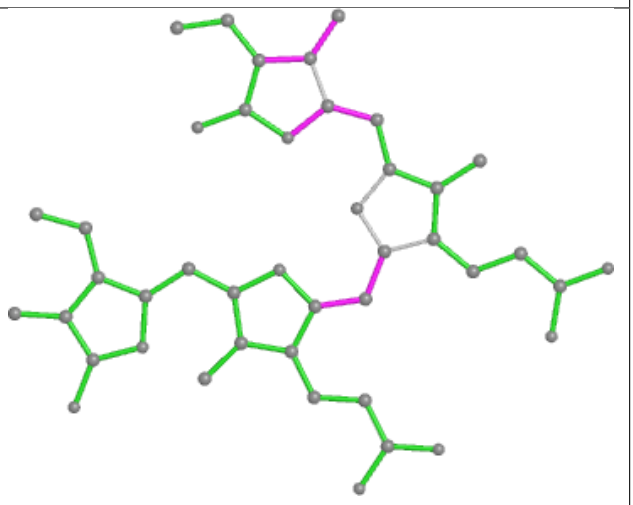

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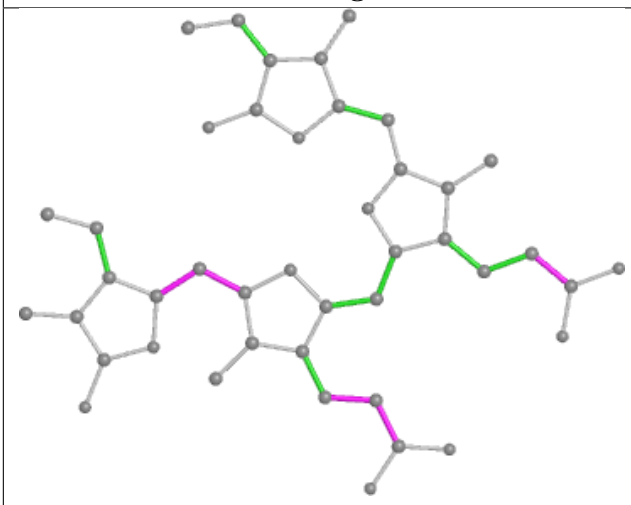

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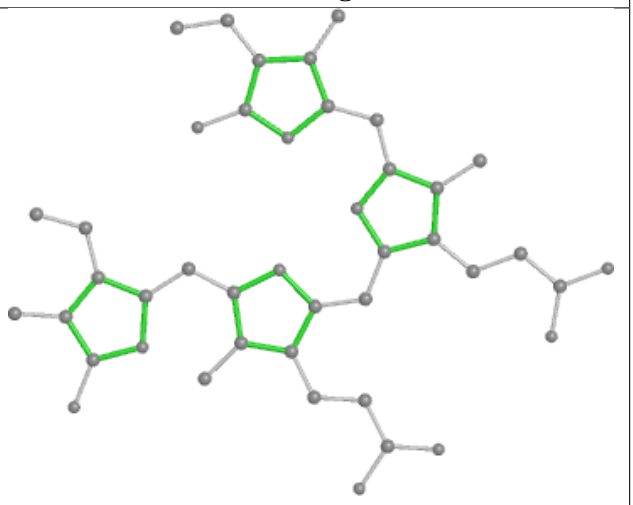

Rings

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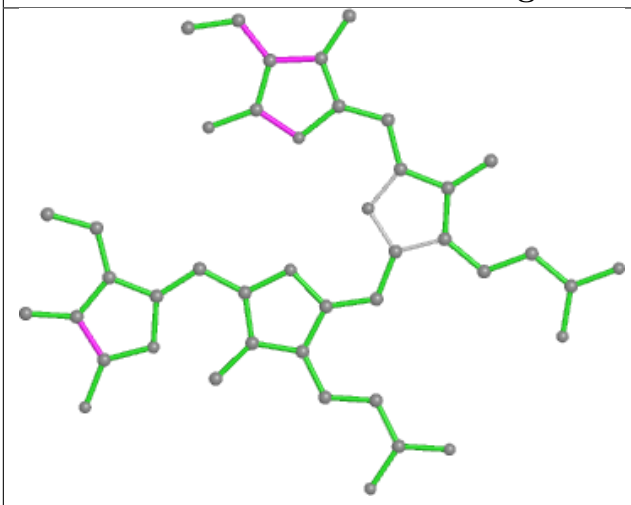

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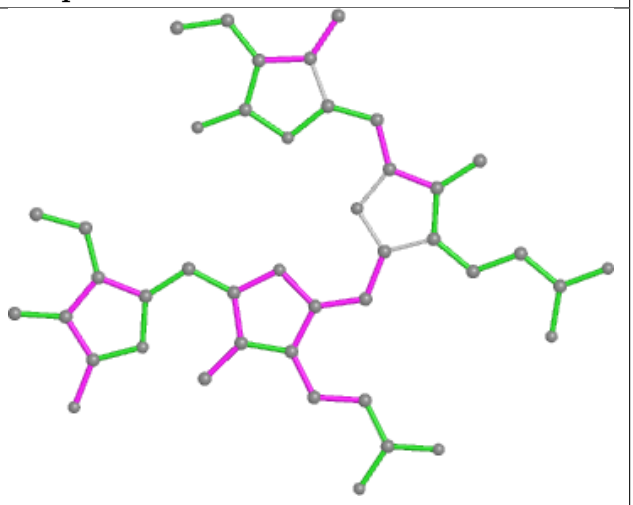

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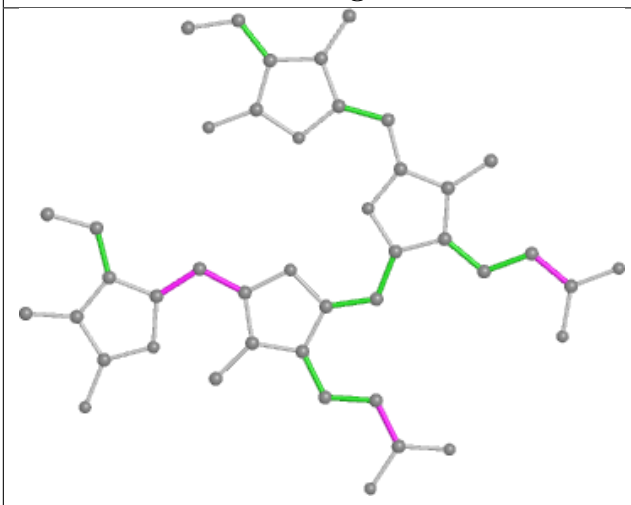

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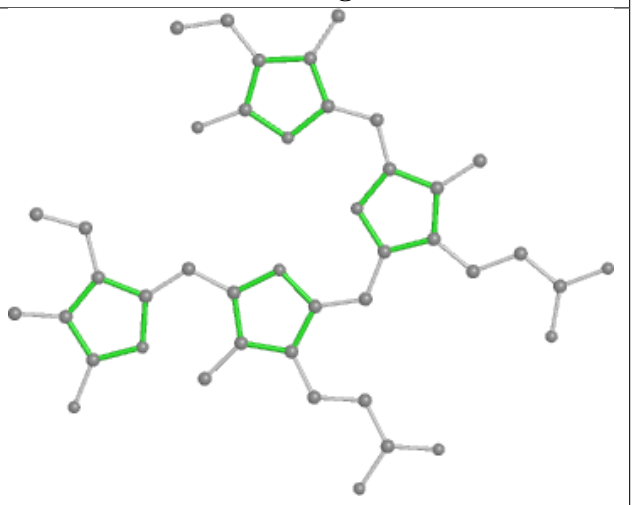
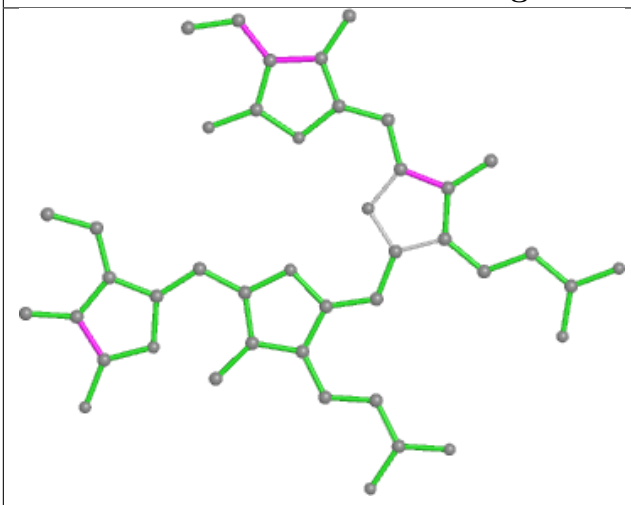


Rings

Ligand PEB hW 202



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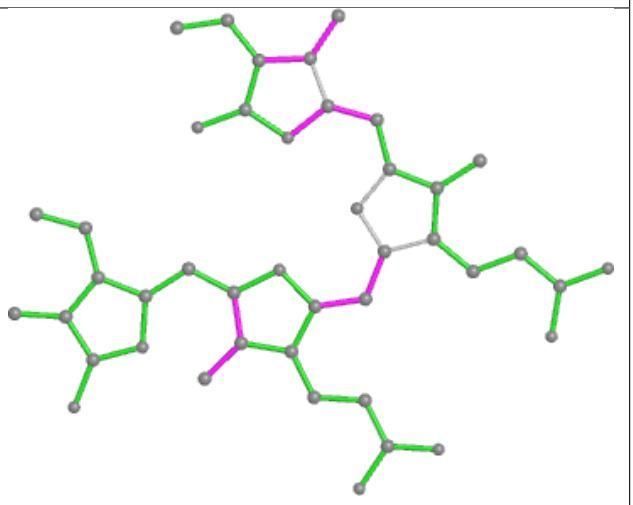

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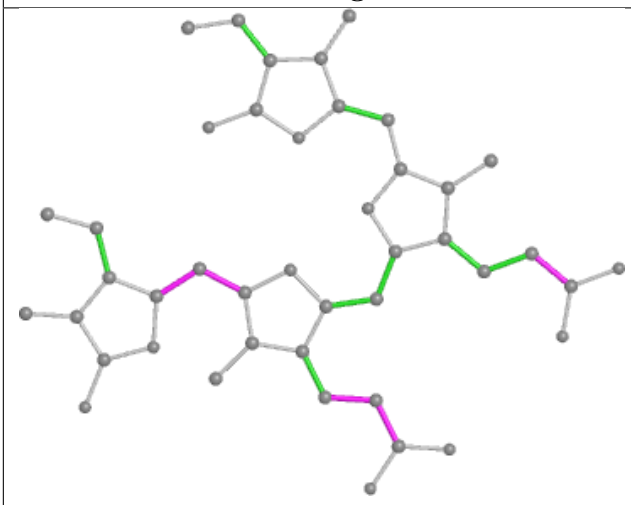

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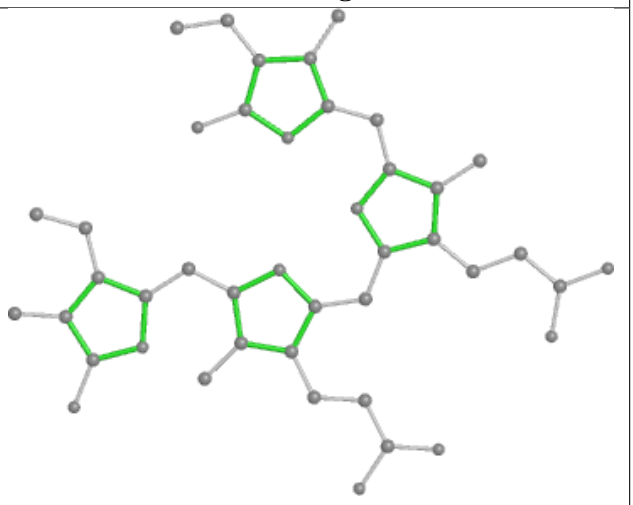
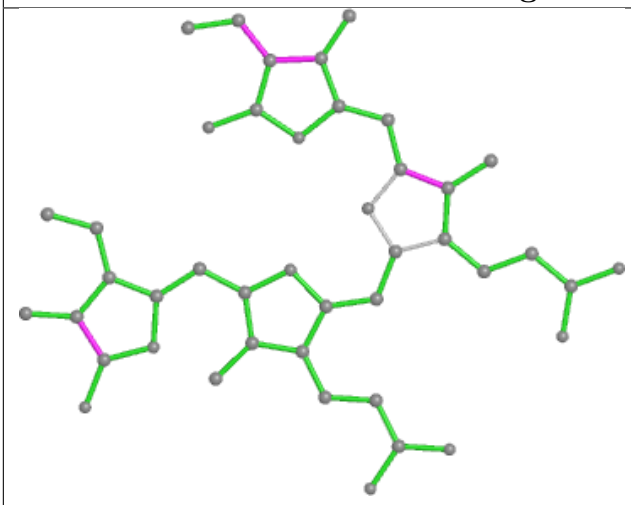


Rings

Ligand PEB g3 202



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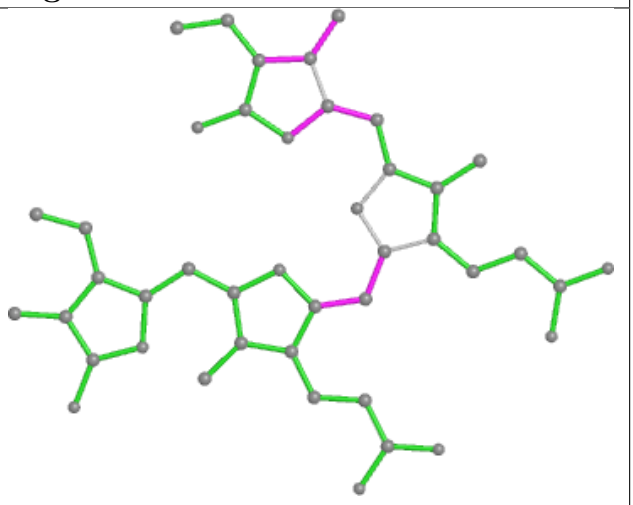

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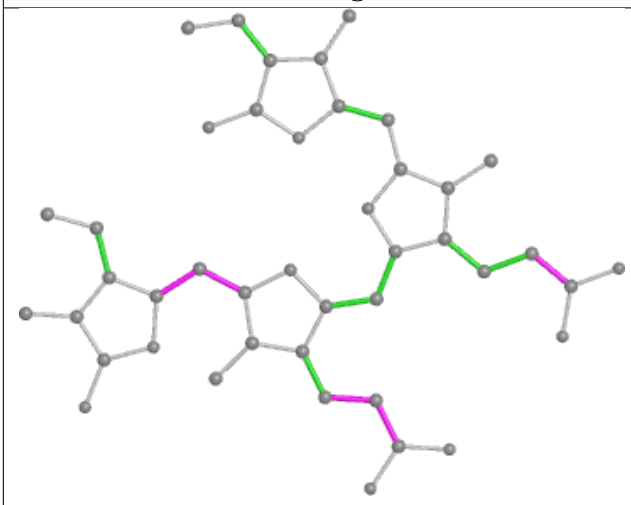

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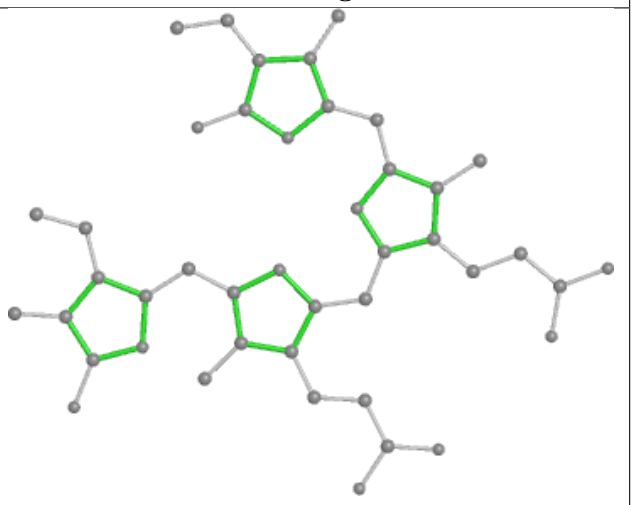
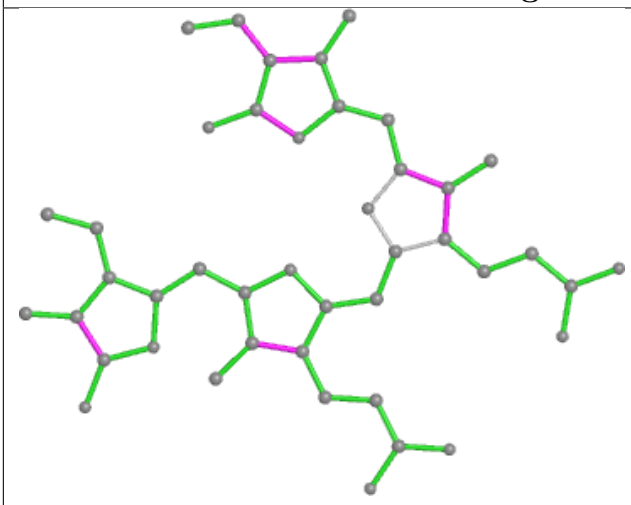


Rings

Ligand PEB r4 201



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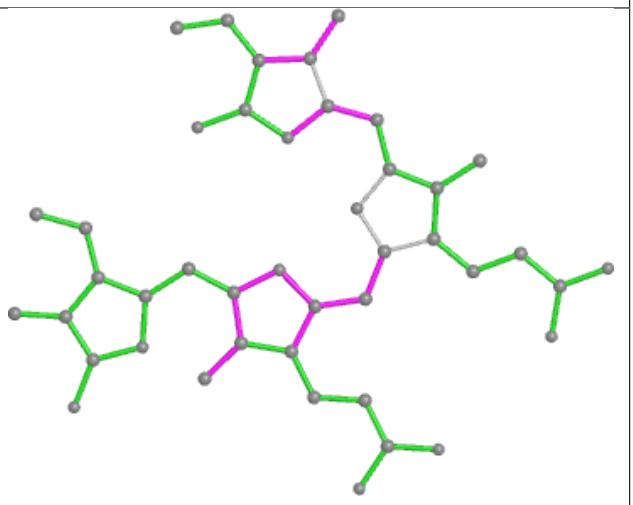

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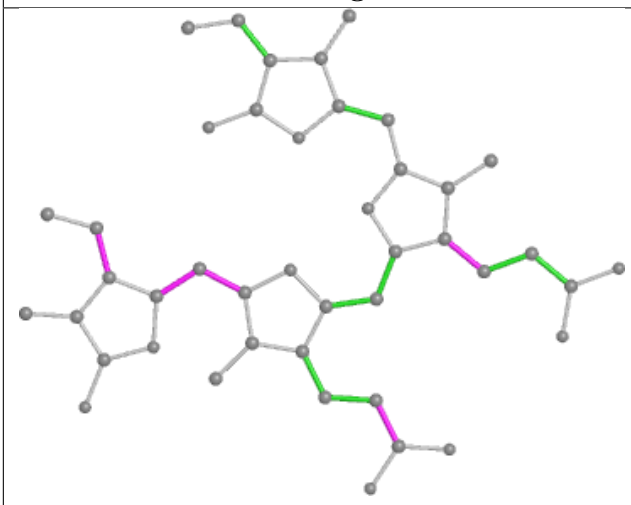

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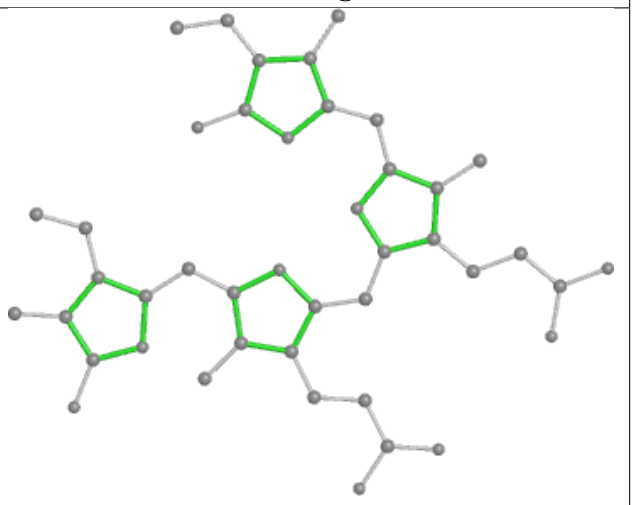
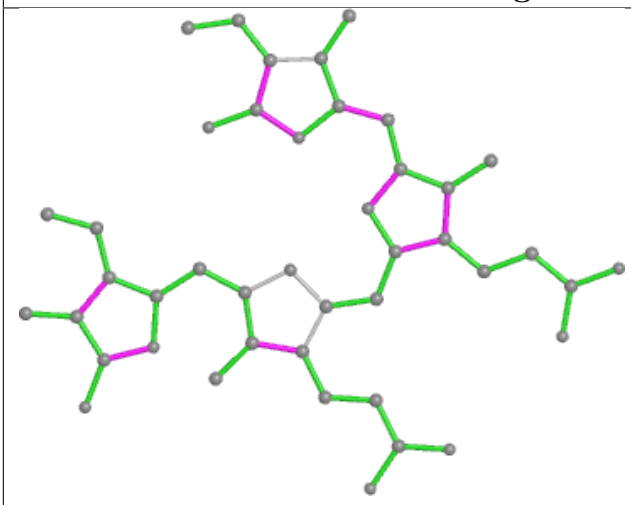


Rings

Ligand PUB hP 203



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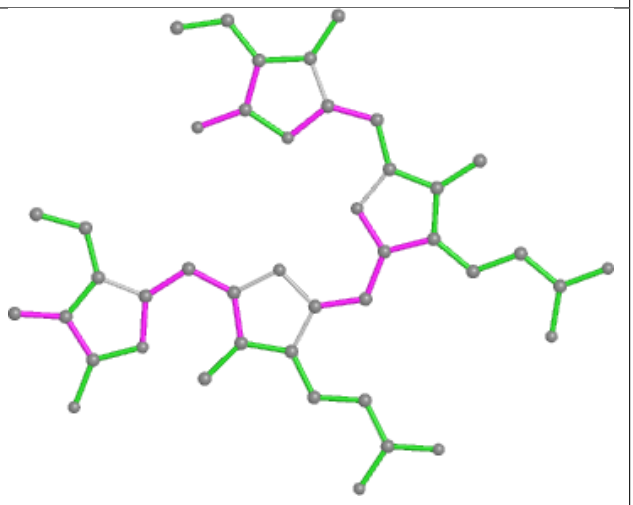

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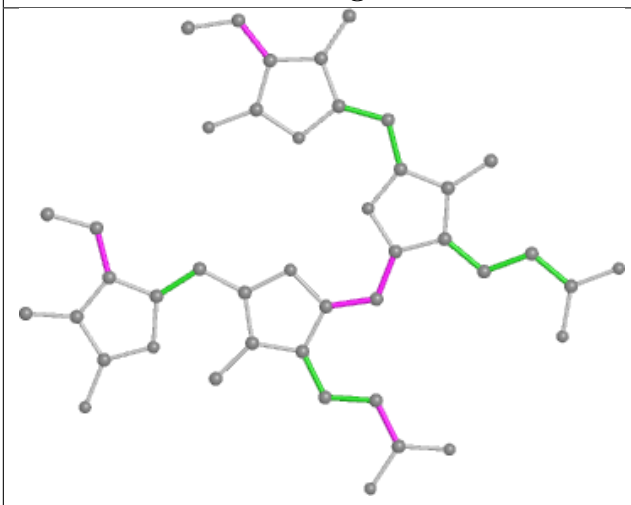

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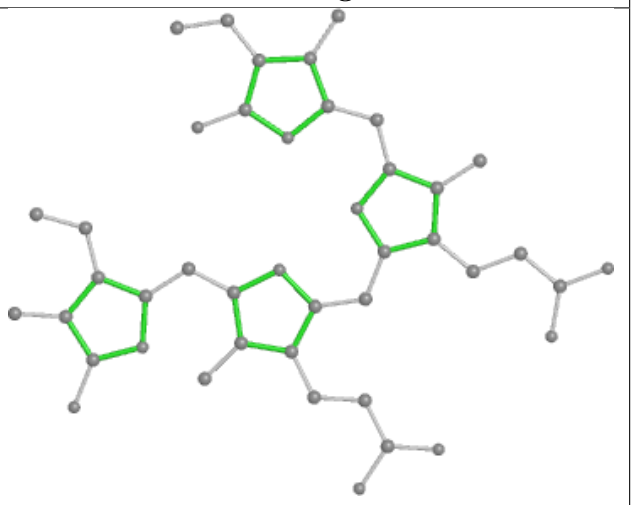

Rings

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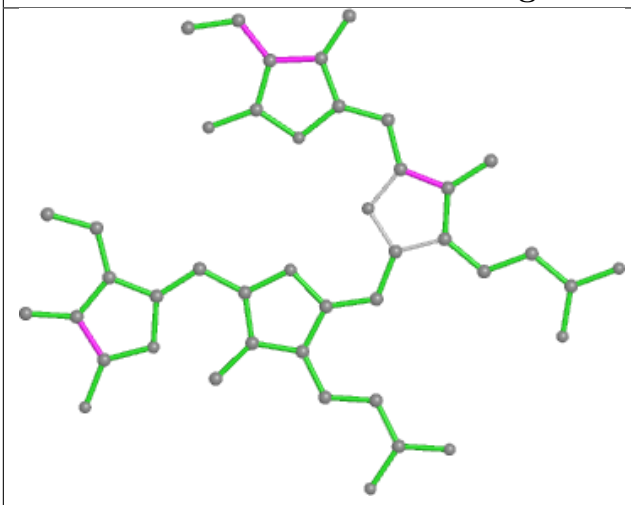

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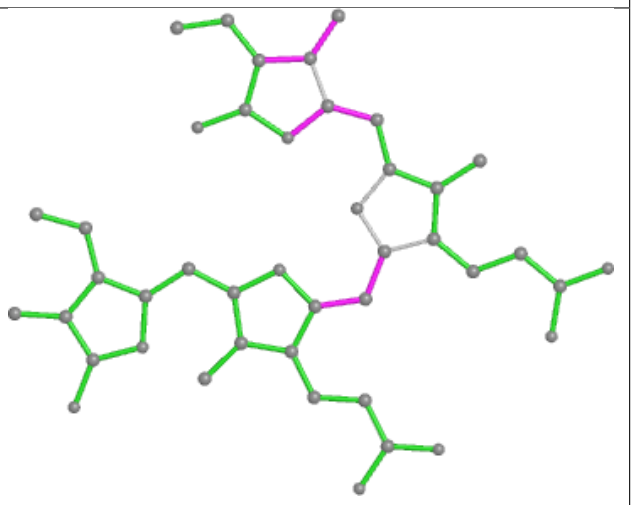

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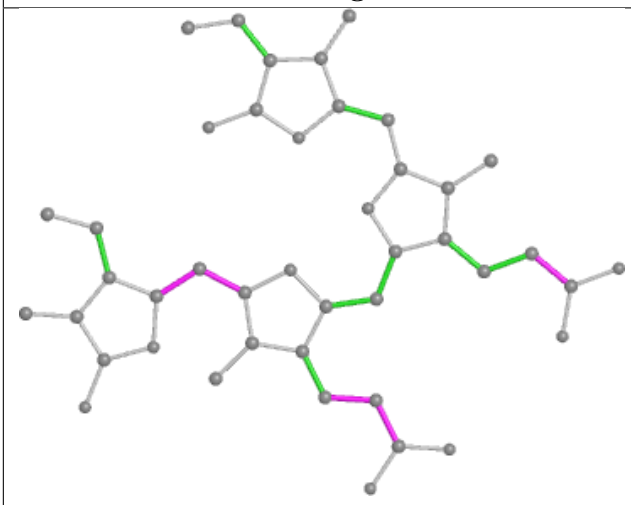

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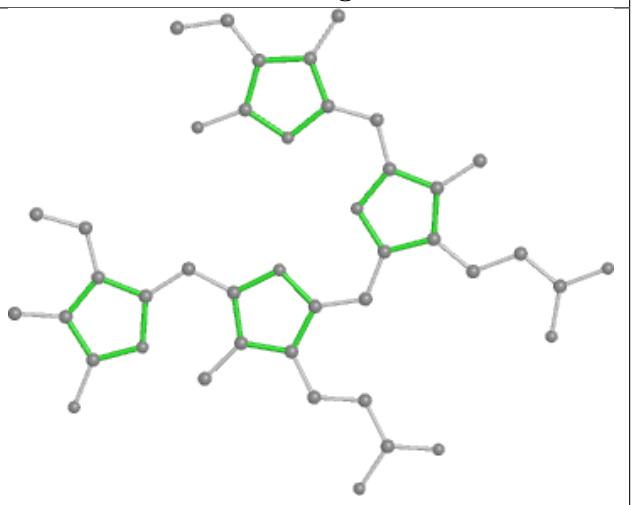
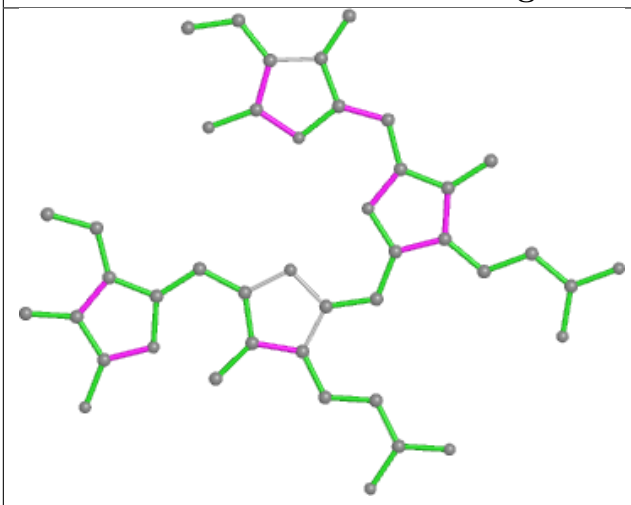


Rings

Ligand PUB 44 305



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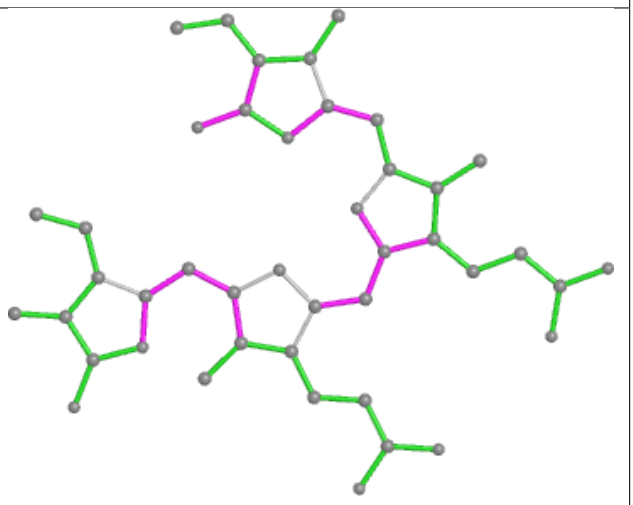
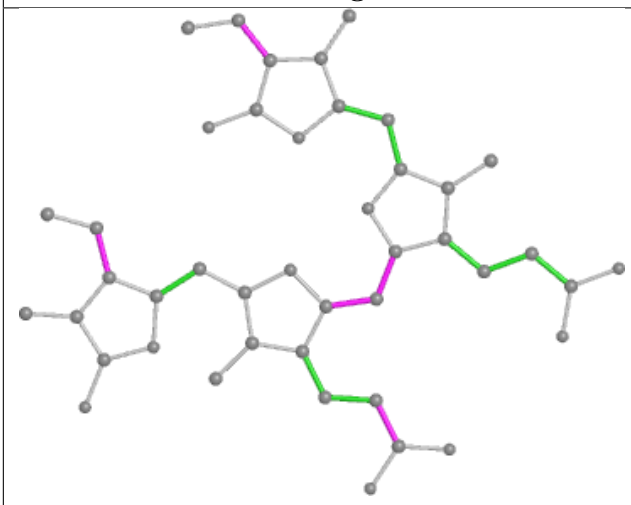


Bond angles



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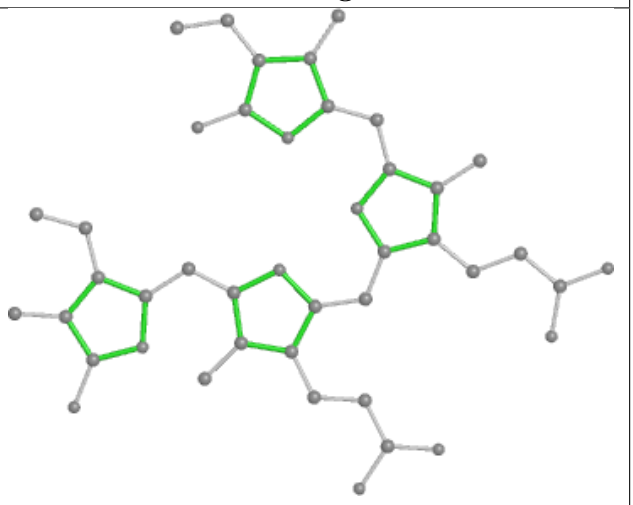
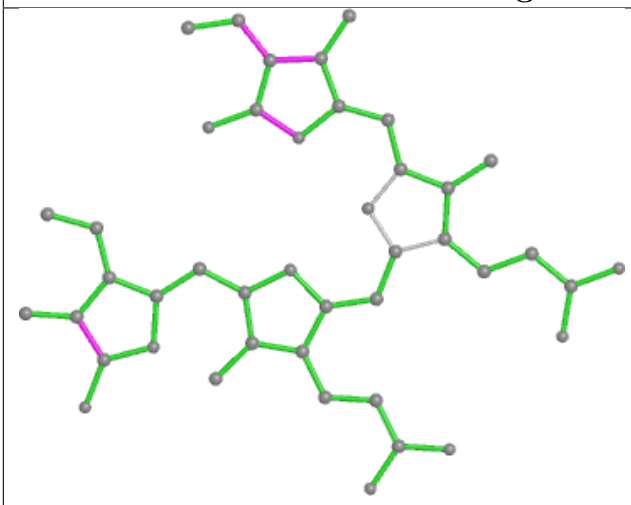


Rings

Ligand PEB B4 201



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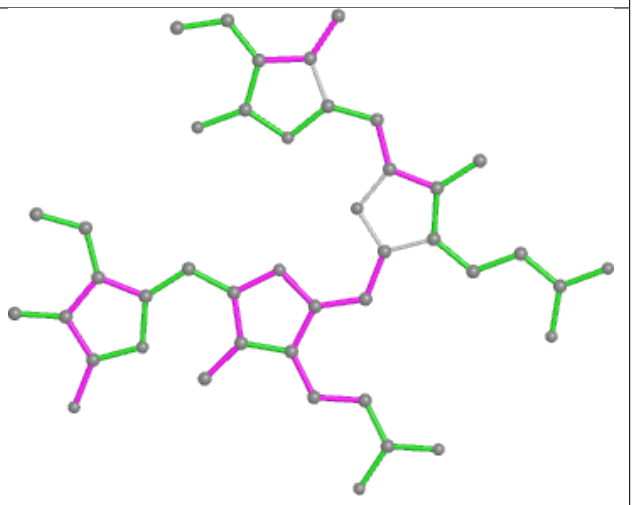
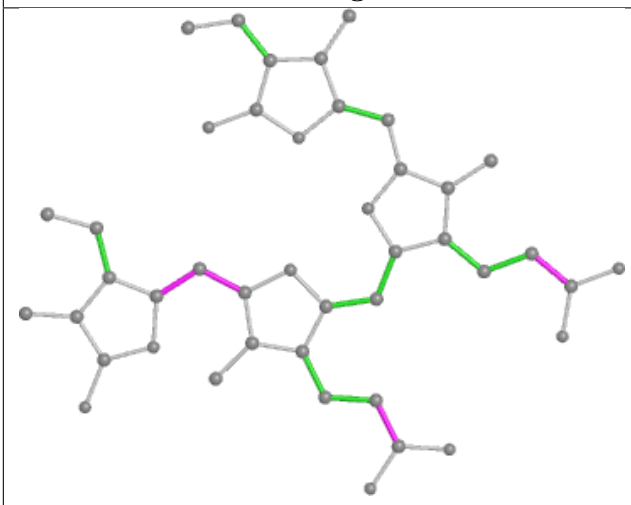


Bond angles



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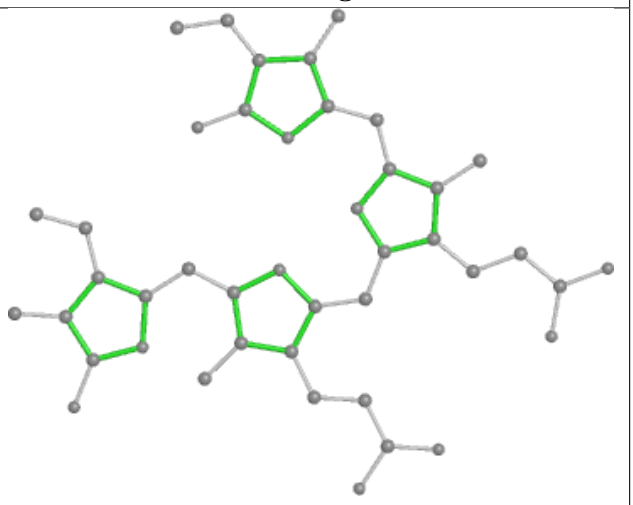
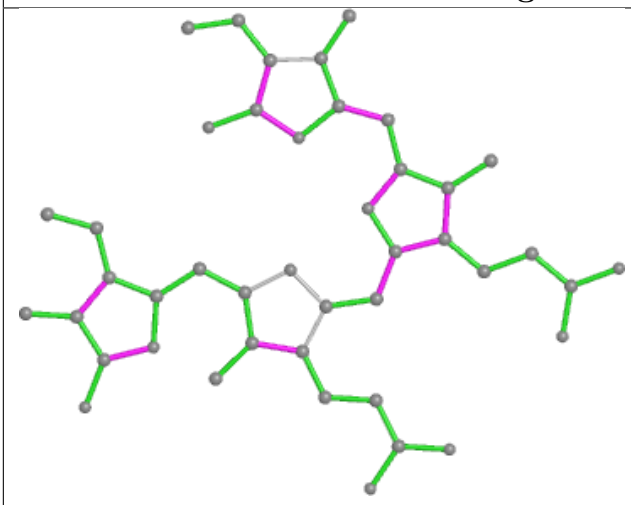


Rings

Ligand PUB fw 203



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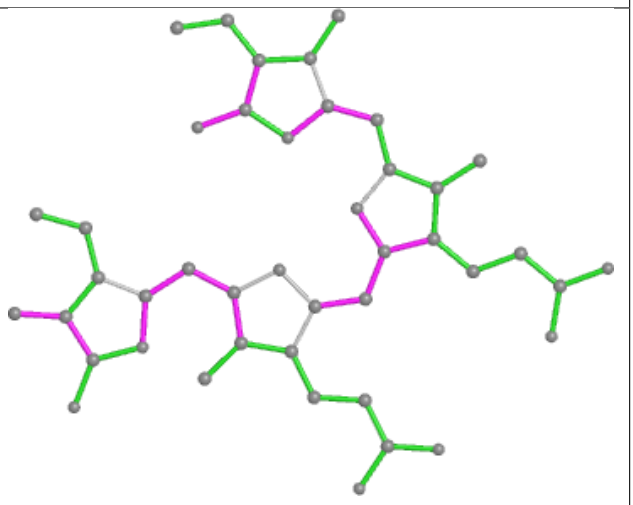
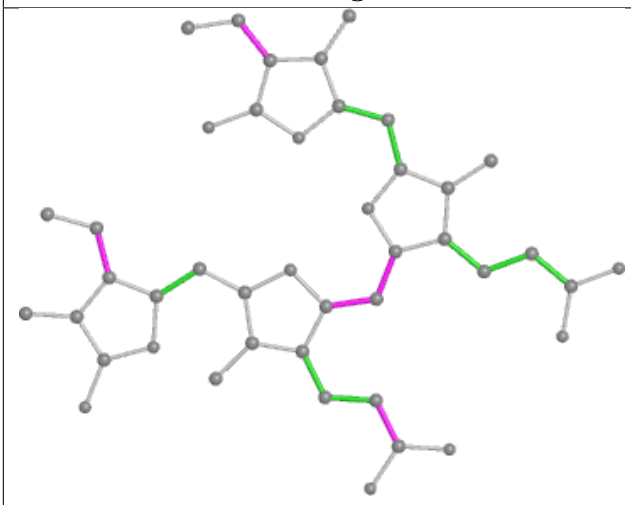
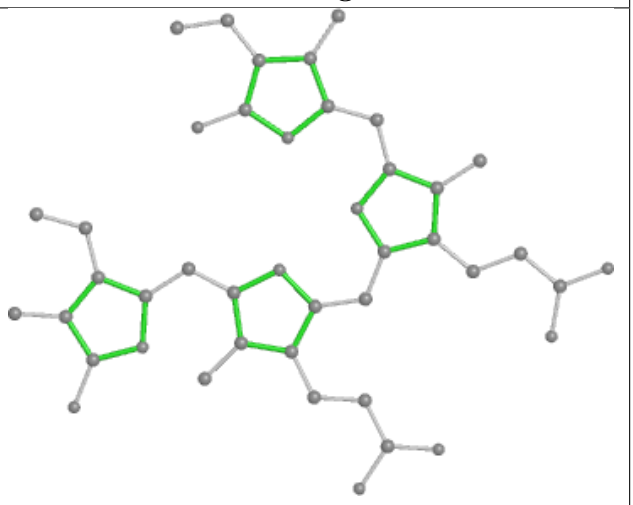


Bond angles

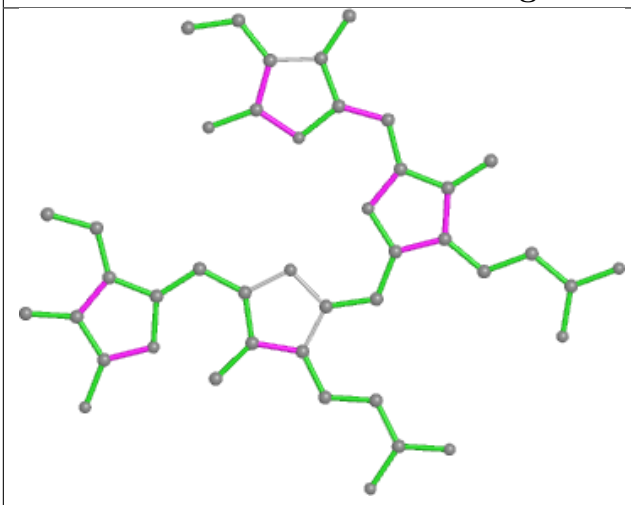


Torsions



Rings

Ligand PUB r2 203



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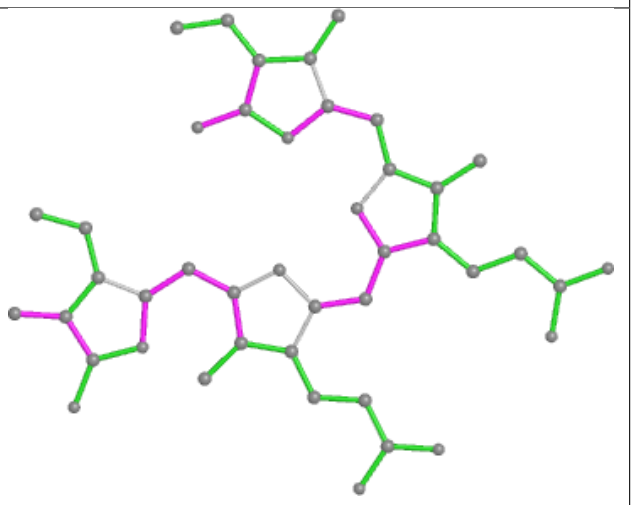

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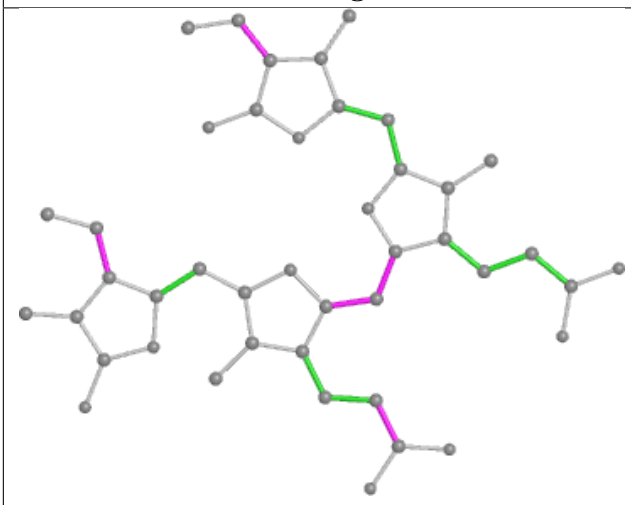

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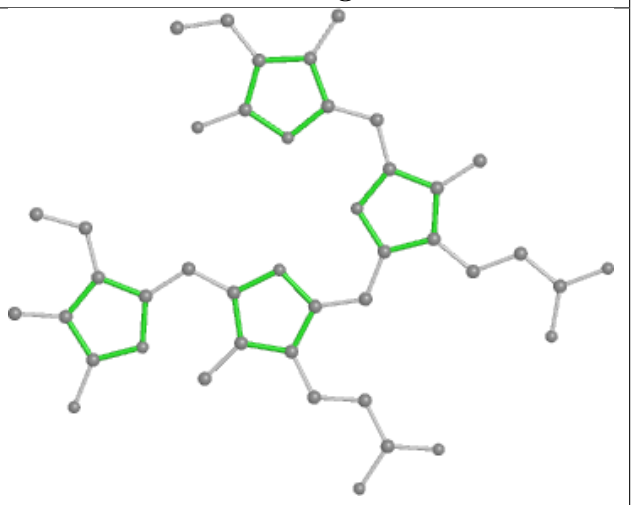
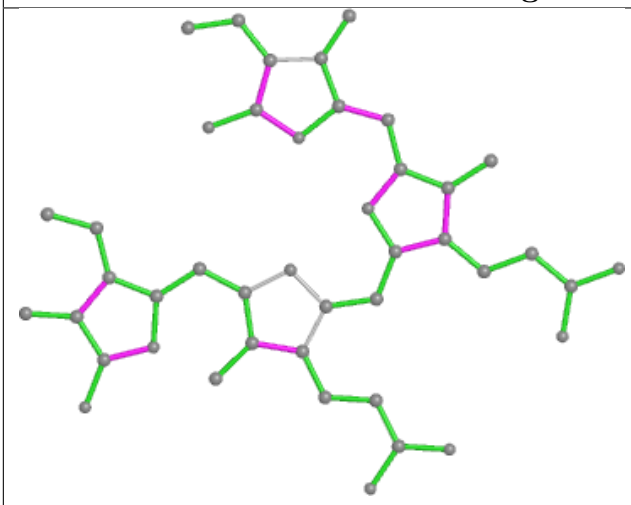


Rings

Ligand PUB fa 202



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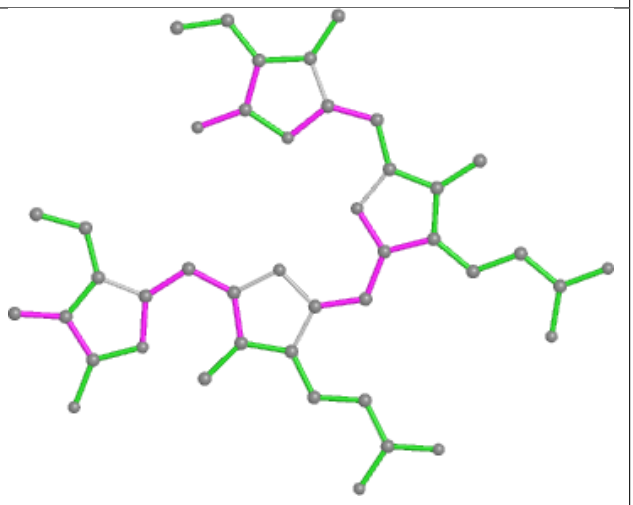

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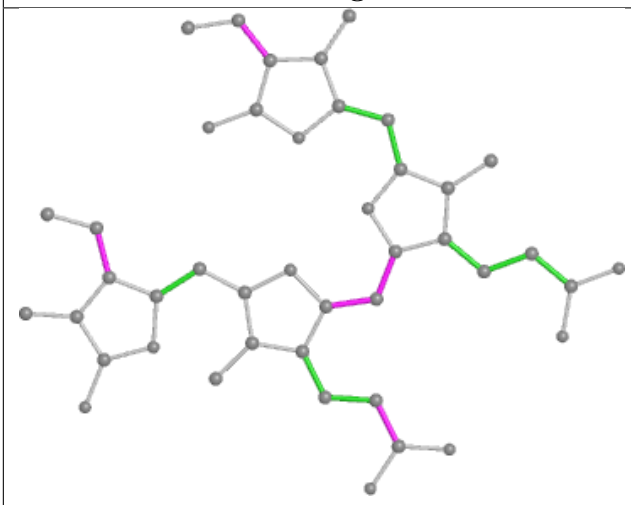

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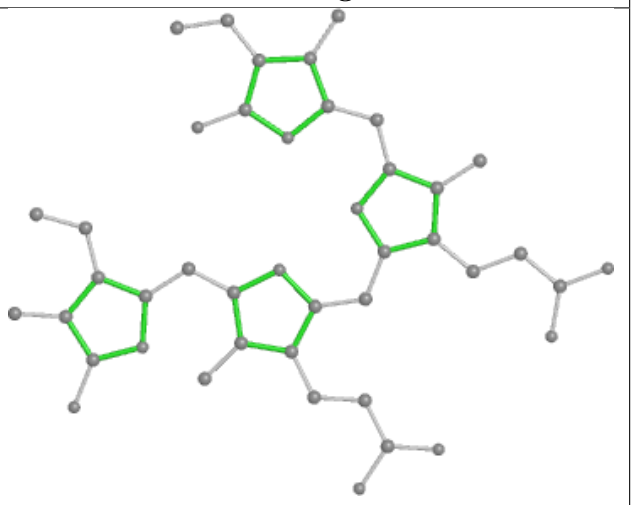
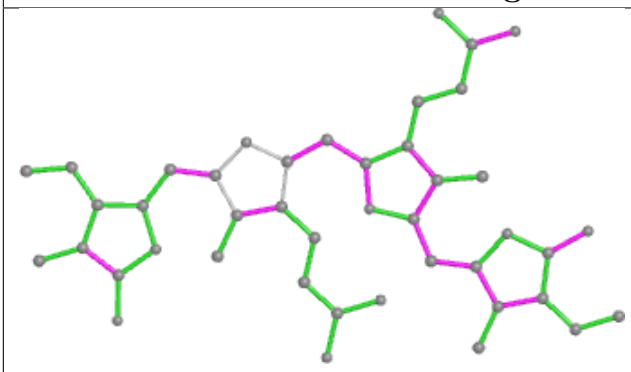


Rings

Ligand CYC R1 1001



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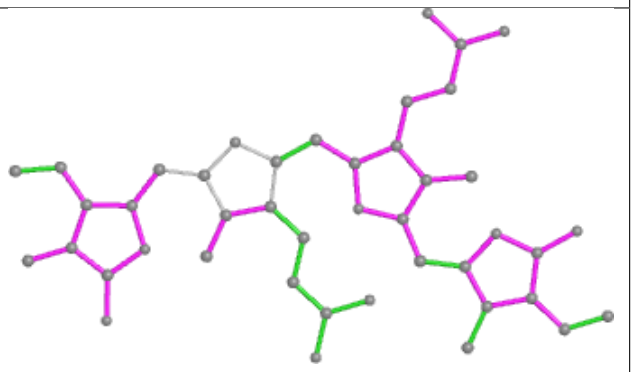

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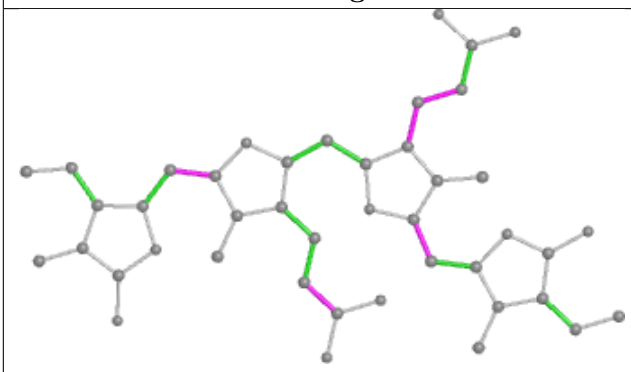

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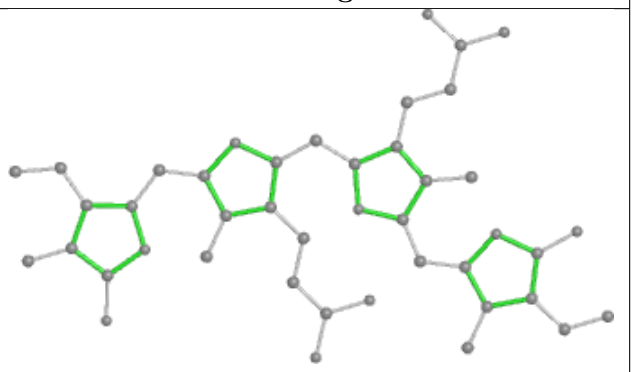
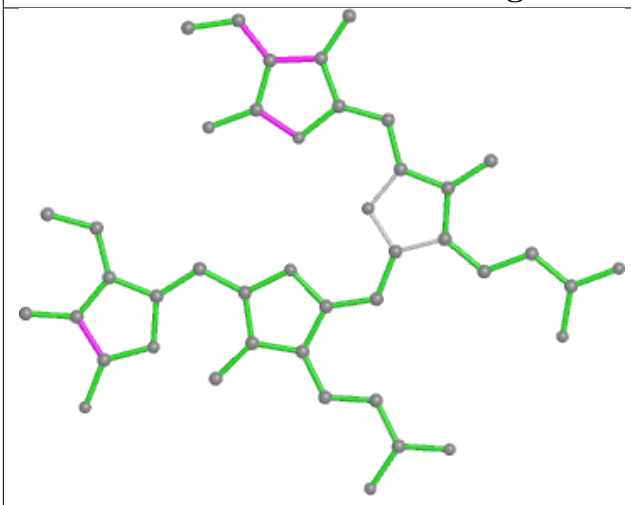


Rings

Ligand PEB Y5 1001



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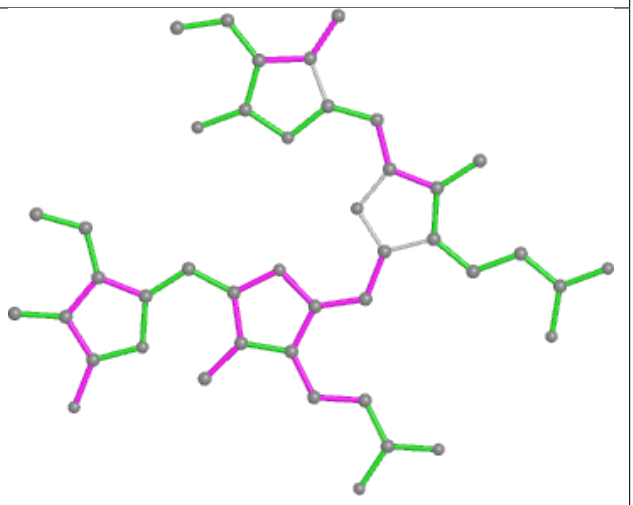

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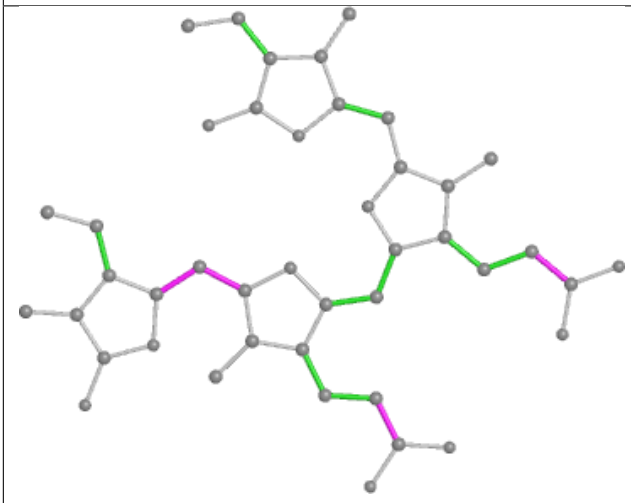

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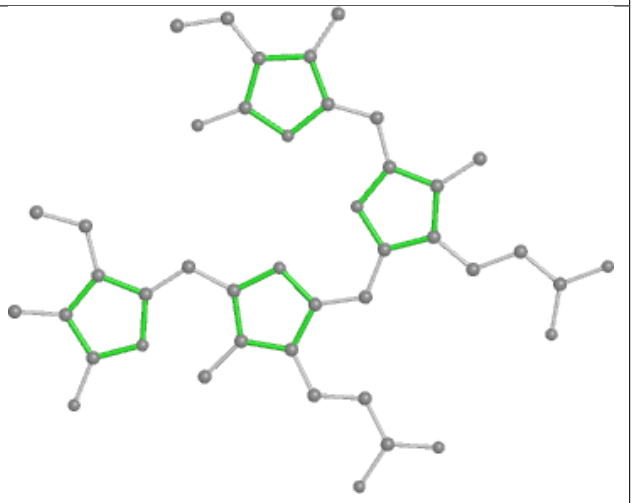

Rings

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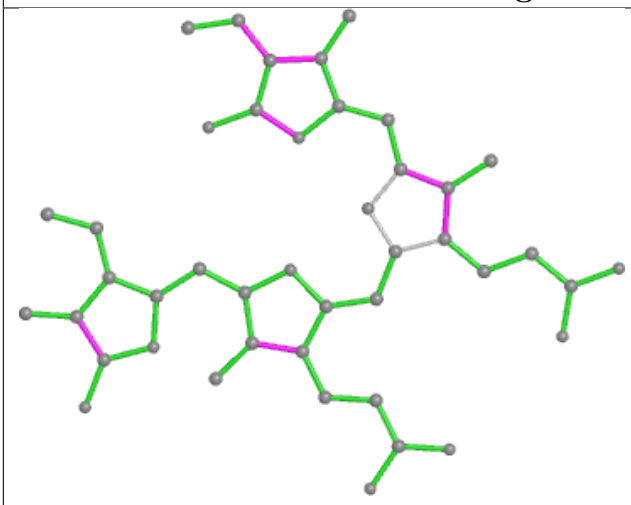

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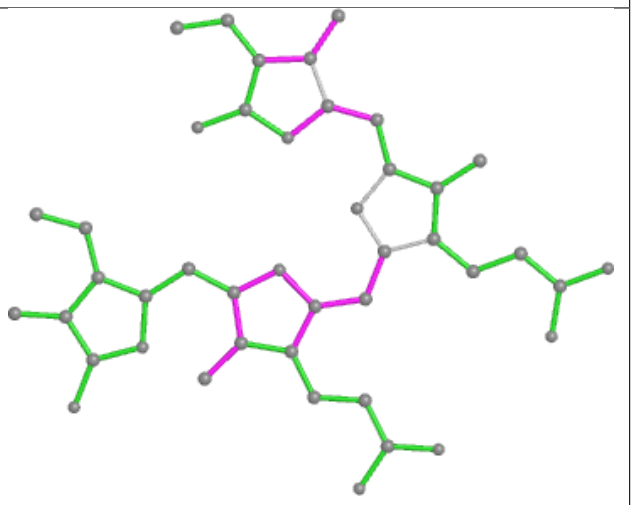

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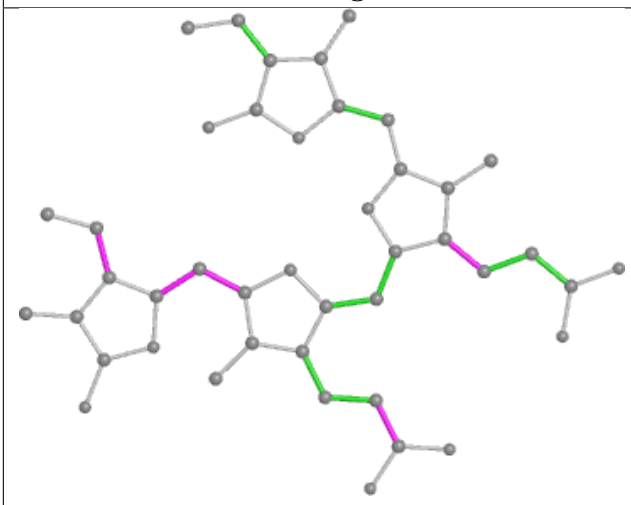

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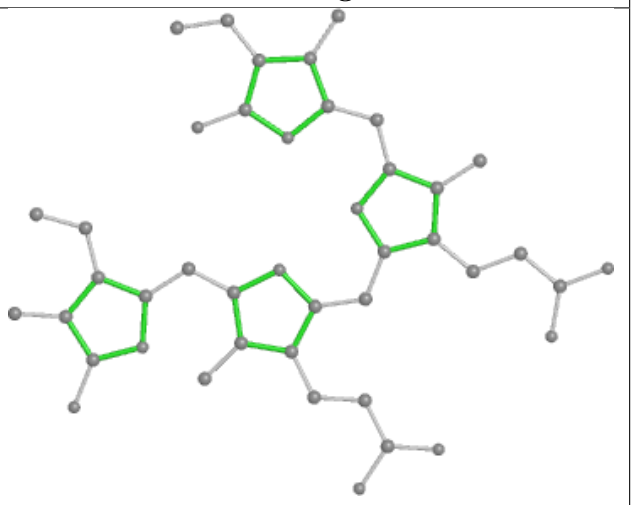
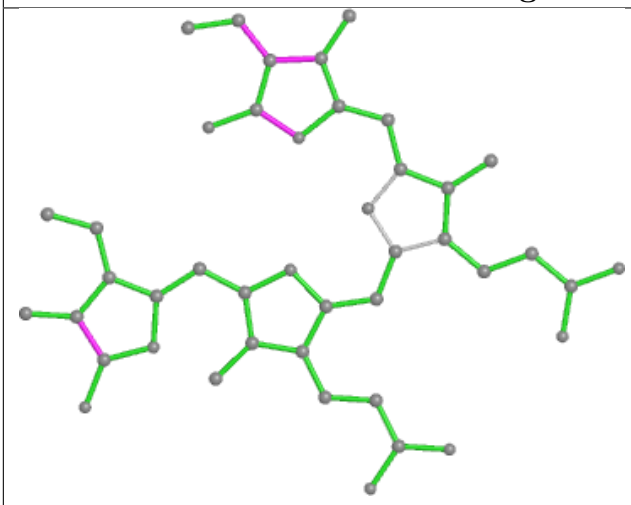


Rings

Ligand PEB x6 202



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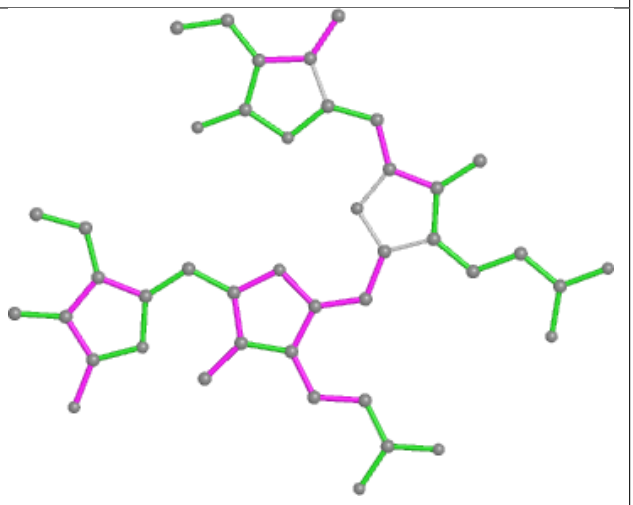

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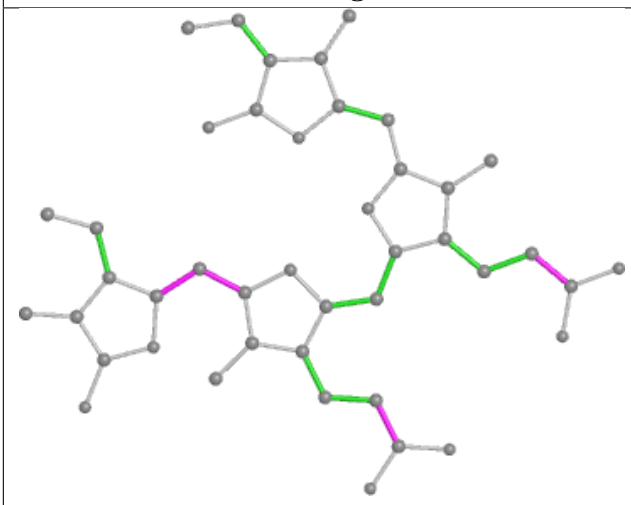

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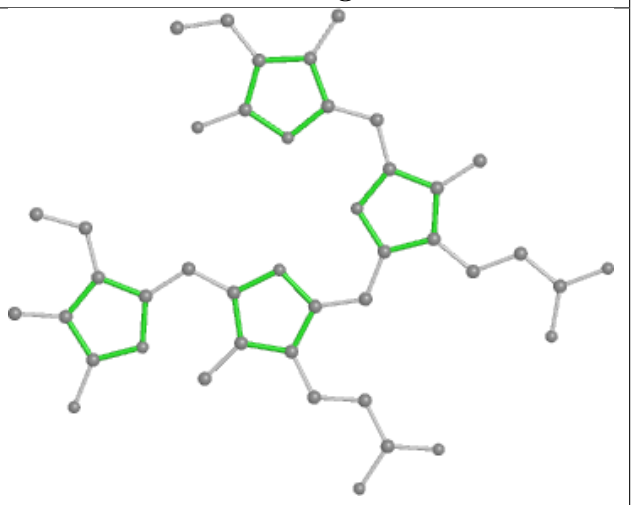

Rings

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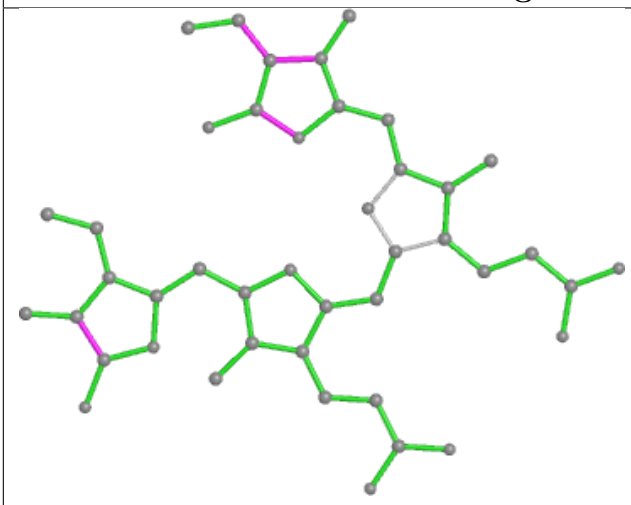

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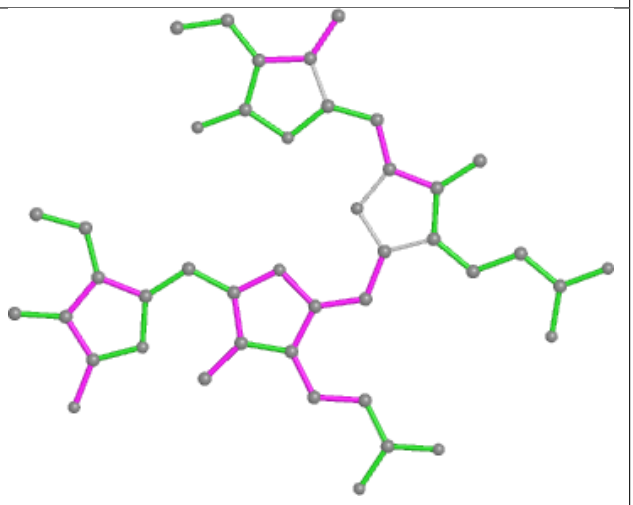

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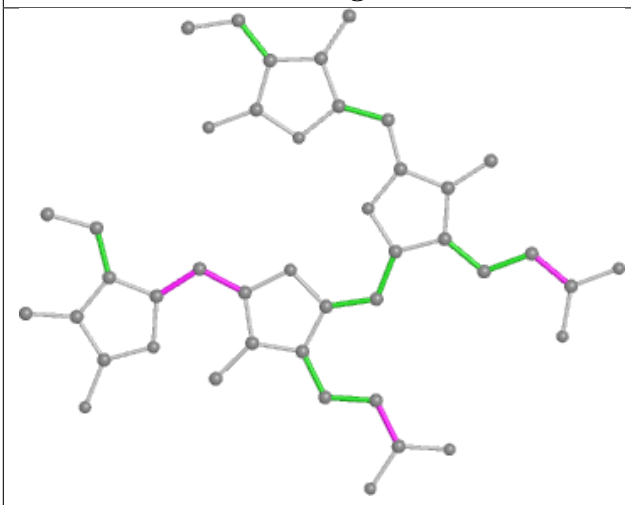

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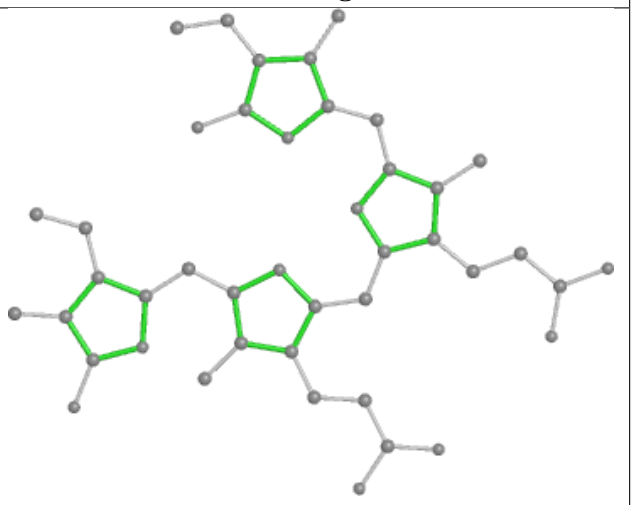

Rings

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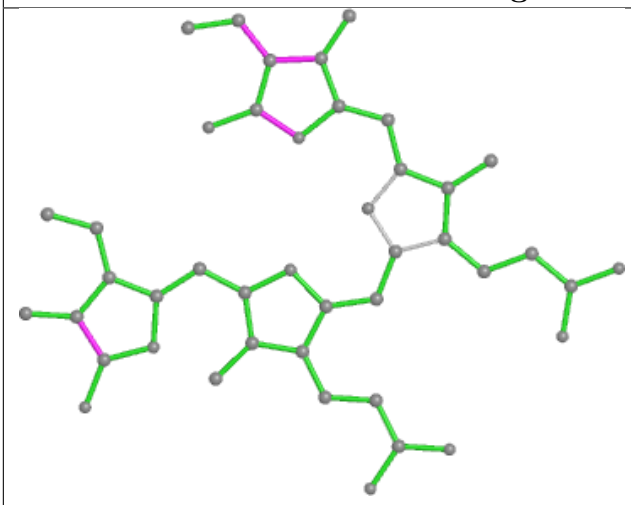

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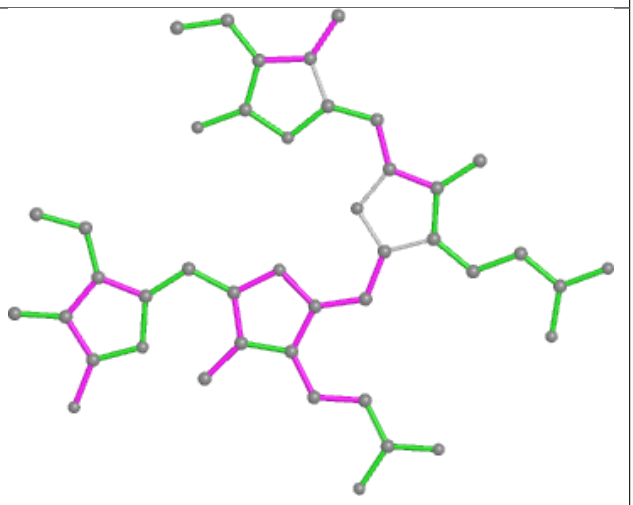

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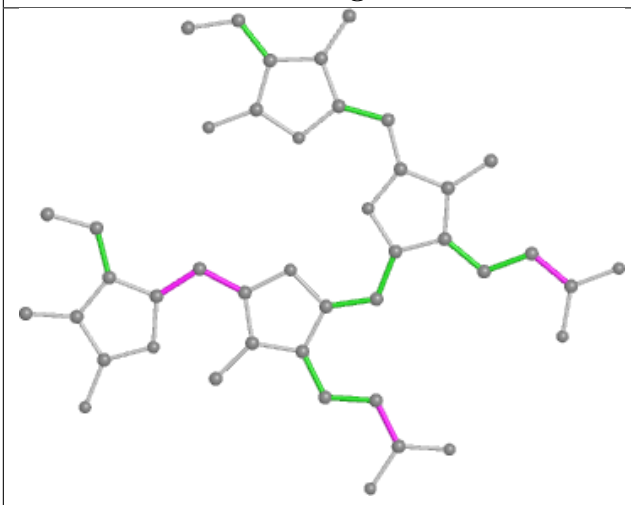

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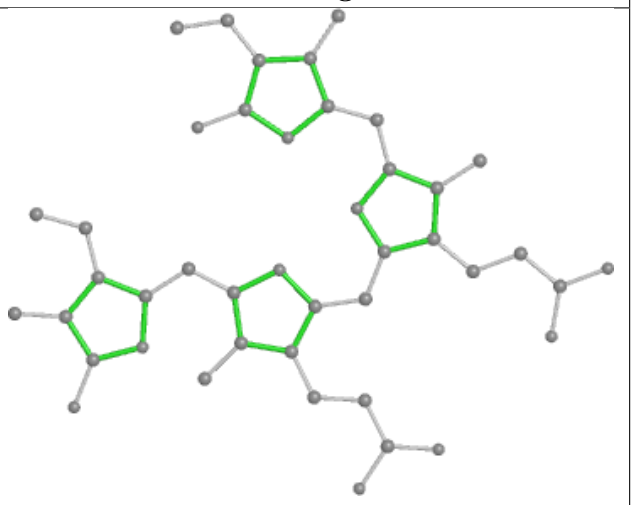
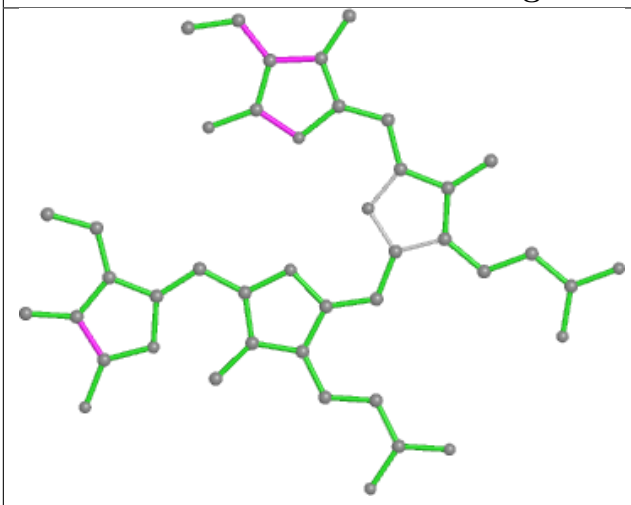


Rings

Ligand PEB cI 201



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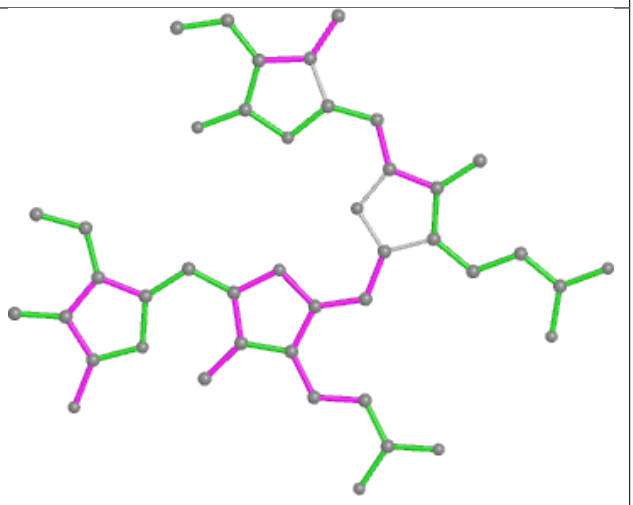

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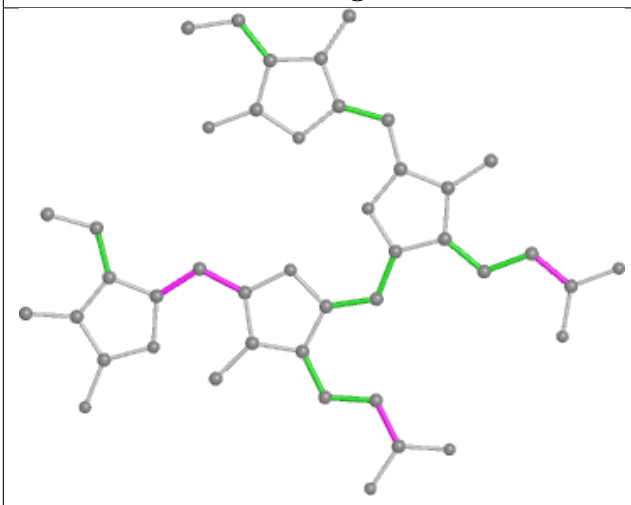

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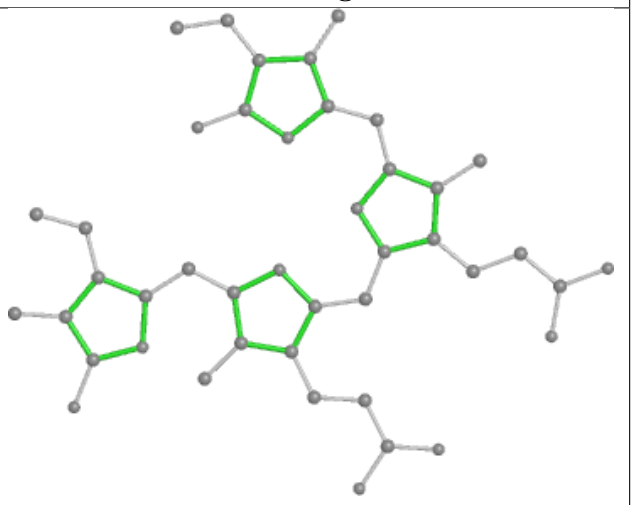

Rings

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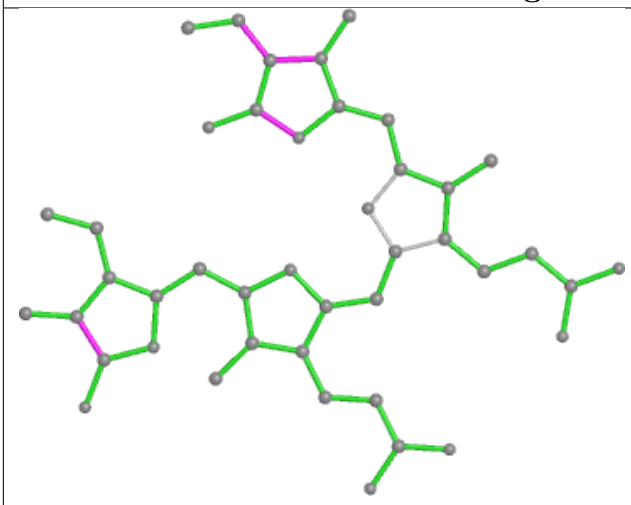

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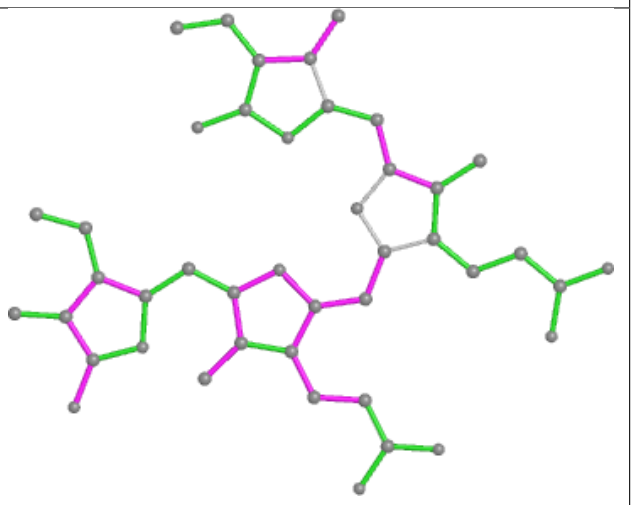

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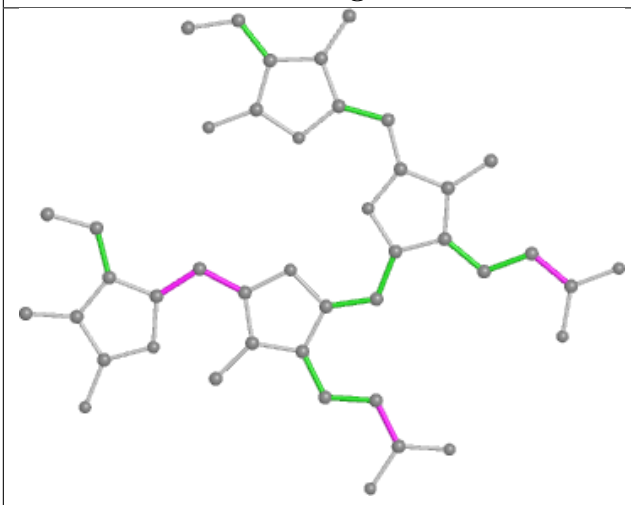

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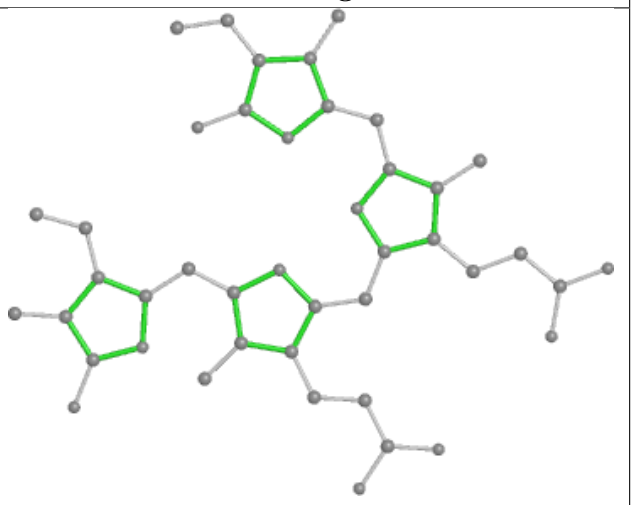
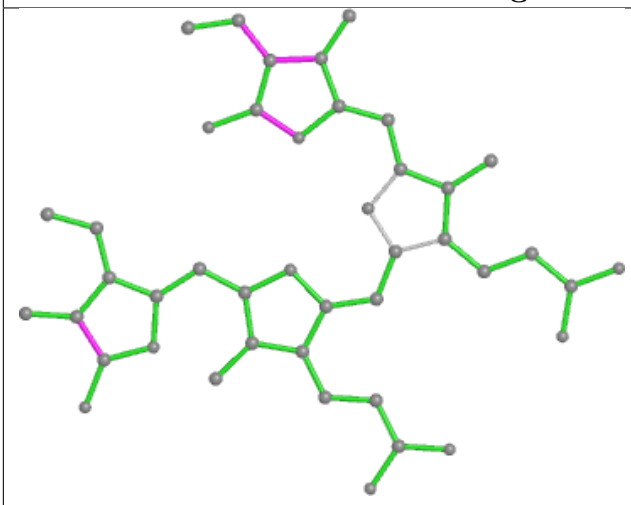


Rings

Ligand PEB W4 202



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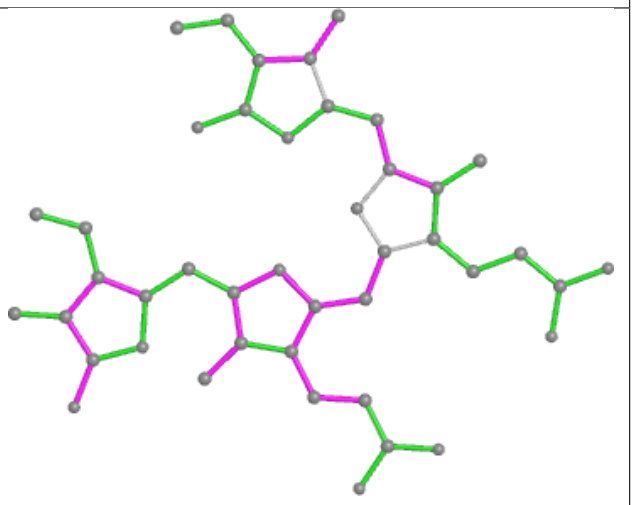

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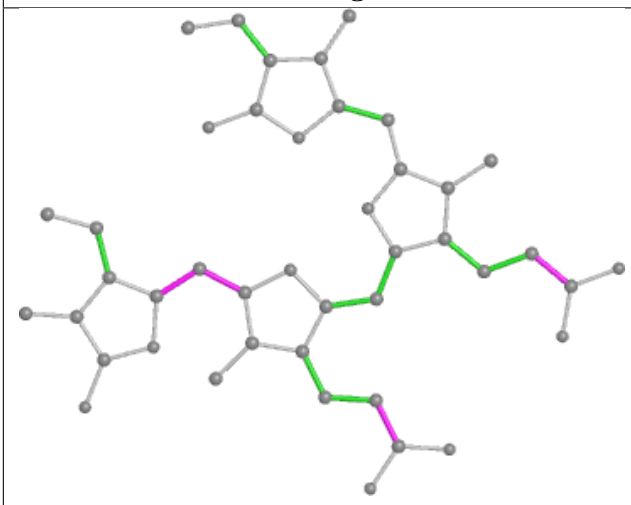

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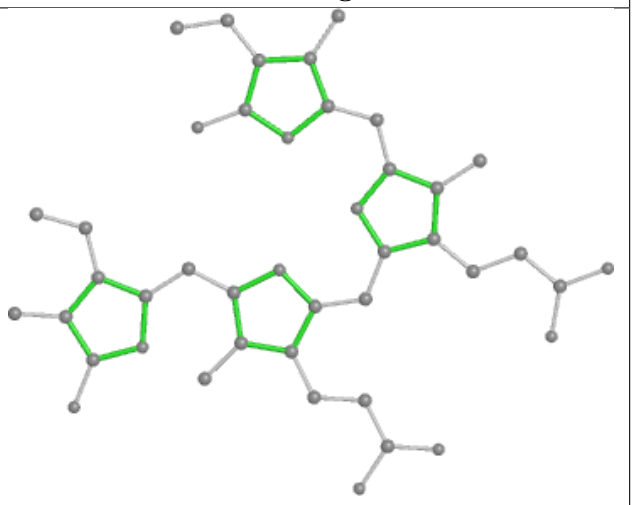
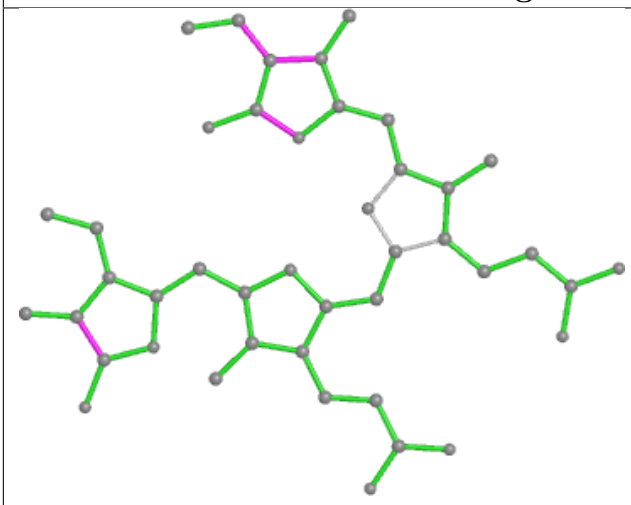


Rings

Ligand PEB aX 402



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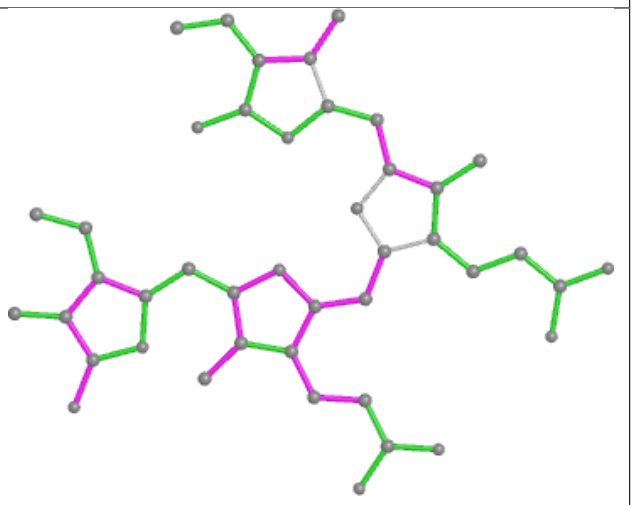
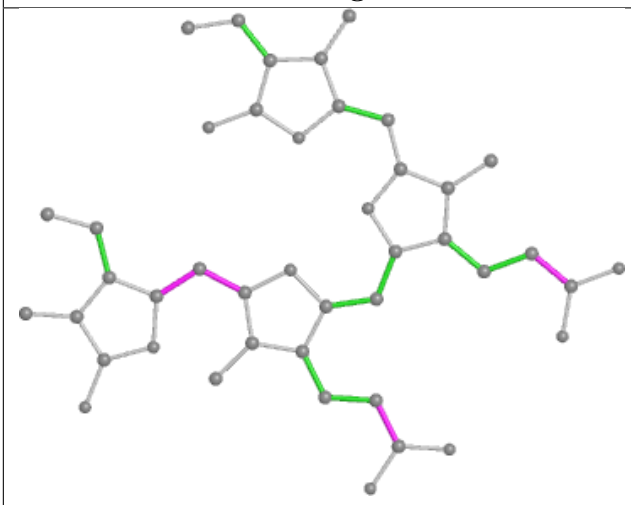


Bond angles



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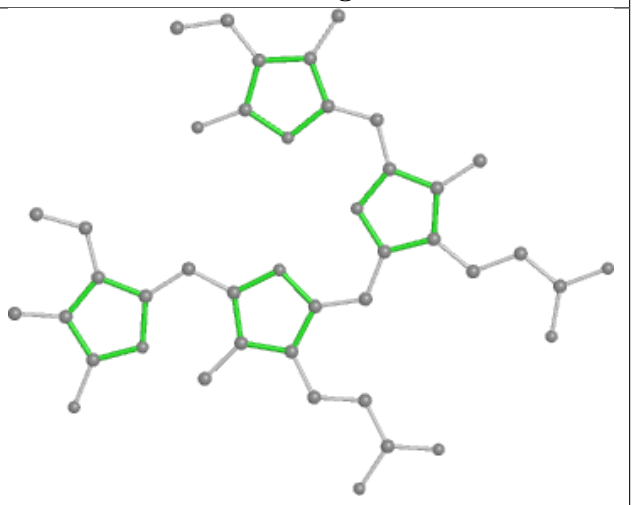
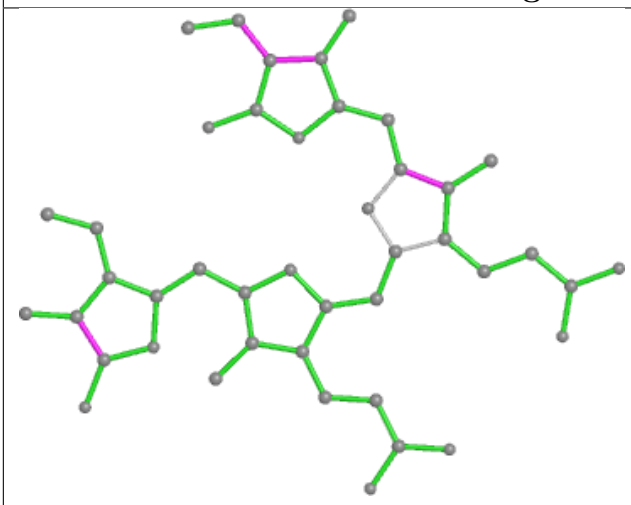
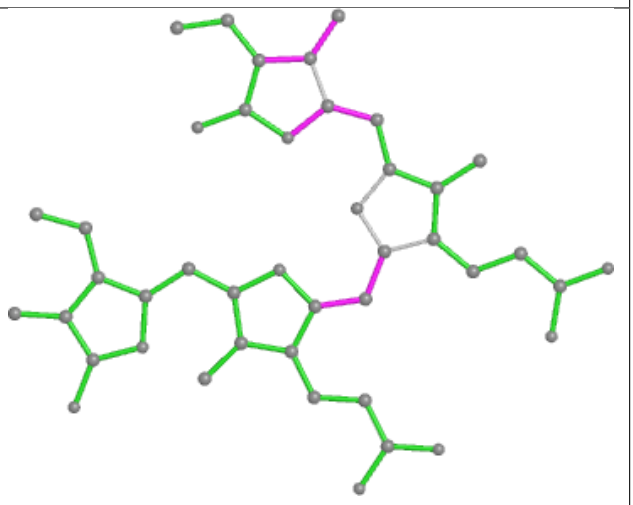


Rings

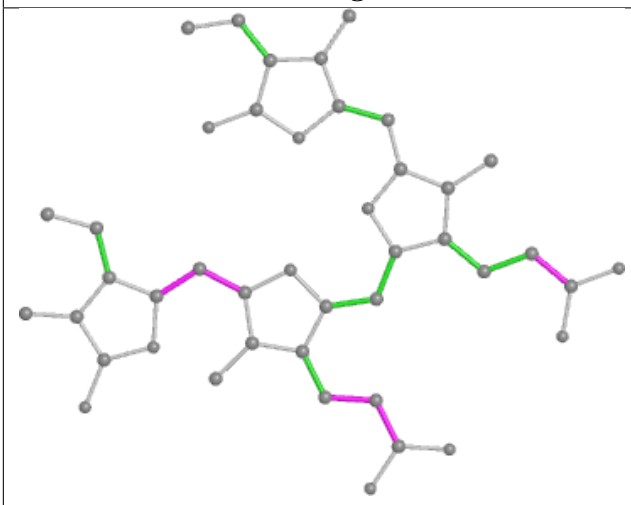
Ligand PEB cI 202



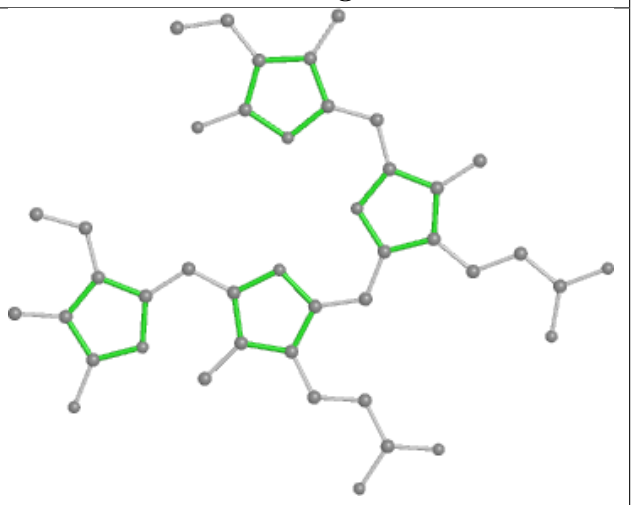
Bond lengths



Bond angles

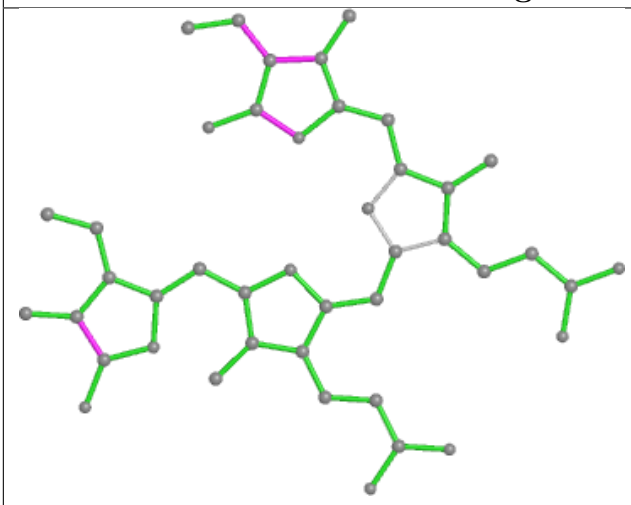


Torsions



Rings

Ligand PEB N8 202



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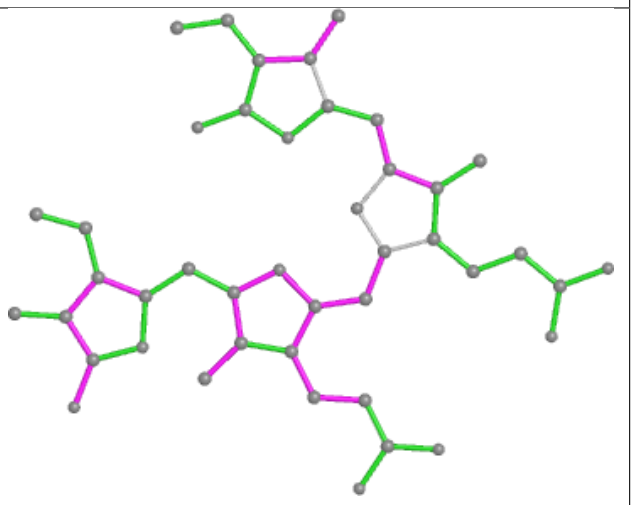

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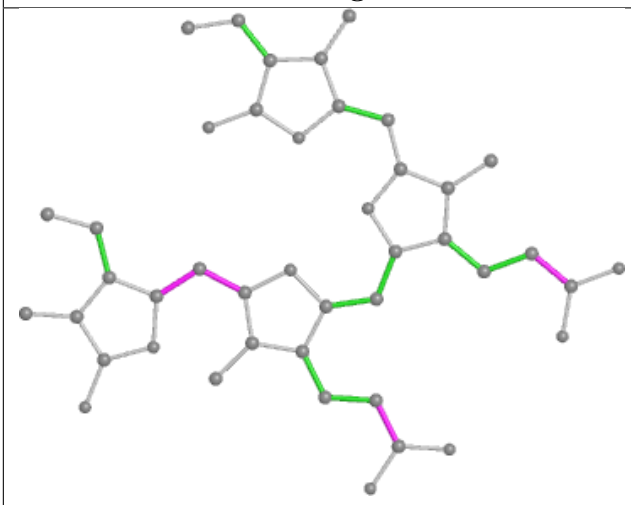

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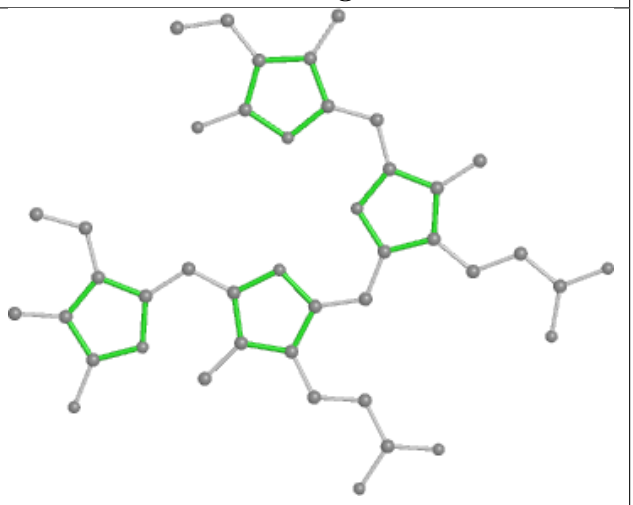
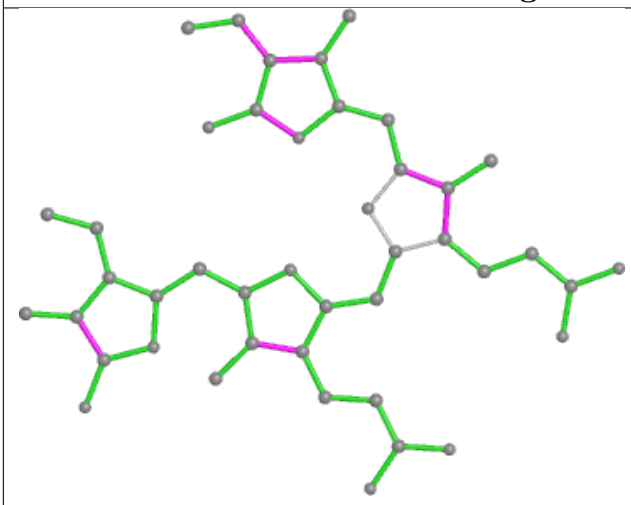


Rings

Ligand PEB ep 202



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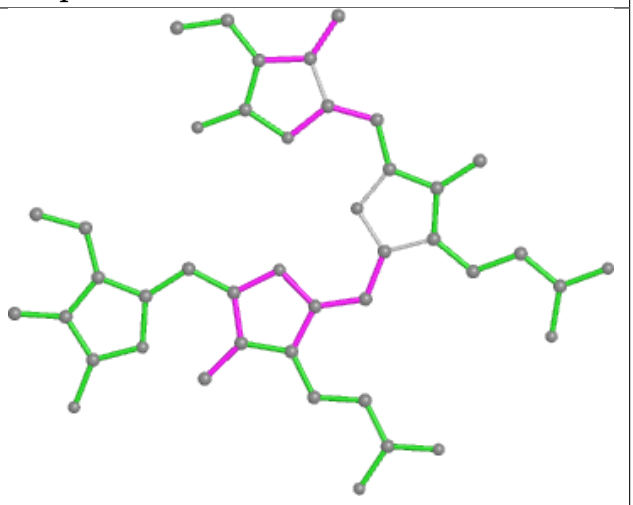

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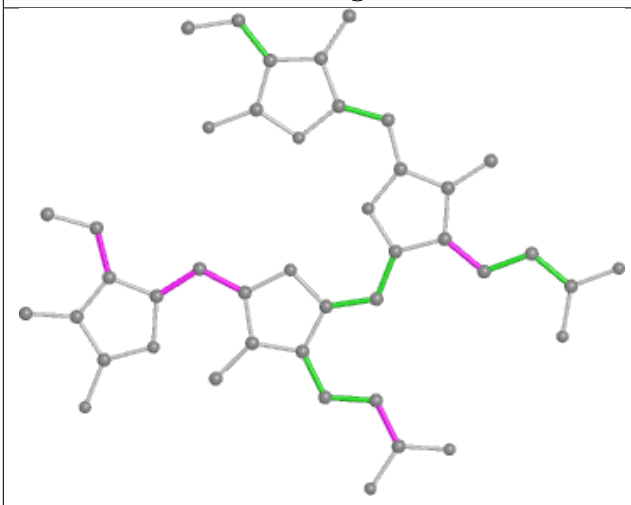

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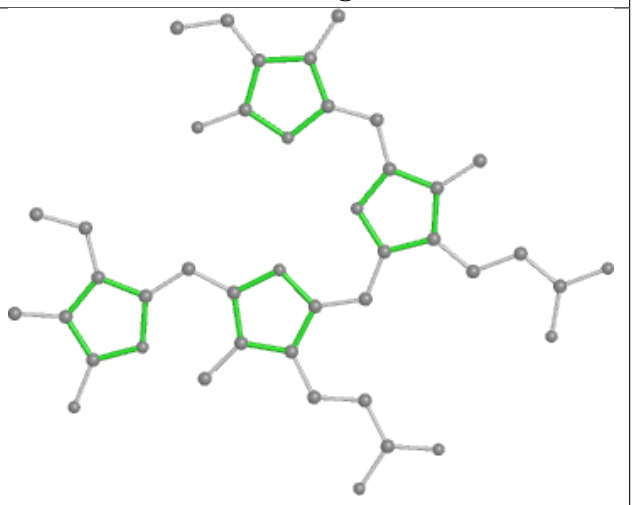
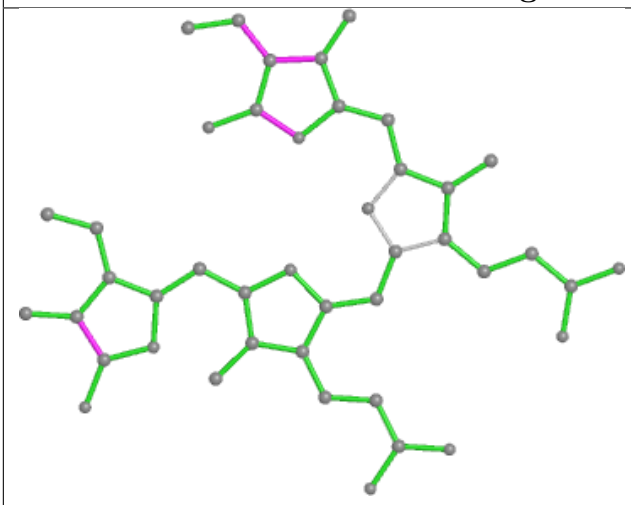


Rings

Ligand PEB 44 301



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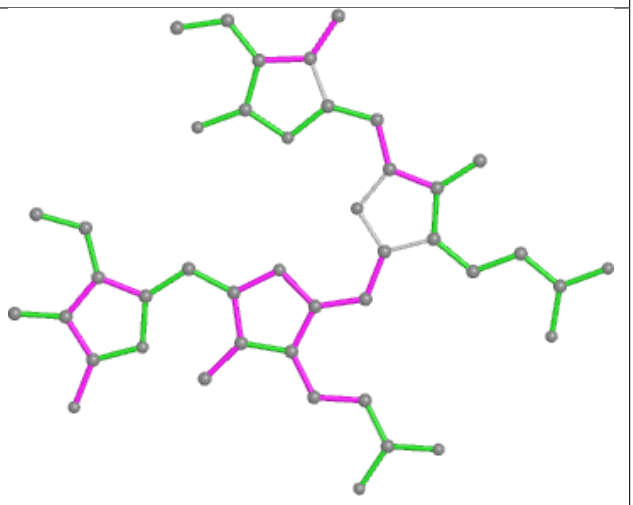

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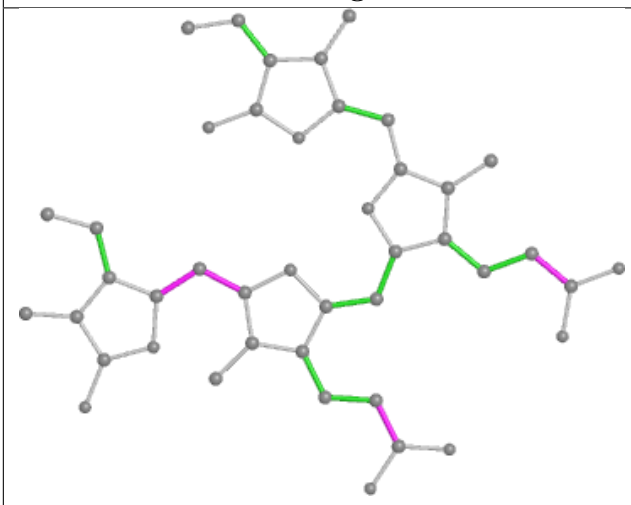

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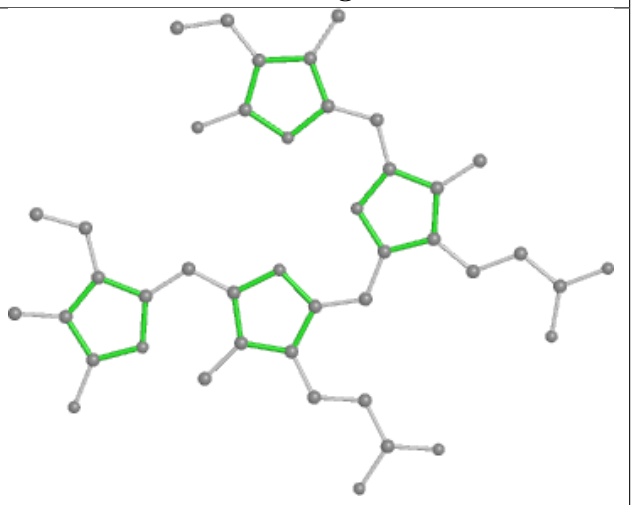
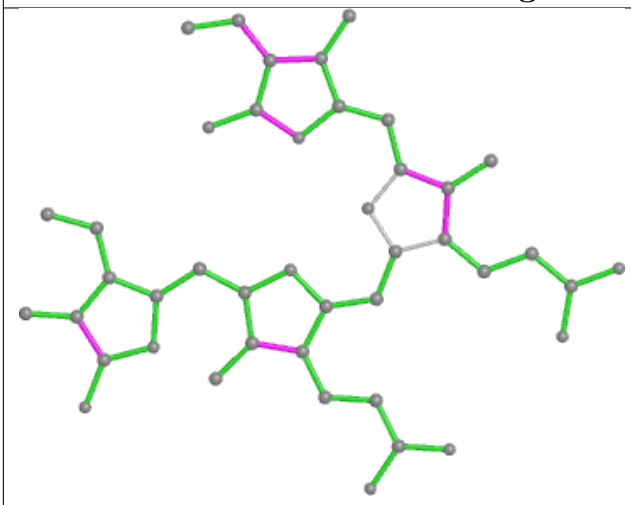


Rings

Ligand PEB h8 202



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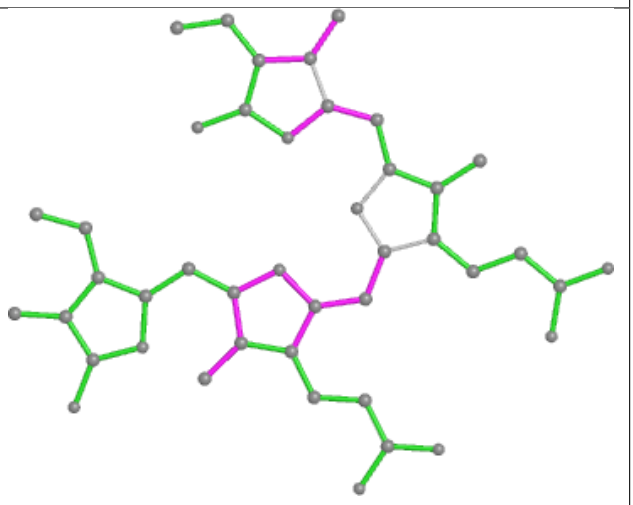

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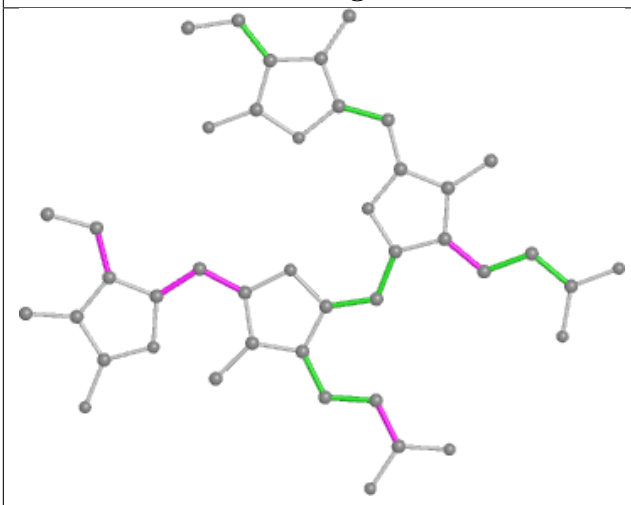

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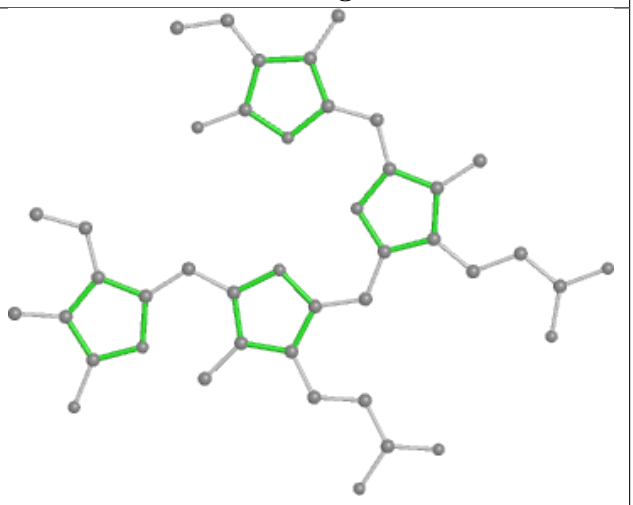
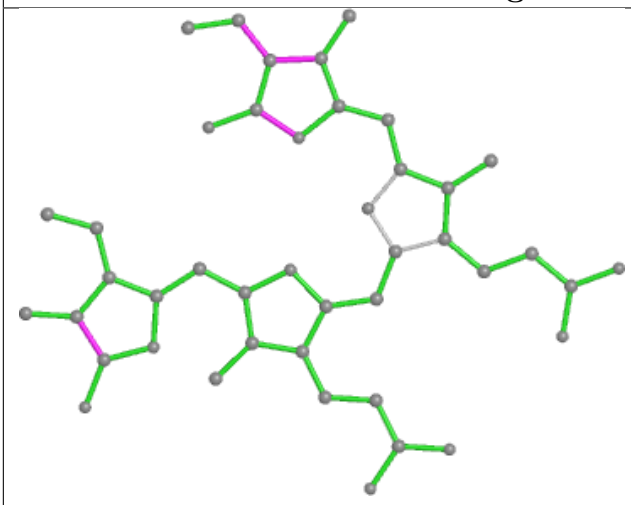


Rings

Ligand PEB w6 1002



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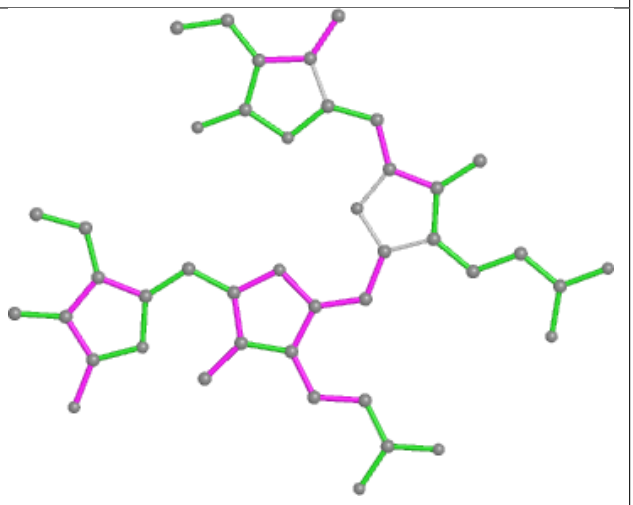
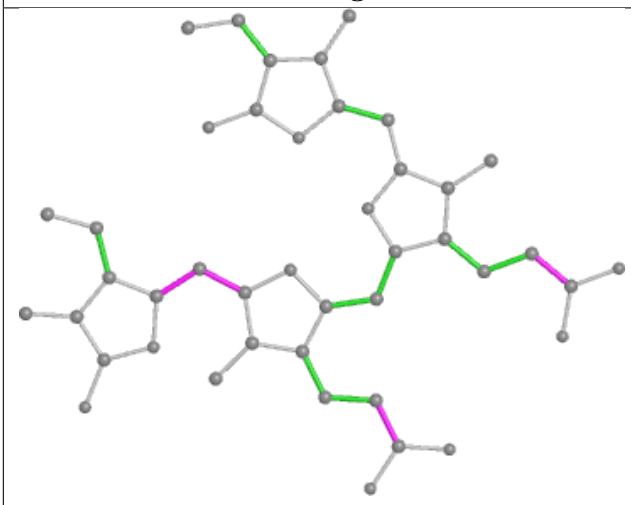


Bond angles



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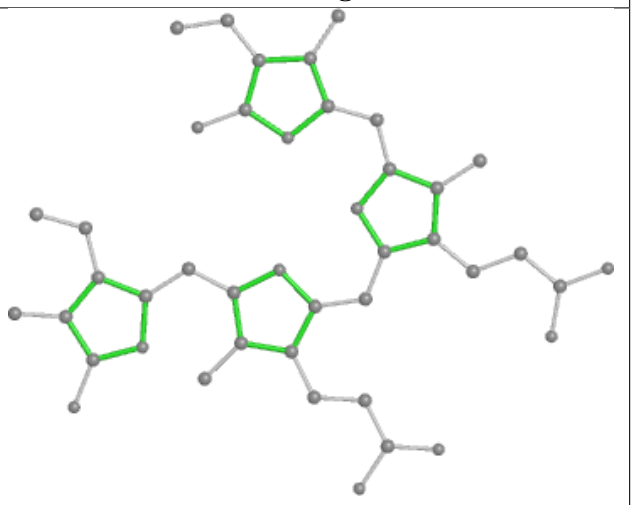
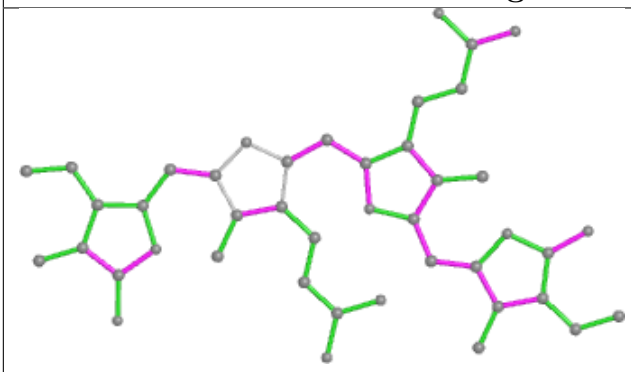


Rings

Ligand CYC b1 1001



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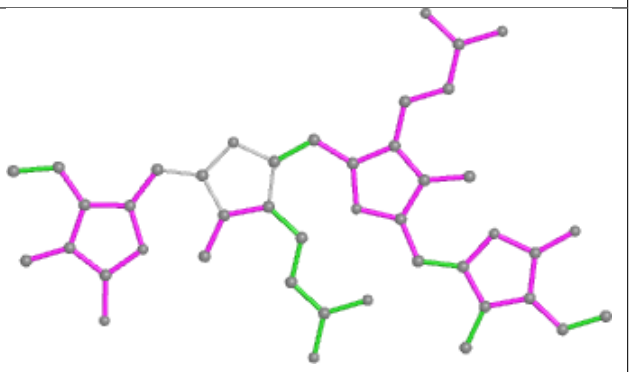

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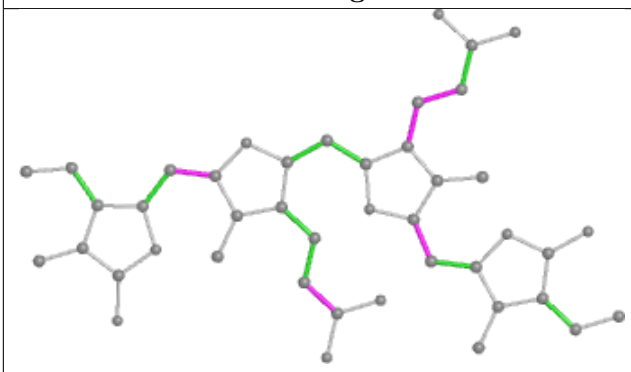

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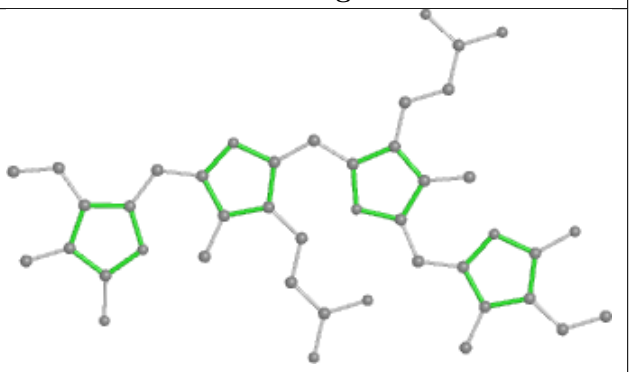
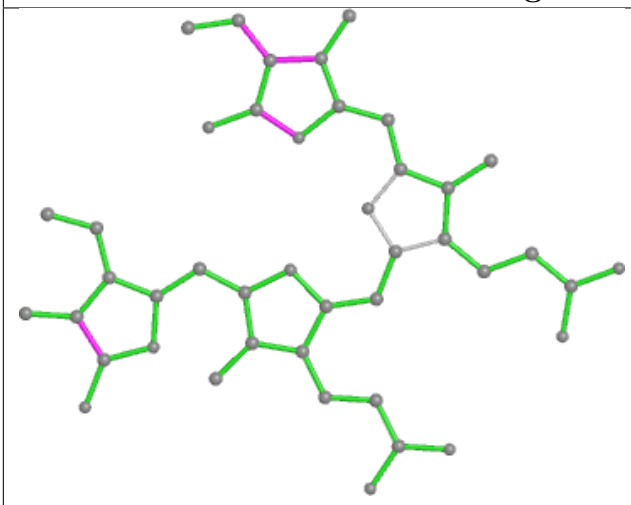


Rings

Ligand PEB cj 201



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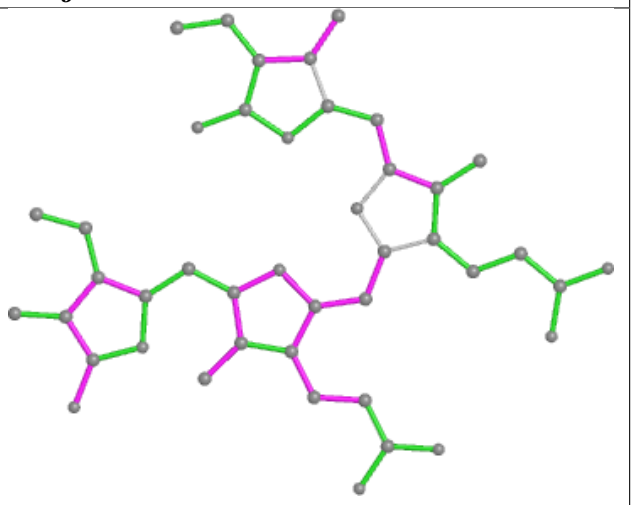

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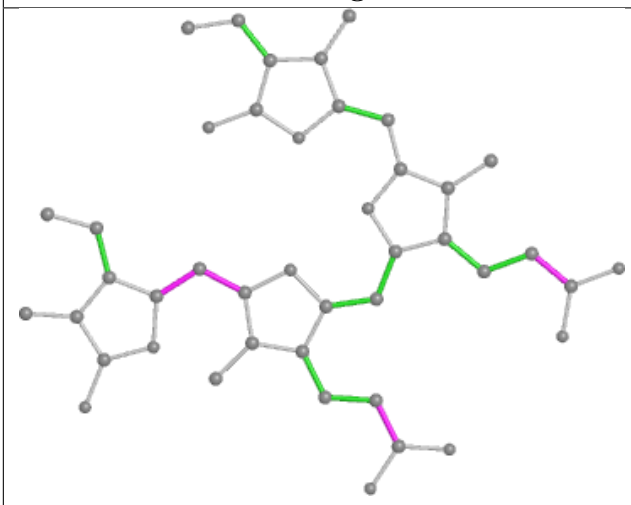

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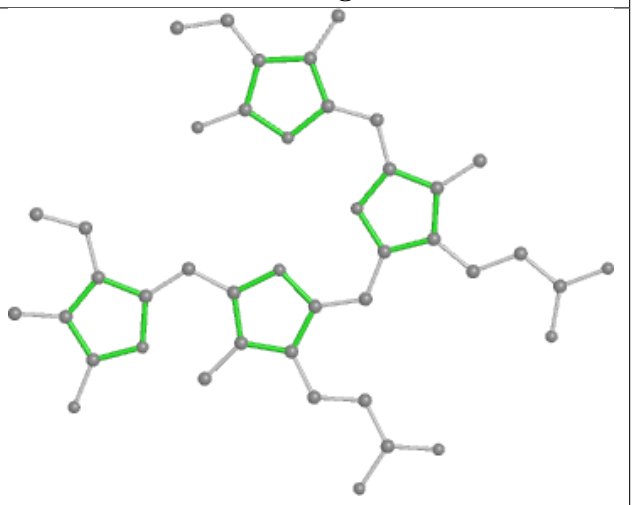
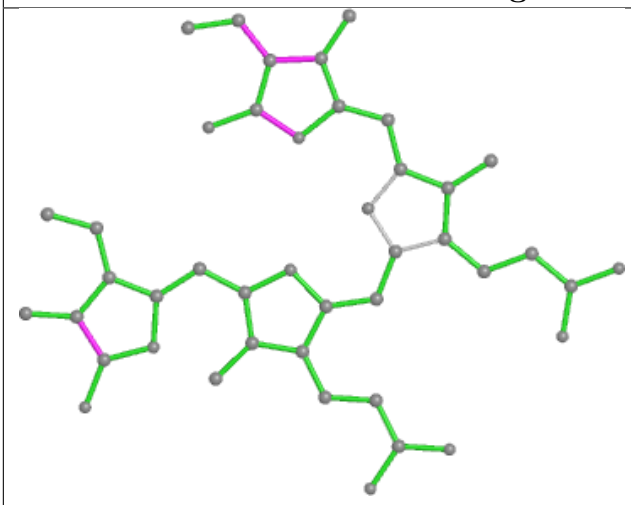


Rings

Ligand PEB dW 202



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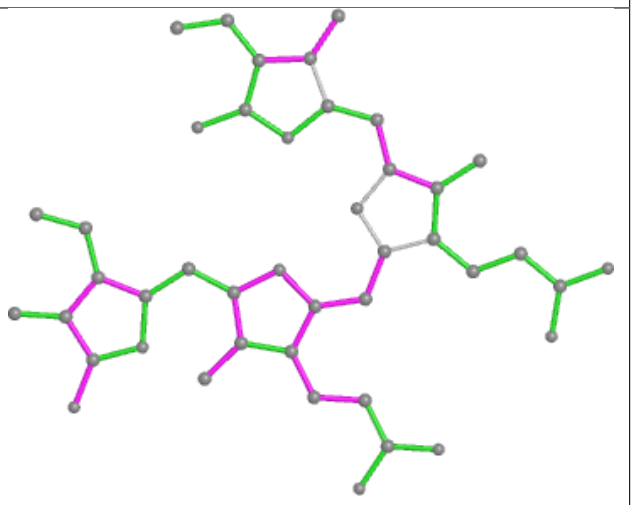
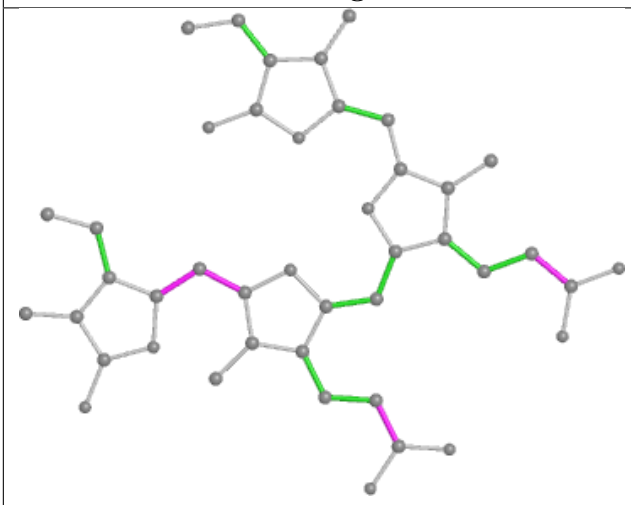


Bond angles



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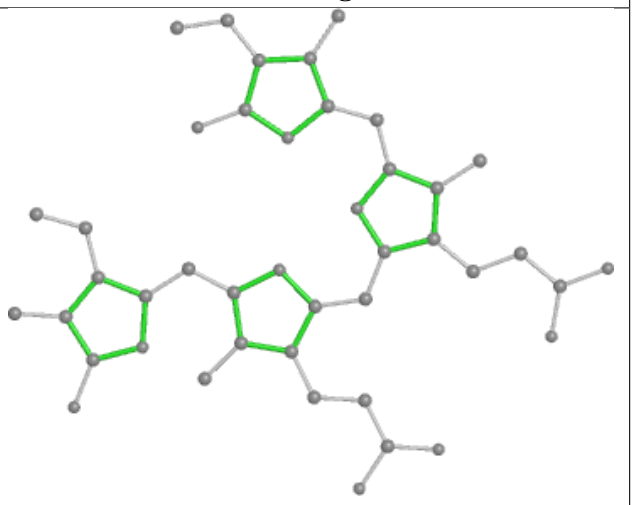
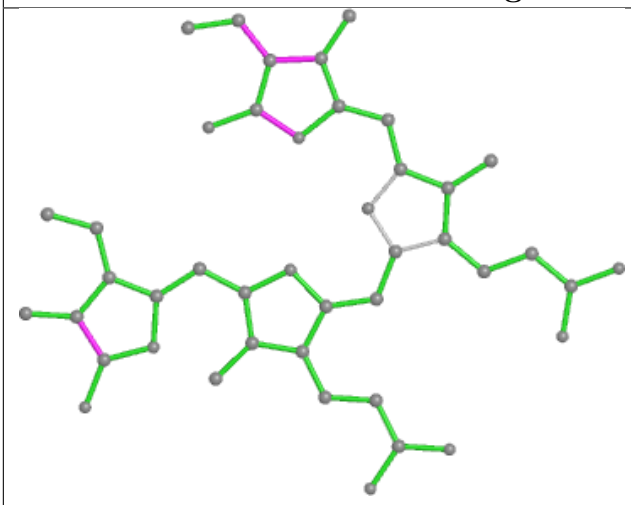


Rings

Ligand PEB m5 1001



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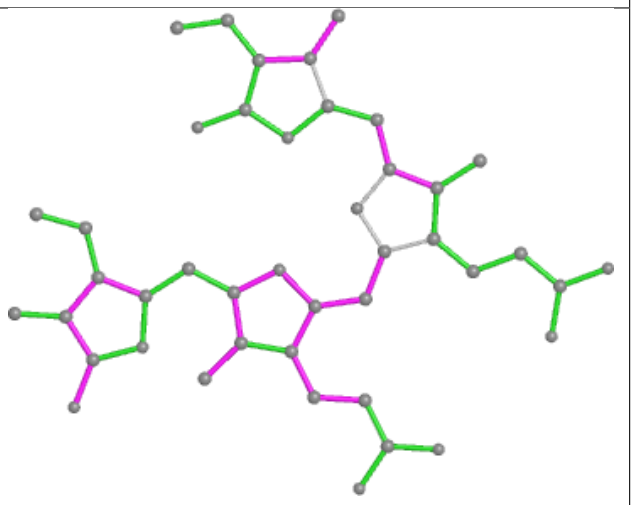

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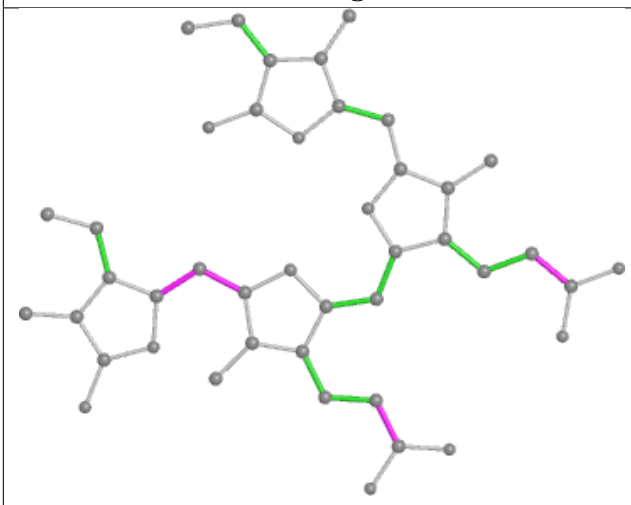

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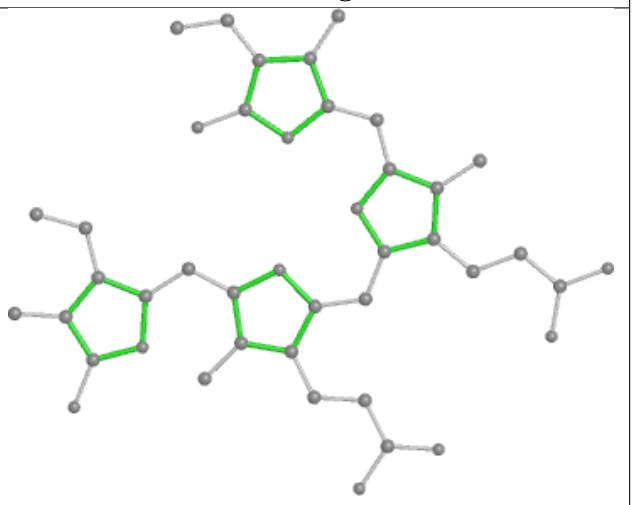
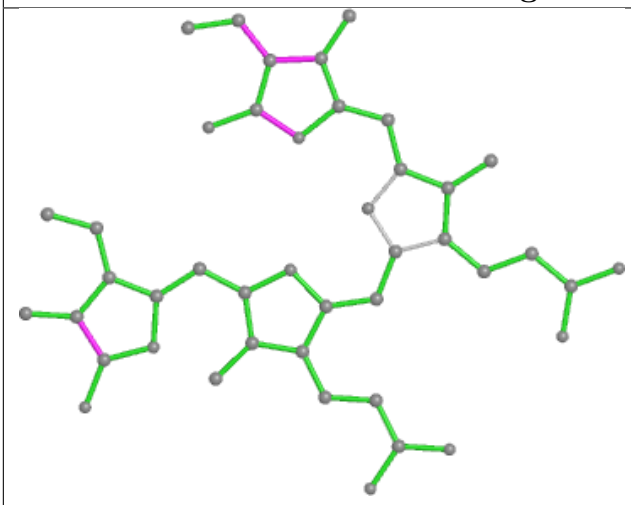


Rings

Ligand PEB av 201



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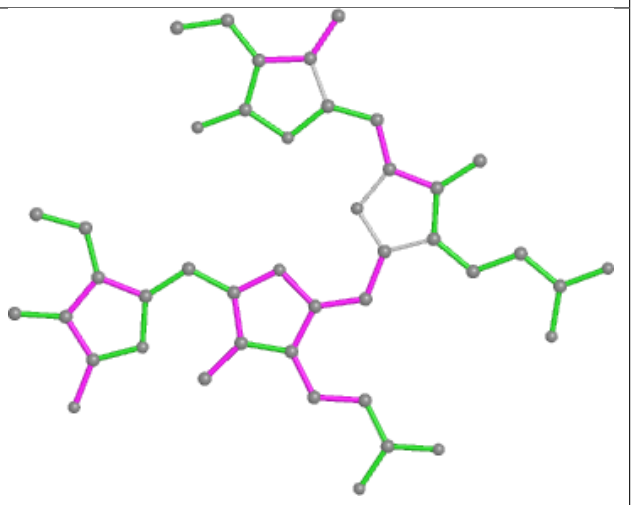

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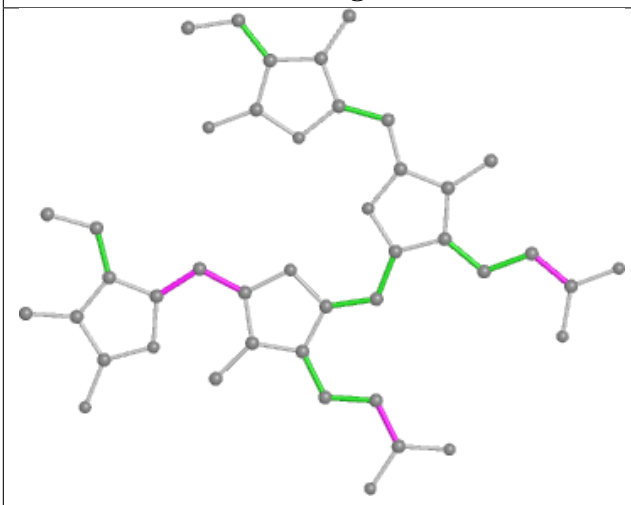

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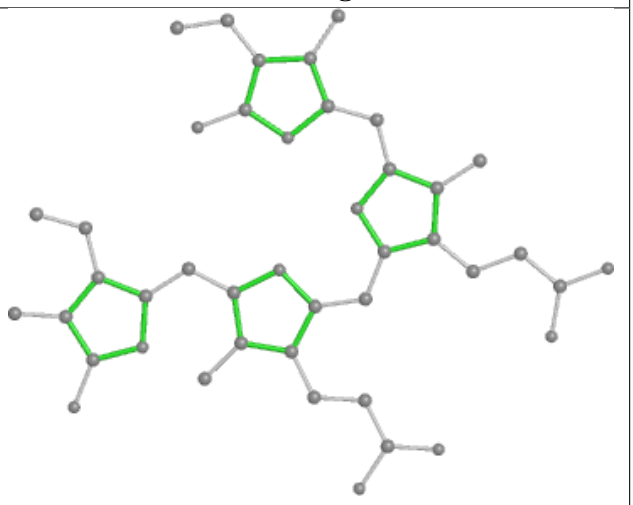
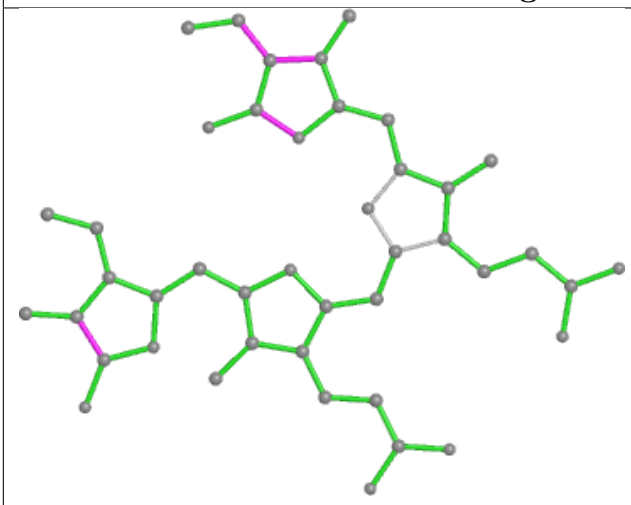


Rings

Ligand PEB dz 401



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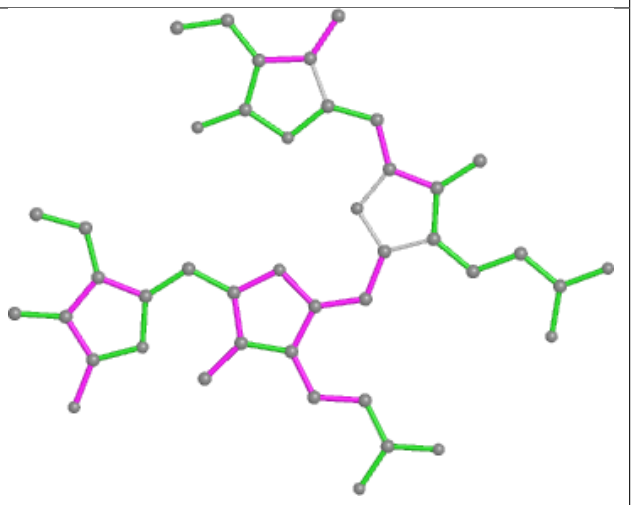

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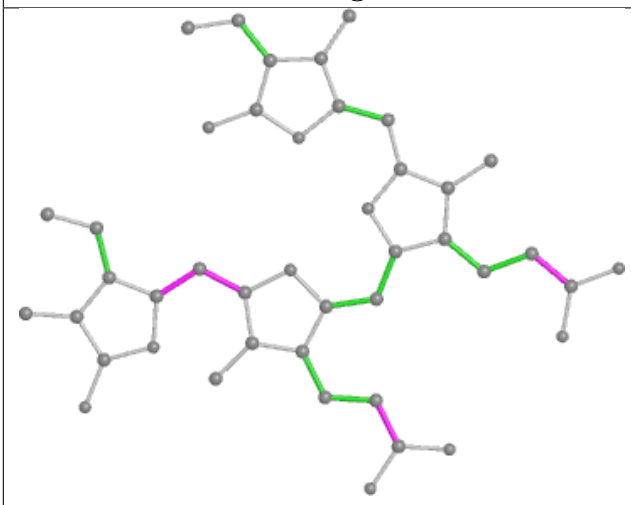

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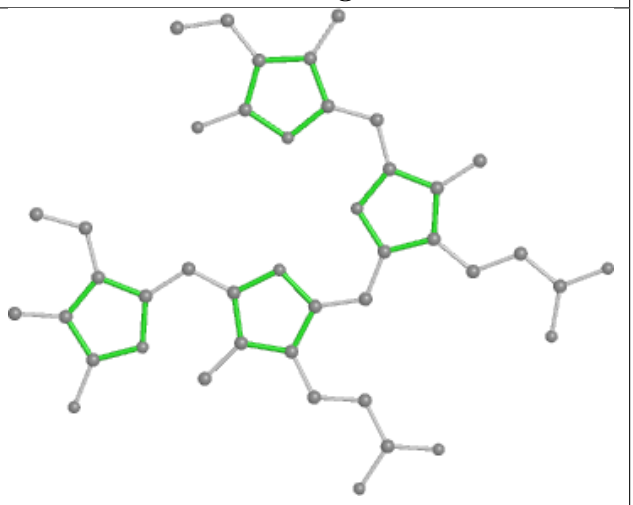
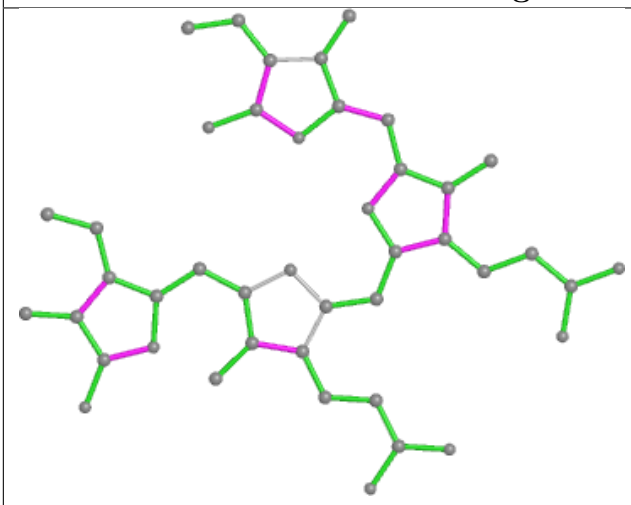


Rings

Ligand PUB N3 203



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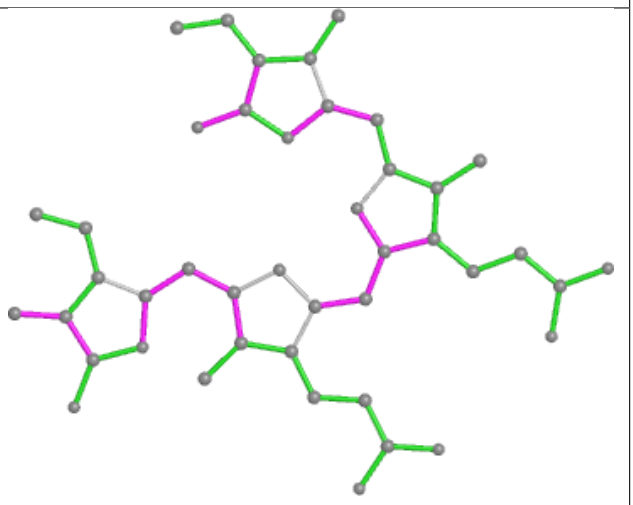
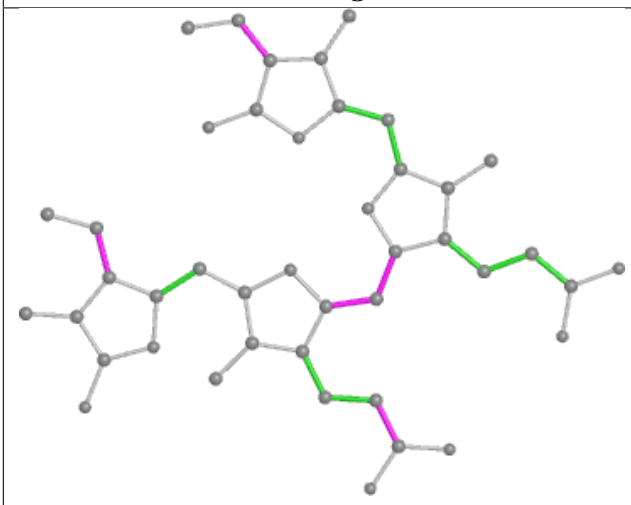


Bond angles



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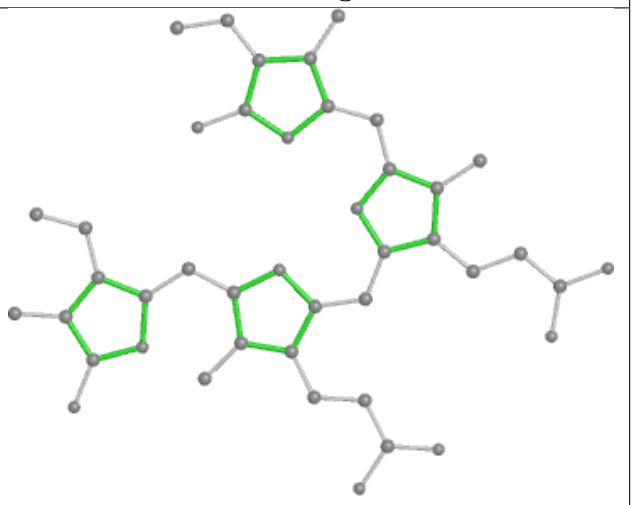
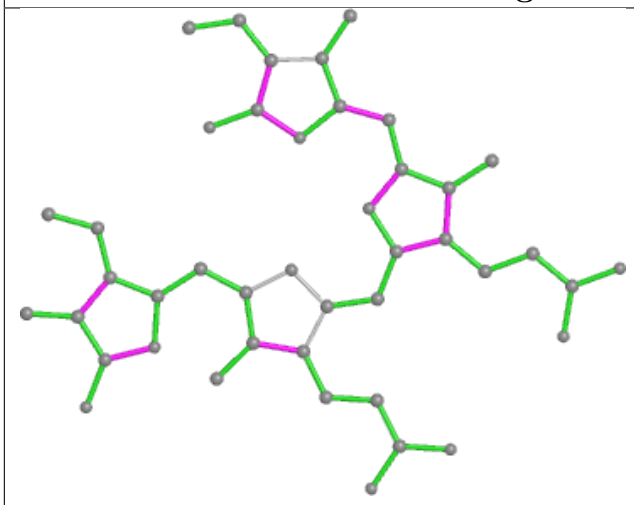
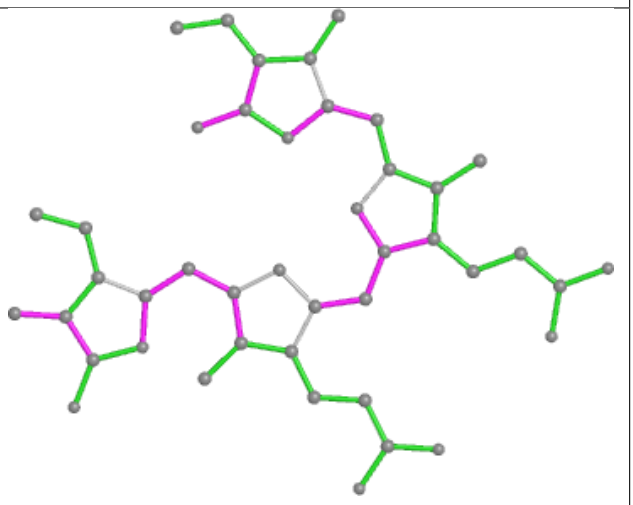


Rings

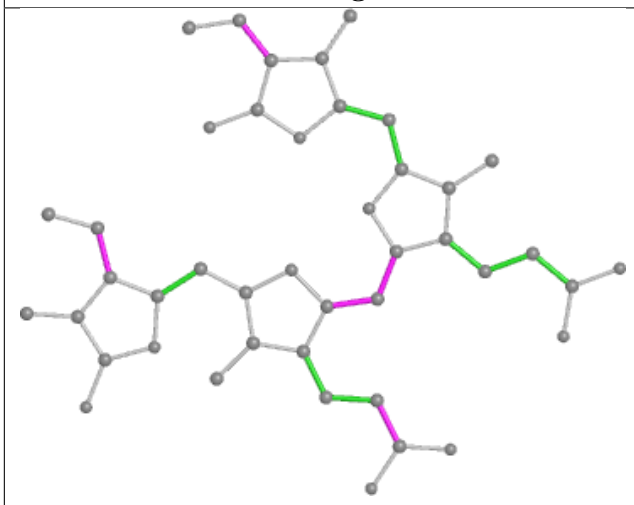
Ligand PUB dL 203



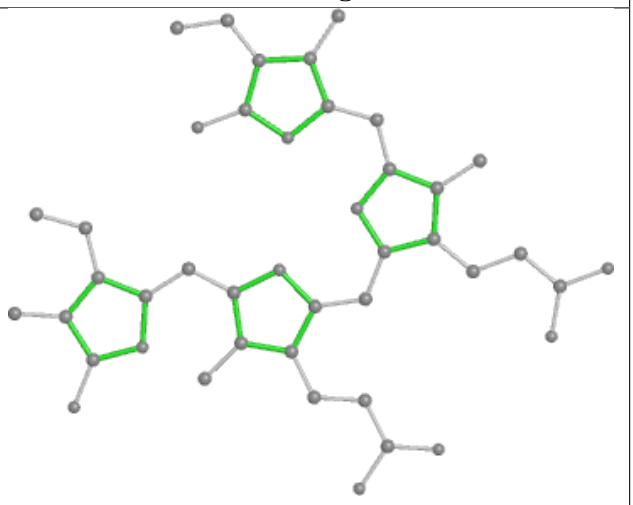
Bond lengths



Bond angles

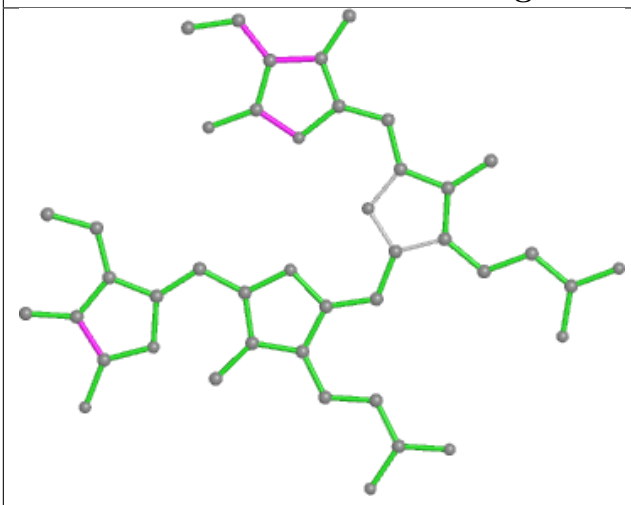


Torsions



Rings

Ligand PEB K8 201



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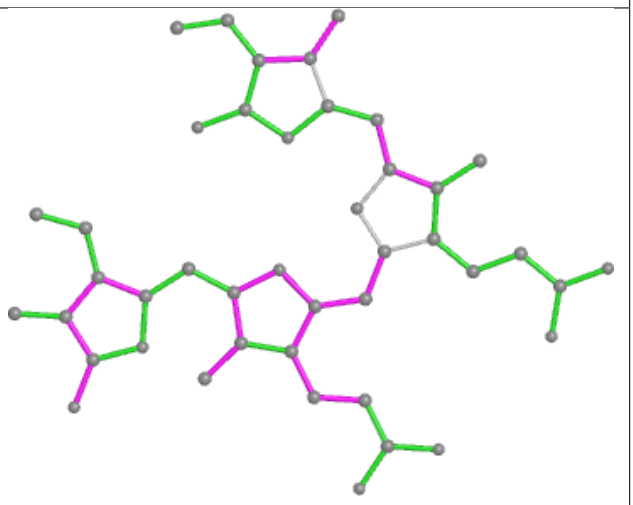

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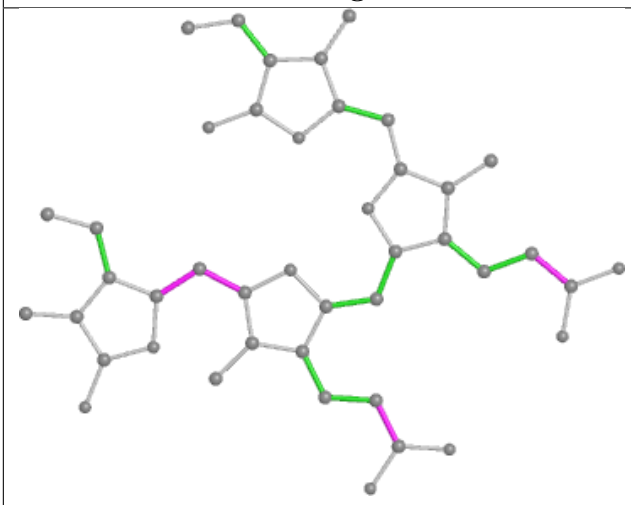

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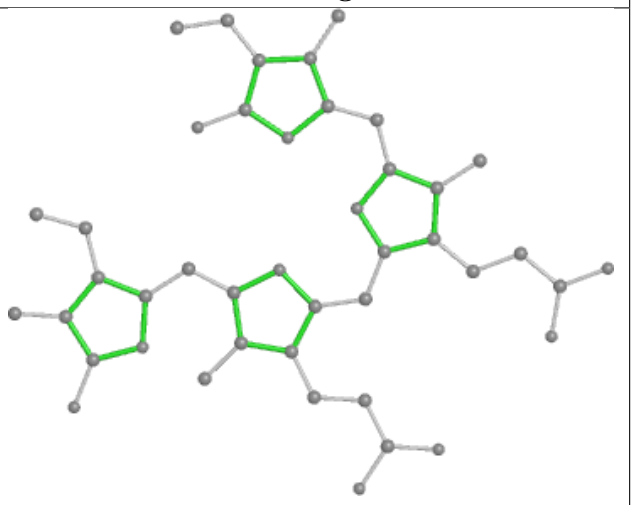
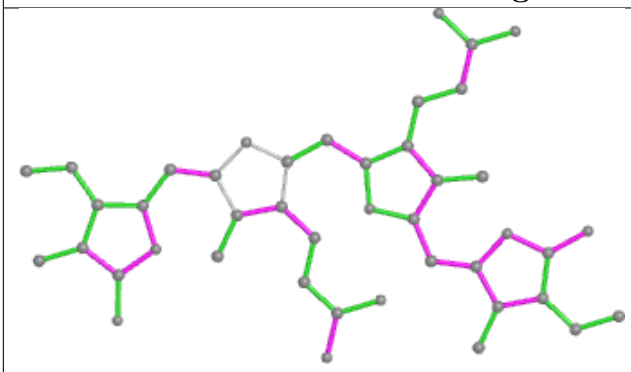


Rings

Ligand CYC H1 201



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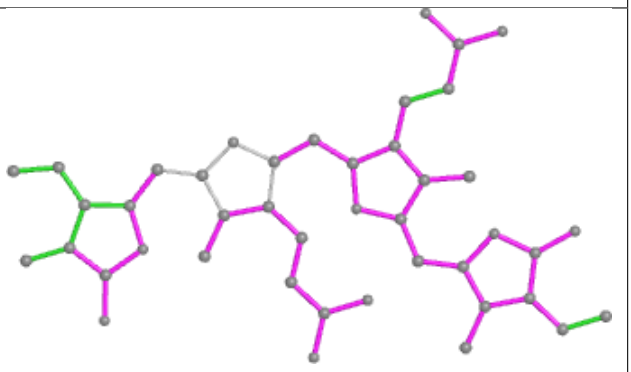

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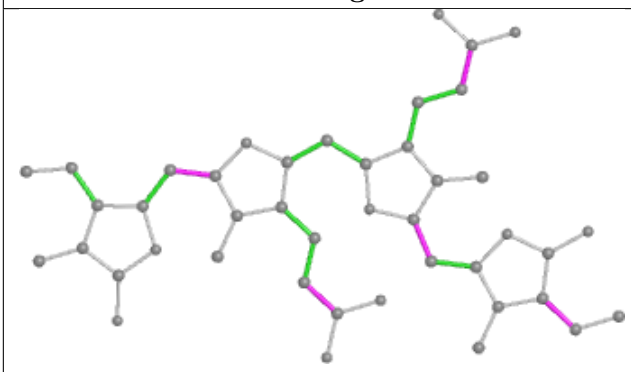

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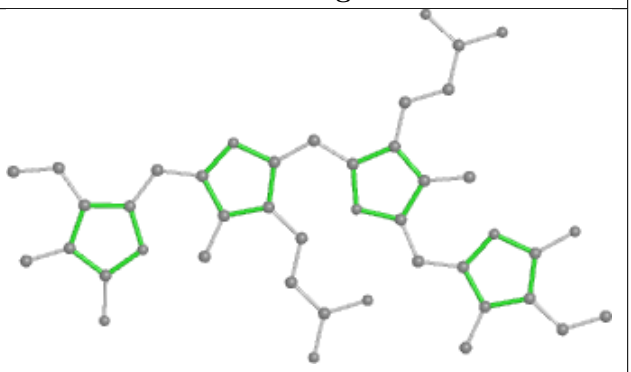
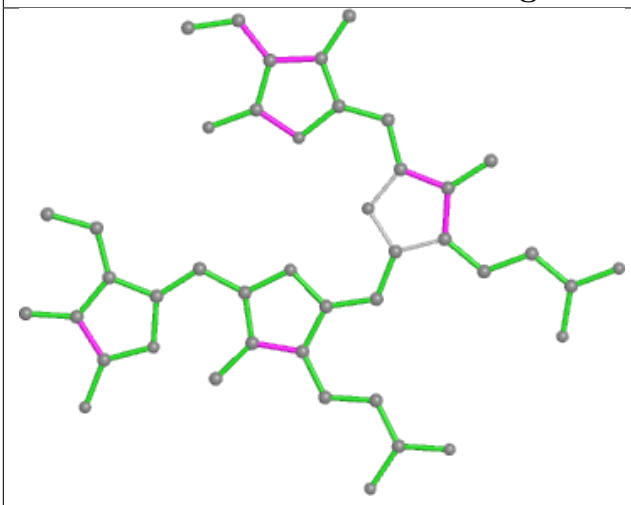


Rings

Ligand PEB ax 201



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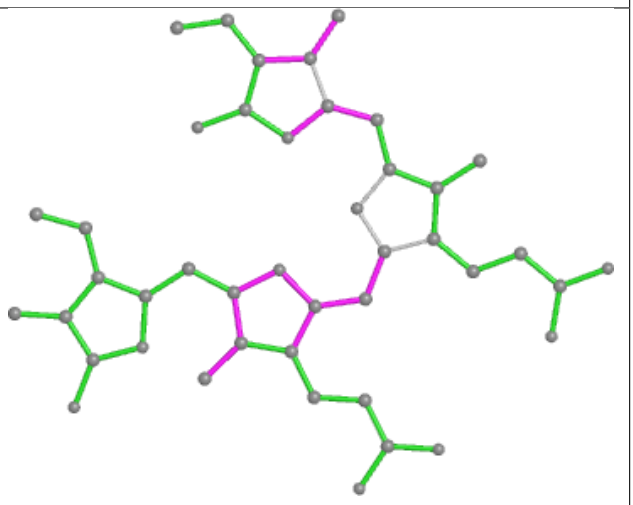

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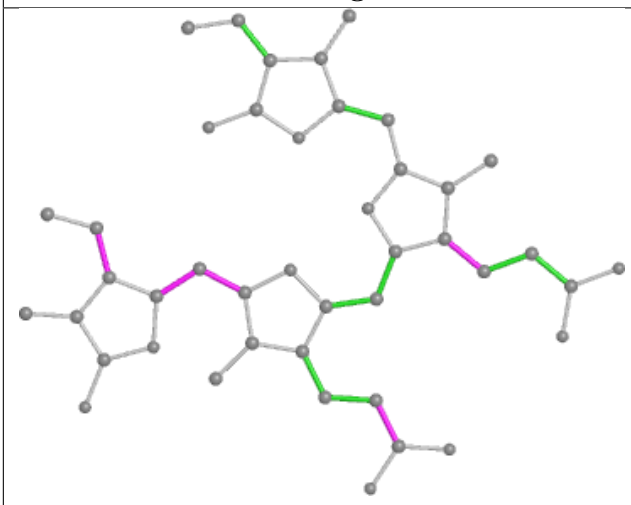

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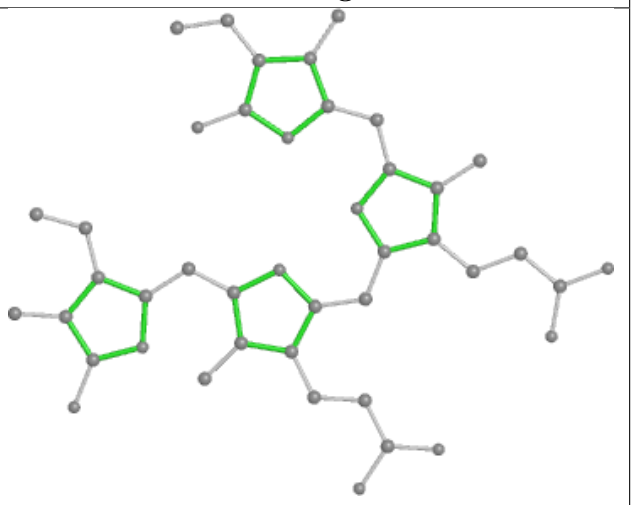
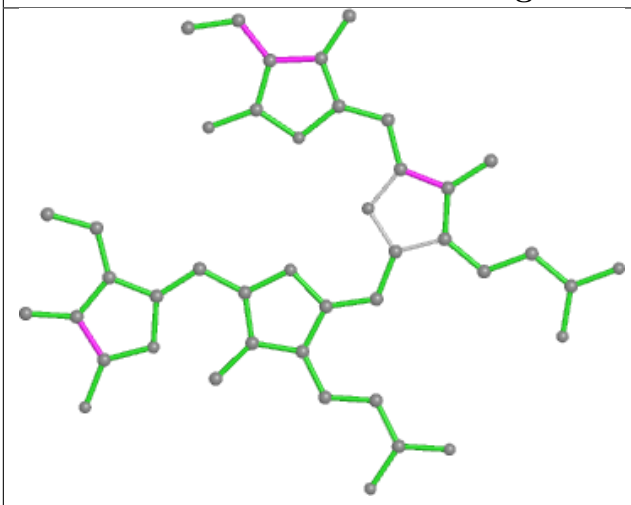


Rings

Ligand PEB R2 201



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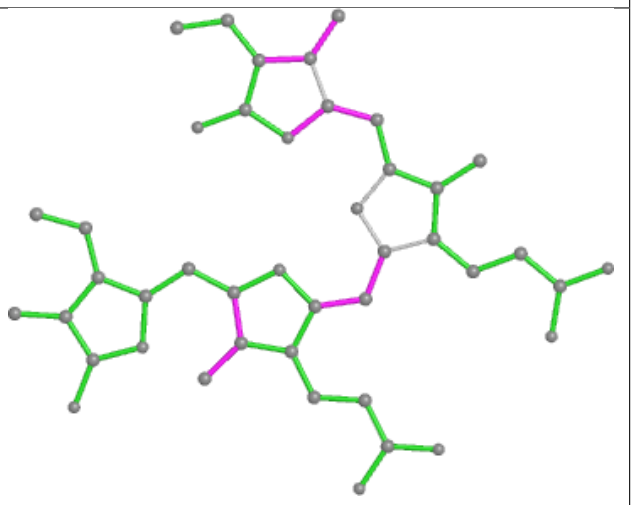

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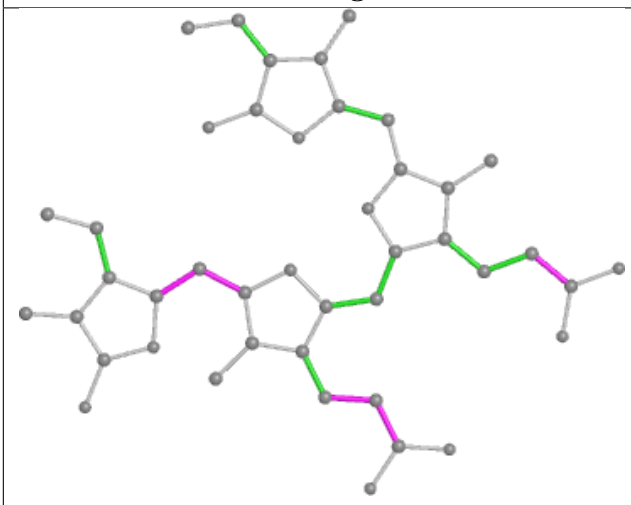

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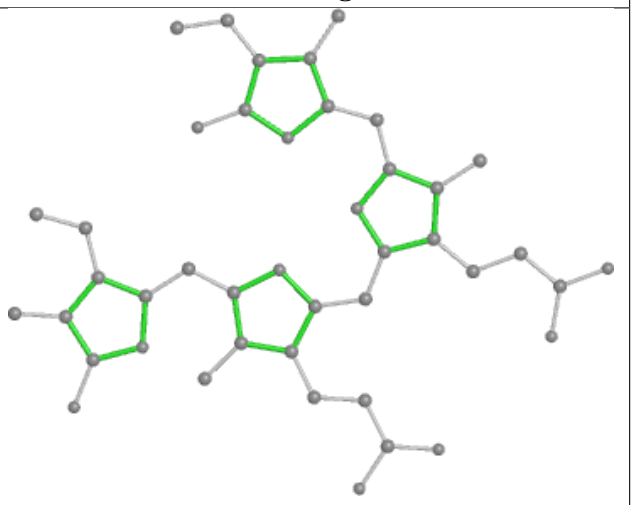
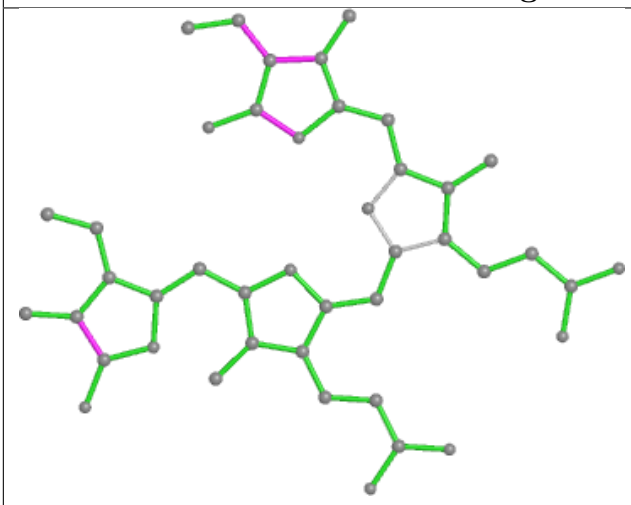


Rings

Ligand PEB a7 201



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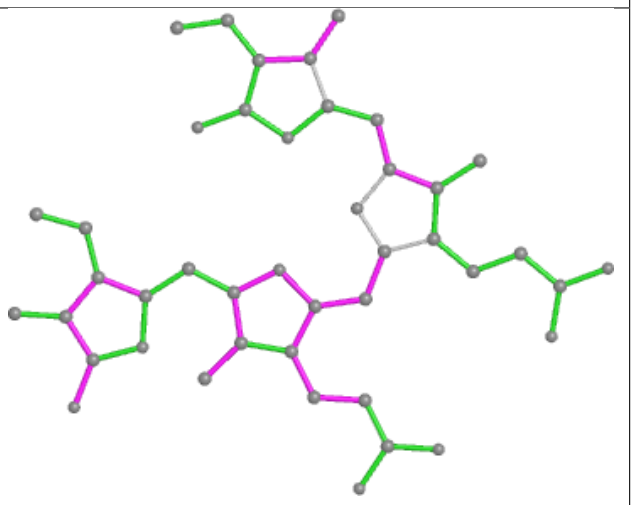

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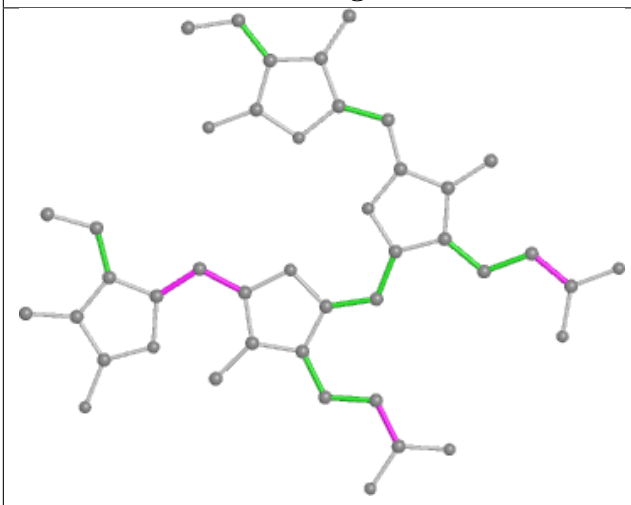

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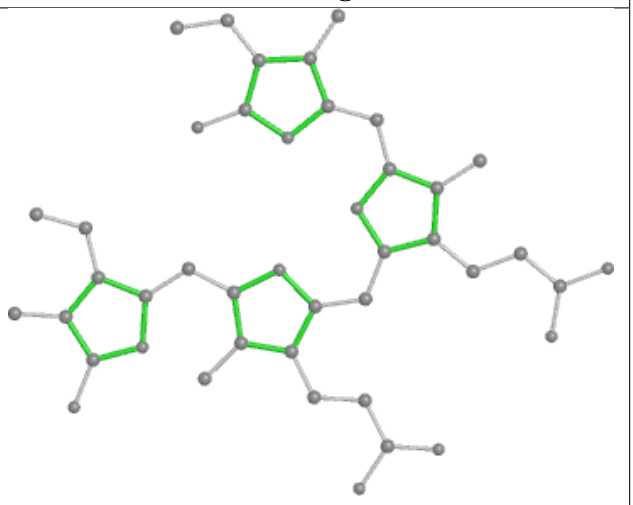

Rings

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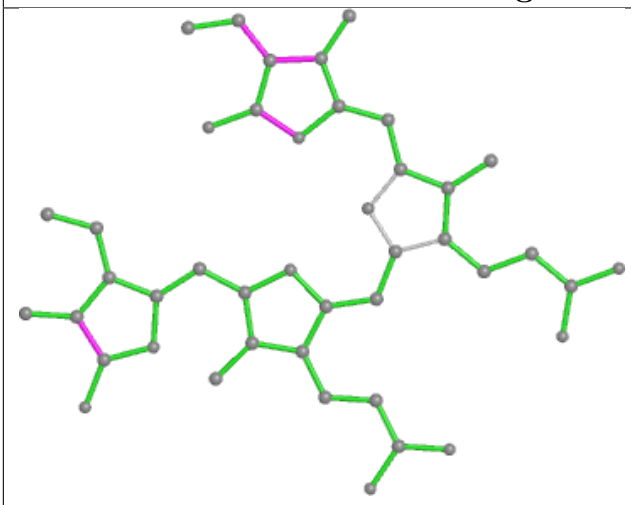

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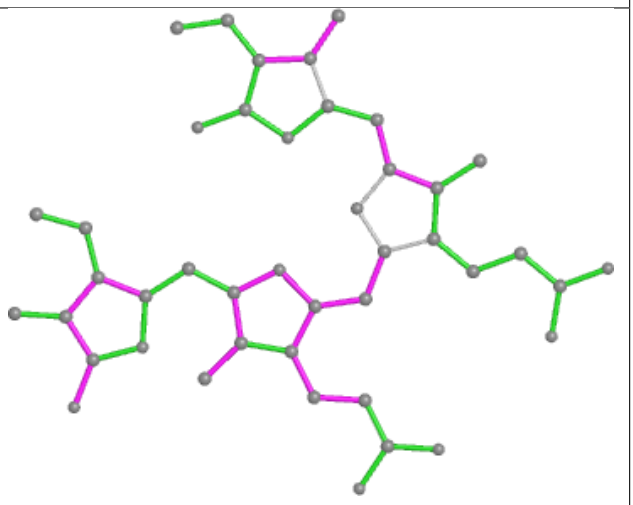

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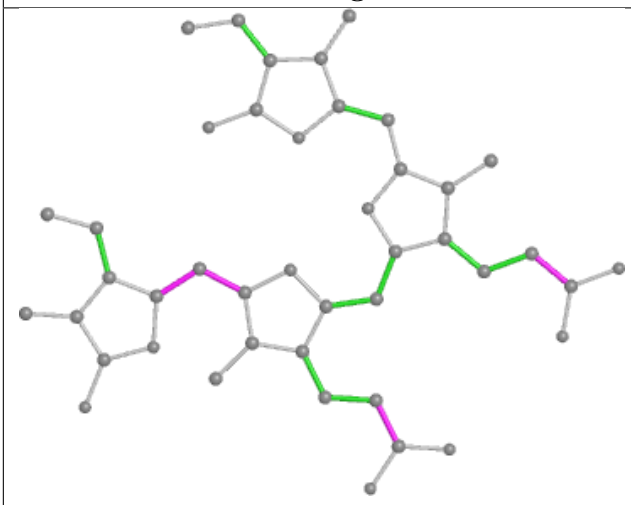

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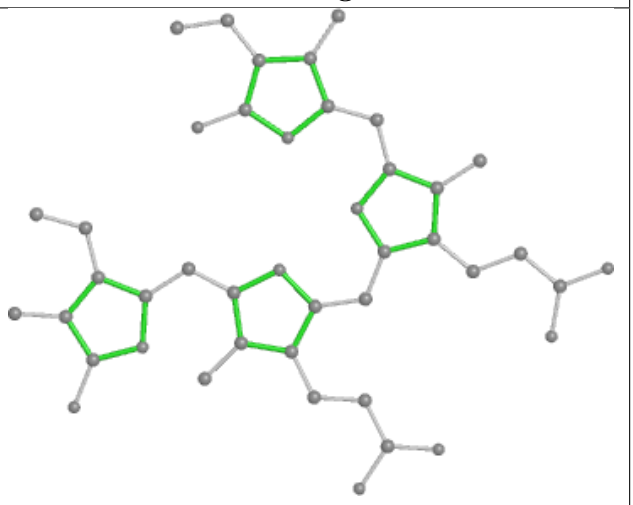
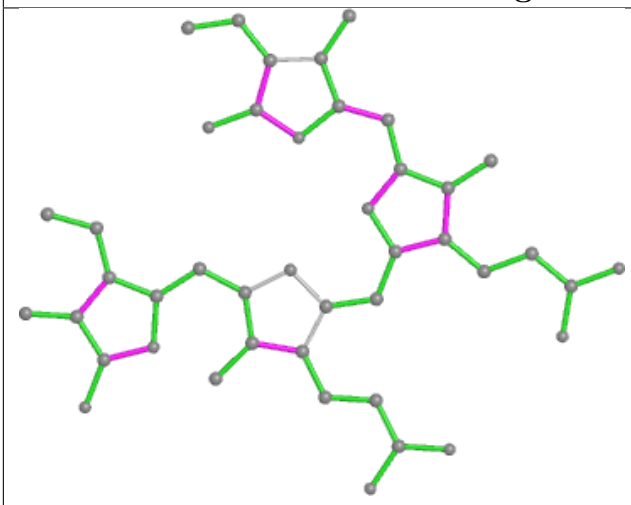


Rings

Ligand PUB bZ 306



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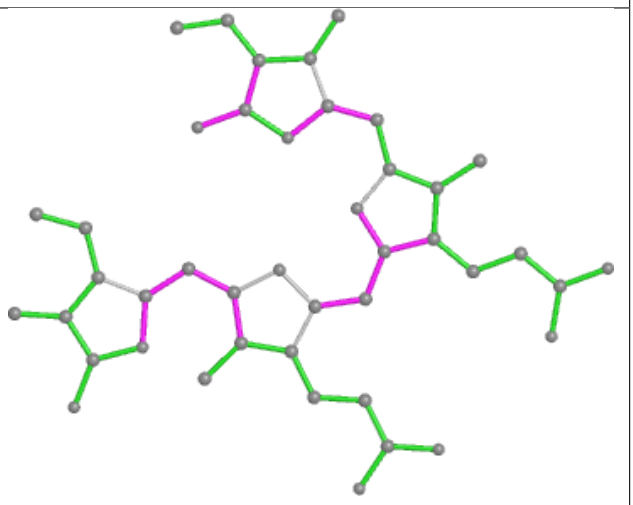

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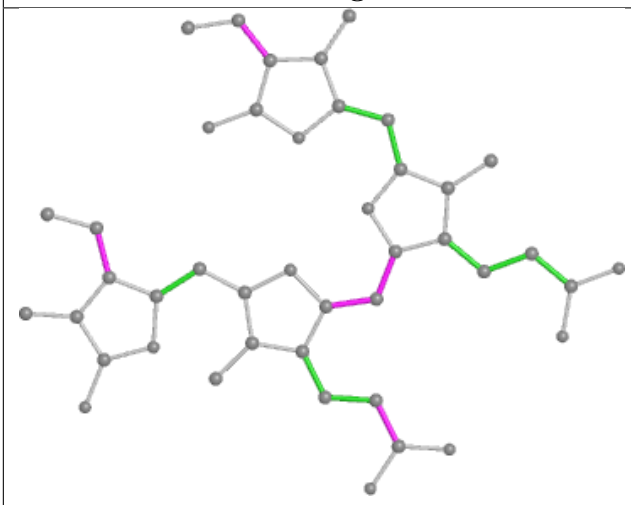

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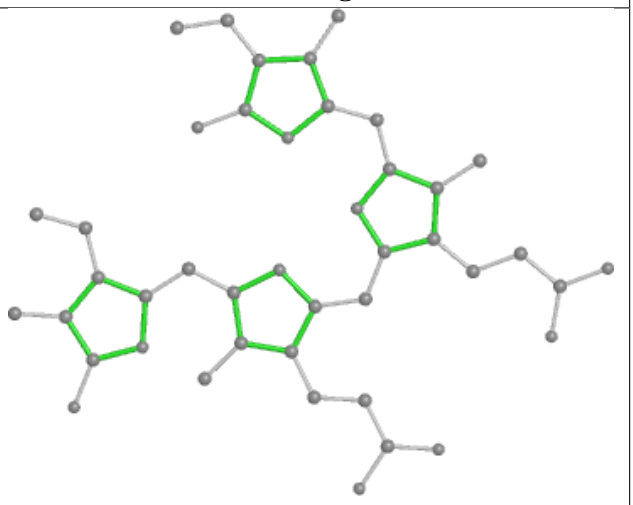
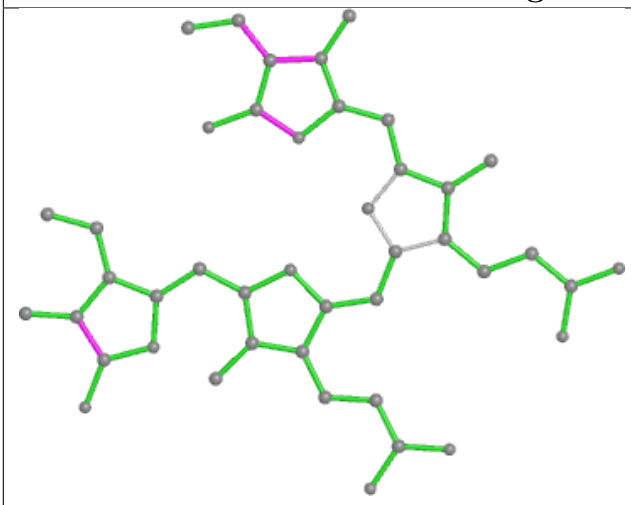


Rings

Ligand PEB fj 201



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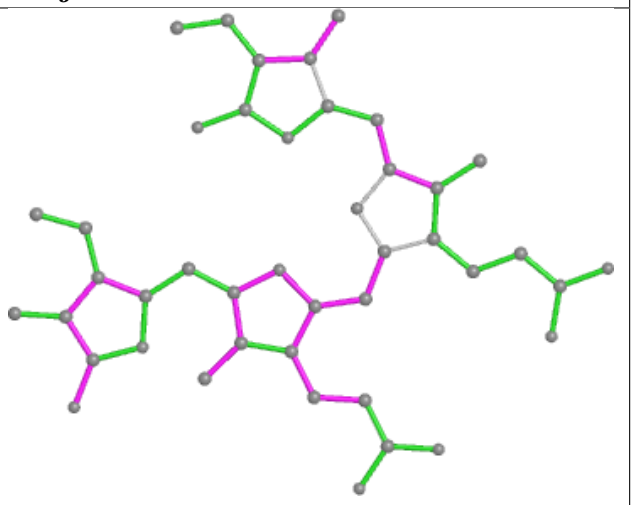

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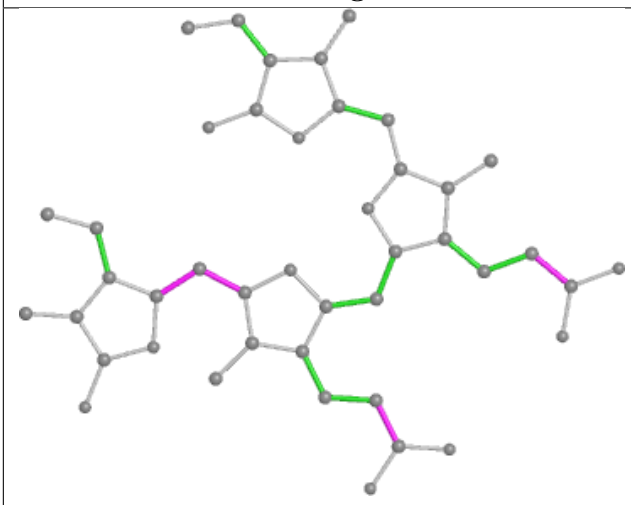

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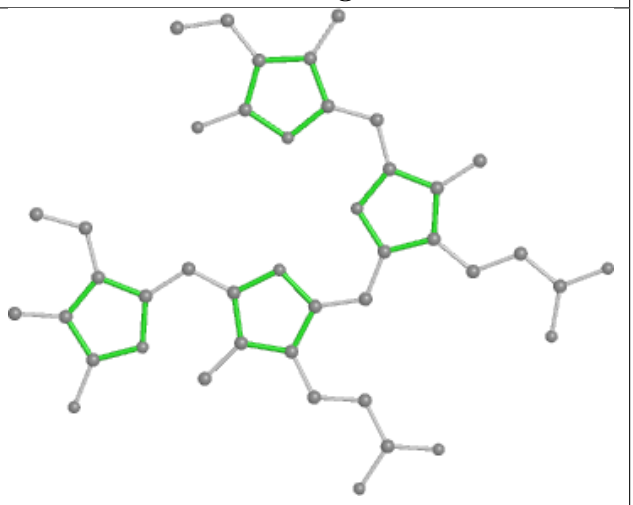
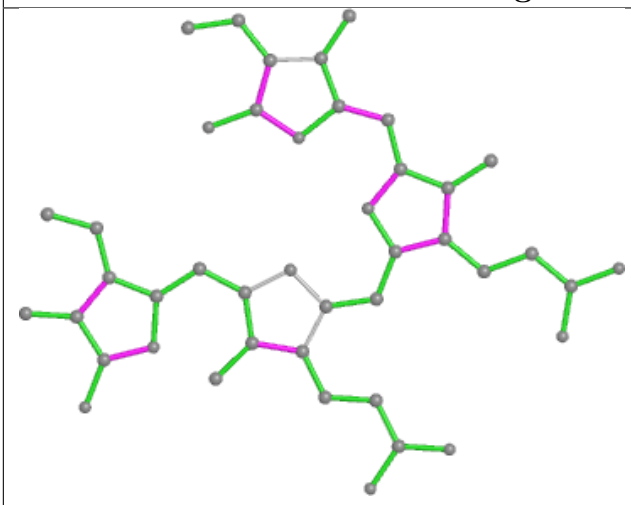


Rings

Ligand PUB T8 305



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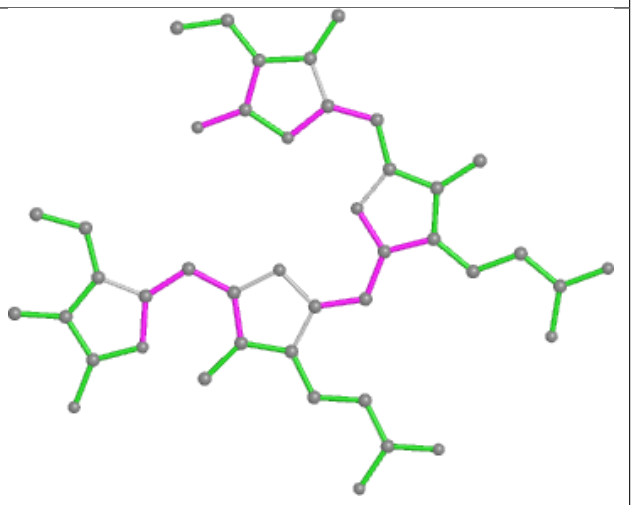

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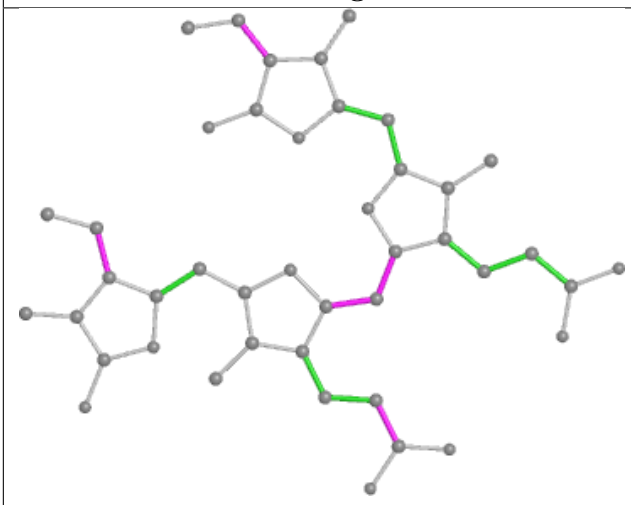

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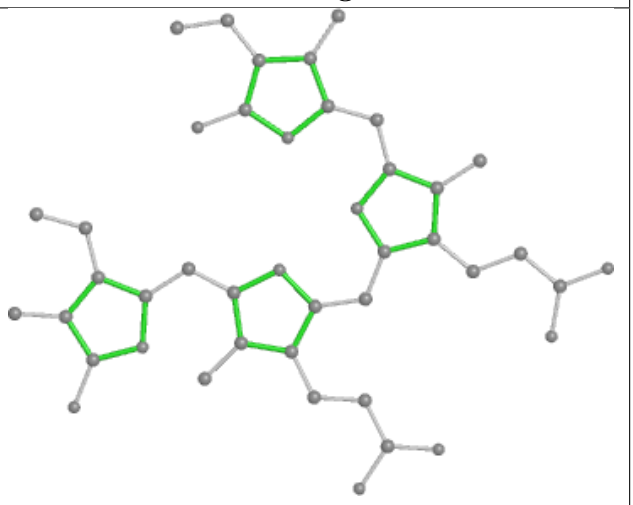
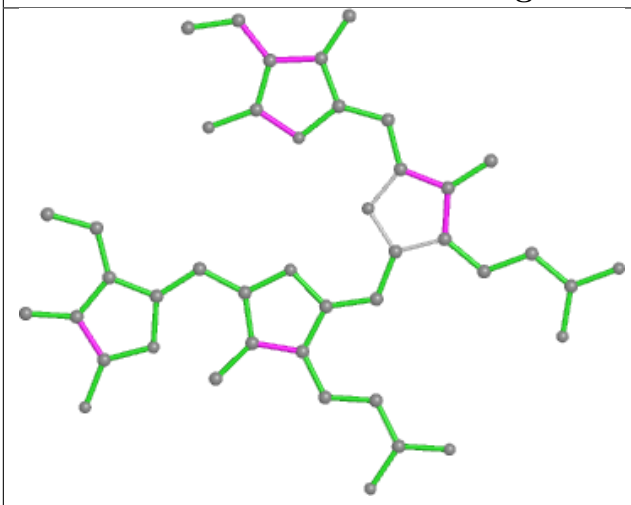


Rings

Ligand PEB R3 202



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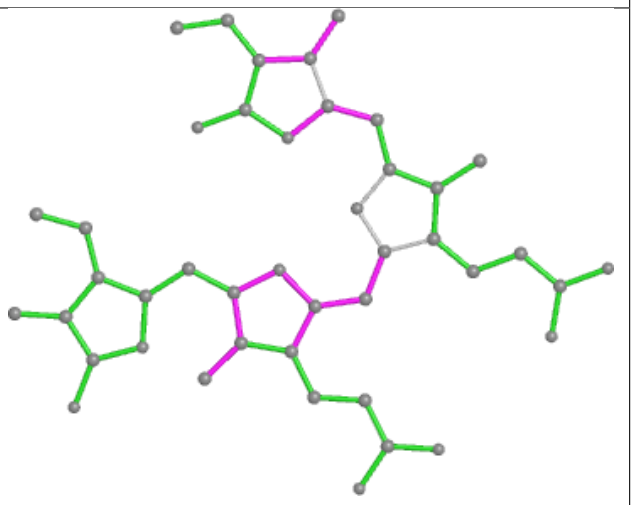

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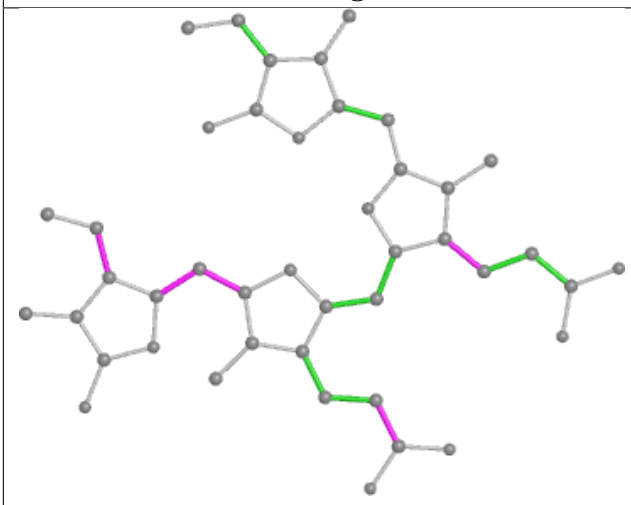

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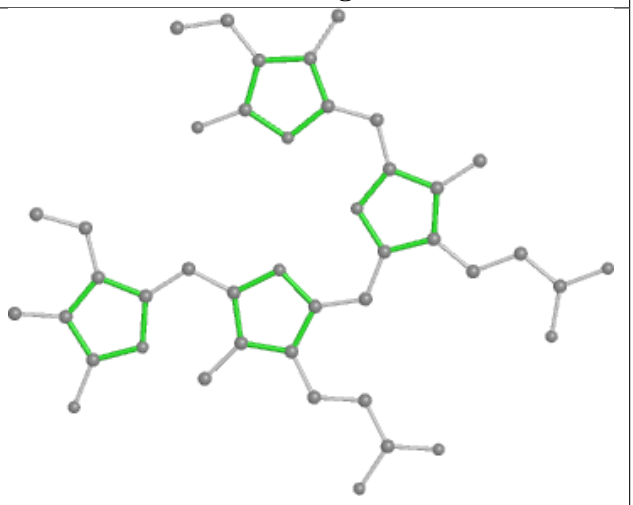
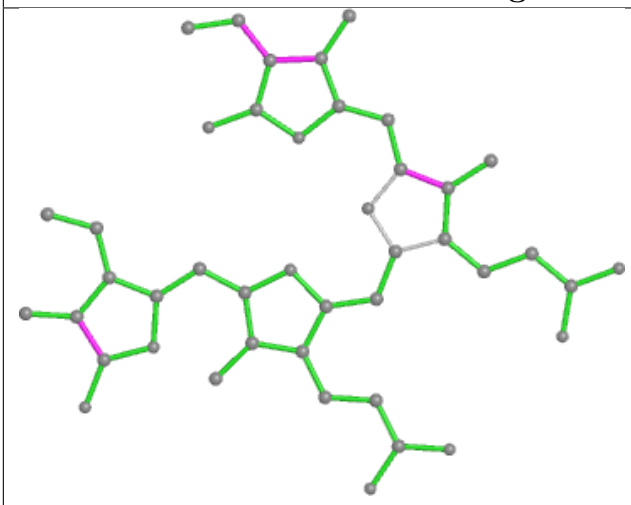


Rings

Ligand PEB Z9 1002



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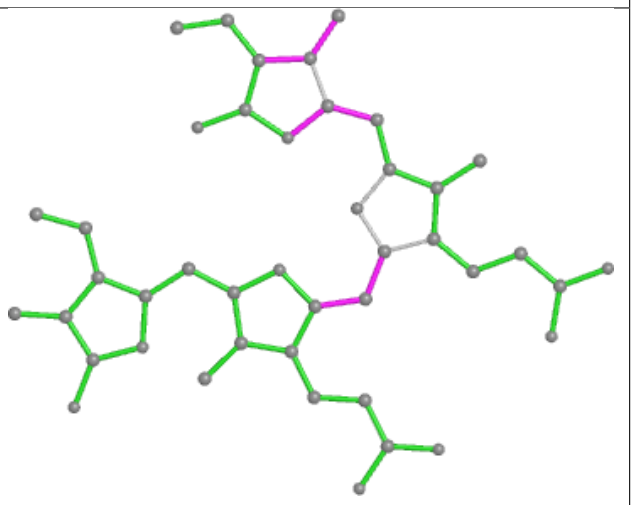

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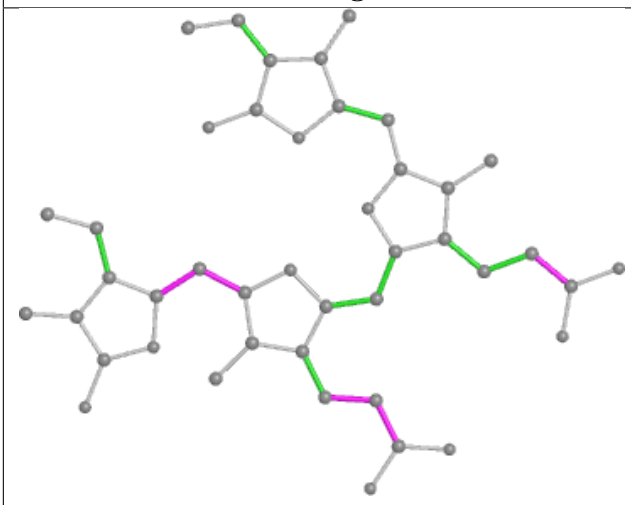

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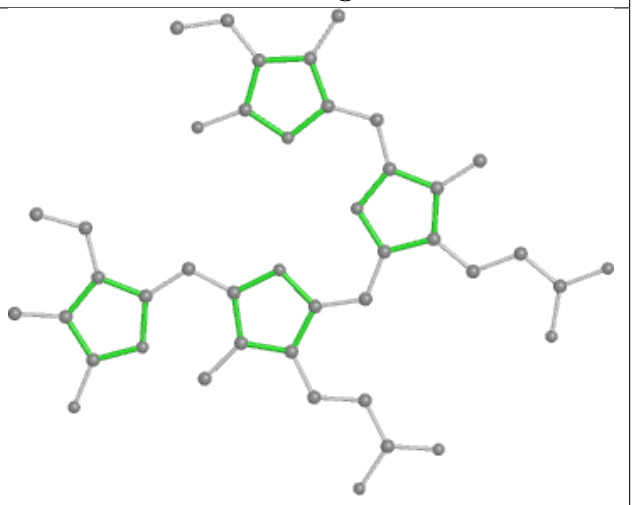
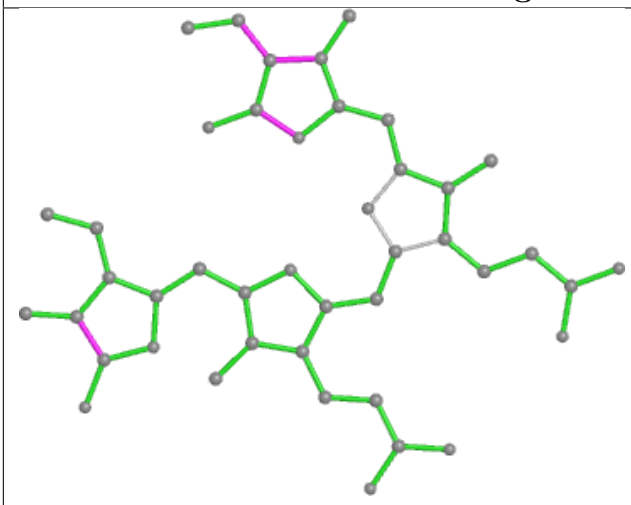


Rings

Ligand PEB hR 201



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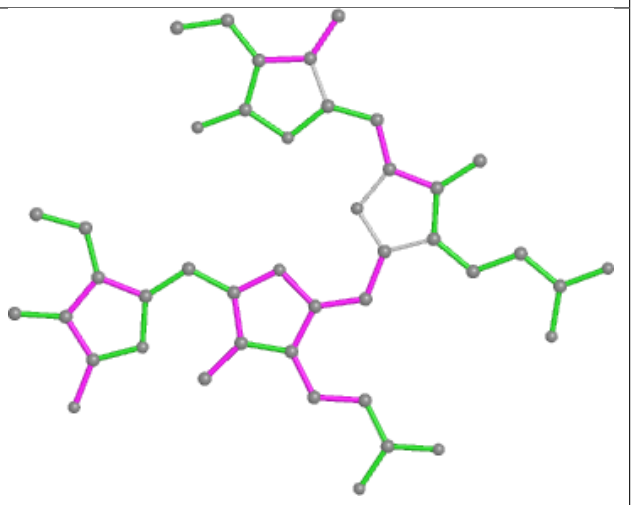
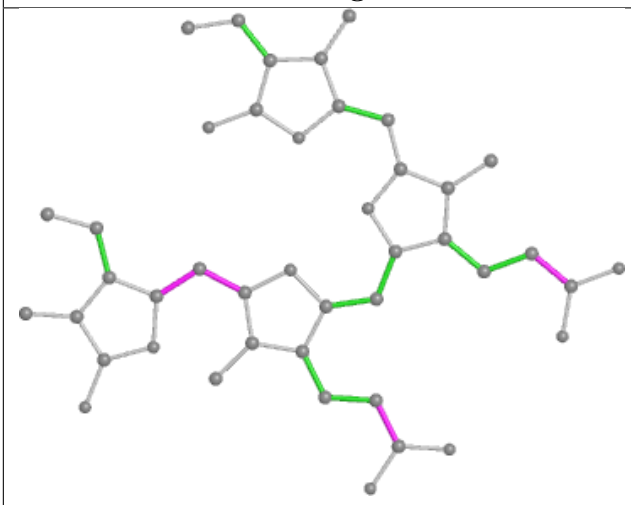


Bond angles



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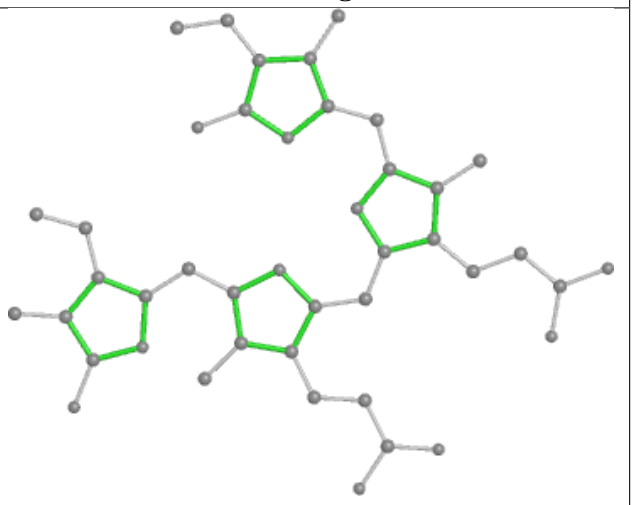
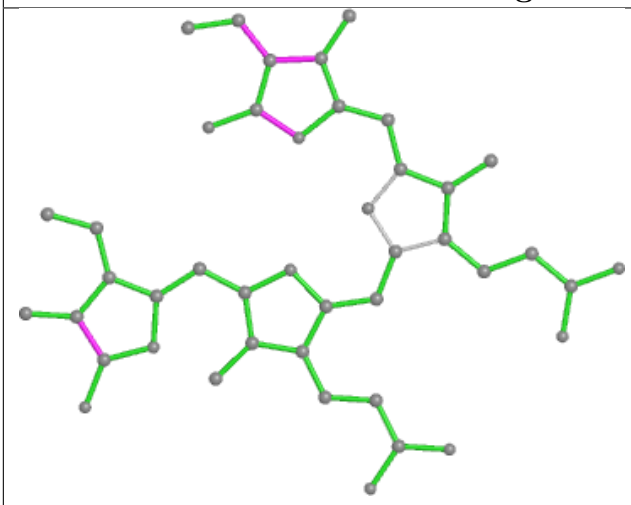


Rings

Ligand PEB R3 201



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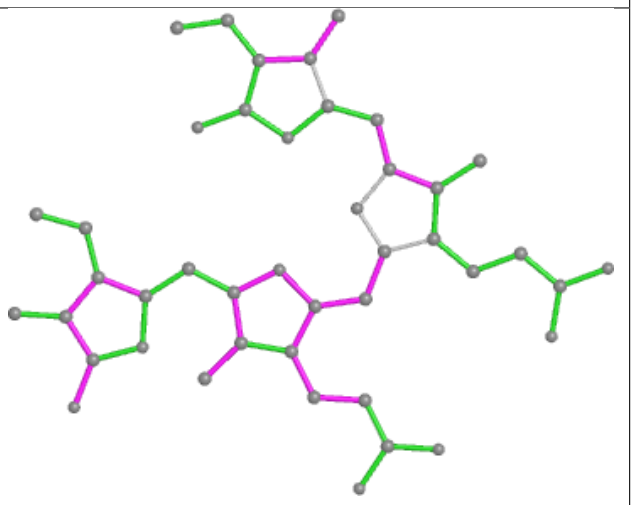
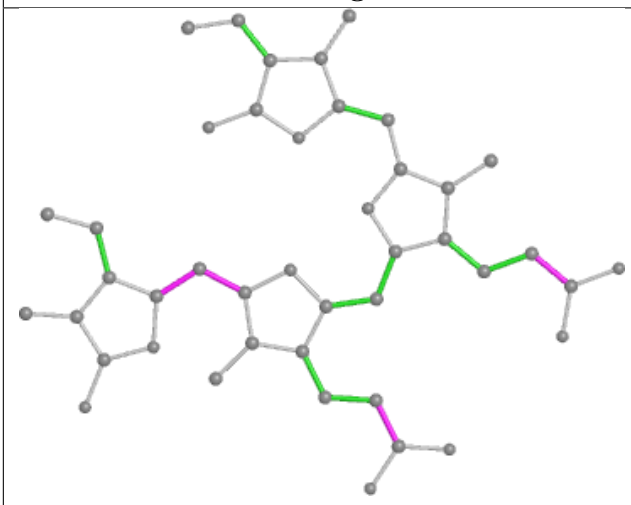
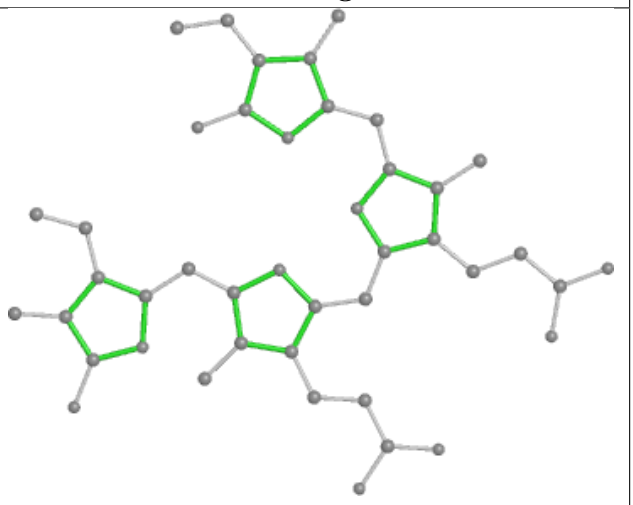


Bond angles

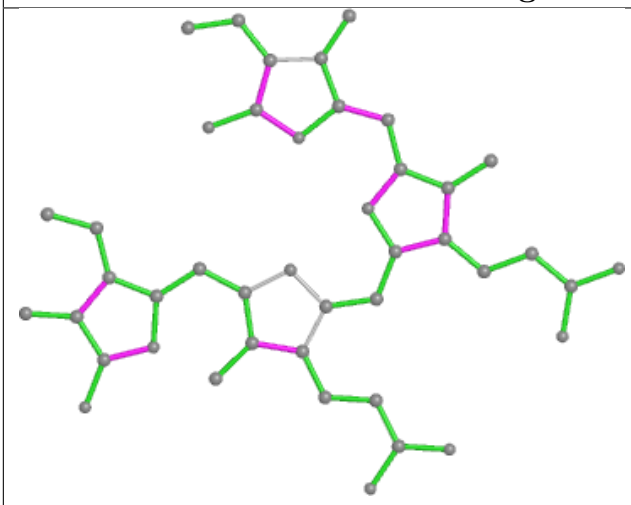


Torsions



Rings

Ligand PUB e9 306



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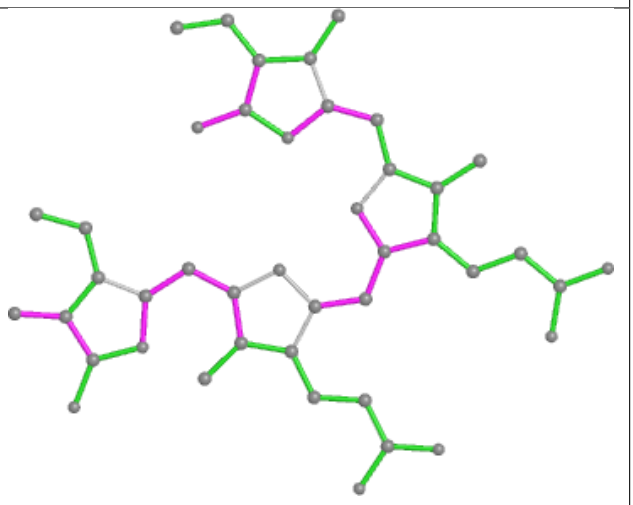
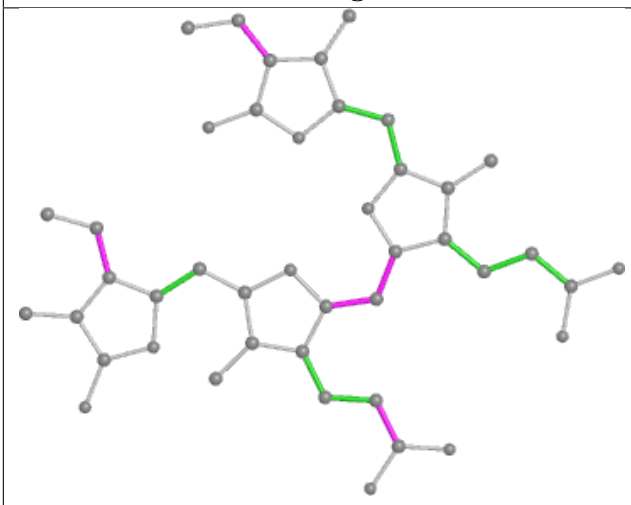


Bond angles



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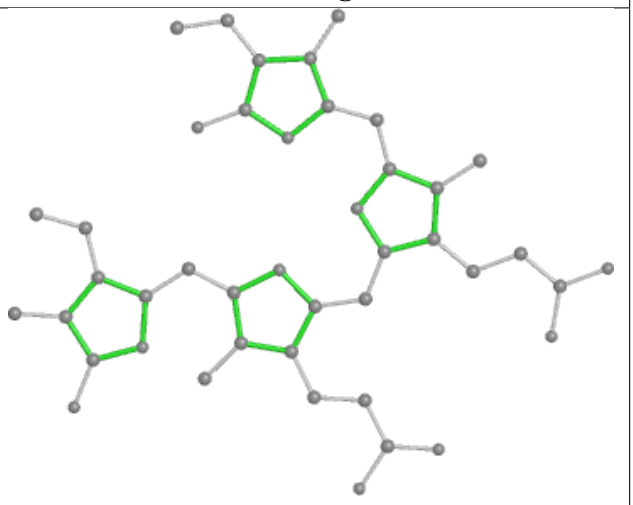
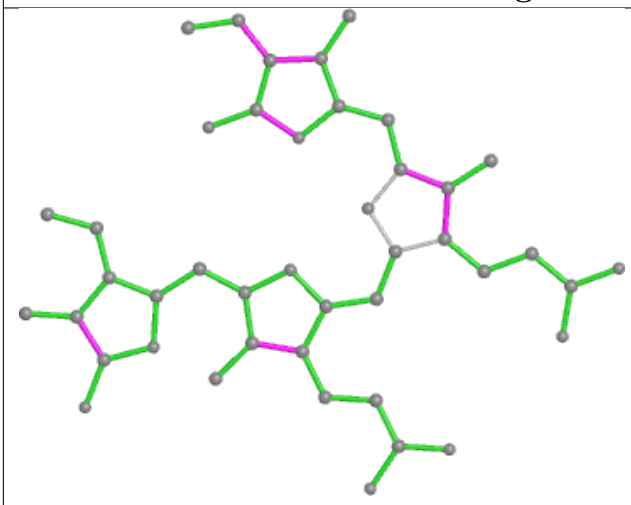


Rings

Ligand PEB bB 202



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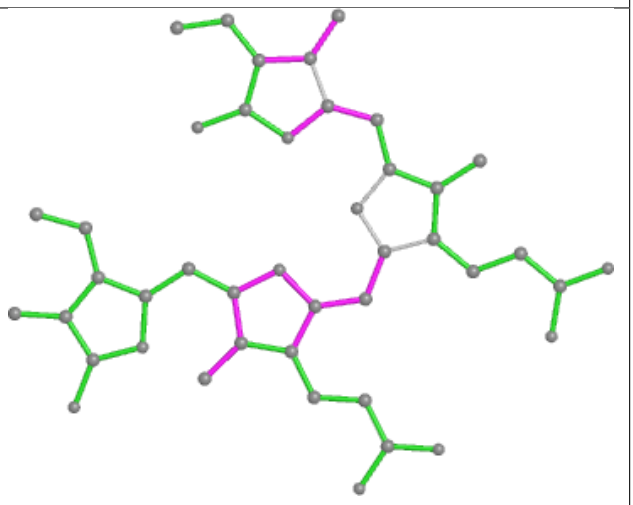

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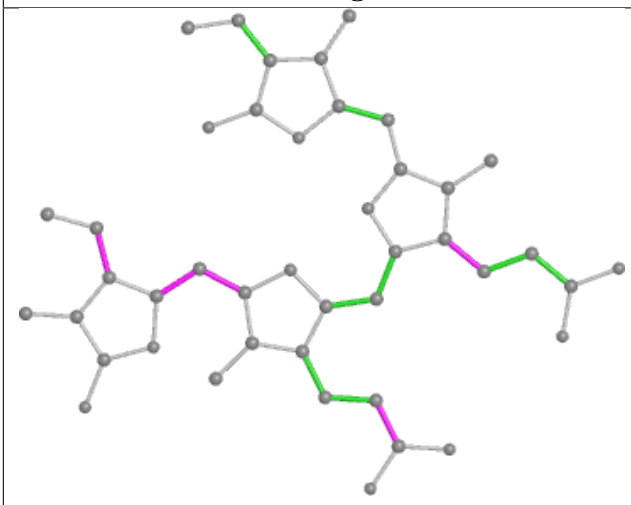

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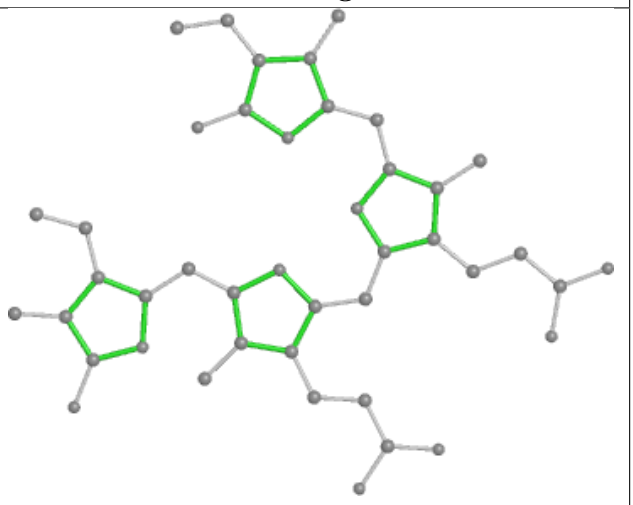
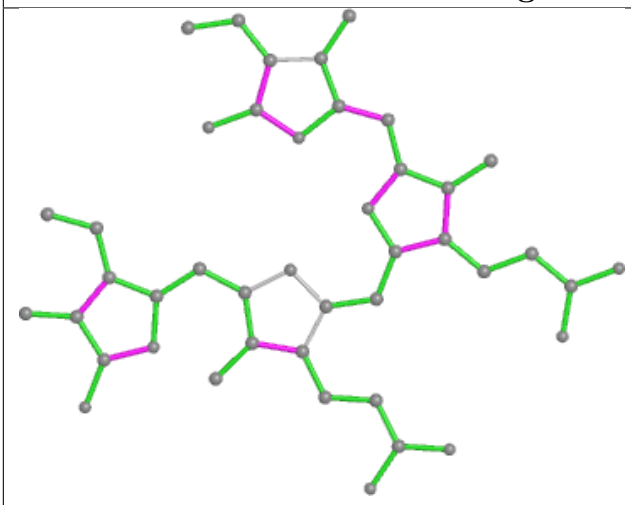


Rings

Ligand PUB o8 203



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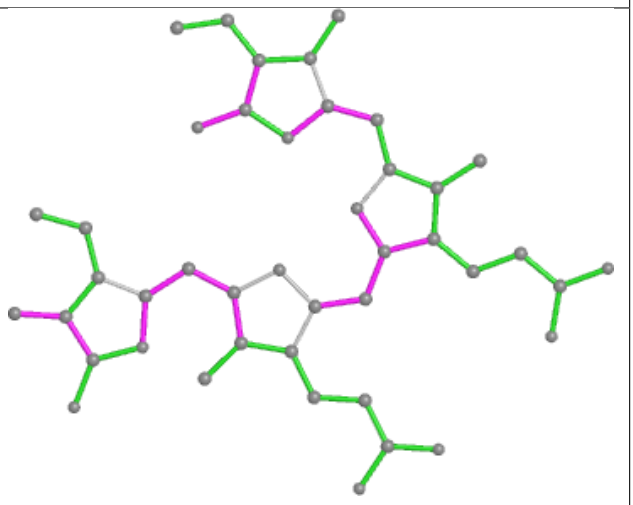

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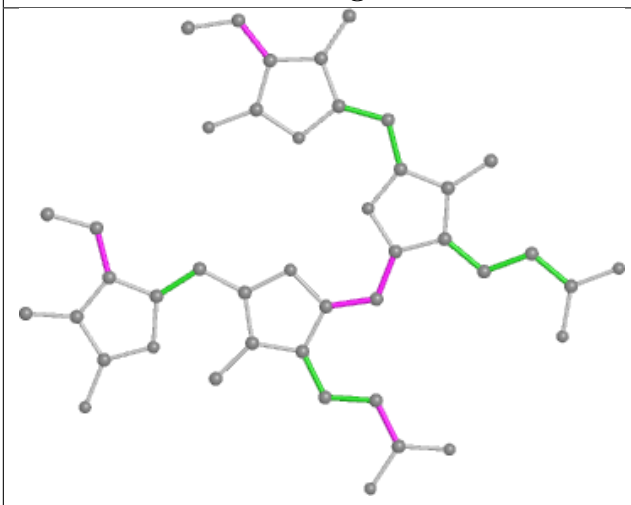

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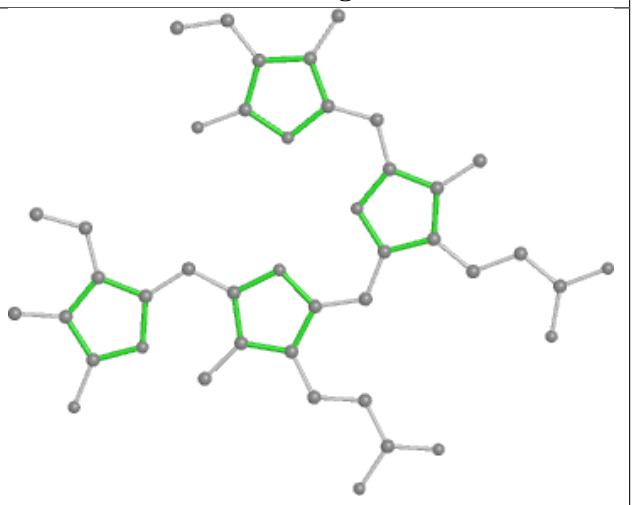
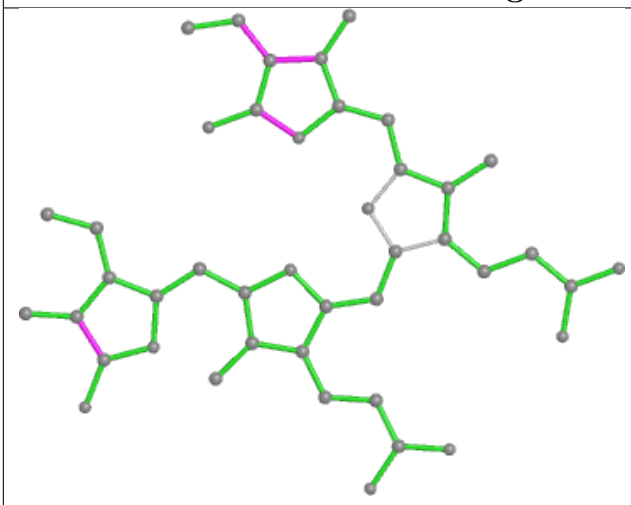


Rings

Ligand PEB Q2 1001



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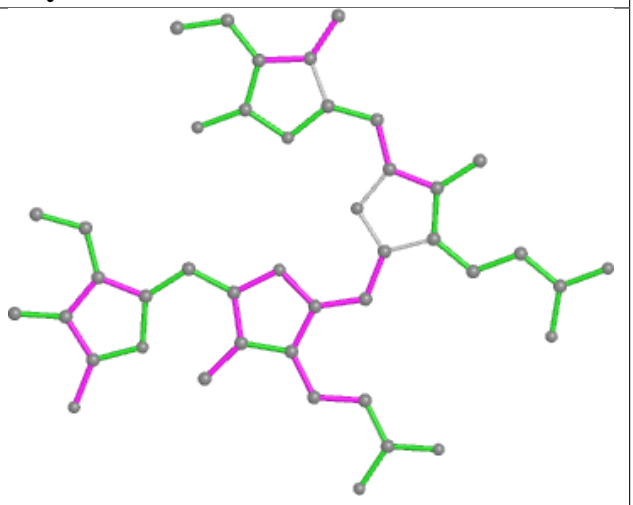

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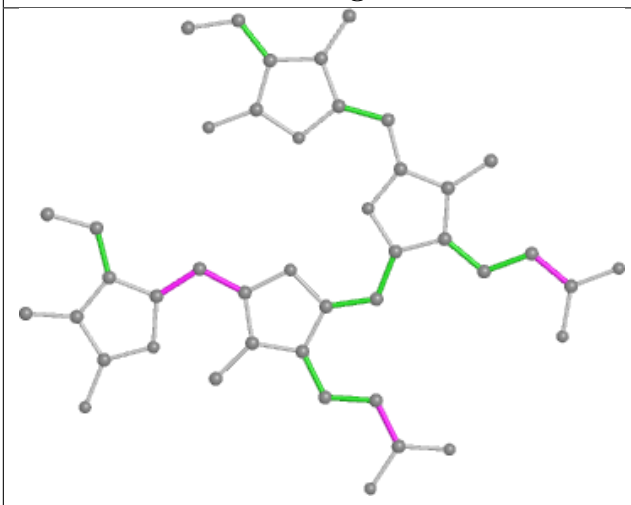

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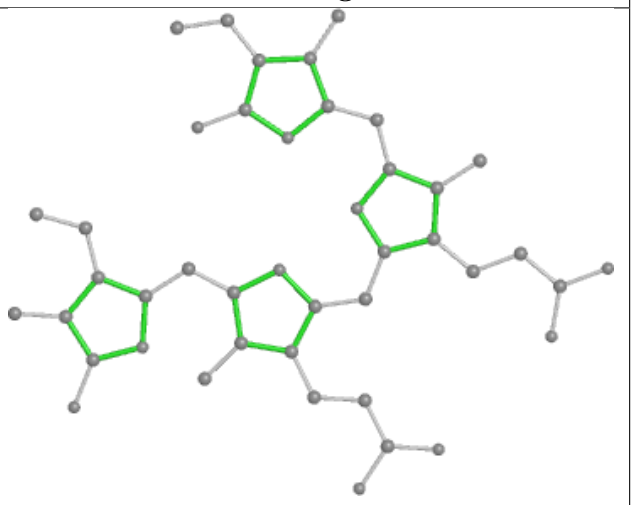
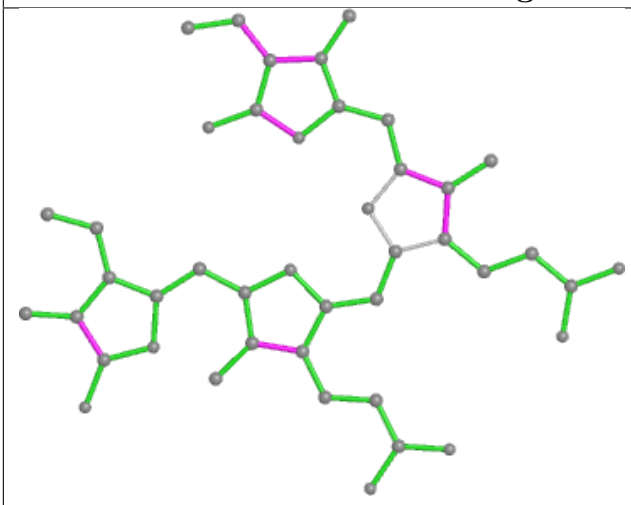


Rings

Ligand PEB P3 202



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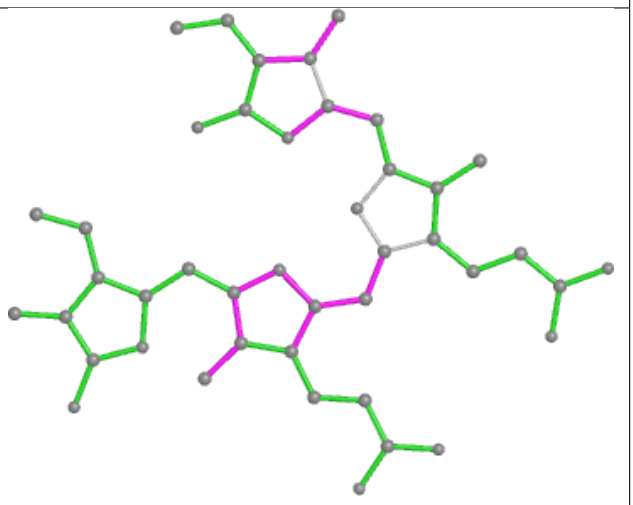

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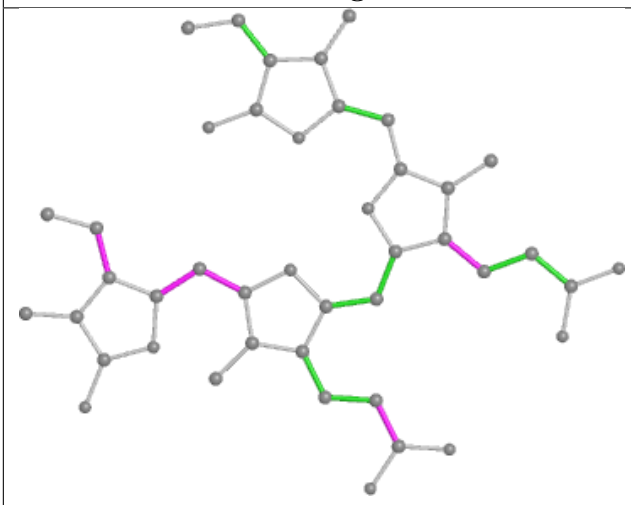

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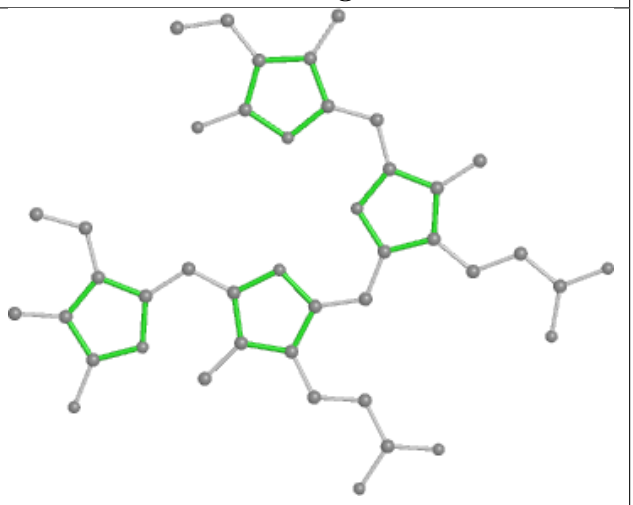

Rings

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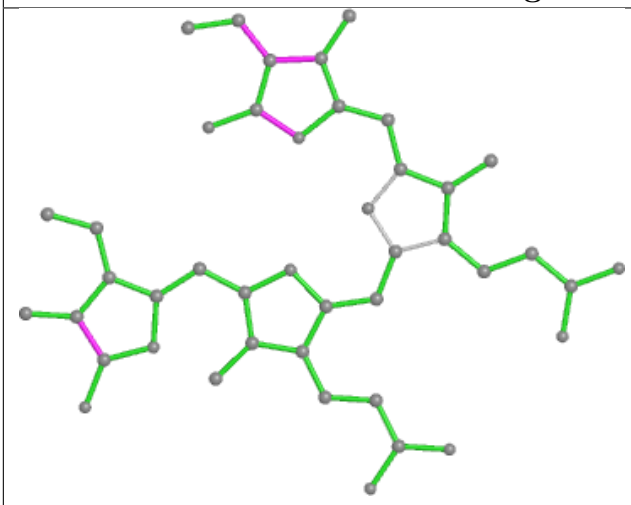

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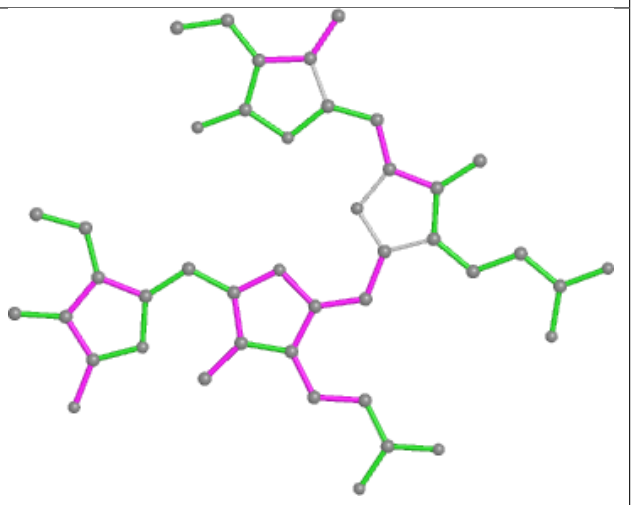

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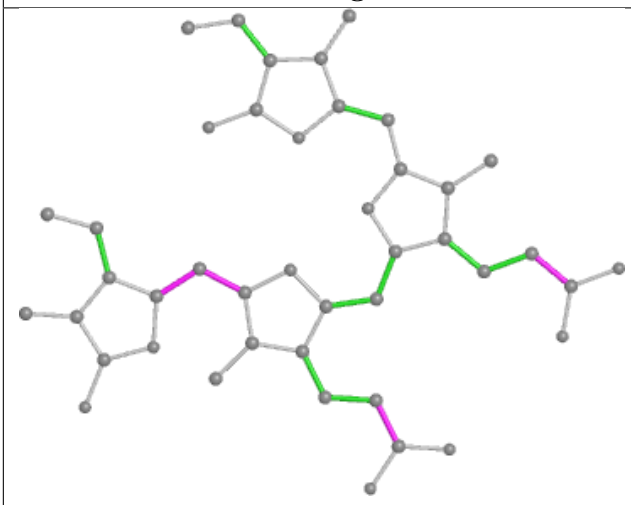

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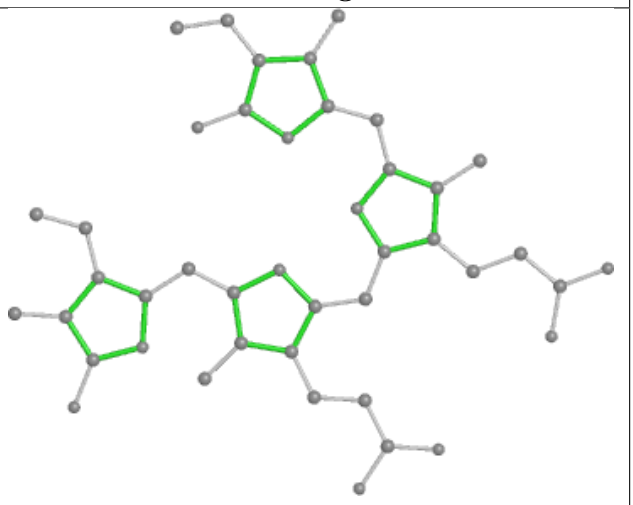

Rings

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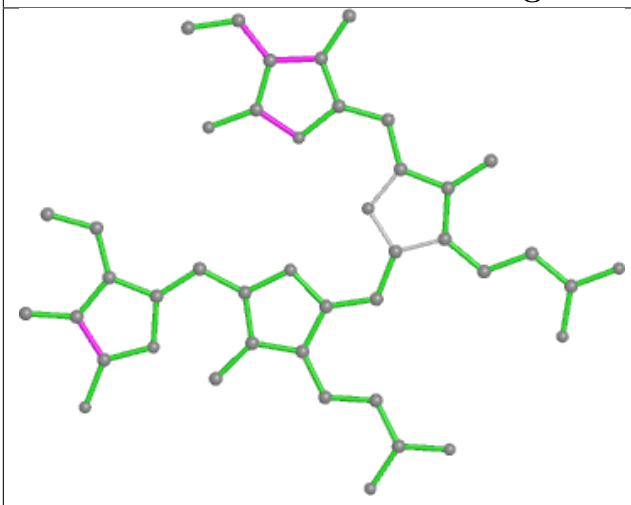

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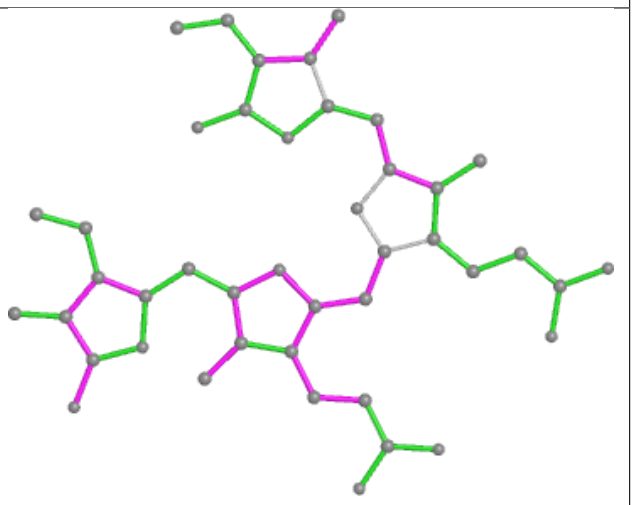

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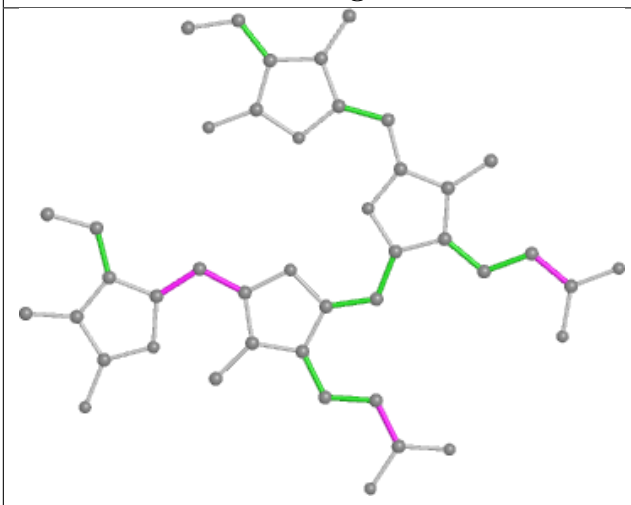

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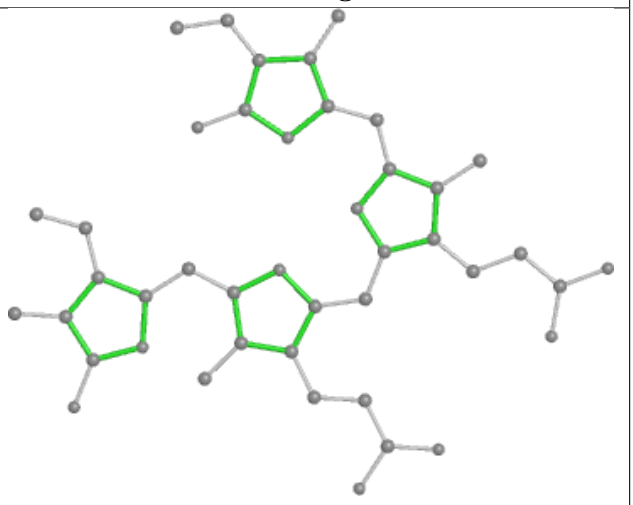
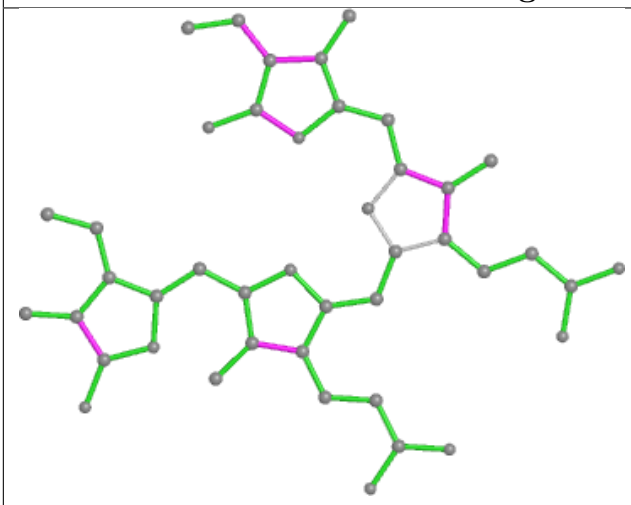


Rings

Ligand PEB n5 202



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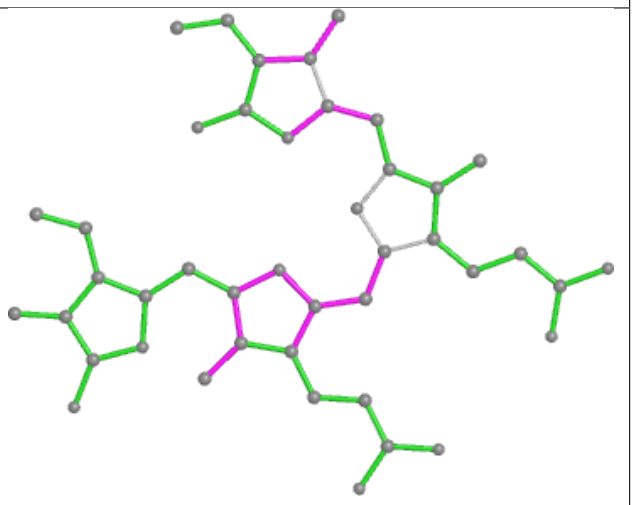

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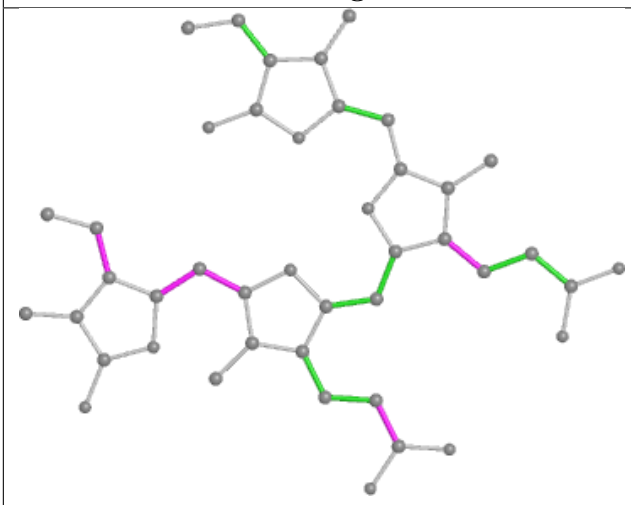

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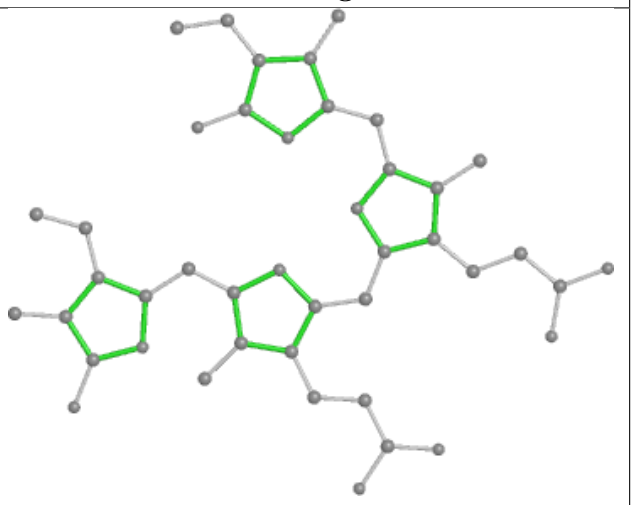

Rings

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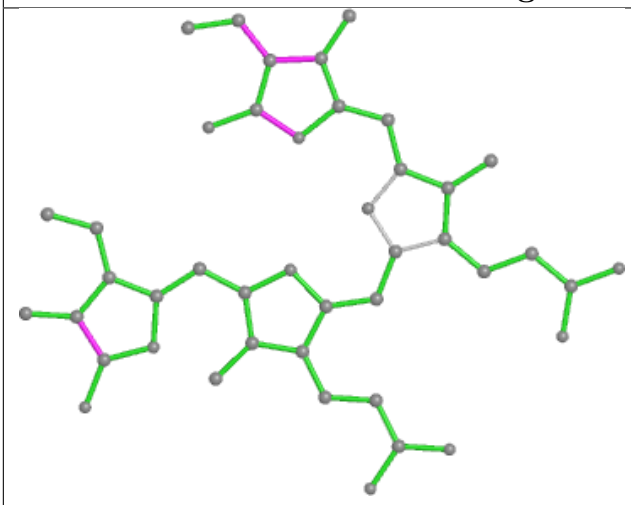

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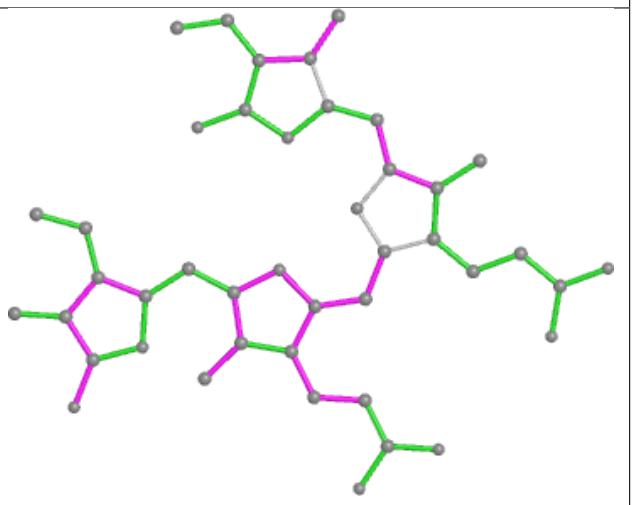

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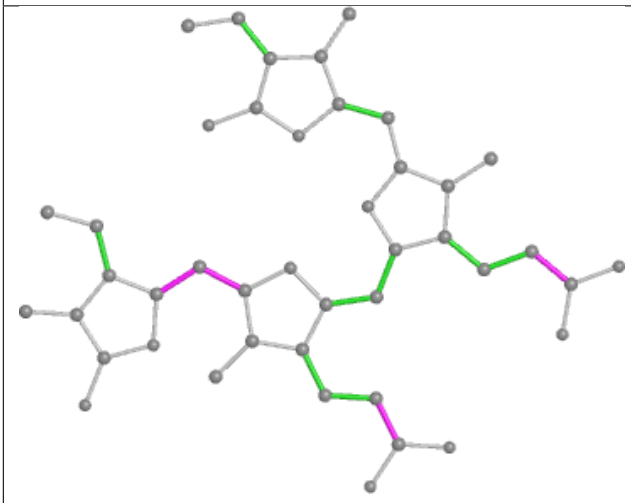

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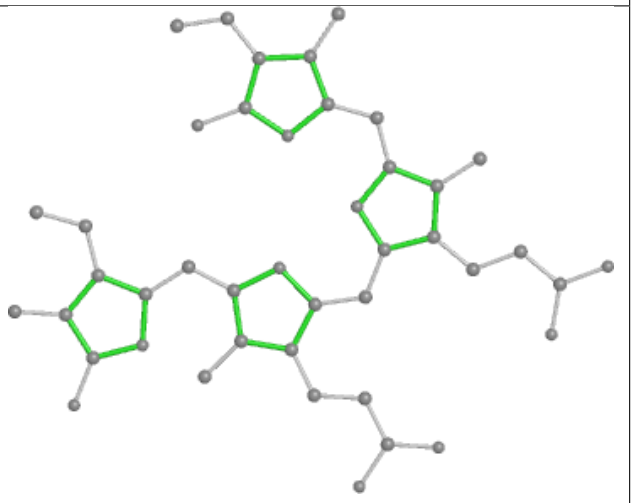
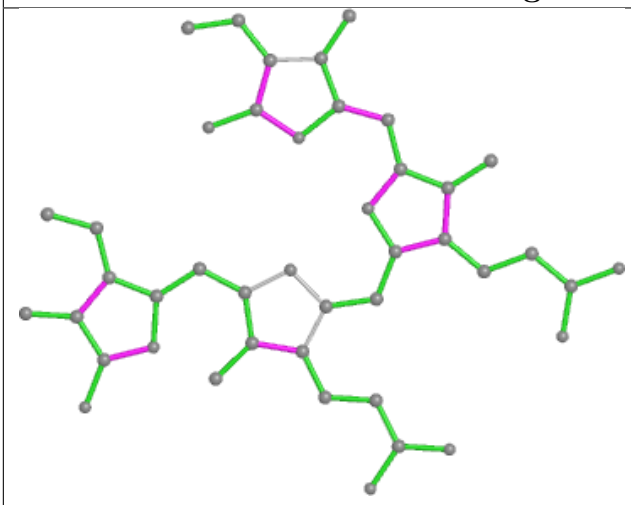


Rings

Ligand PUB lr 203



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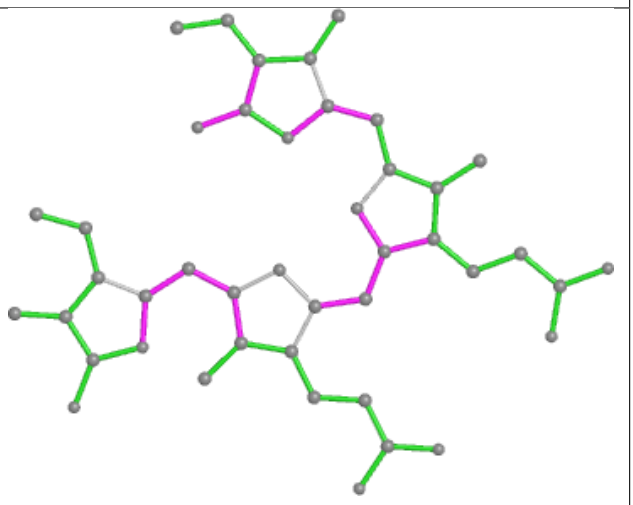

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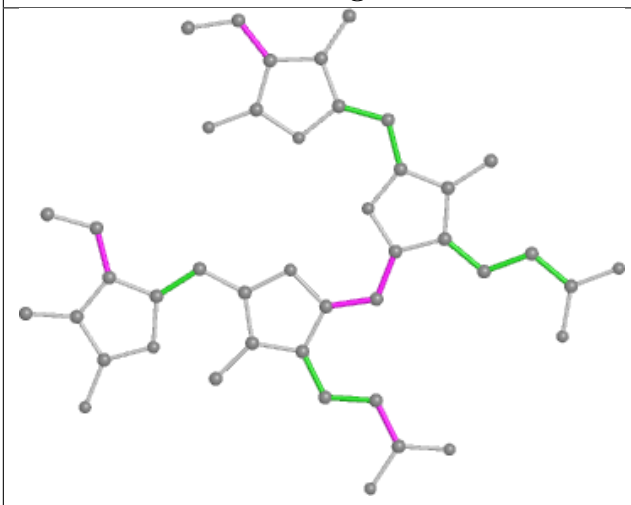

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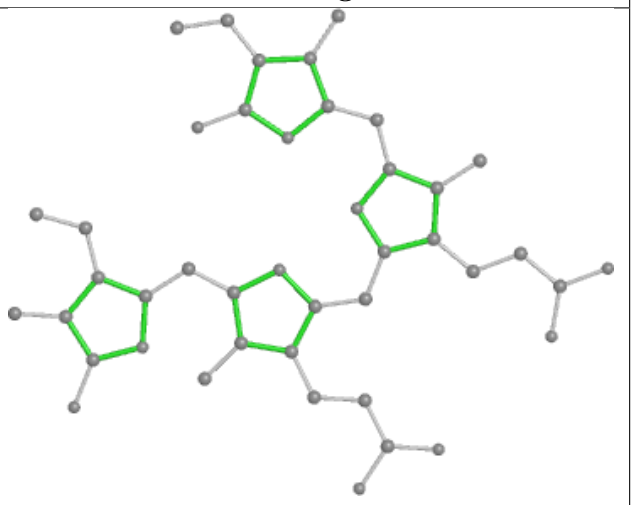
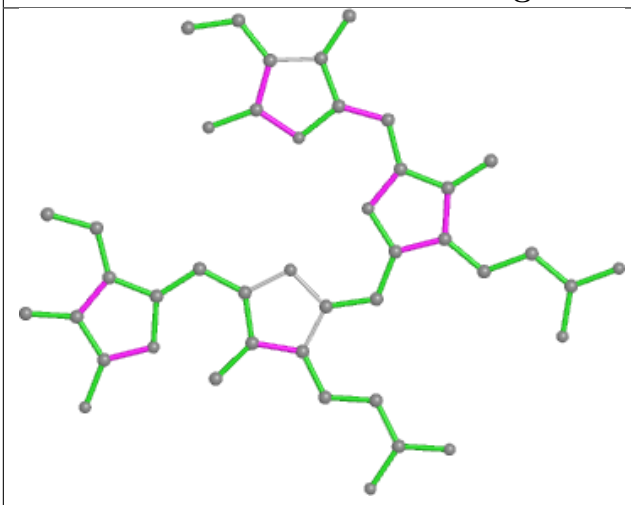


Rings

Ligand PUB hV 203



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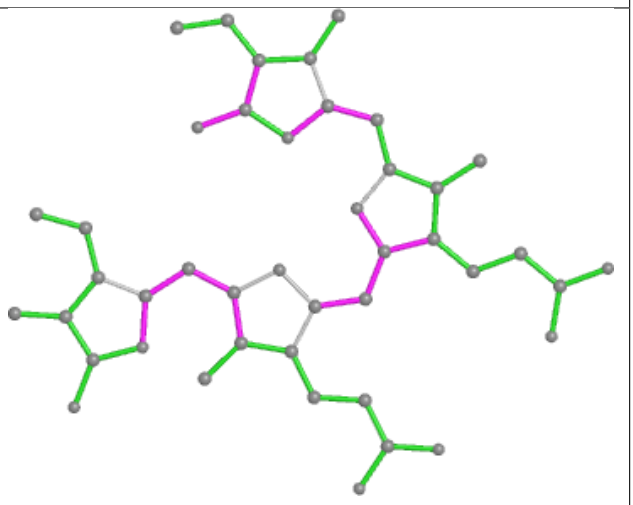
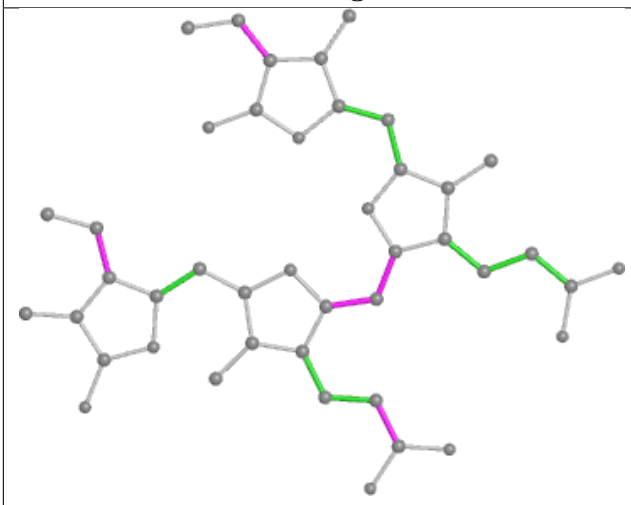


Bond angles



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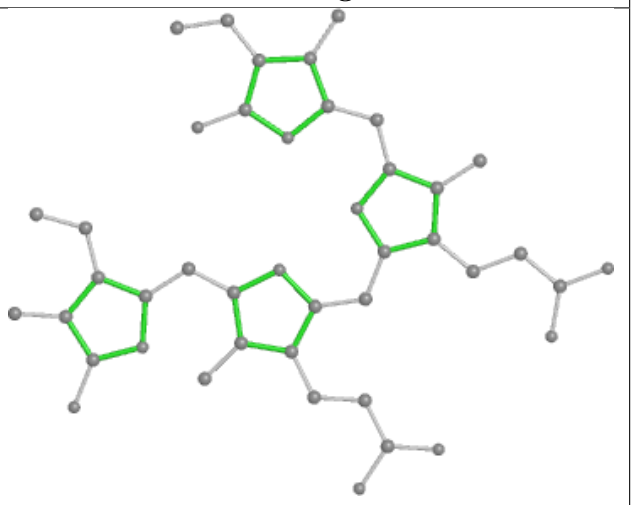
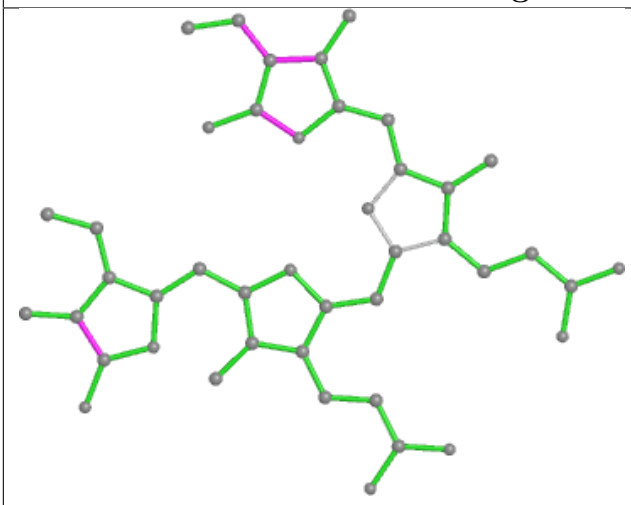


Rings

Ligand PEB M2 201



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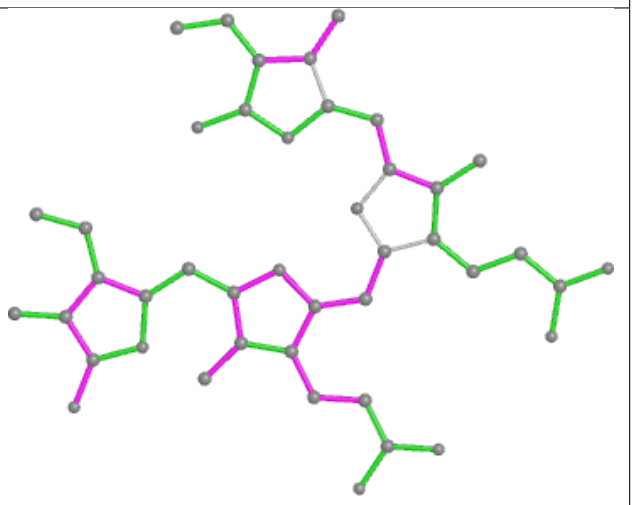
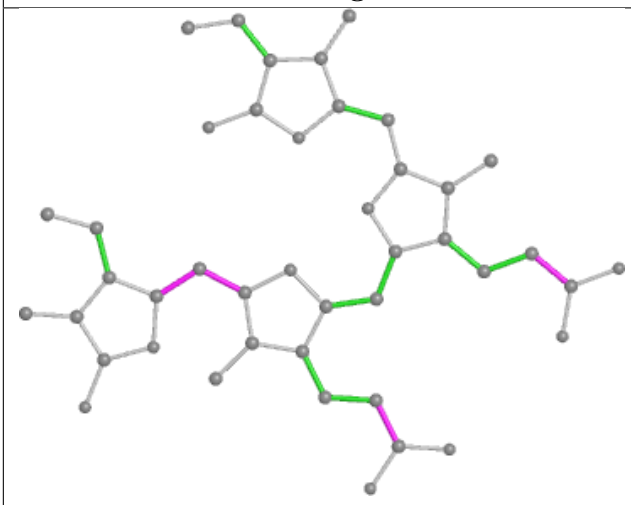


Bond angles



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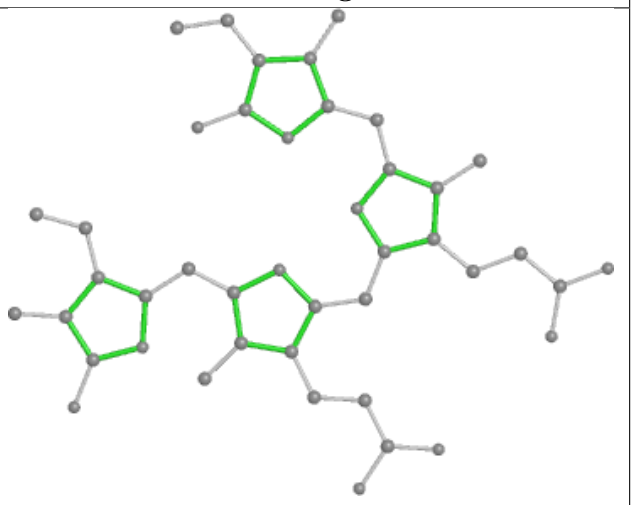
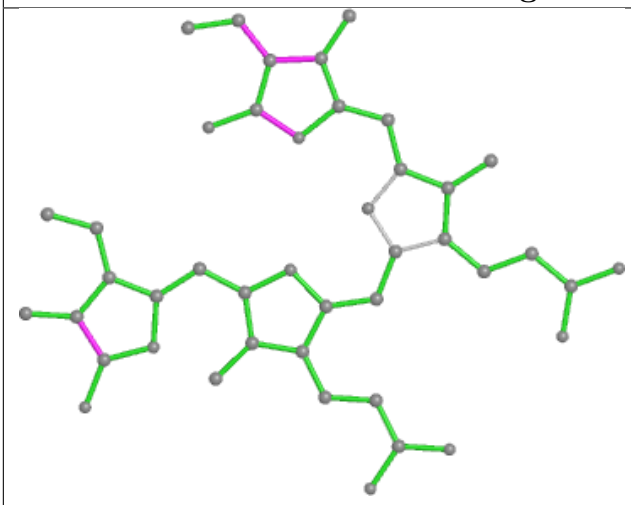


Rings

Ligand PEB o6 201



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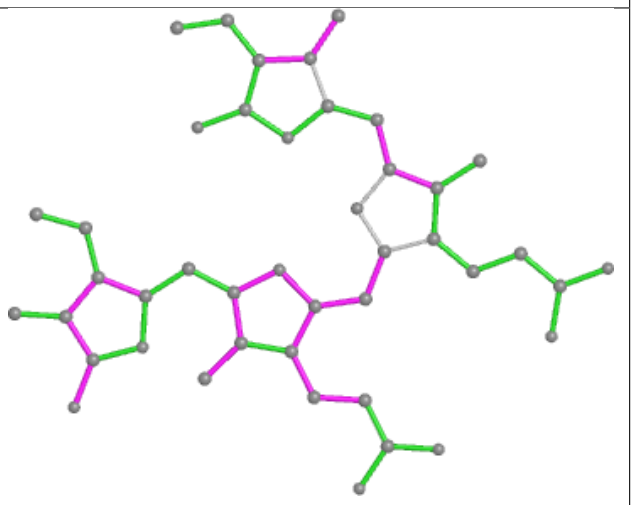
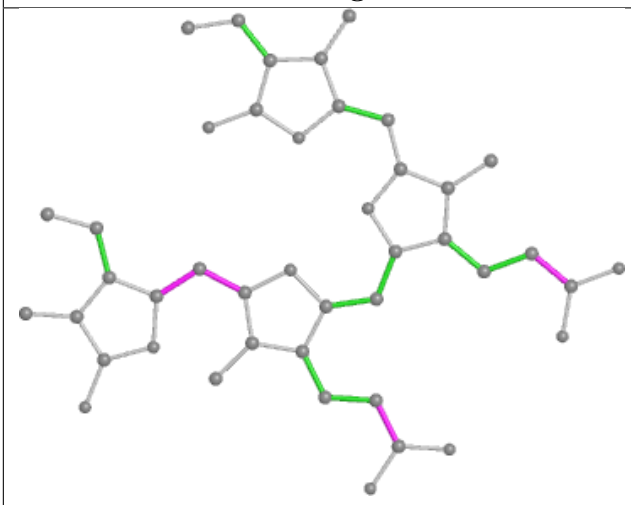


Bond angles



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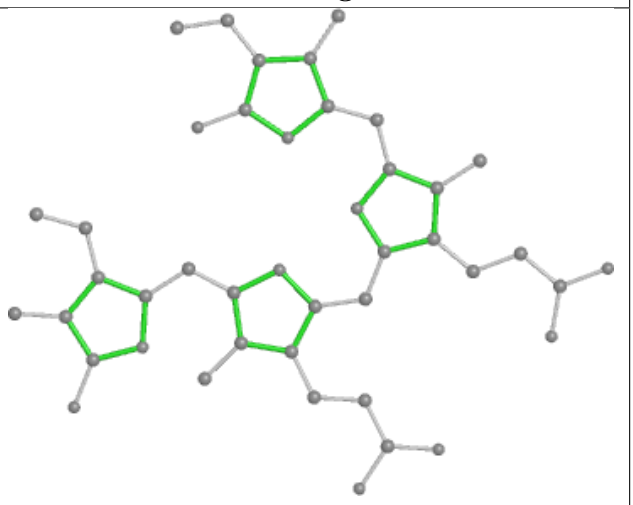
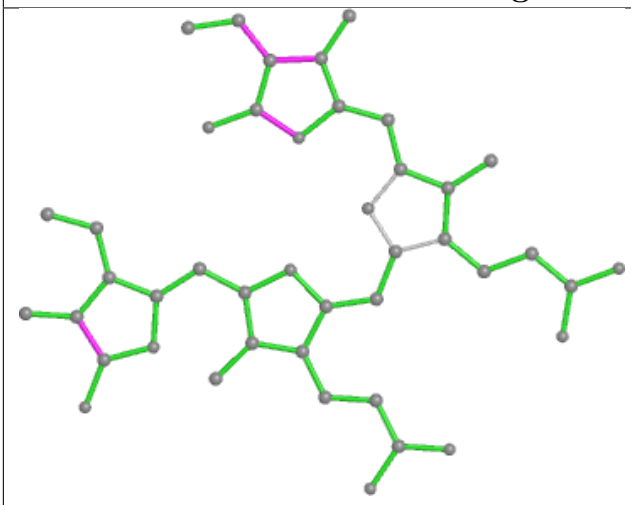


Rings

Ligand PEB M9 201



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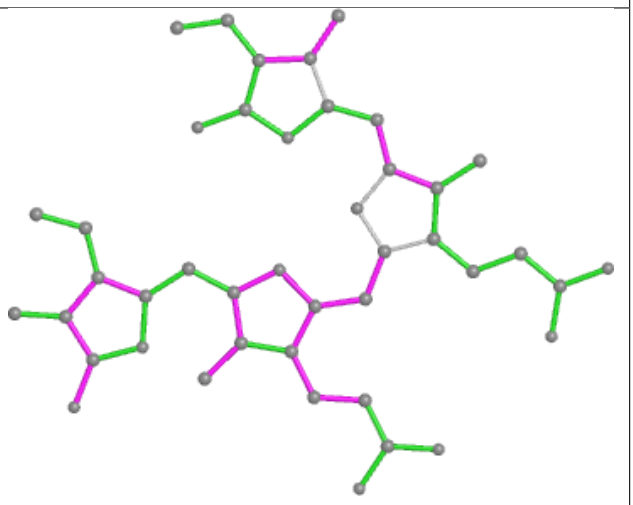

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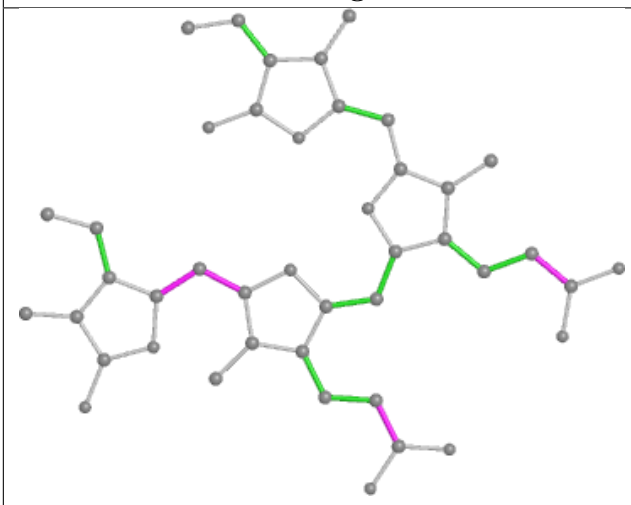
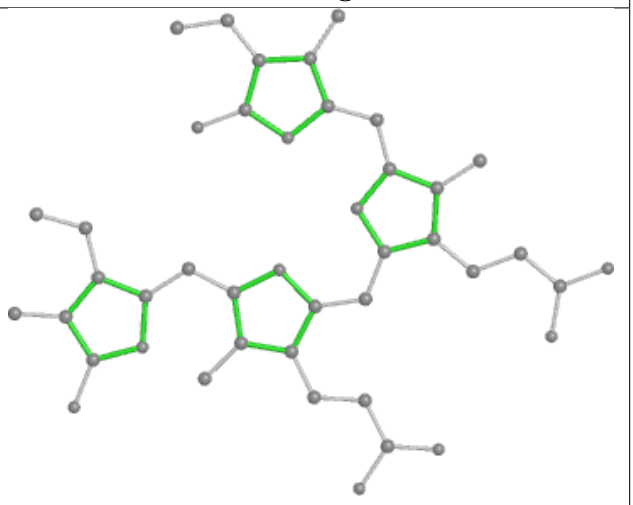
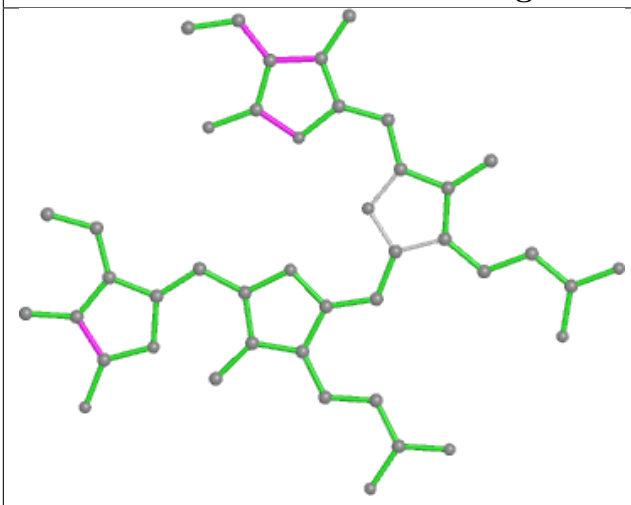


Torsions



Rings

Ligand PEB aA 202



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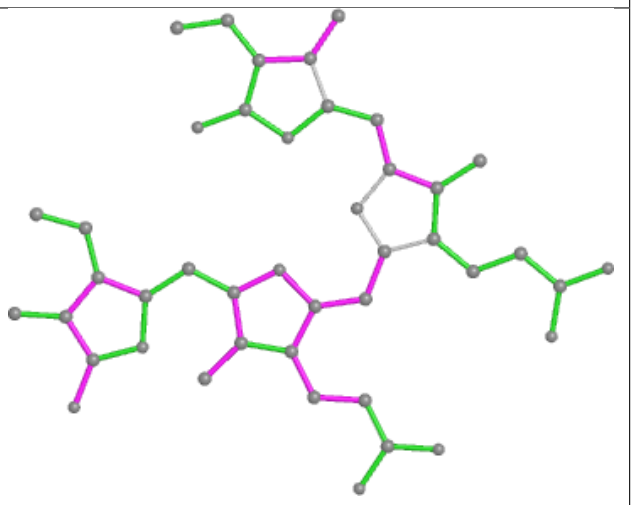

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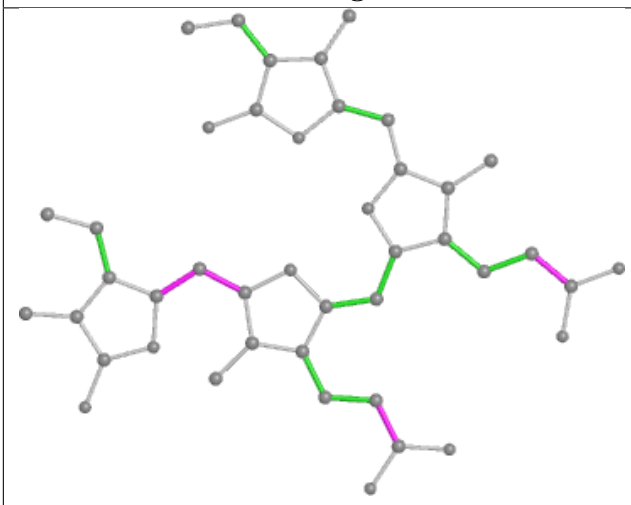

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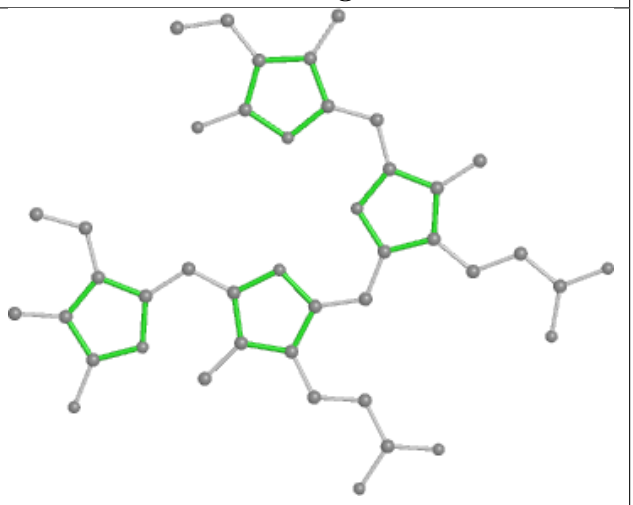
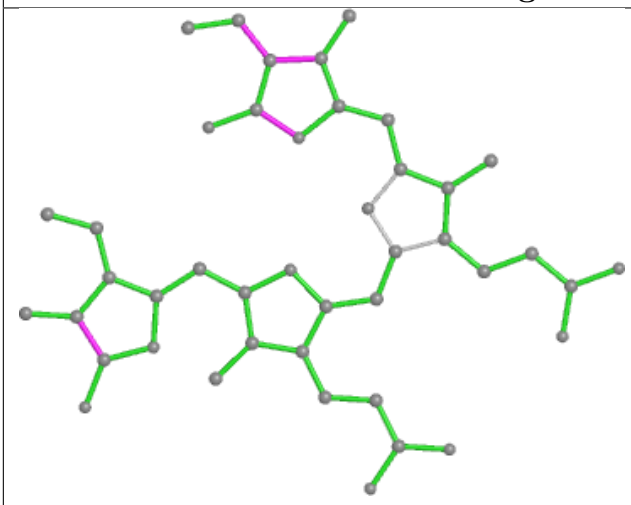


Rings

Ligand PEB dy 401



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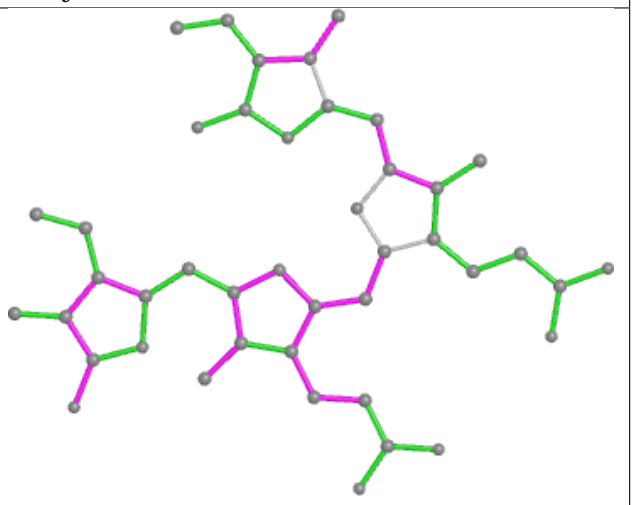

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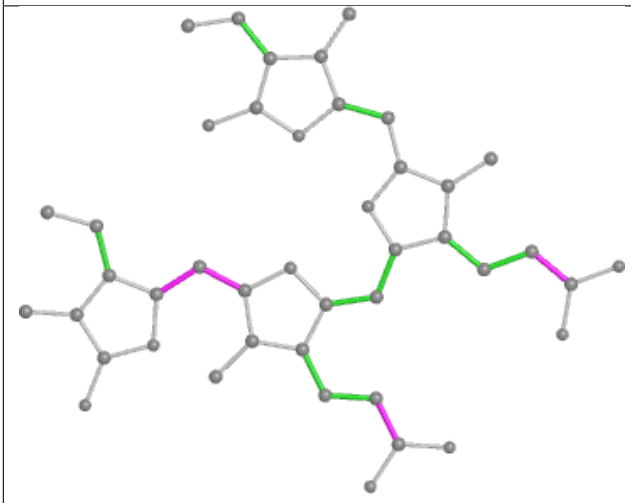

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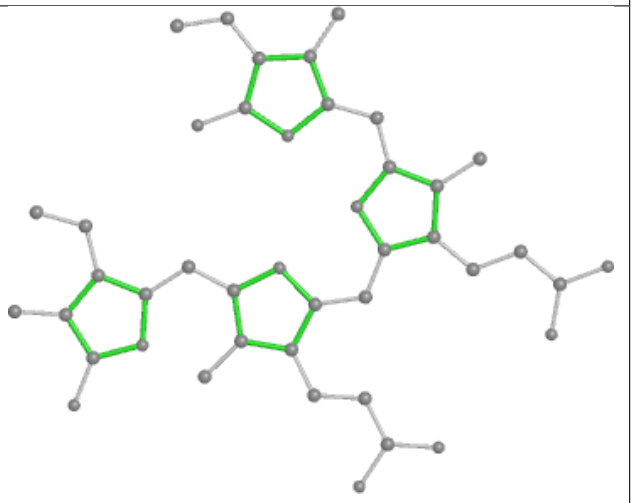

Rings

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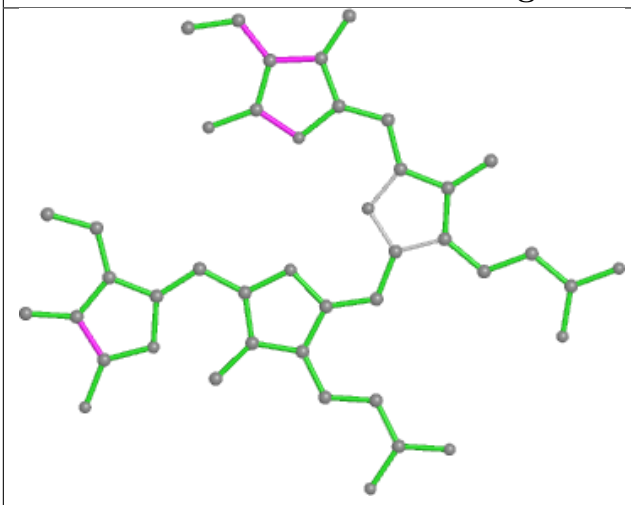

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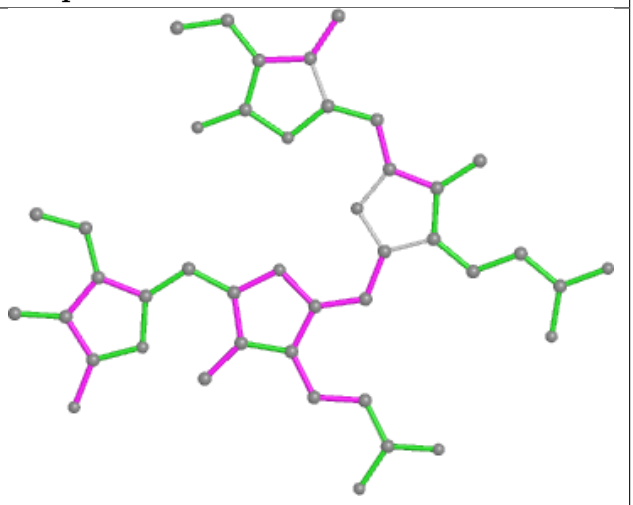

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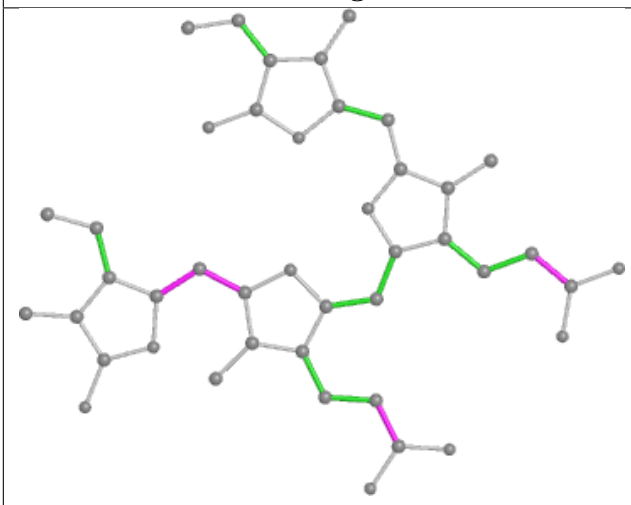

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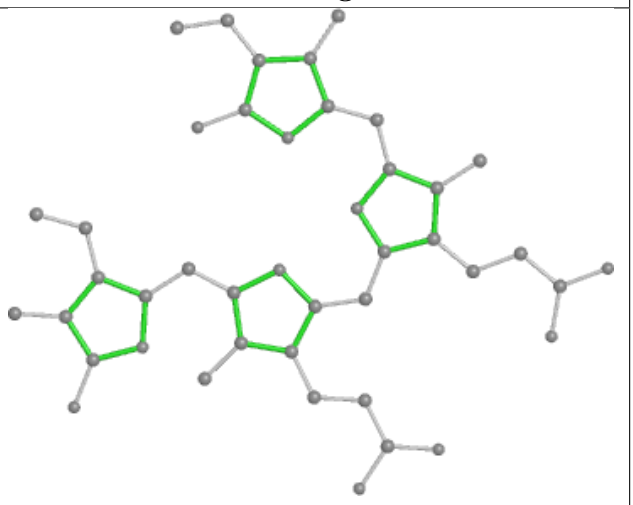
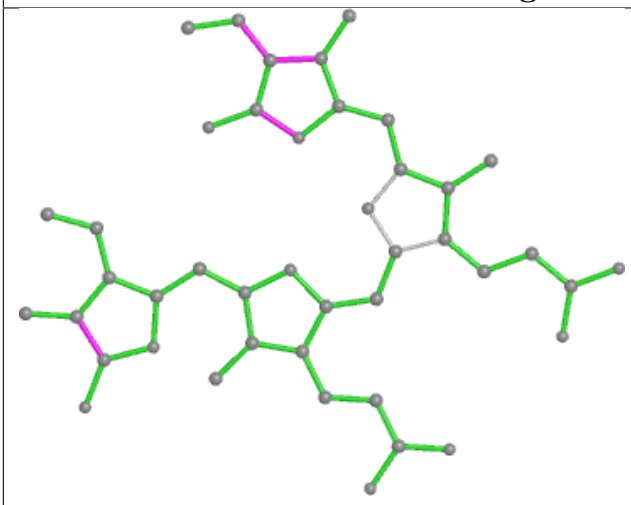


Rings

Ligand PEB J9 201



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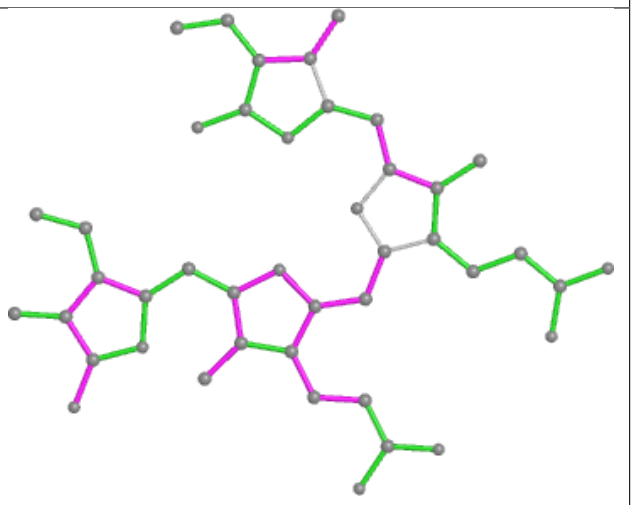

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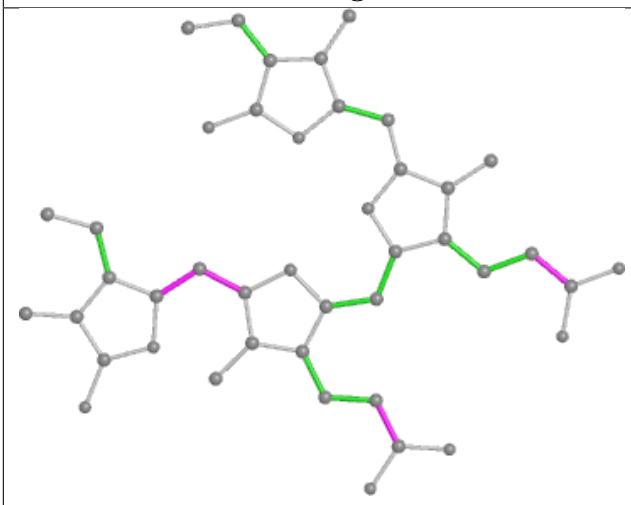

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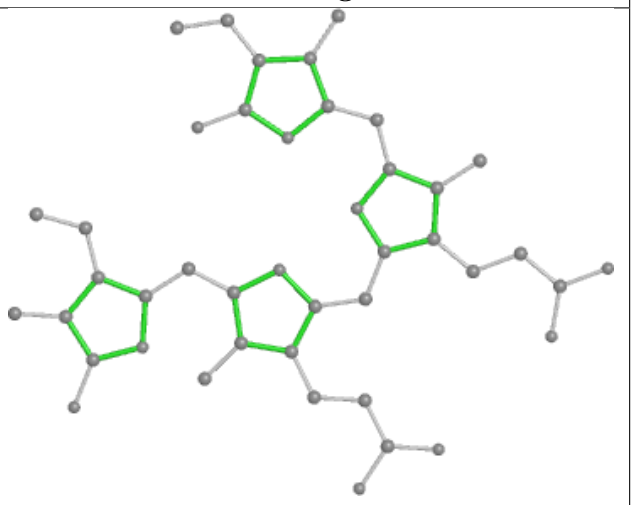
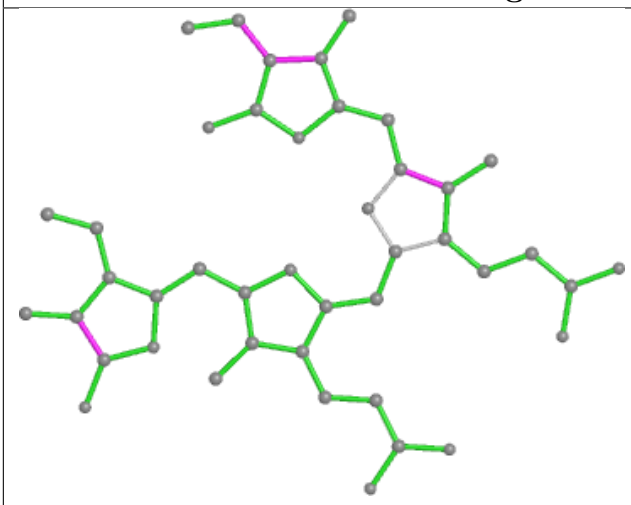


Rings

Ligand PEB K9 1002



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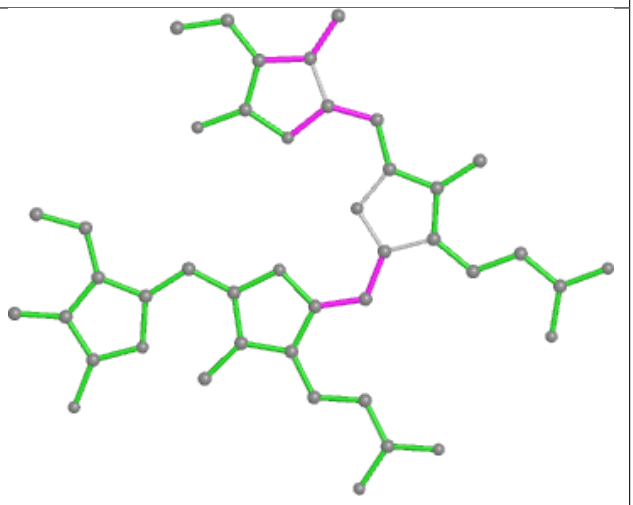

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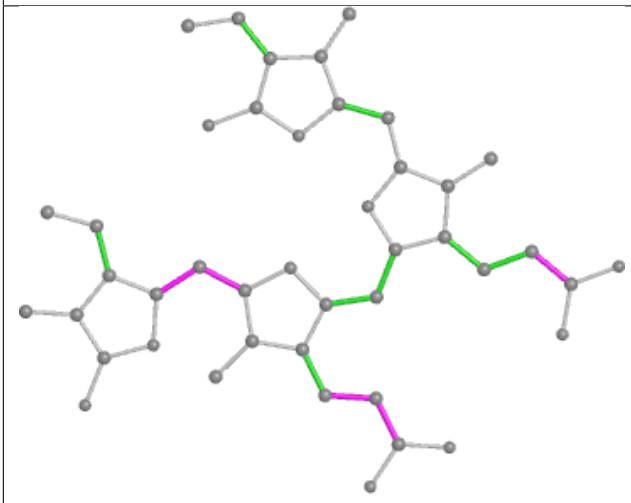

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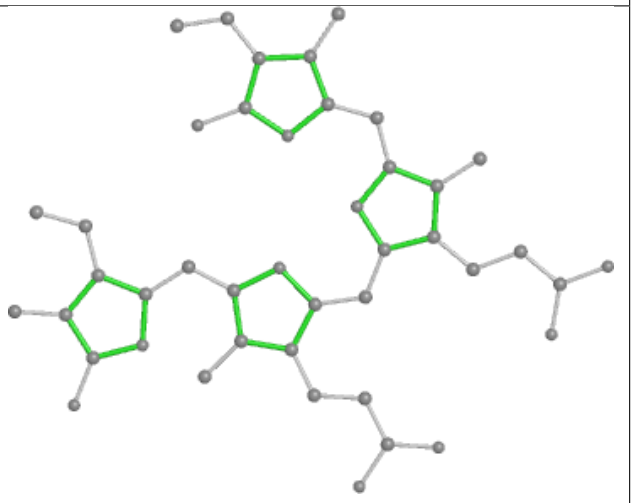

Rings

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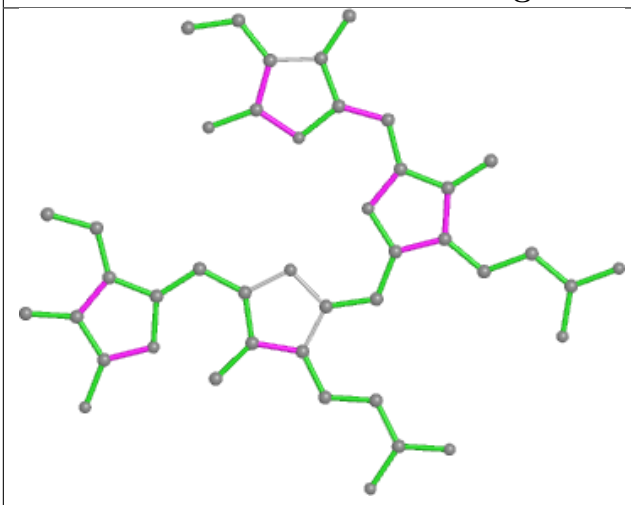

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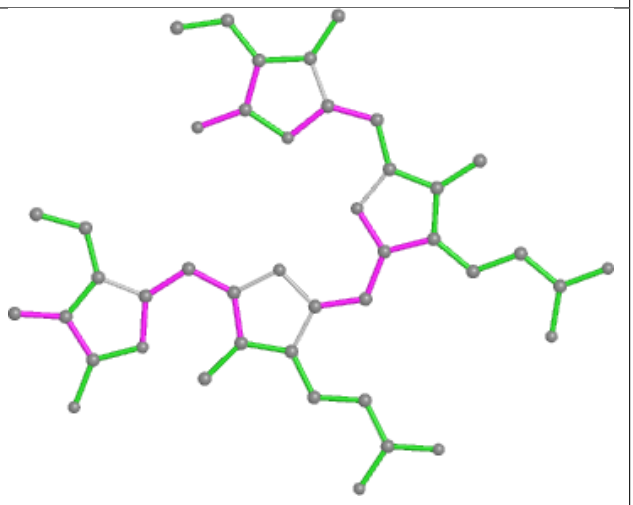

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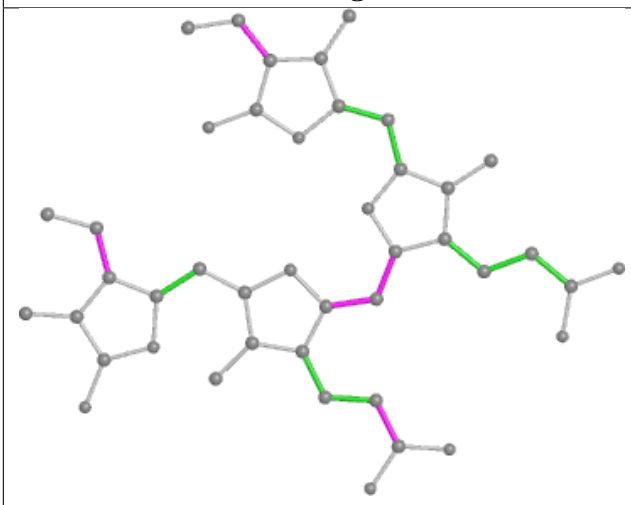

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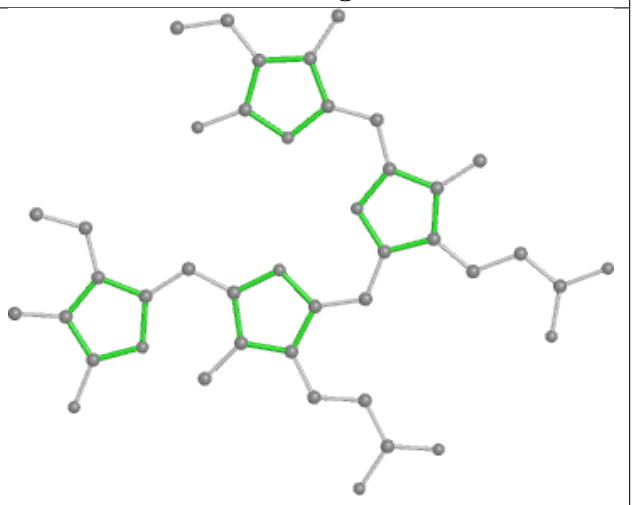

Rings

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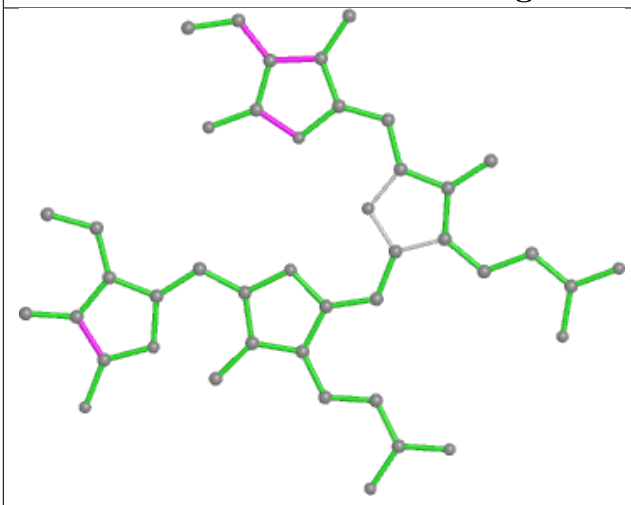

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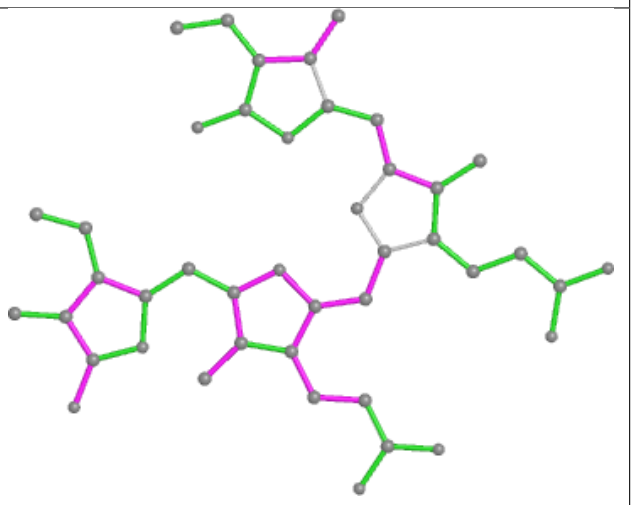

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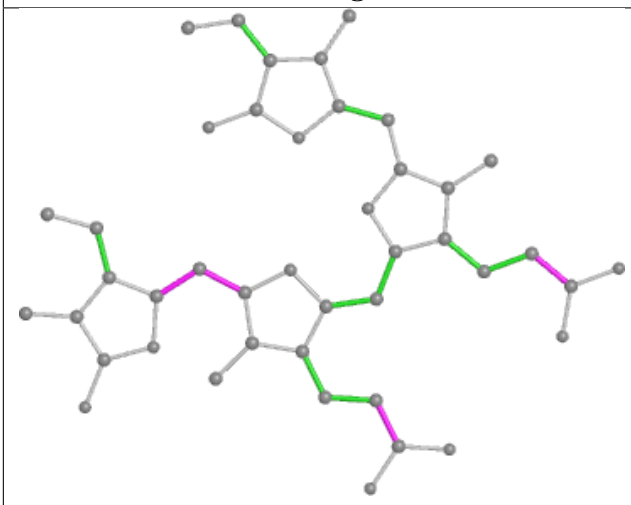

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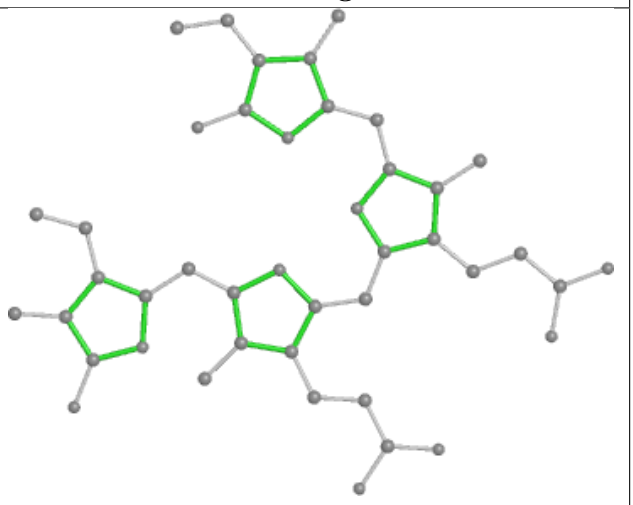

Rings

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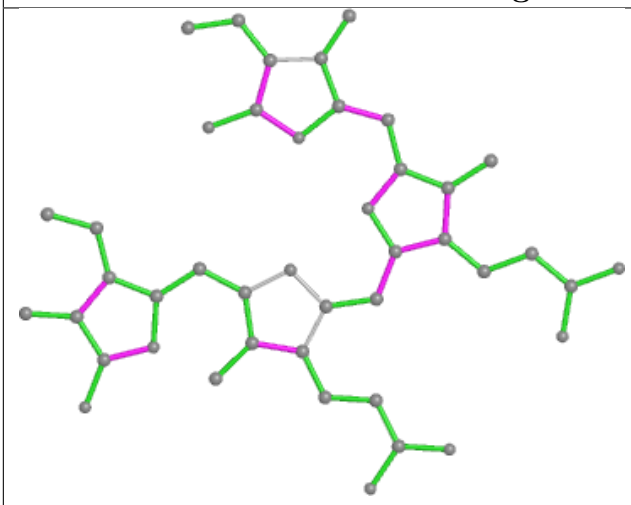

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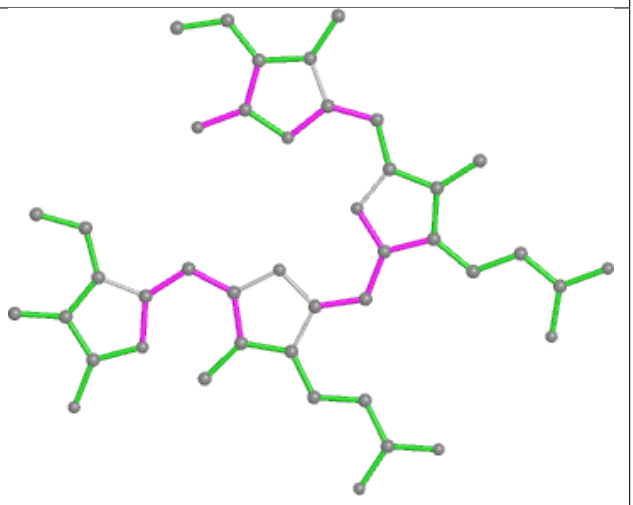

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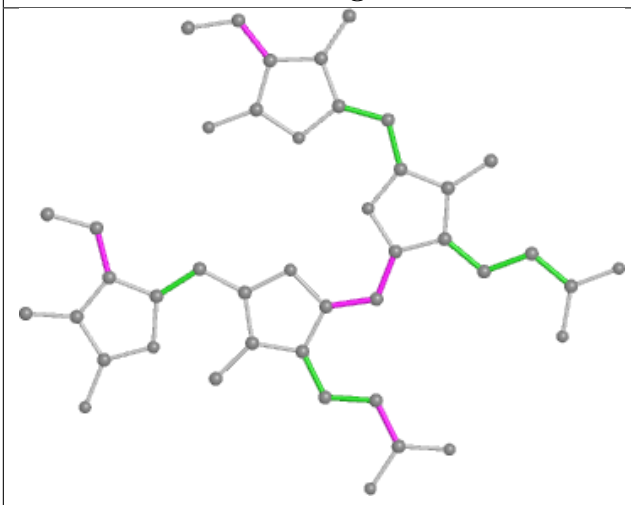

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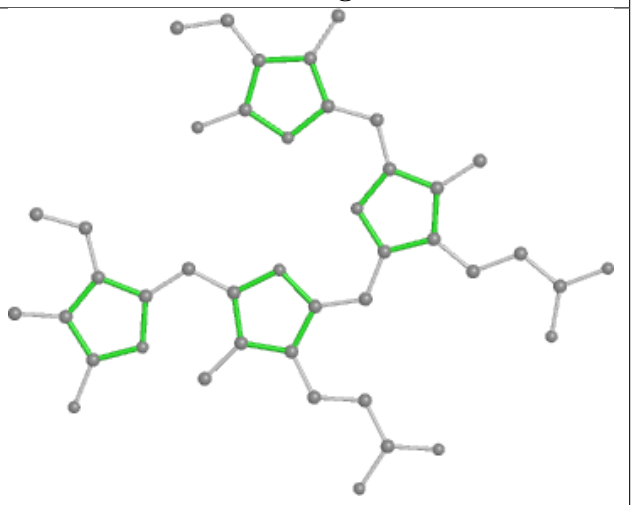

Rings

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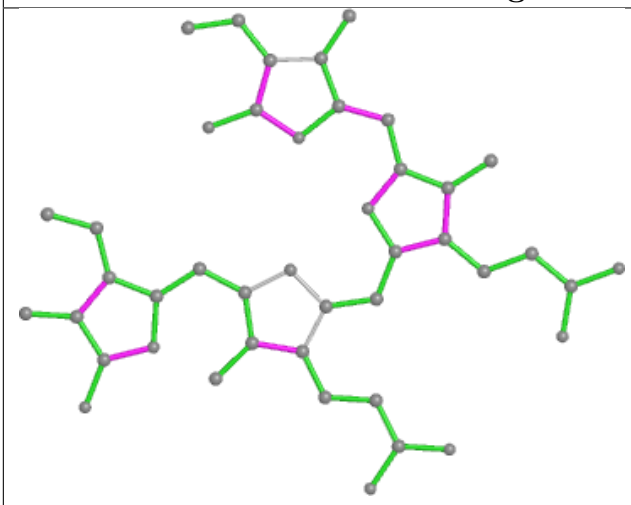

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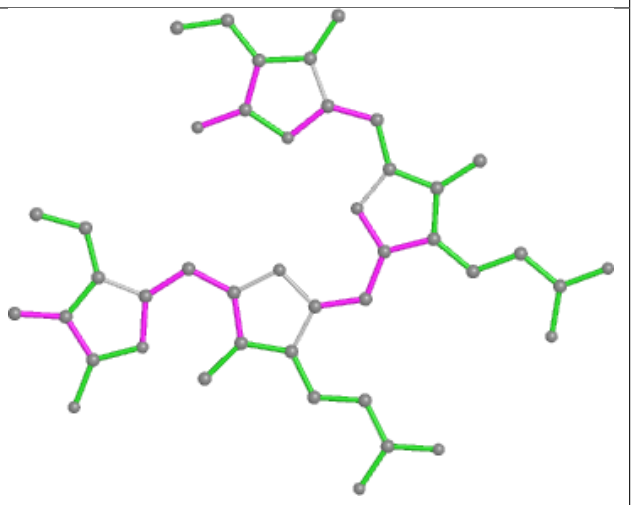

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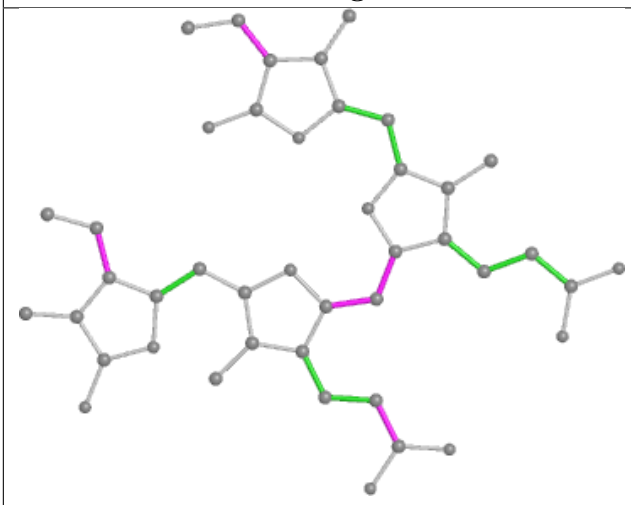

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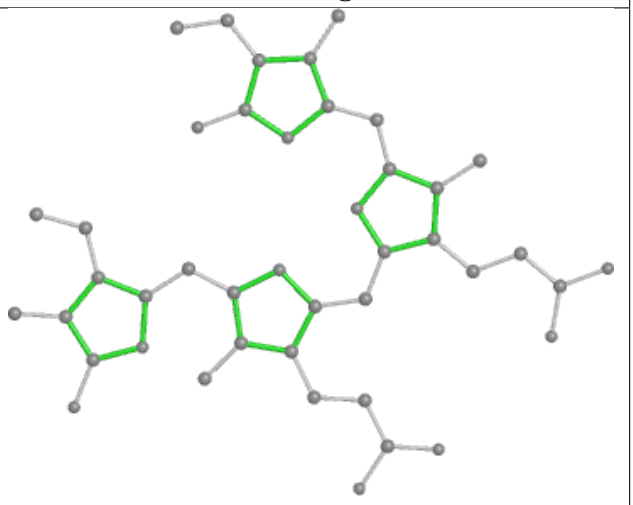

Rings

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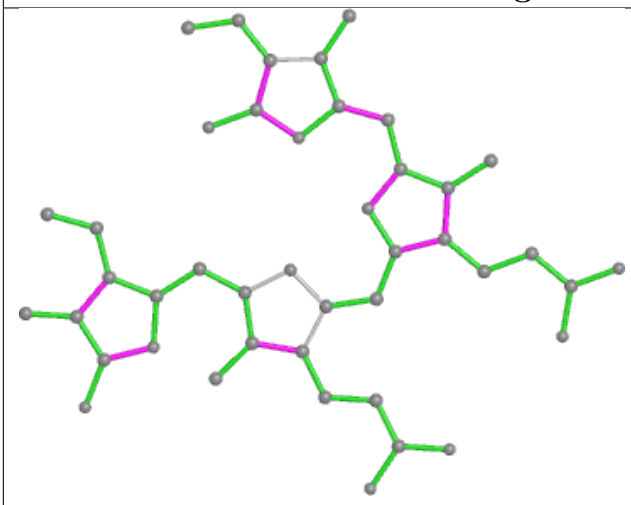

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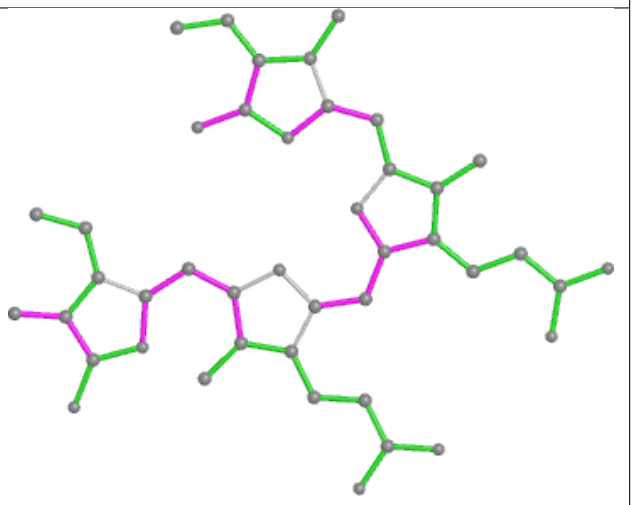

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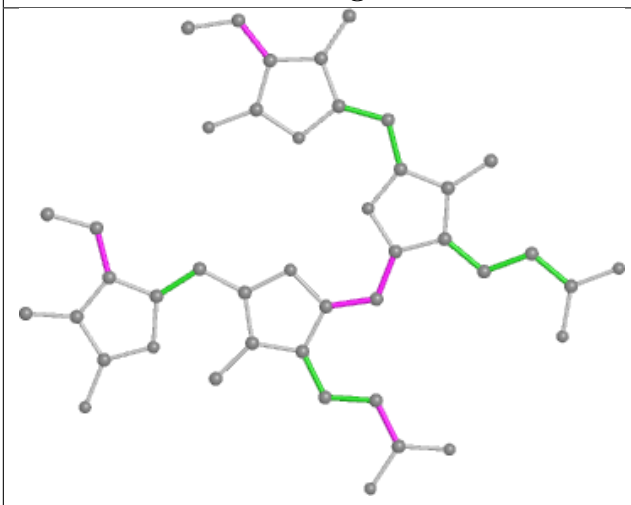

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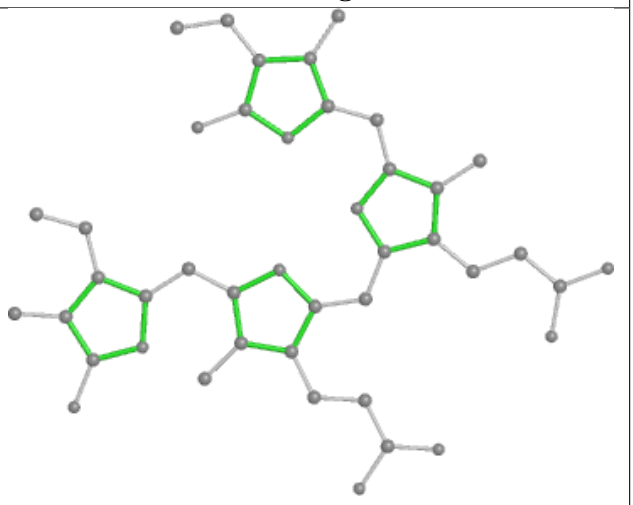
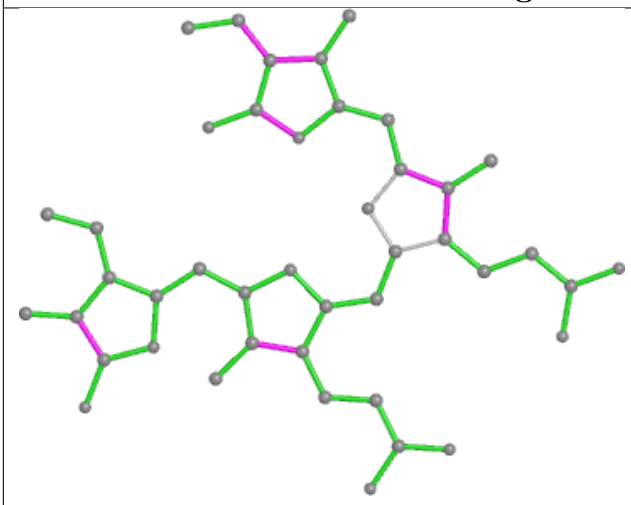


Rings

Ligand PEB A1 301



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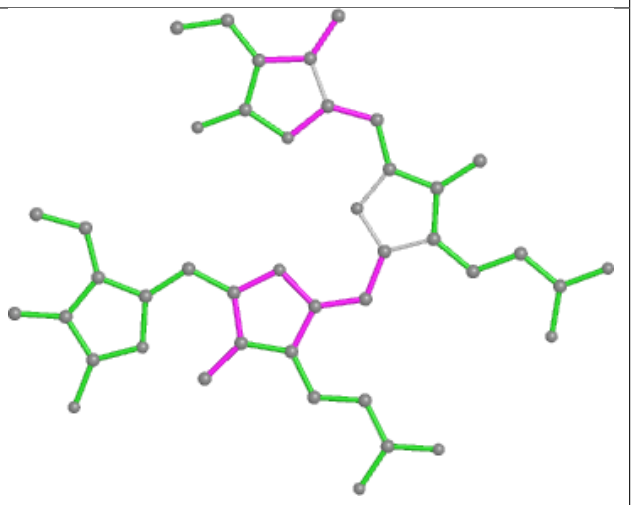

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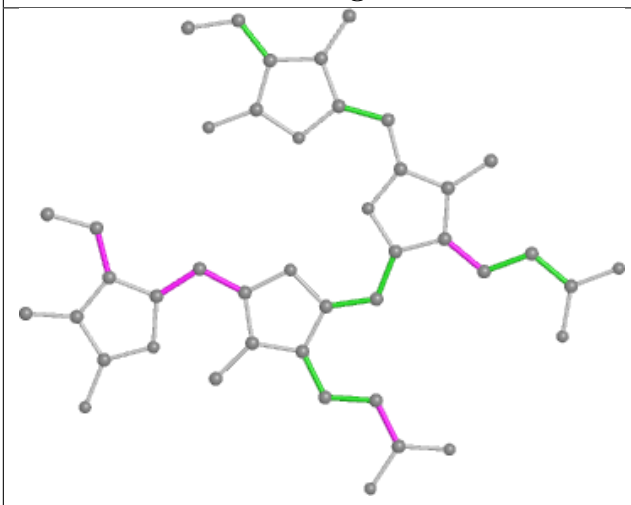

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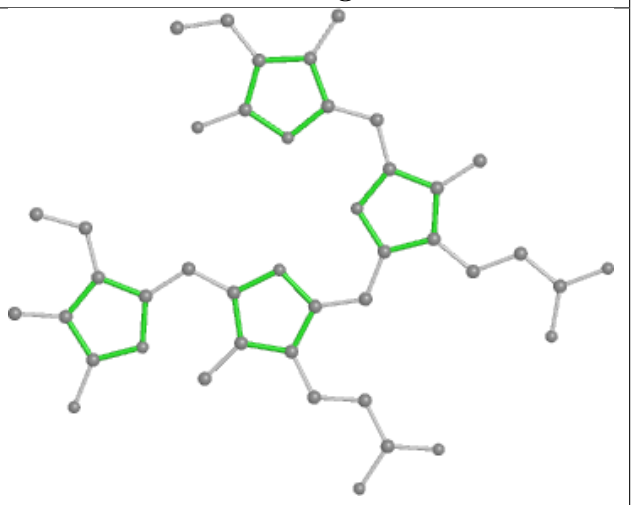

Rings

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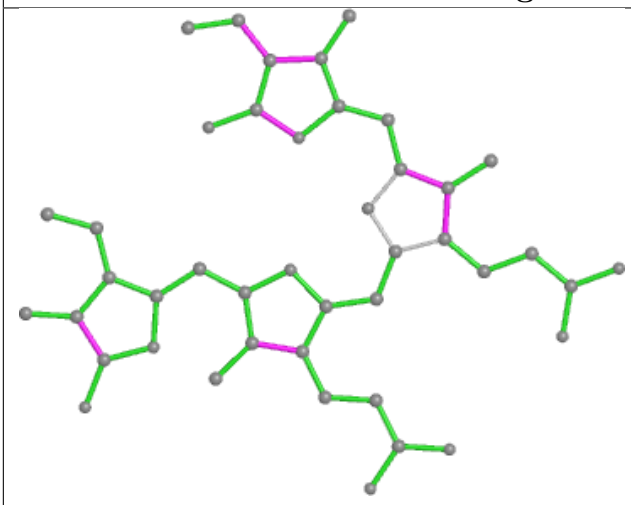

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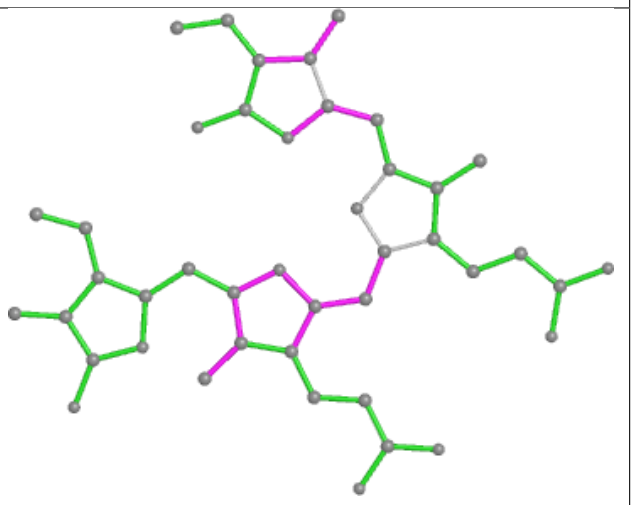

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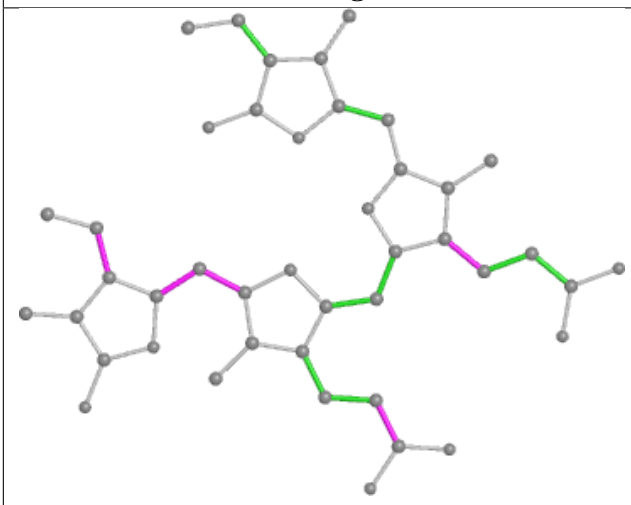

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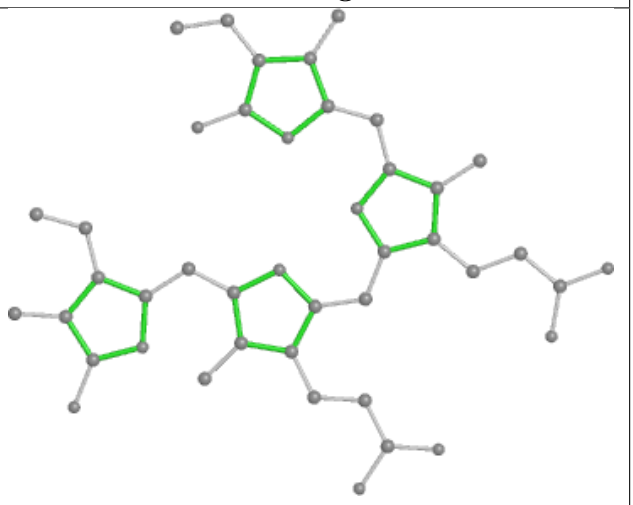
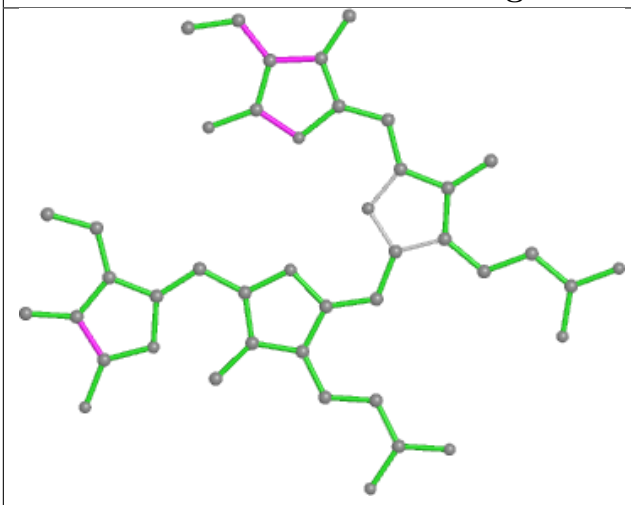


Rings

Ligand PEB aK 1001



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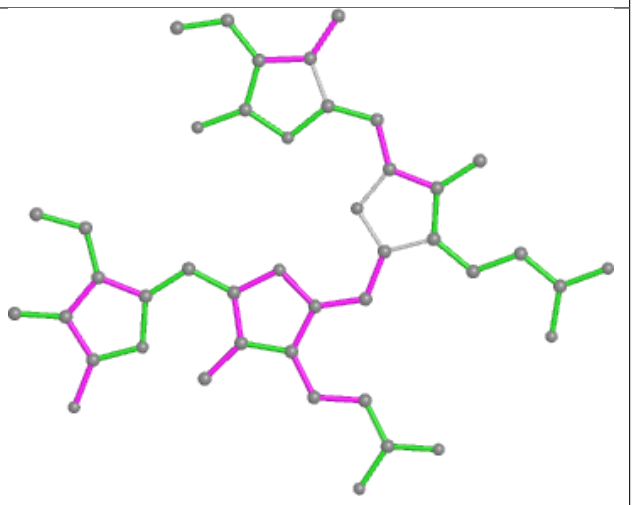
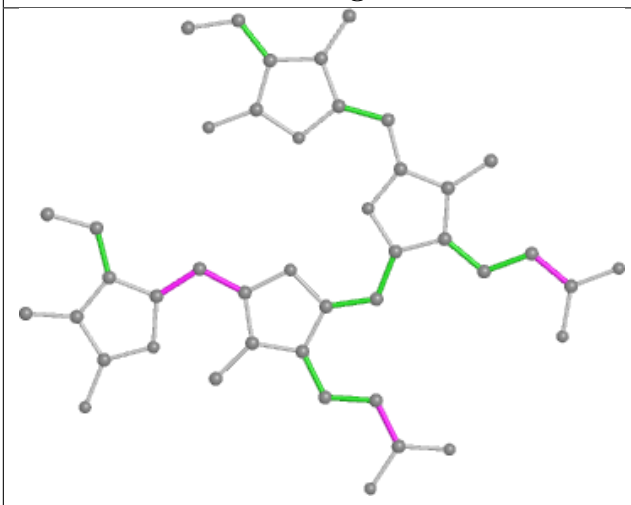
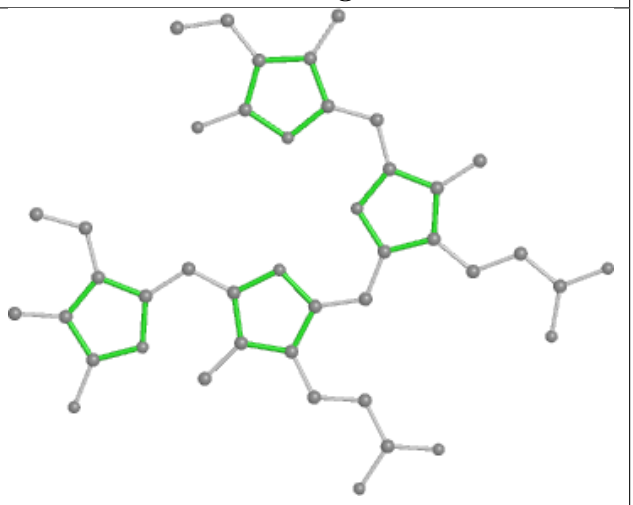


Bond angles

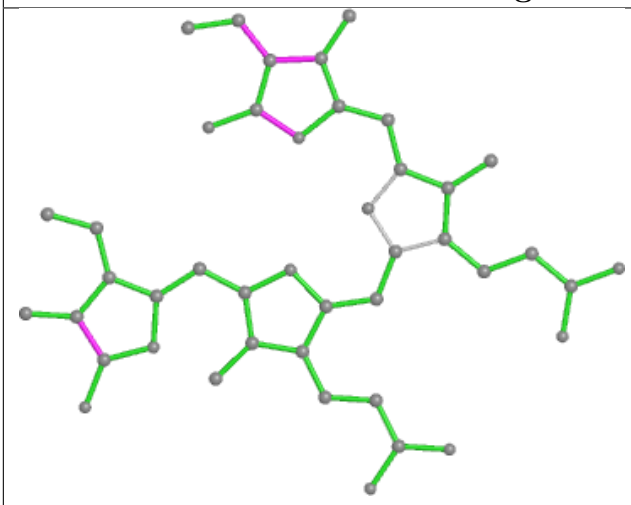


Torsions



Rings

Ligand PEB K3 201



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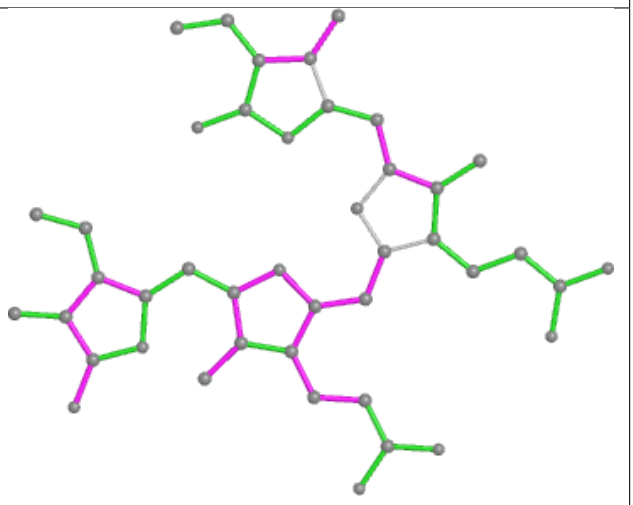

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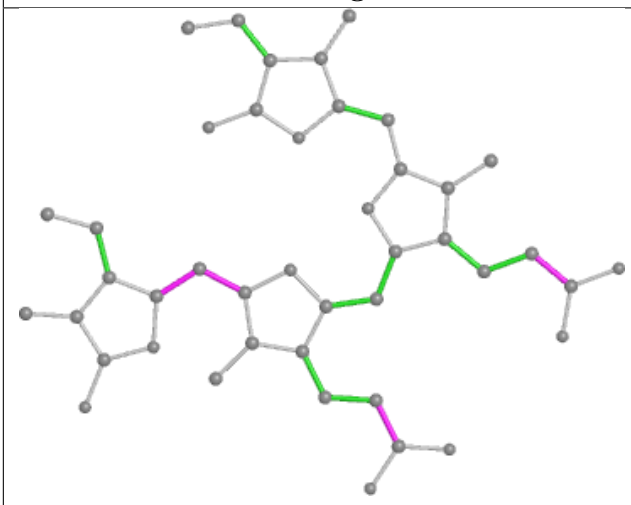

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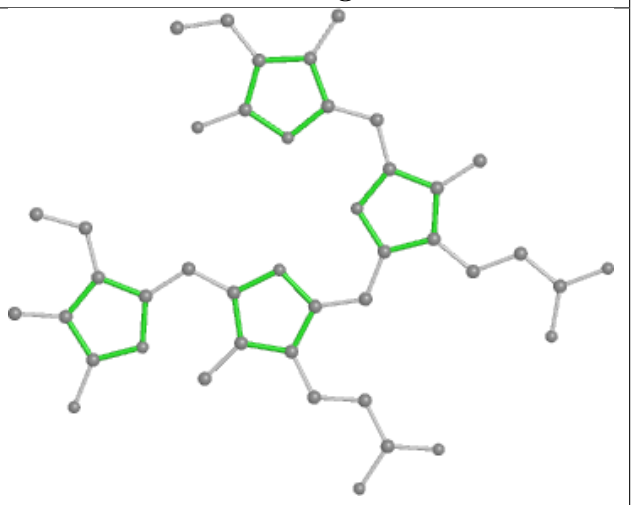
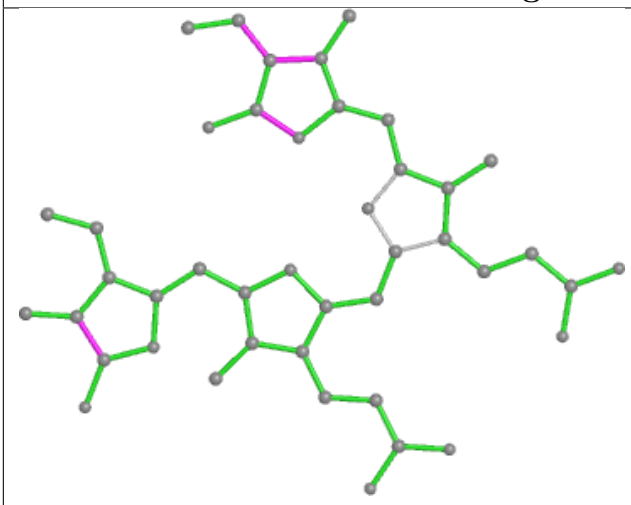


Rings

Ligand PEB fv 201



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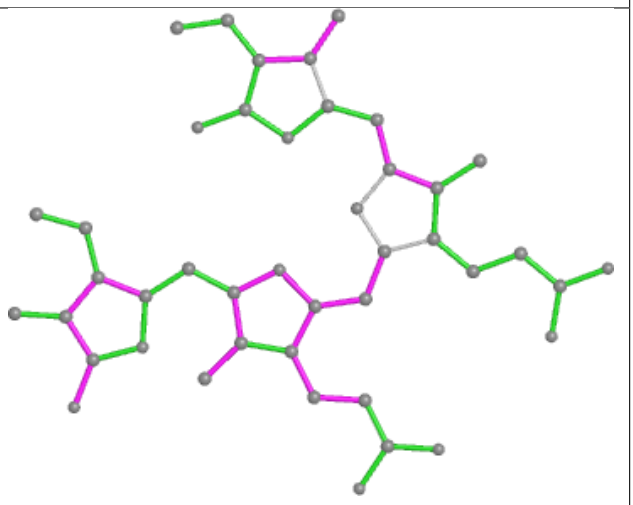

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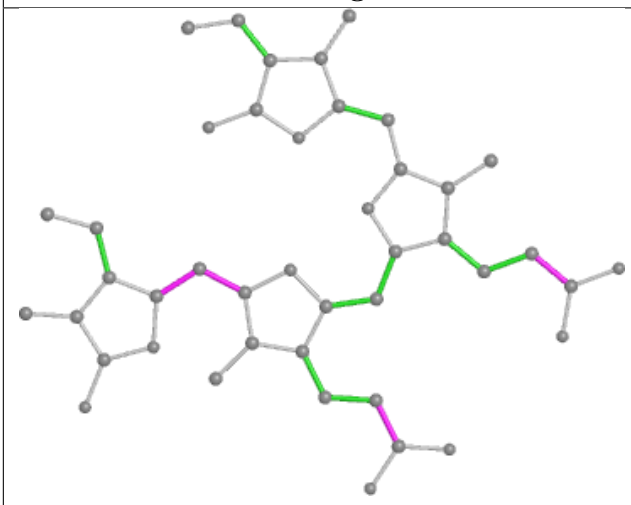

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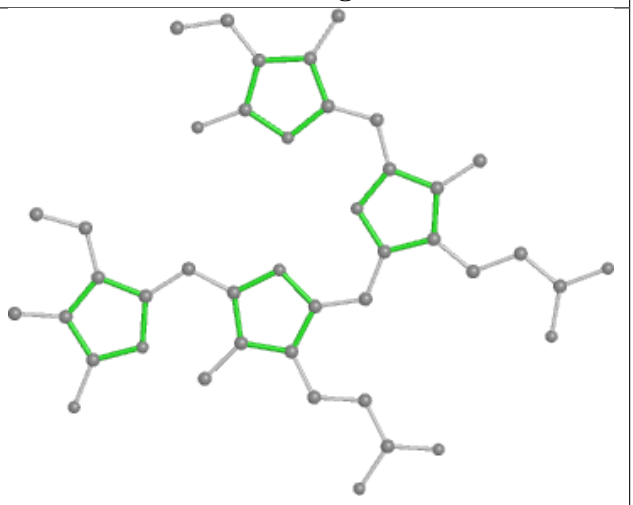
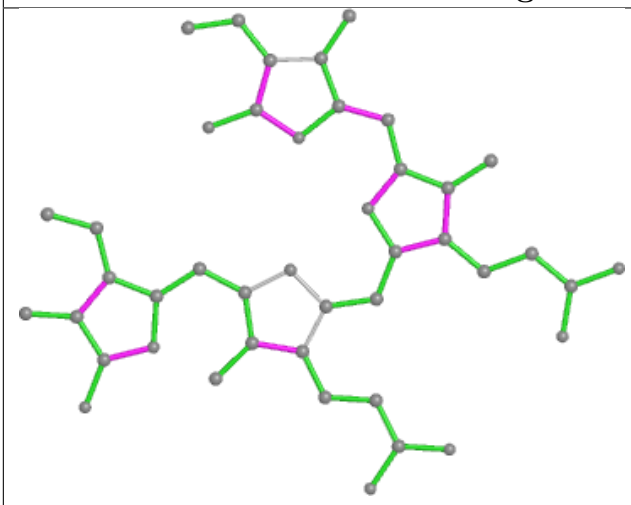


Rings

Ligand PUB d7 203



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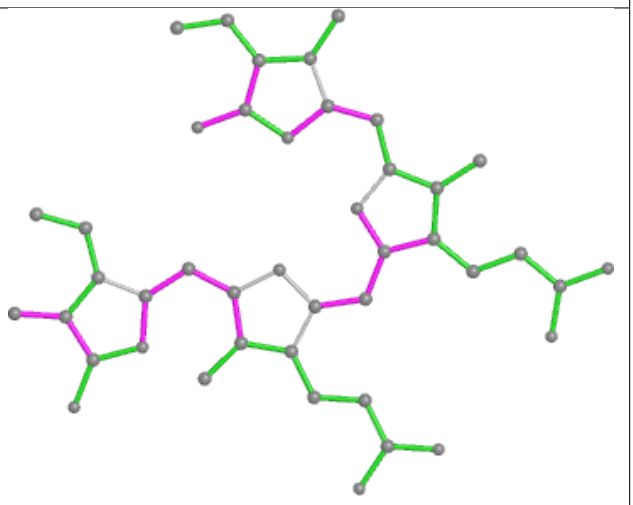

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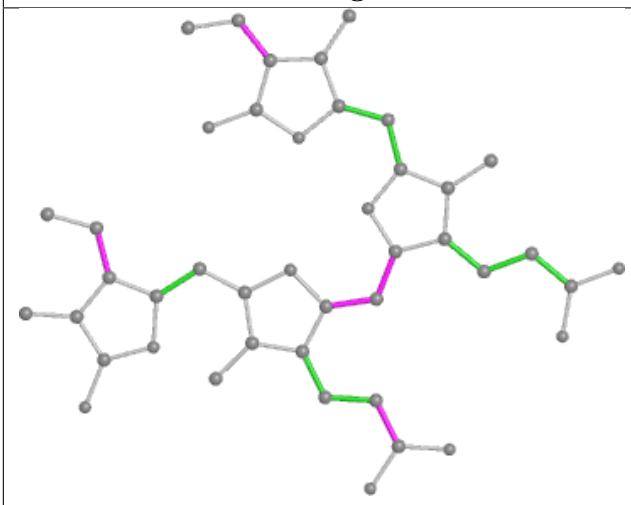

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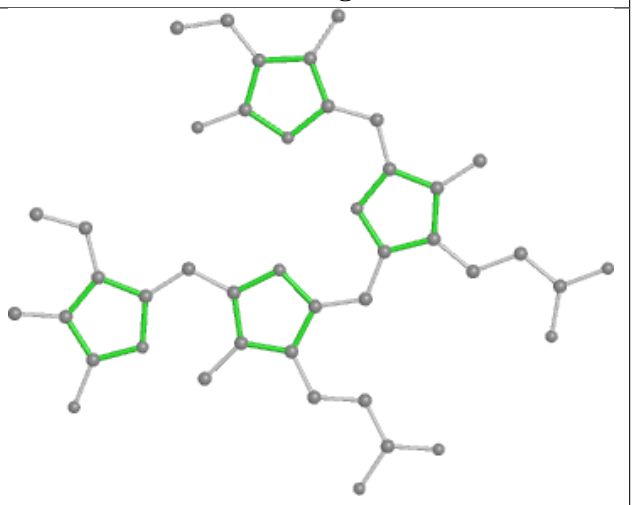
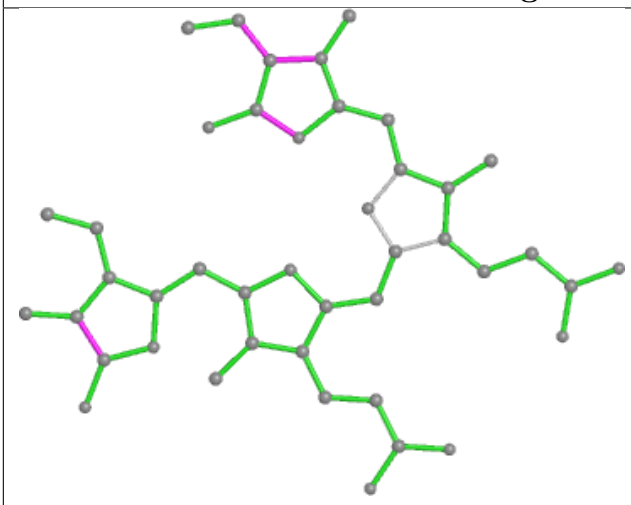


Rings

Ligand PEB e7 201



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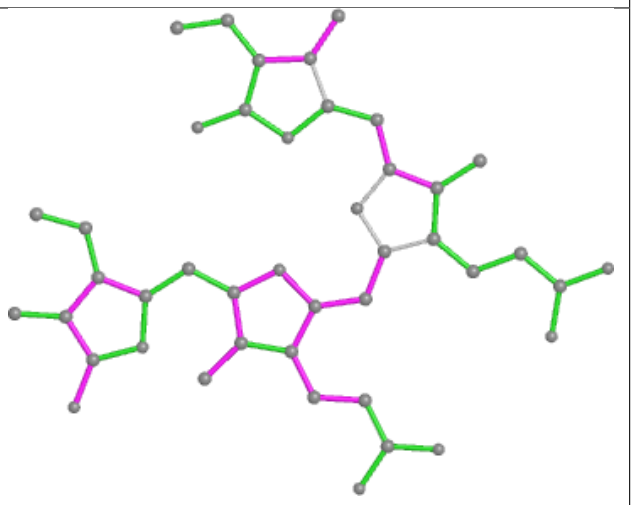

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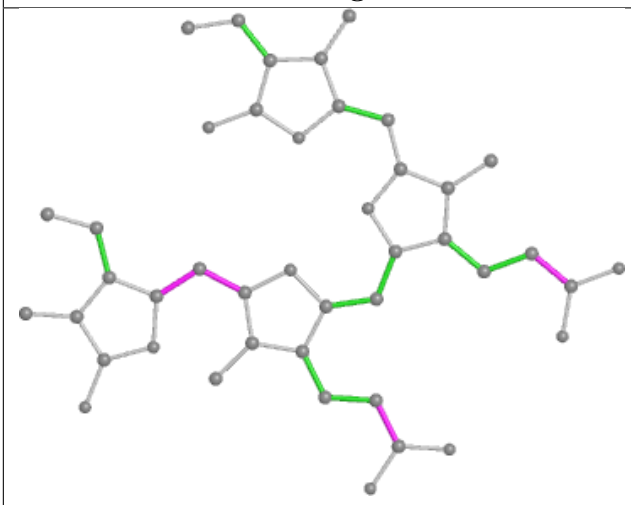

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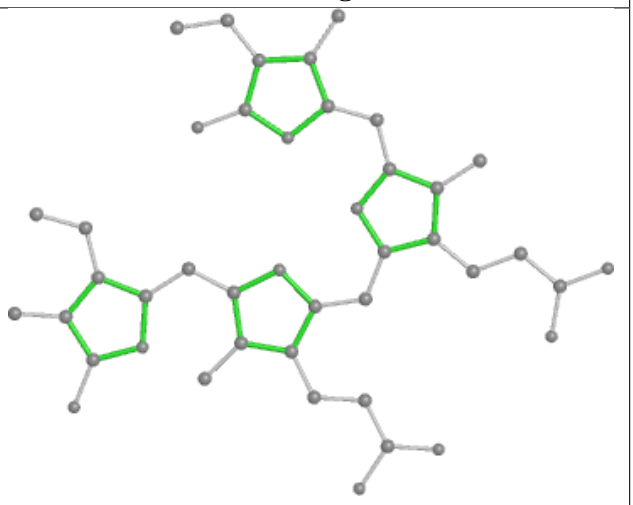
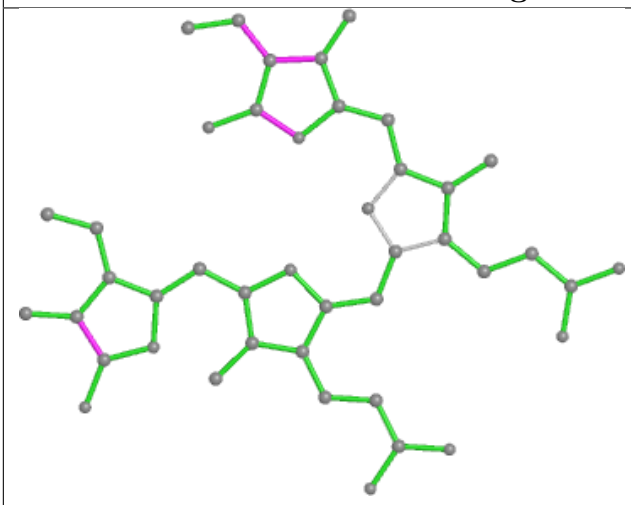


Rings

Ligand PEB ba 1001



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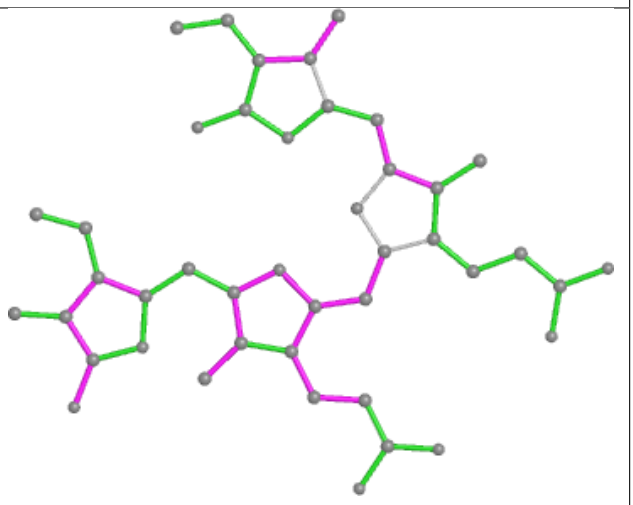

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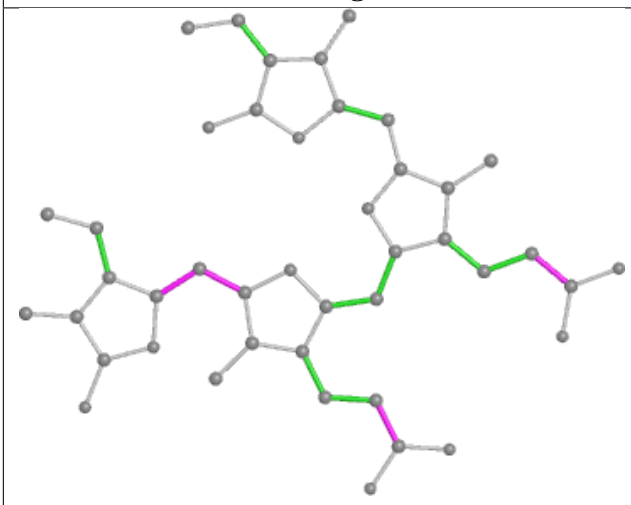

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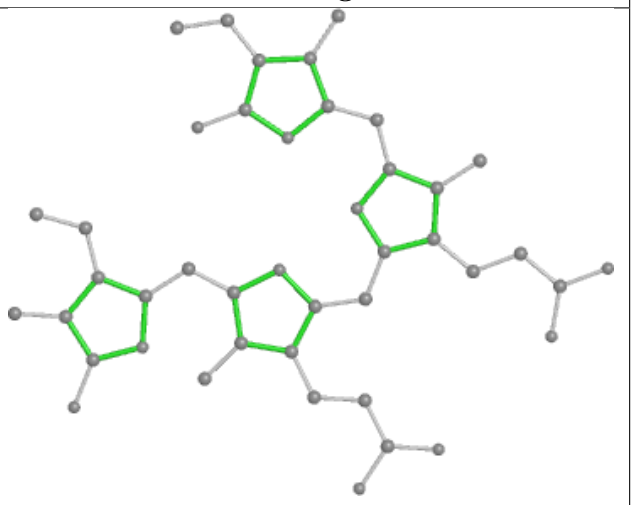

Rings

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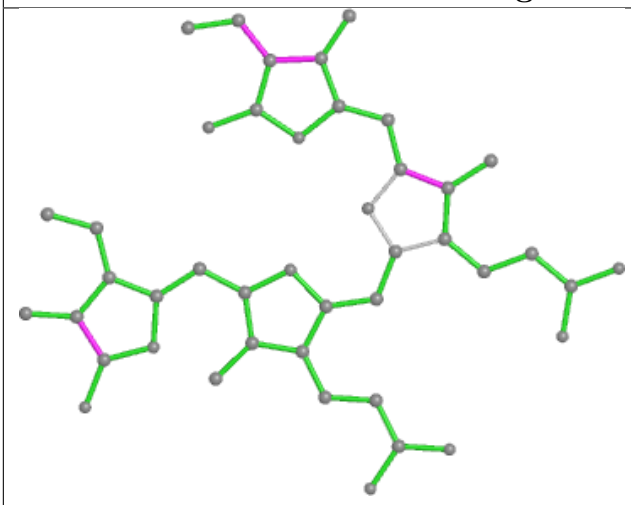

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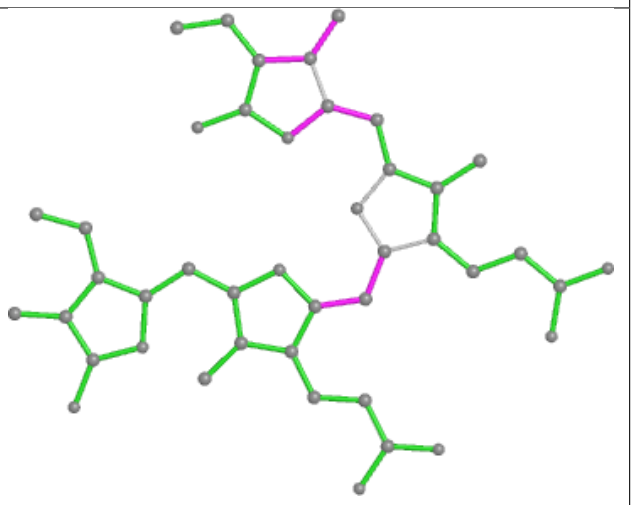

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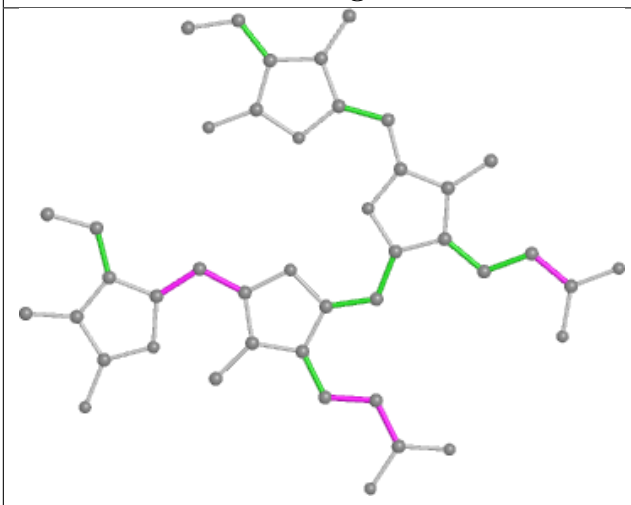

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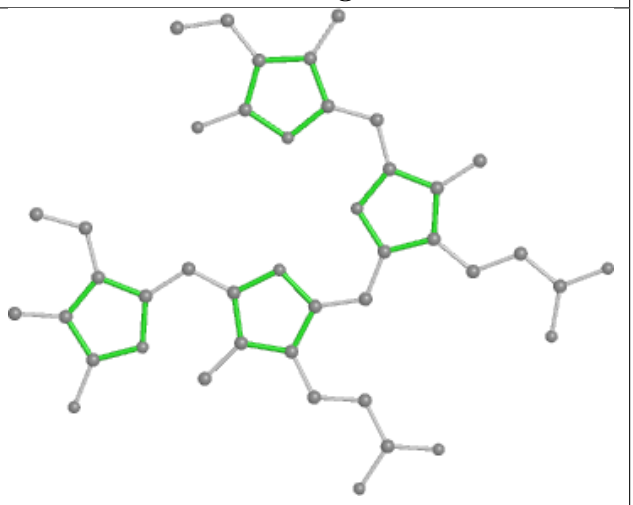

Rings

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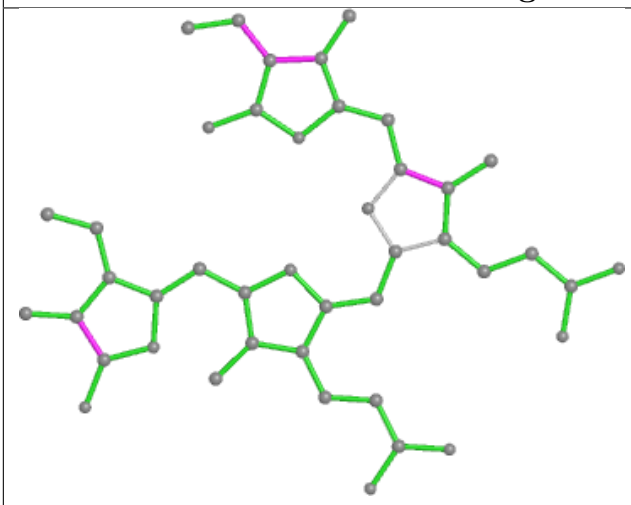

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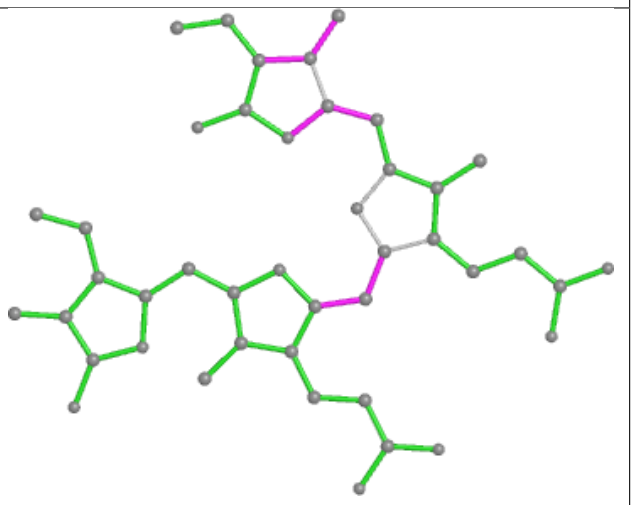

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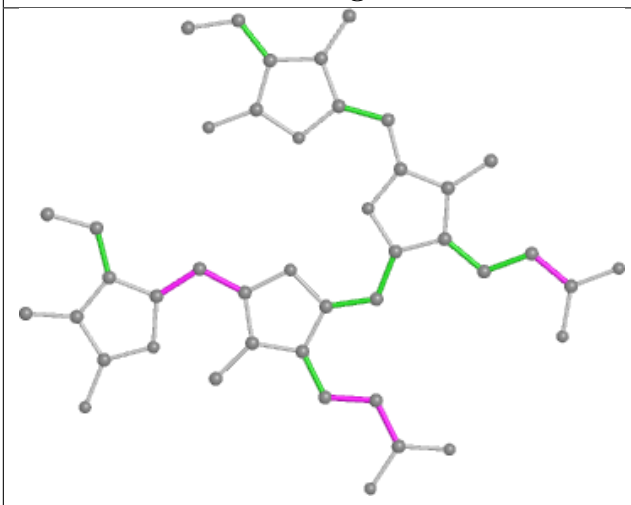

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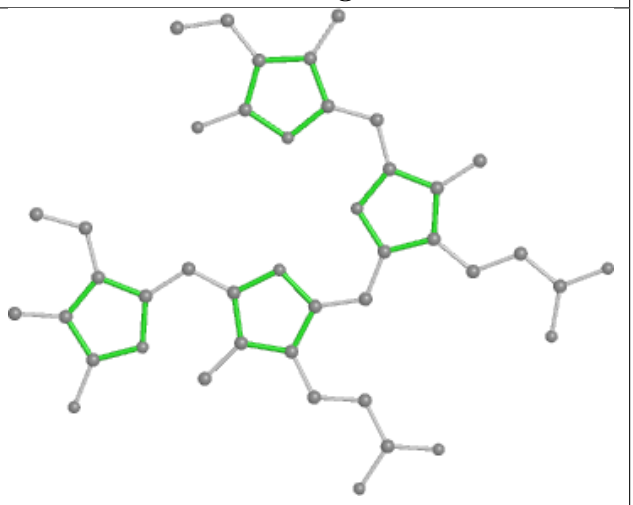
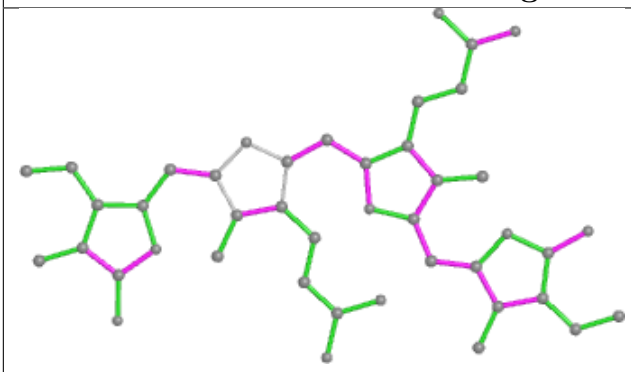


Rings

Ligand CYC f1 201



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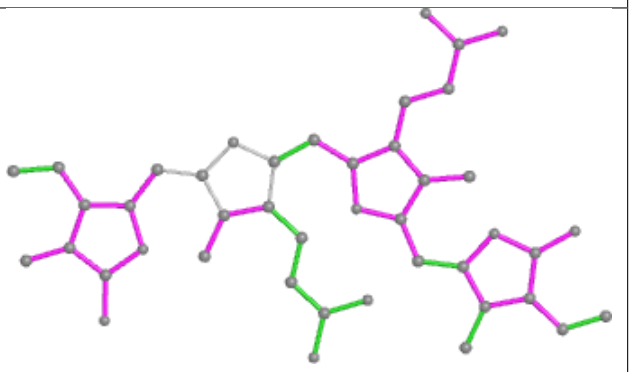

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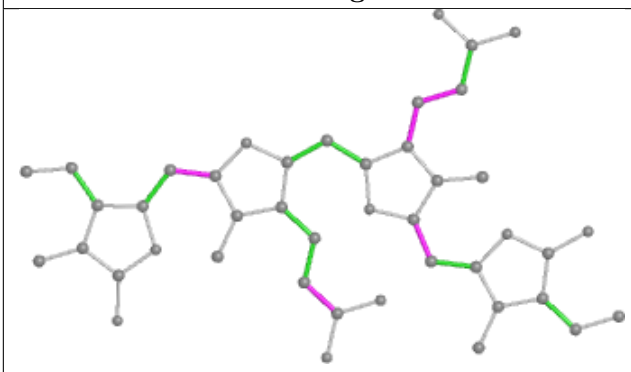

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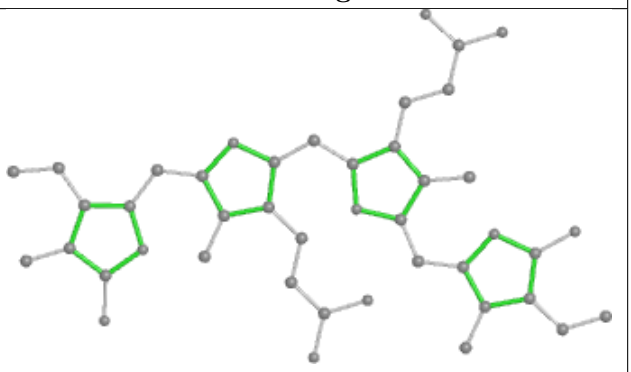

Rings

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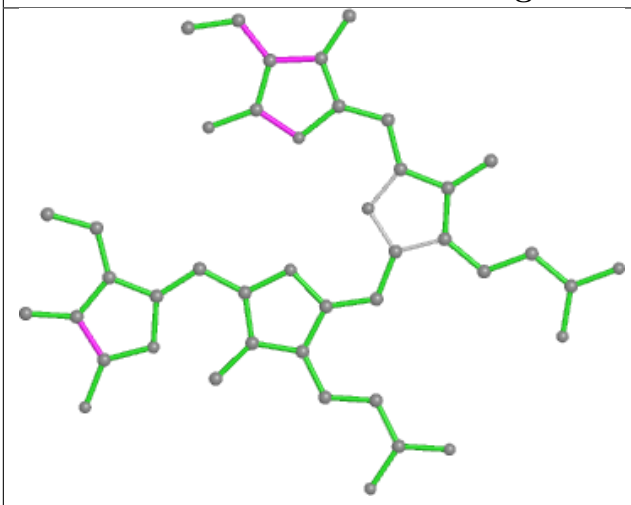

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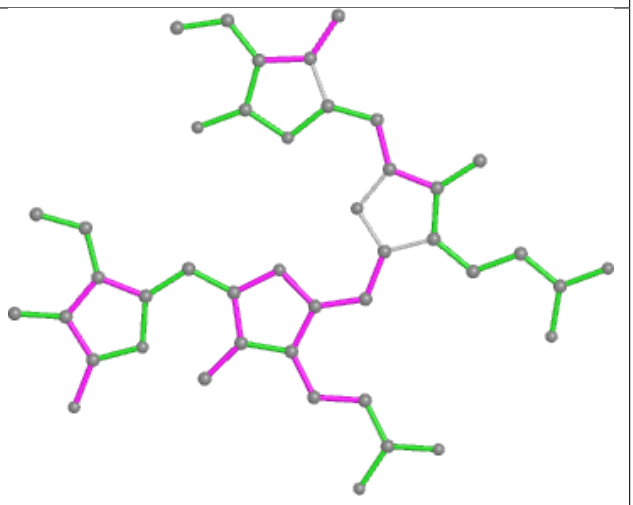

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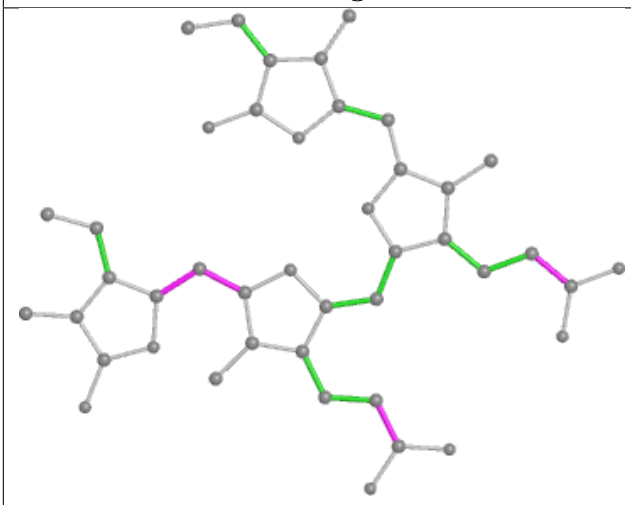

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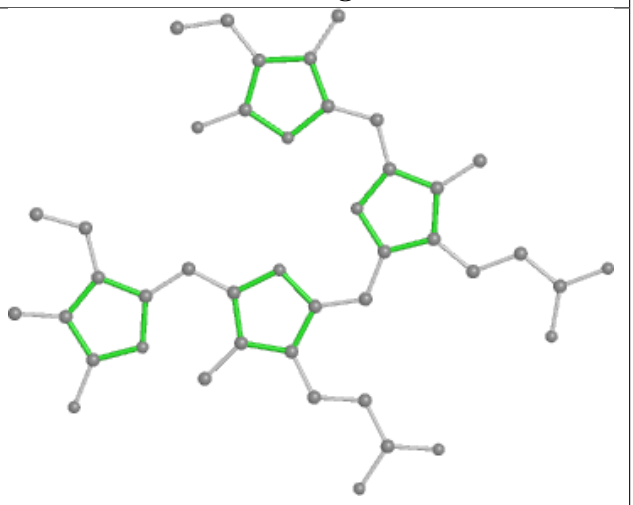
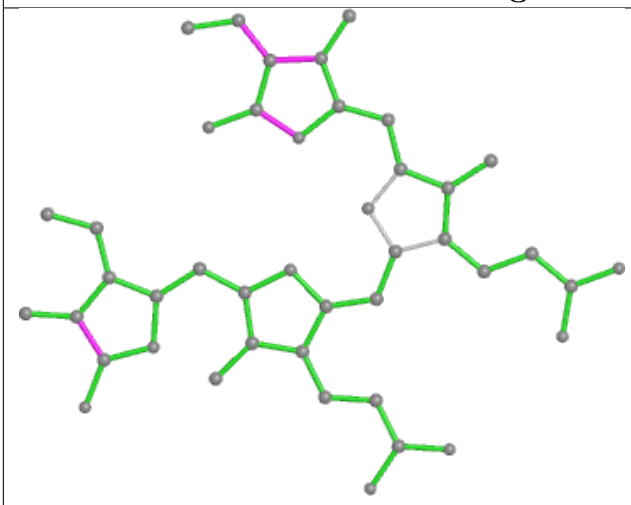


Rings

Ligand PEB by 1002



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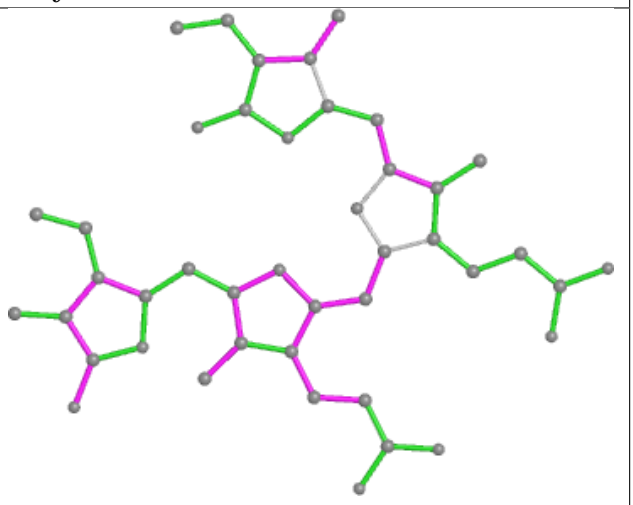

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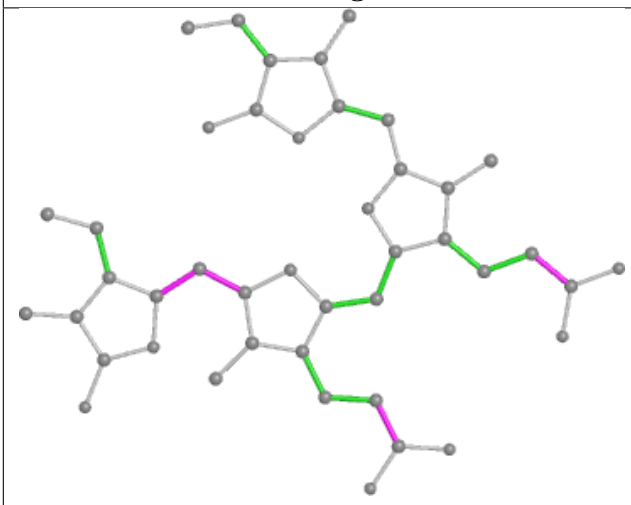

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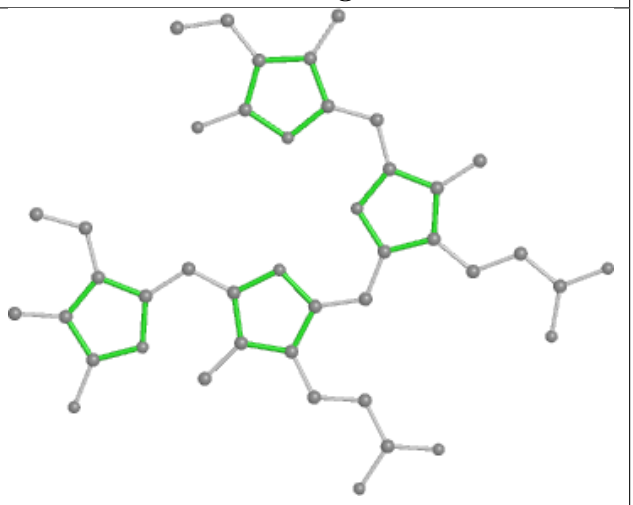

Rings

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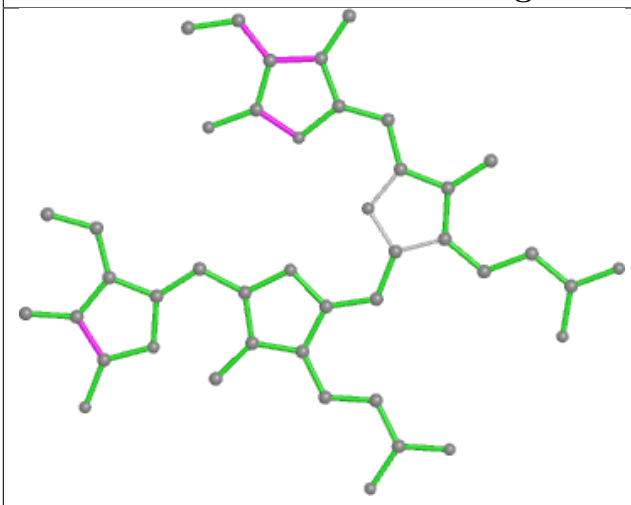

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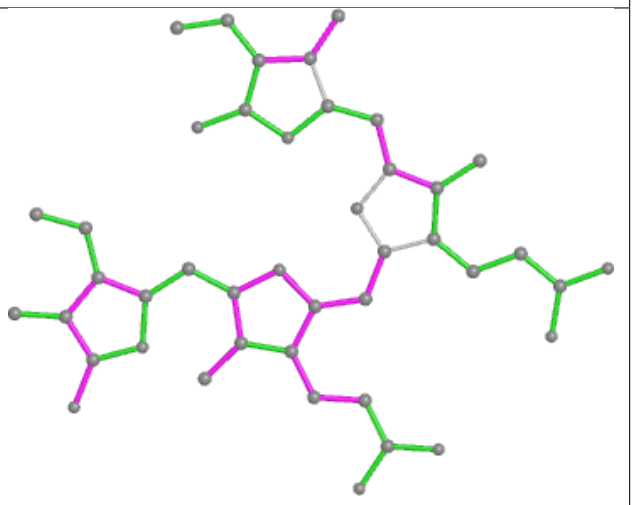

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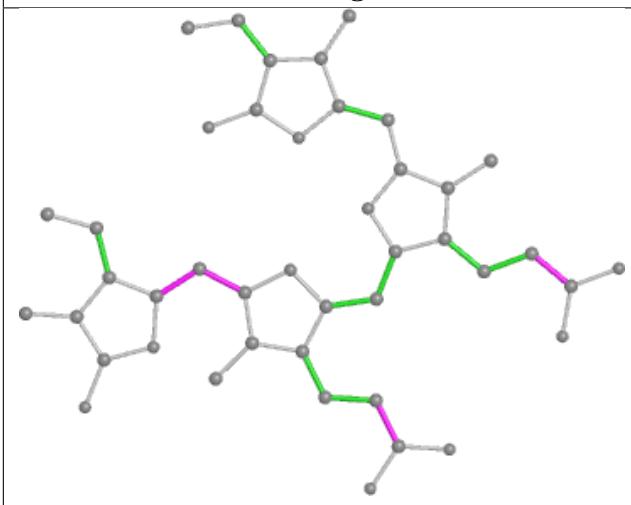

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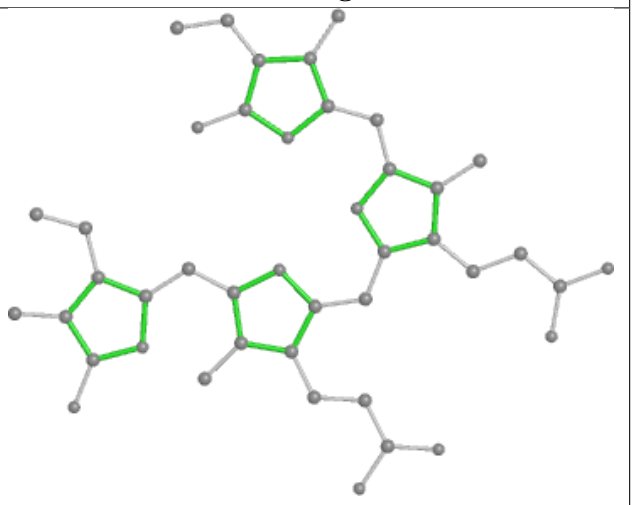

Rings

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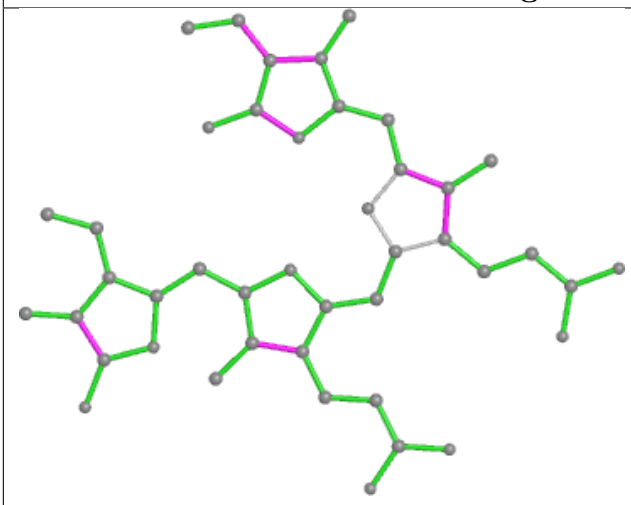

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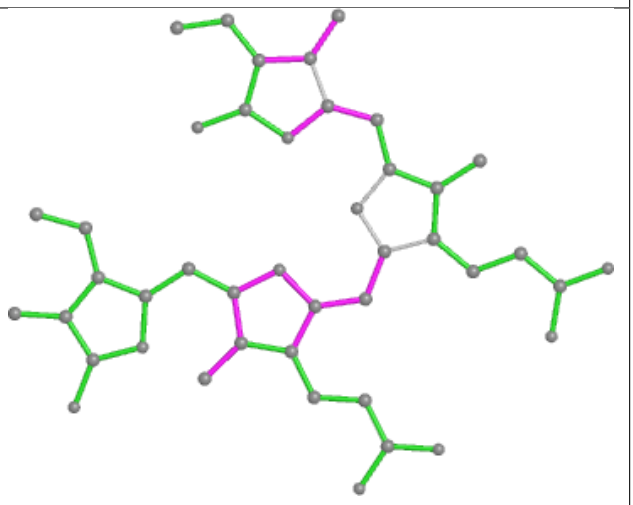

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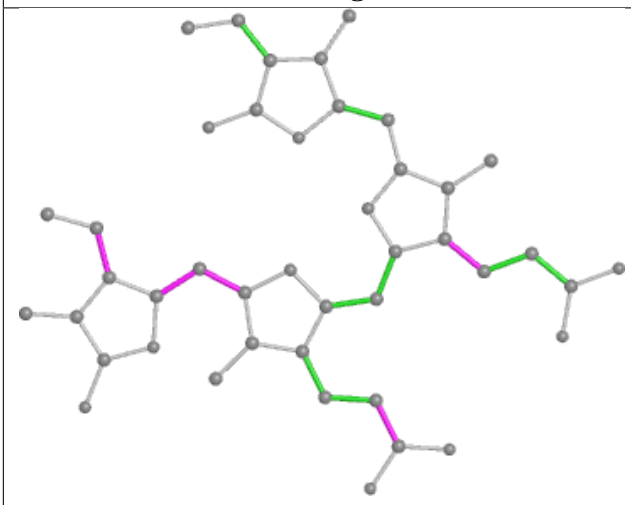

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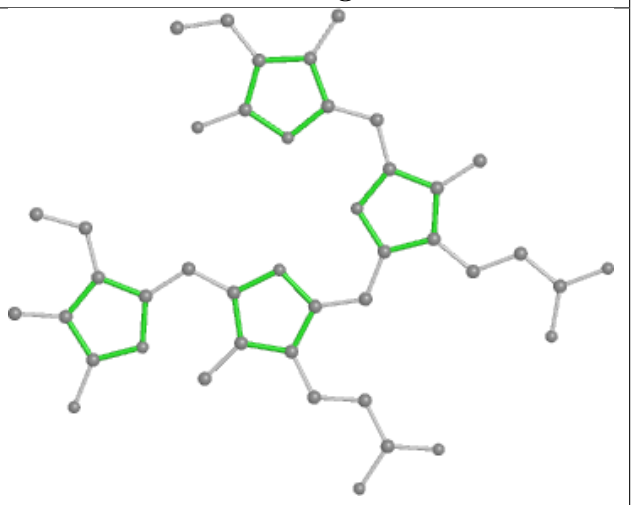

Rings

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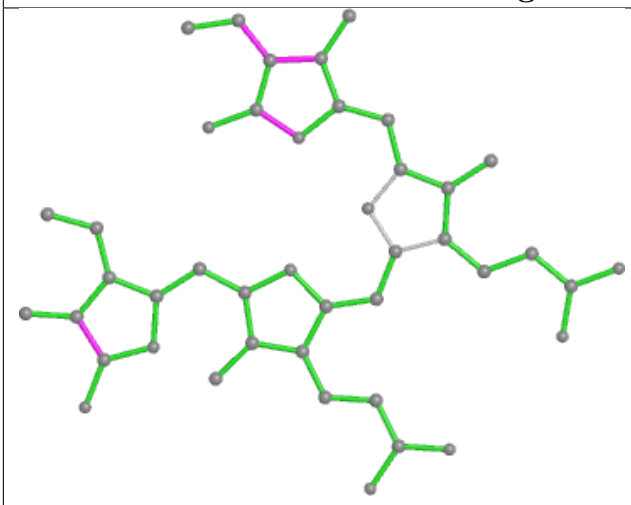

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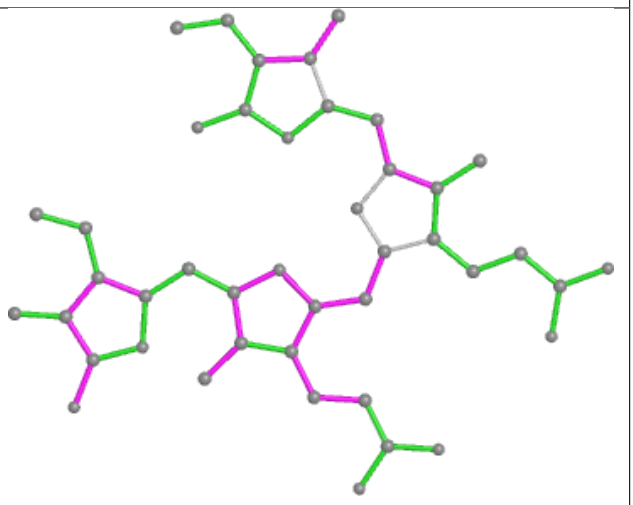

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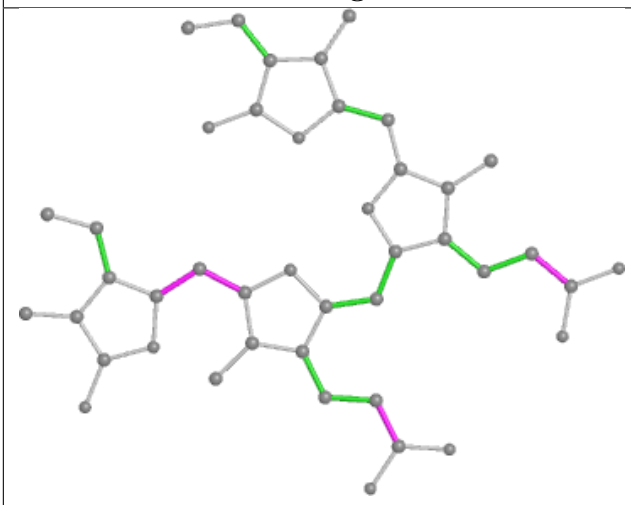
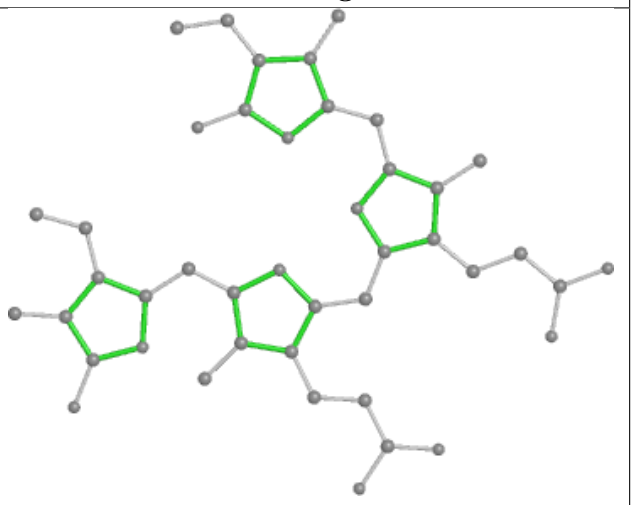
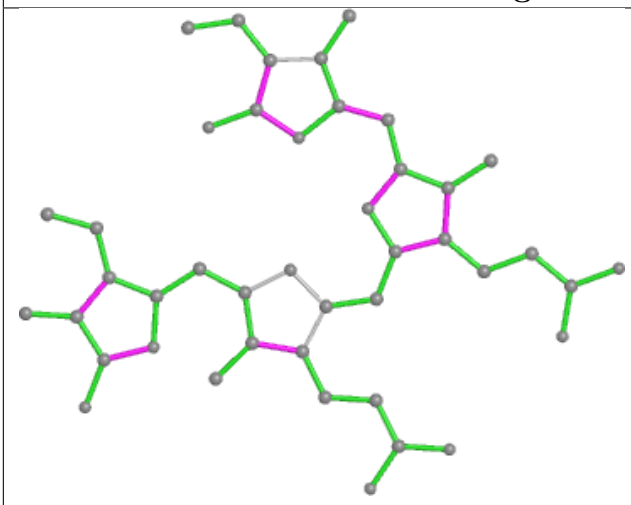


Torsions



Rings

Ligand PUB C2 304



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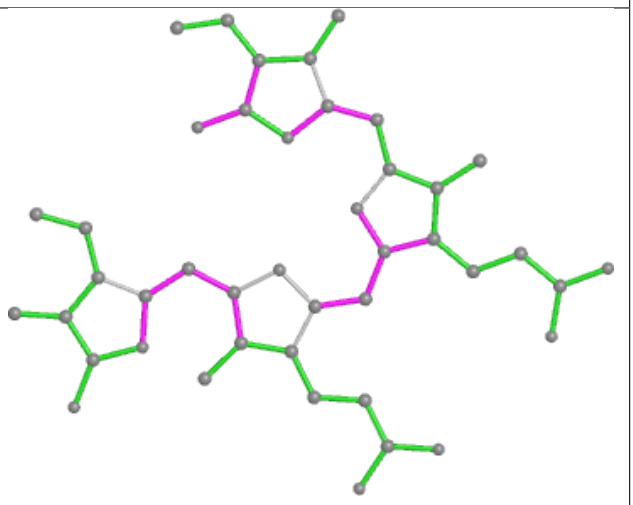

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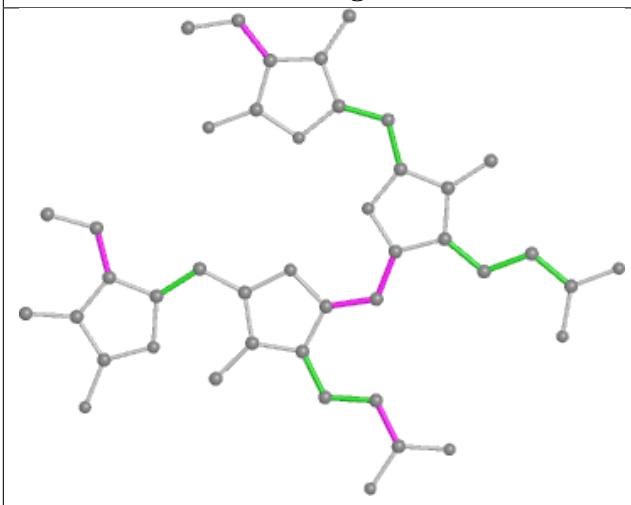

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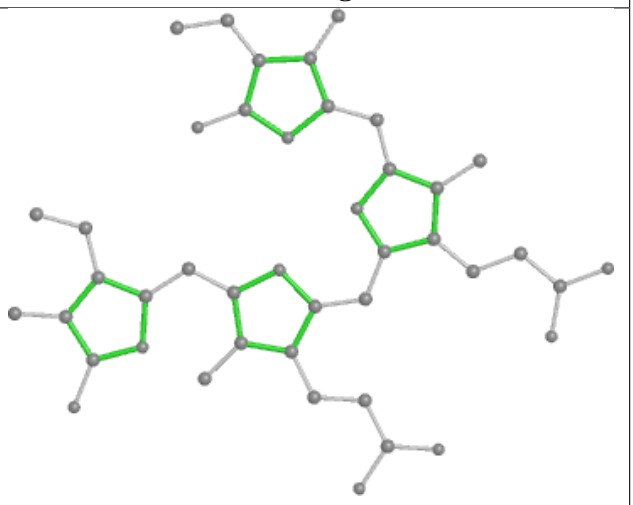
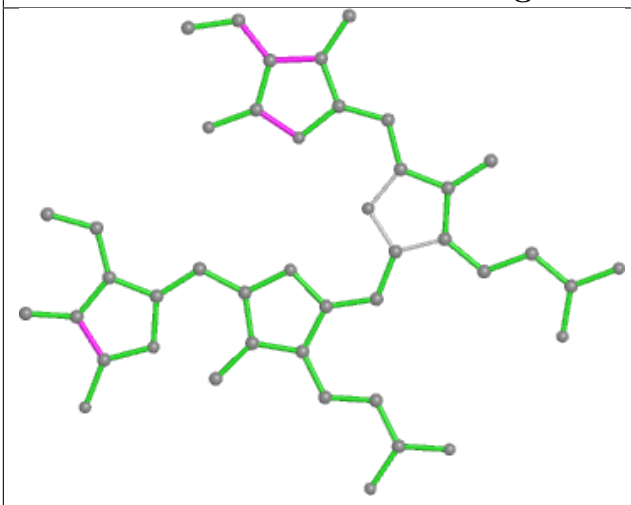


Rings

Ligand PEB hQ 201



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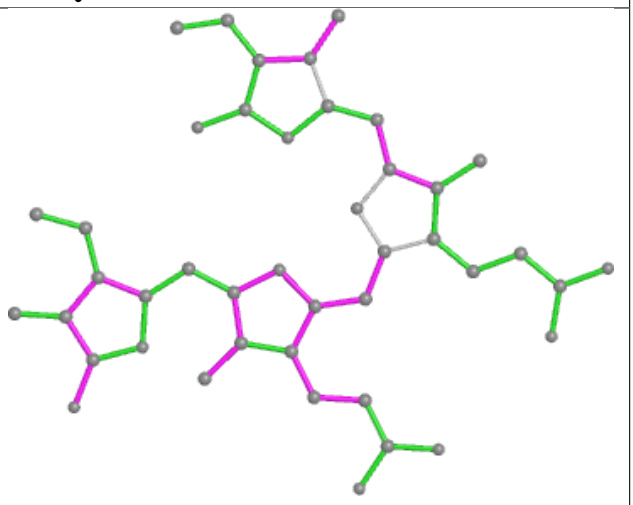

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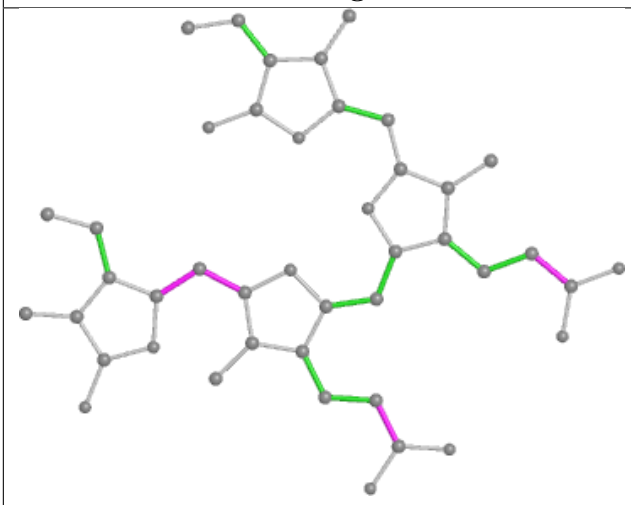

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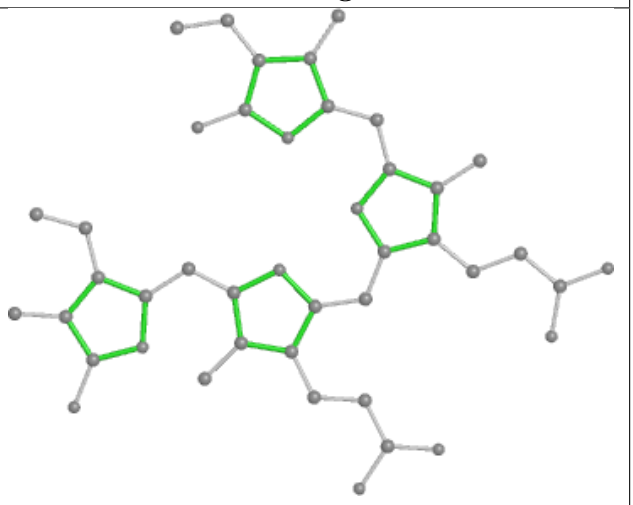
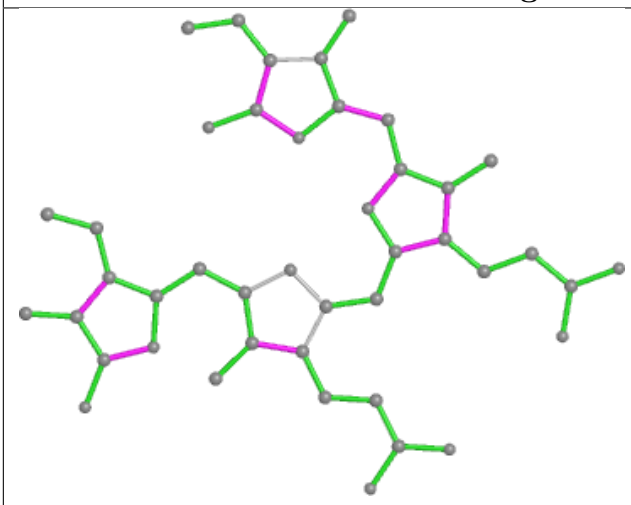


Rings

Ligand PUB dj 203



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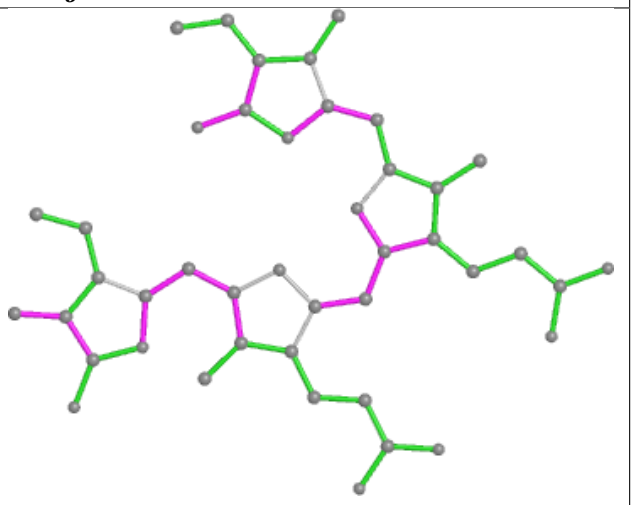

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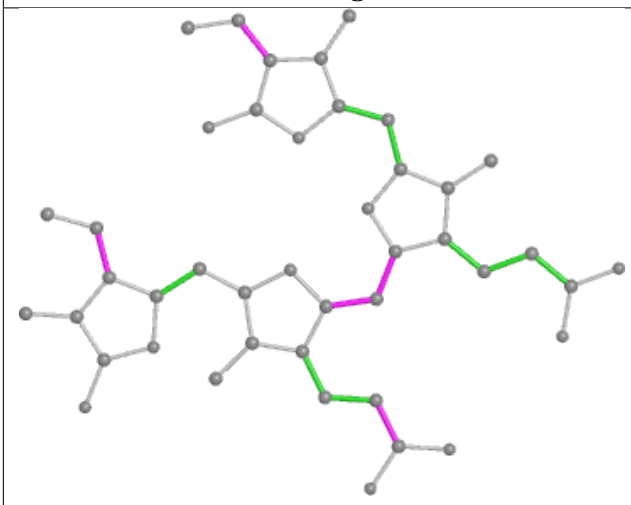

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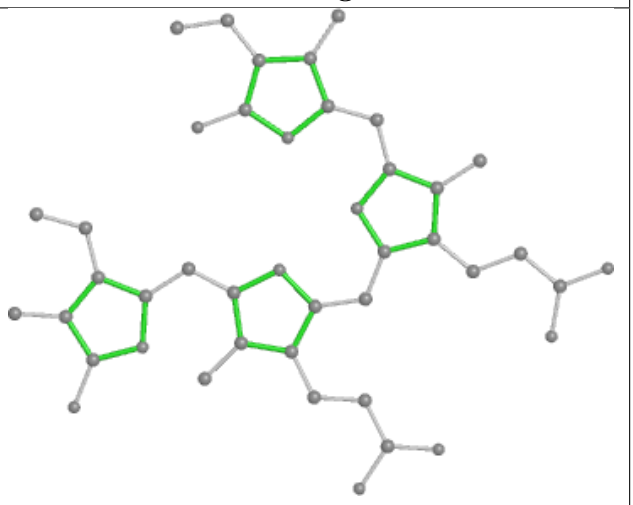
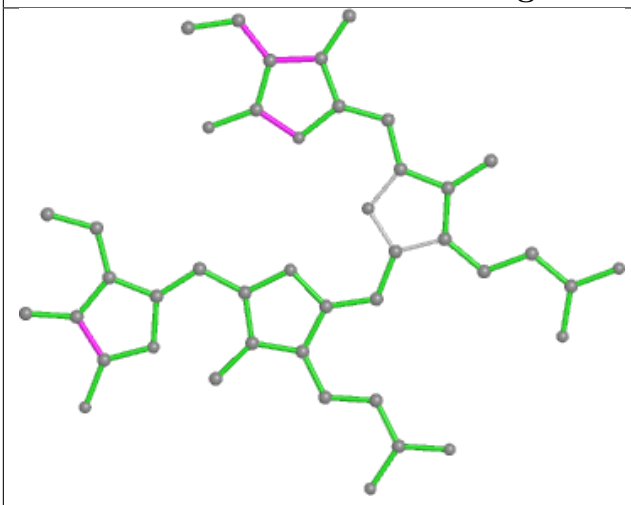


Rings

Ligand PEB F9 201



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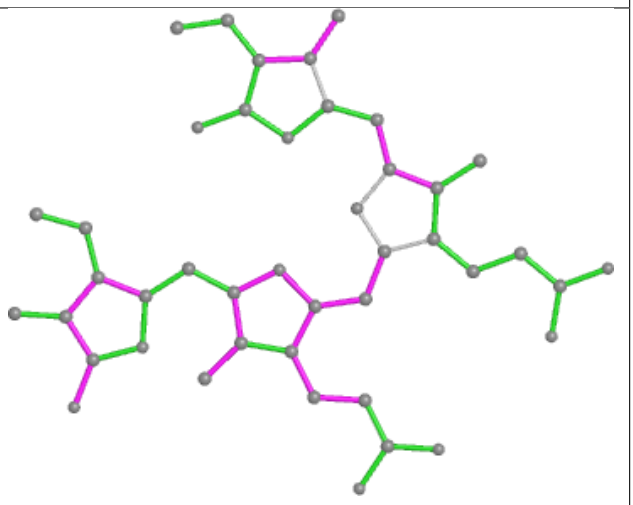

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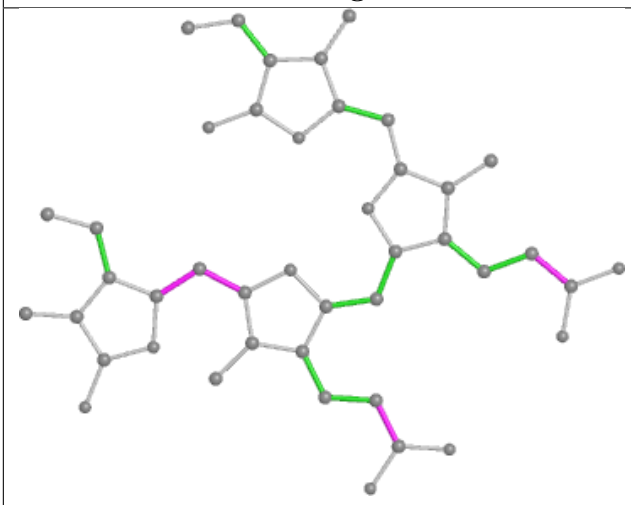

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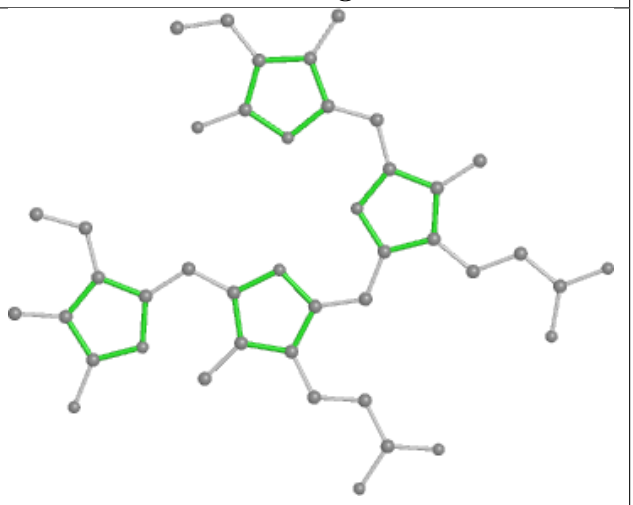

Rings

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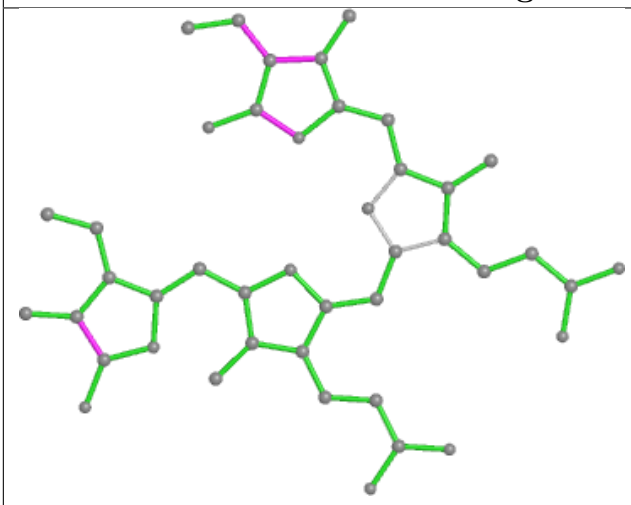

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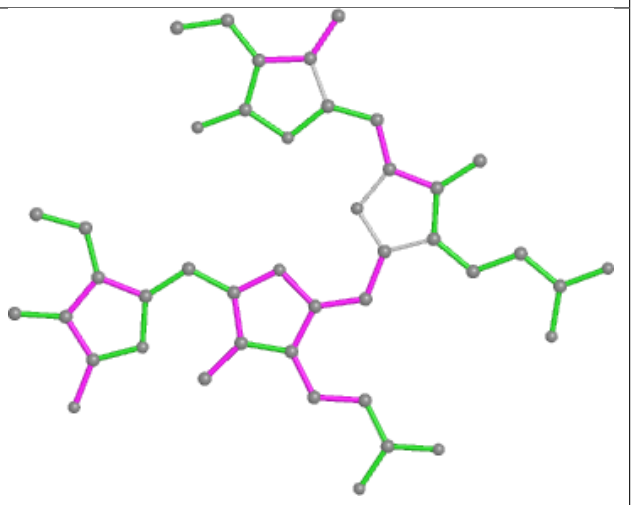

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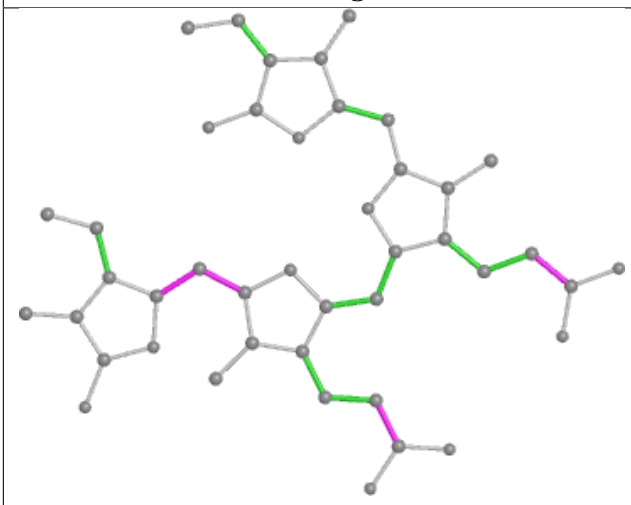

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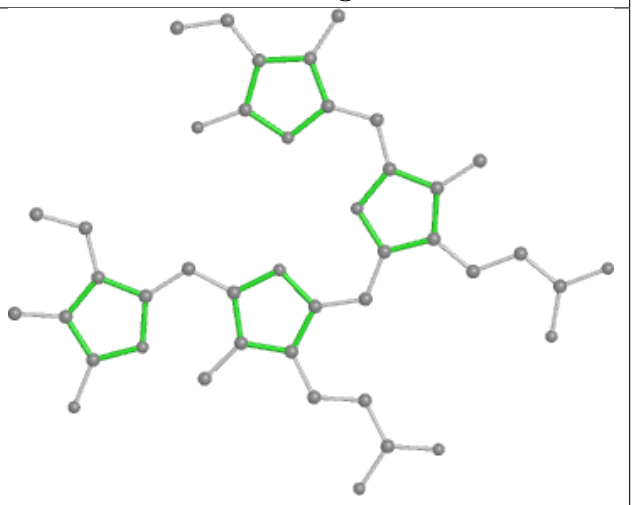

Rings

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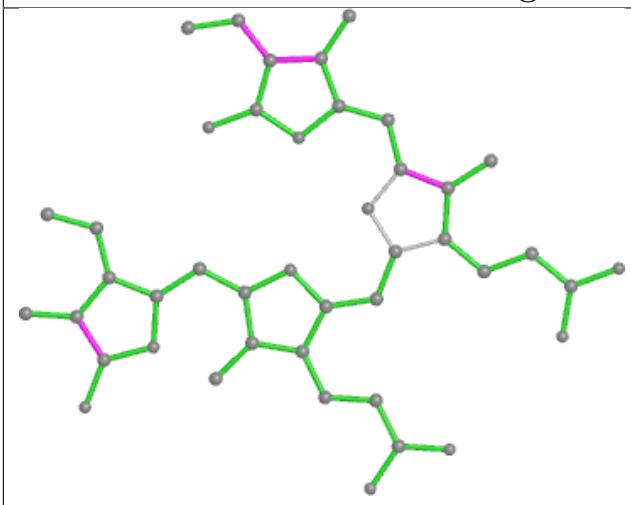

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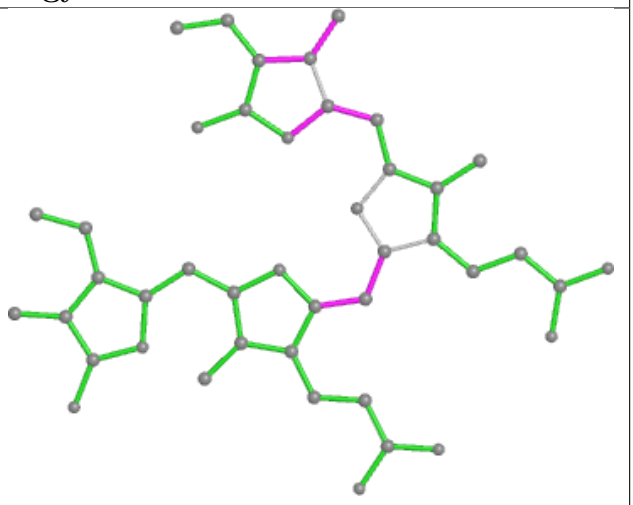

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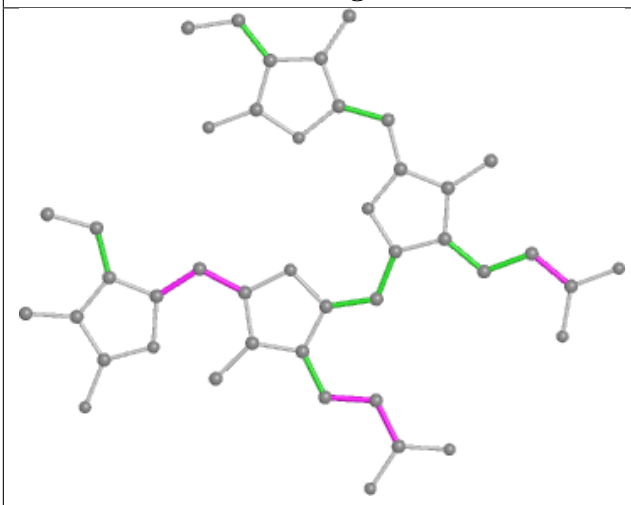

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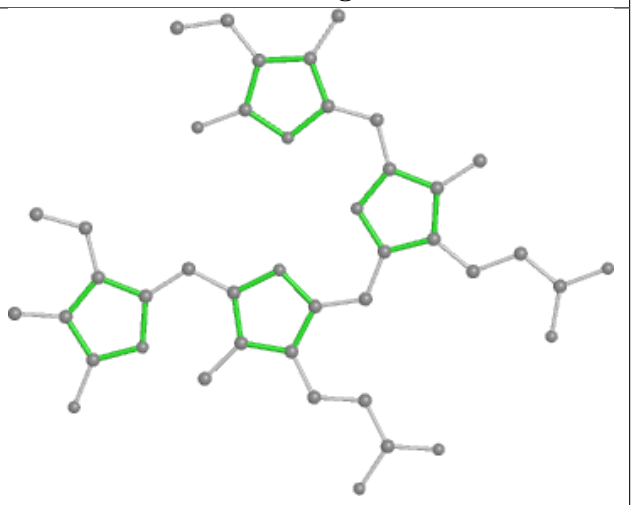
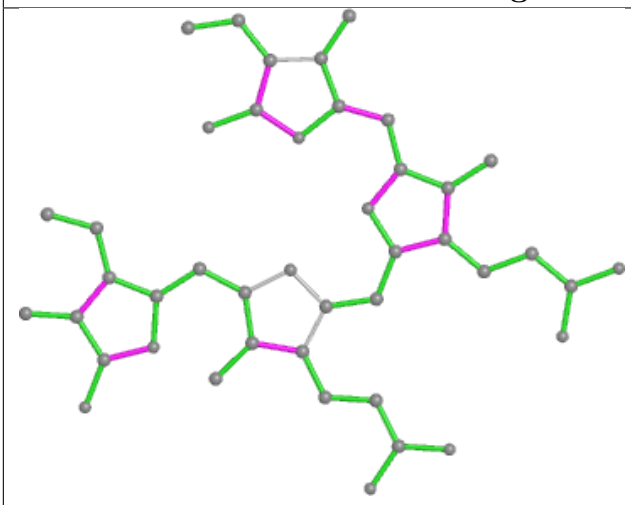


Rings

Ligand PUB iF 1003



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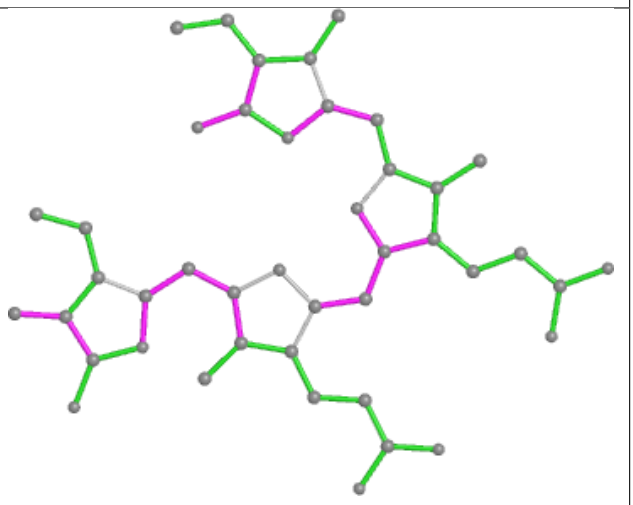

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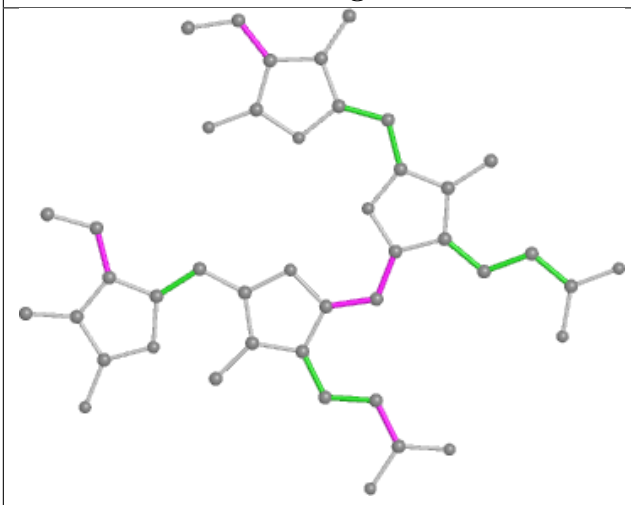

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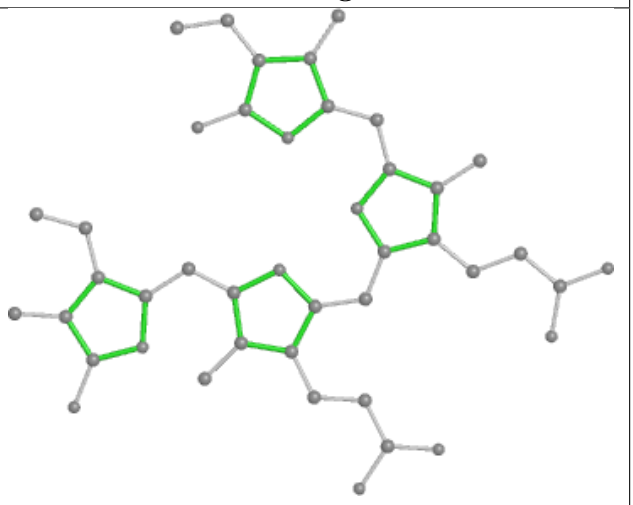
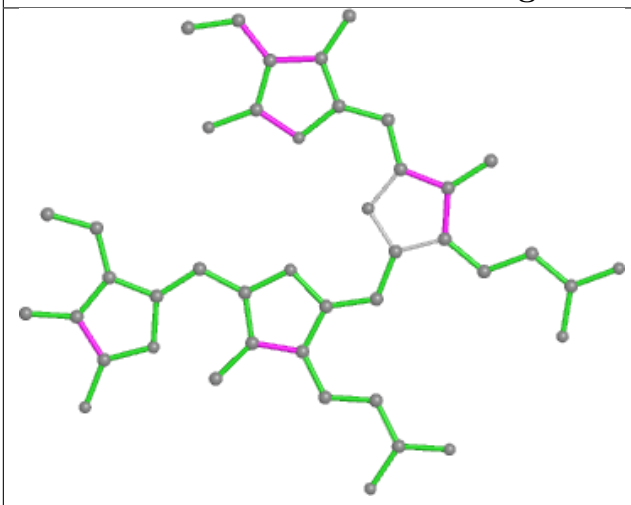


Rings

Ligand PEB bJ 202



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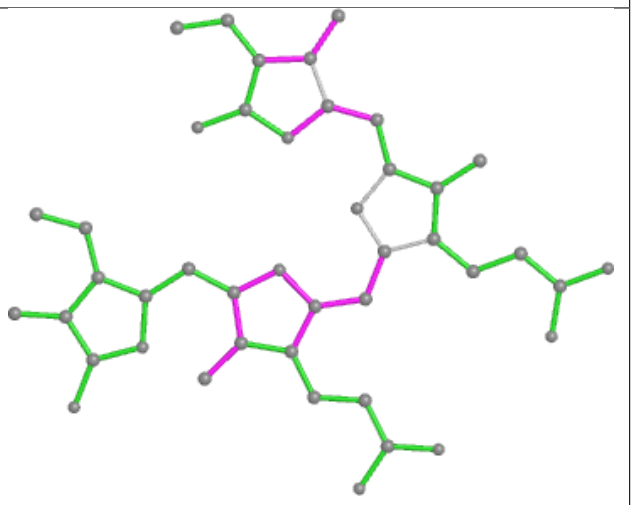

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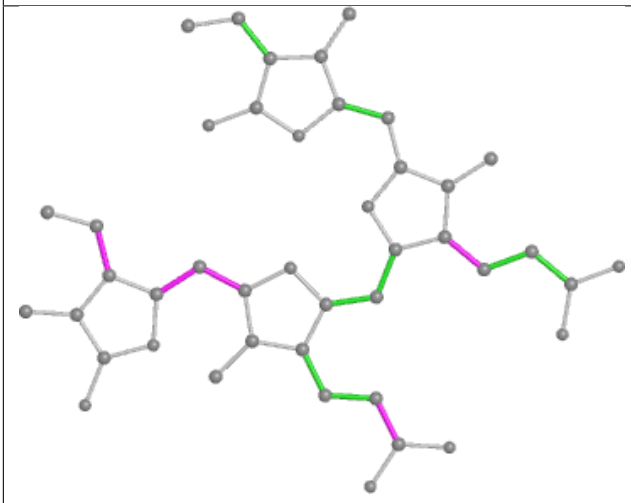

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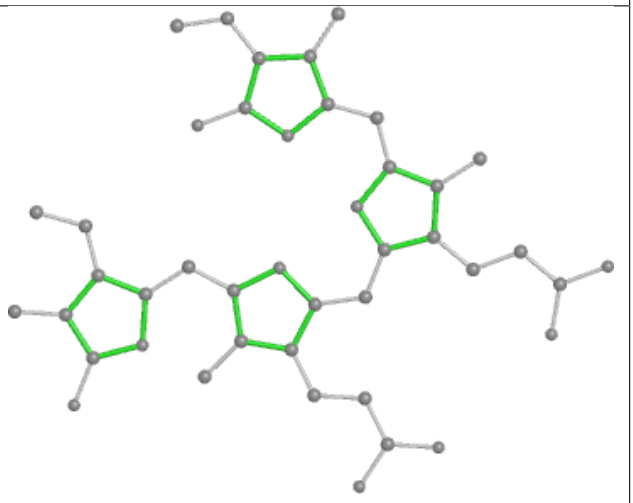

Rings

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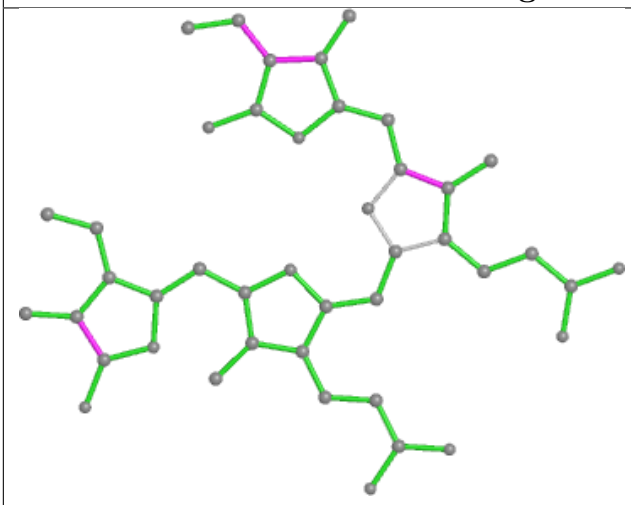

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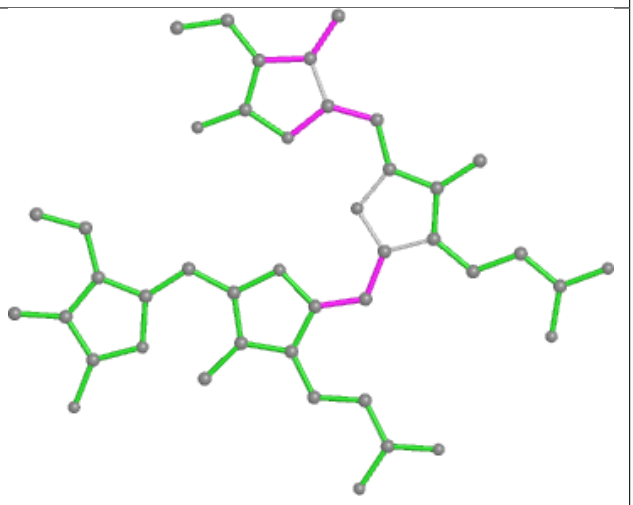

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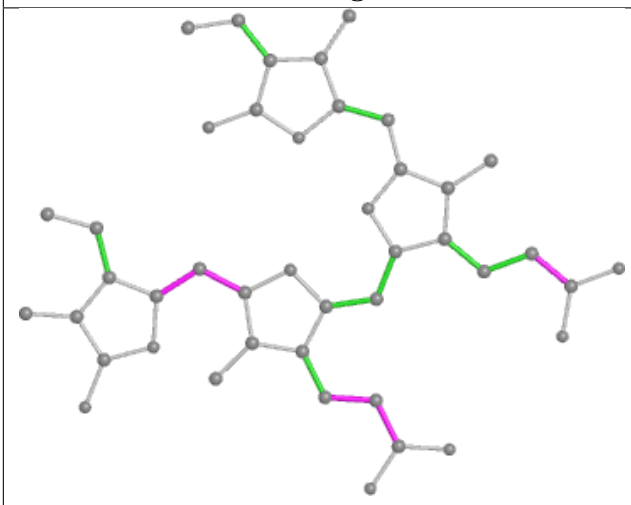

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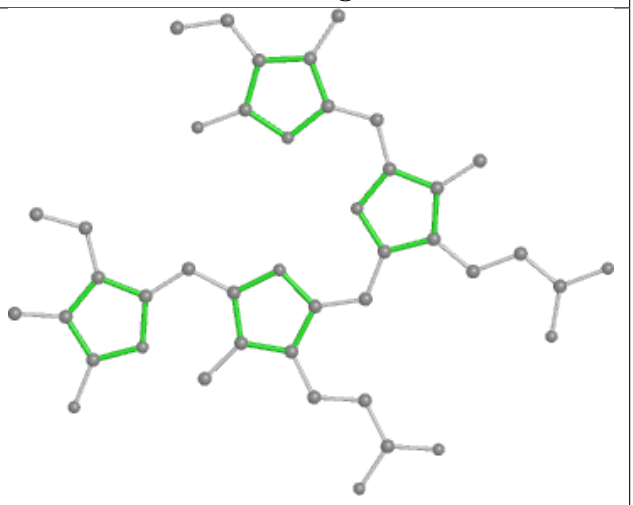
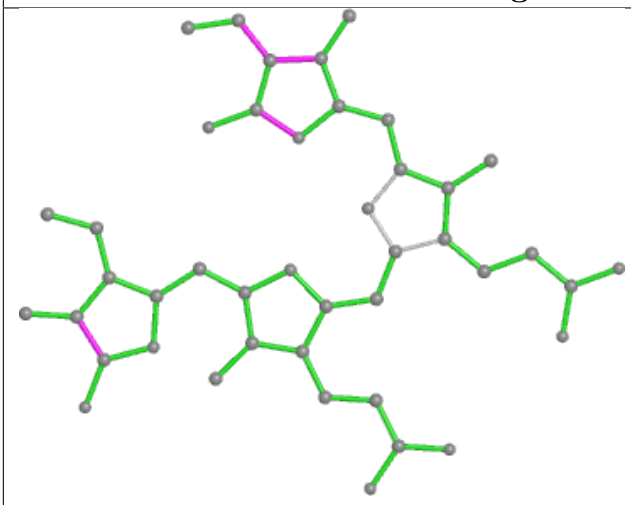


Rings

Ligand PEB 34 1003



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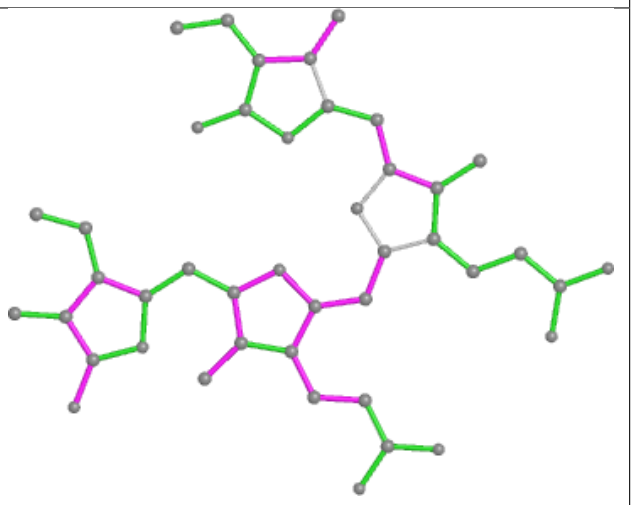

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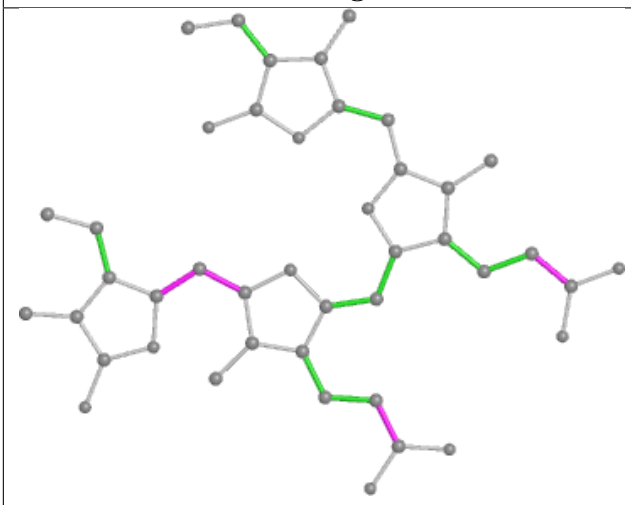

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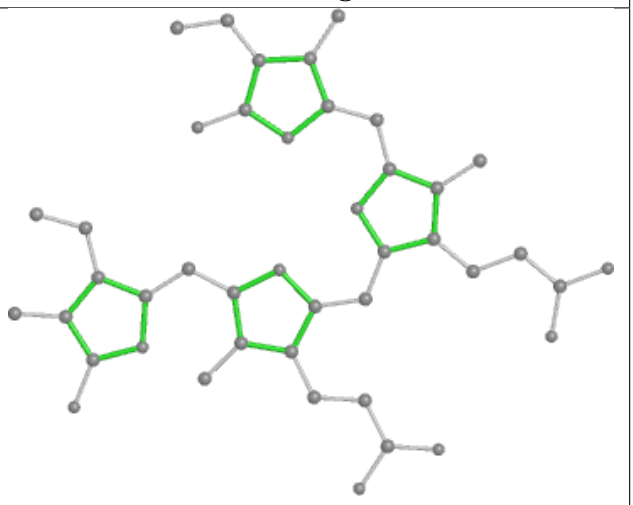
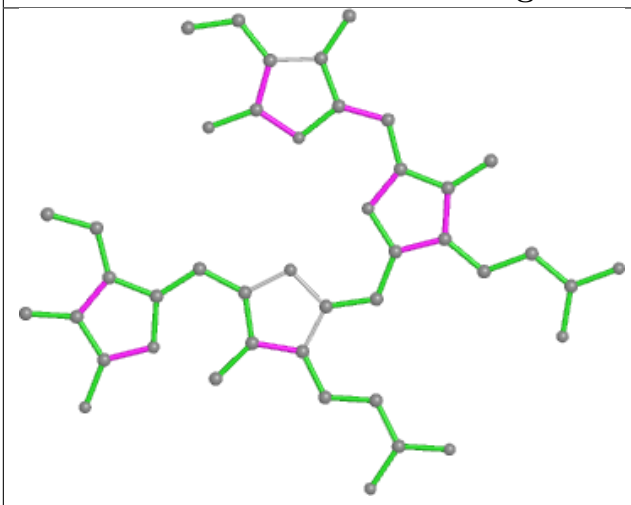


Rings

Ligand PUB p9 203



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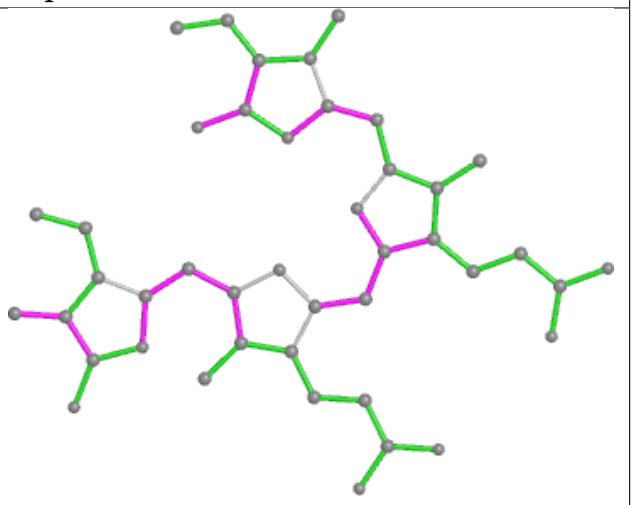

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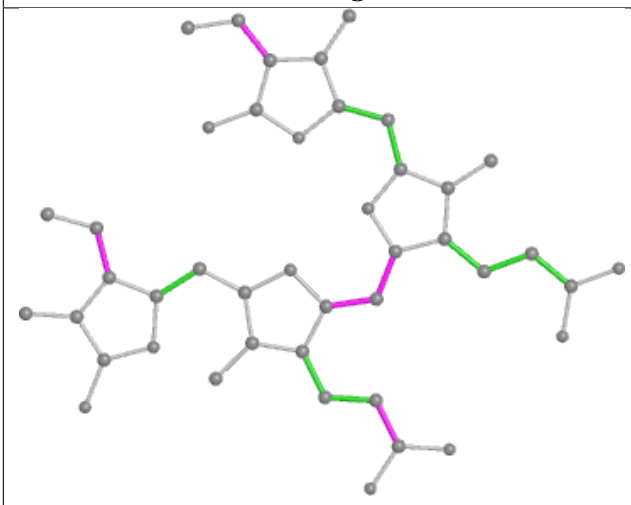

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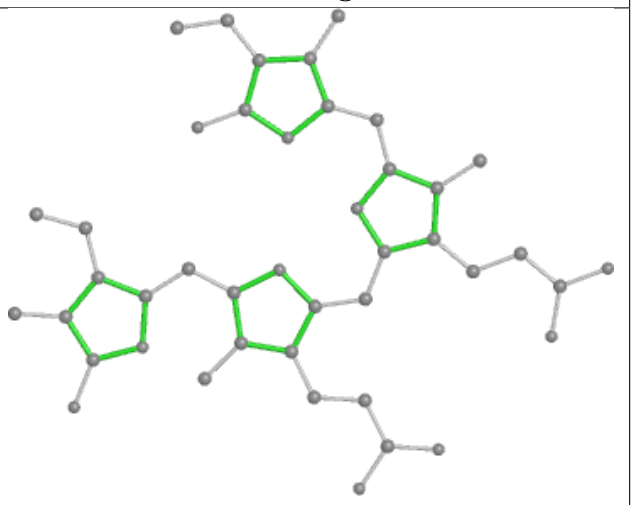
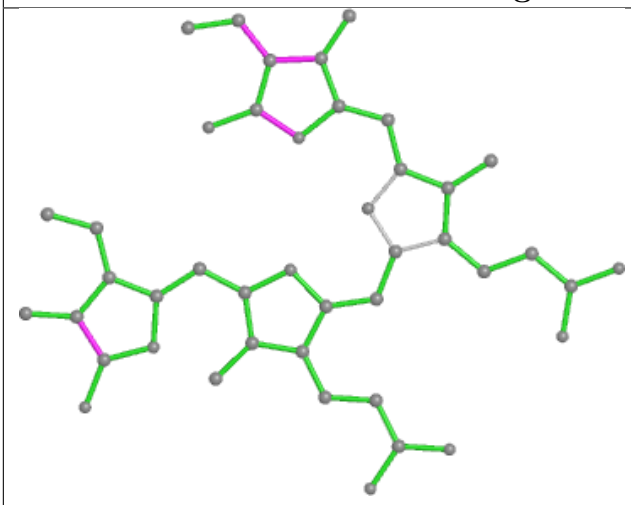


Rings

Ligand PEB m6 202



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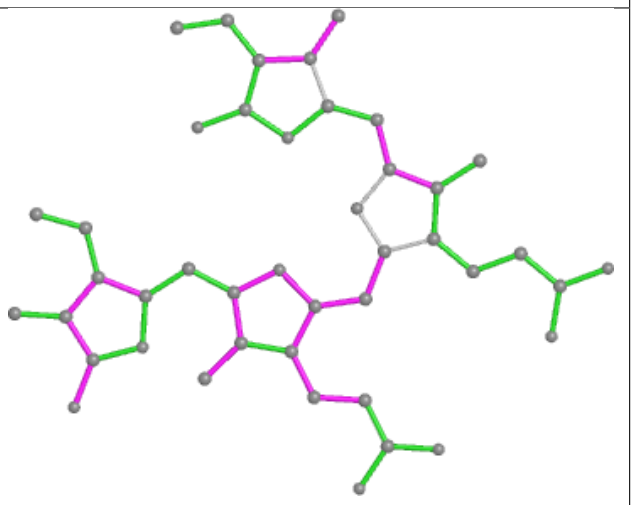

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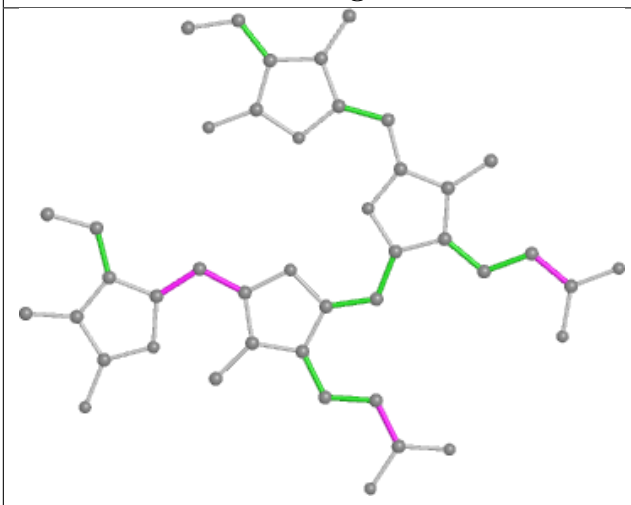

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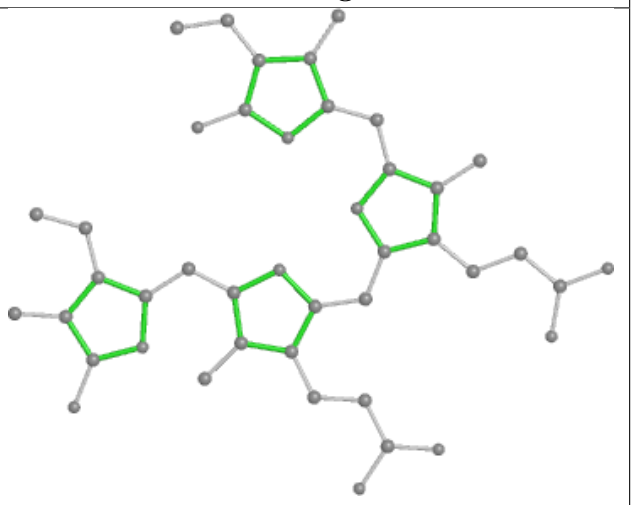
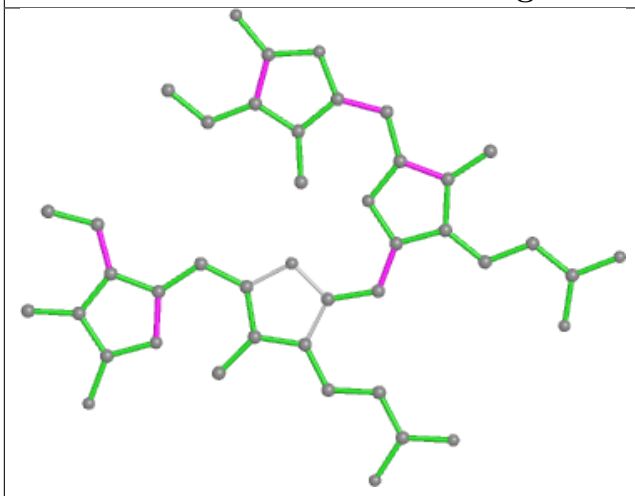


Rings

Ligand PVN d8 303



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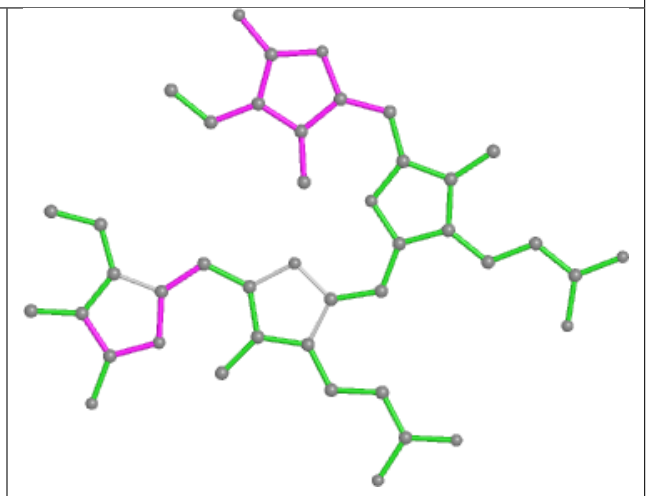
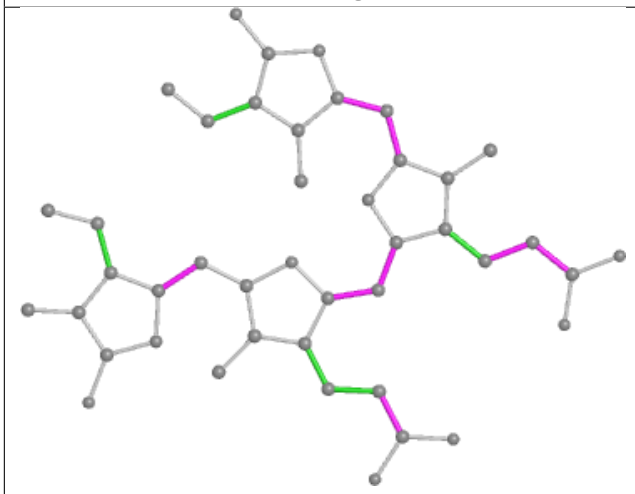


Bond angles



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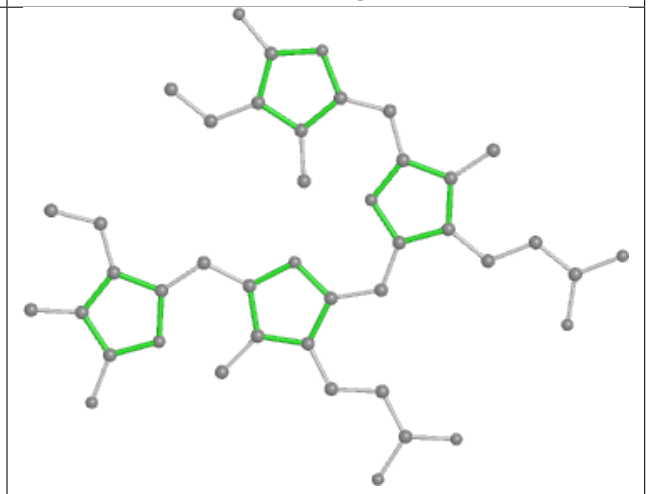
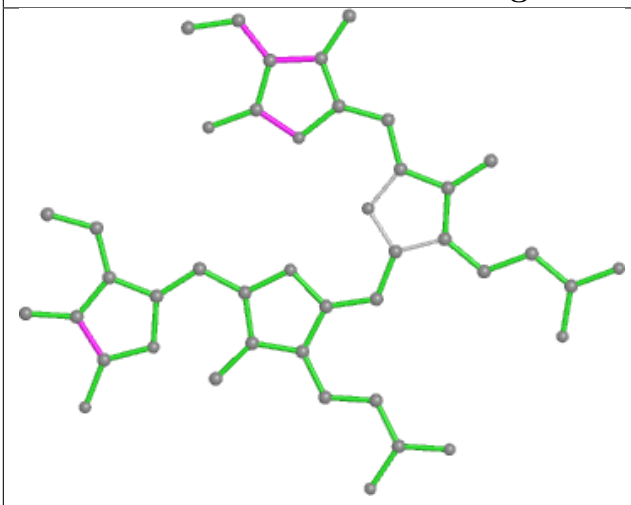
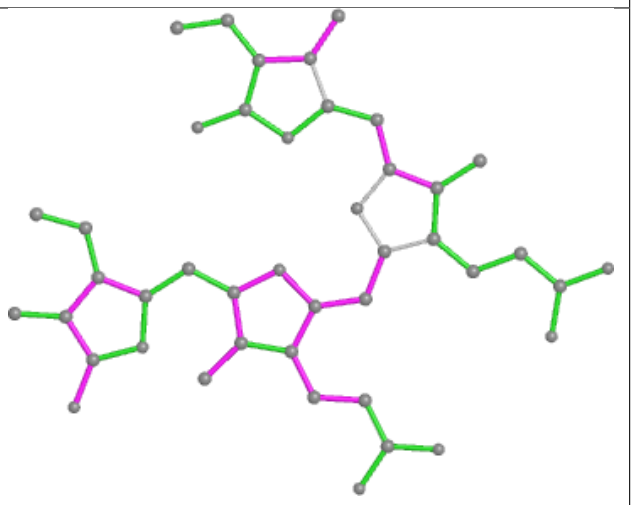


Rings

Ligand PEB W6 201



Bond lengths



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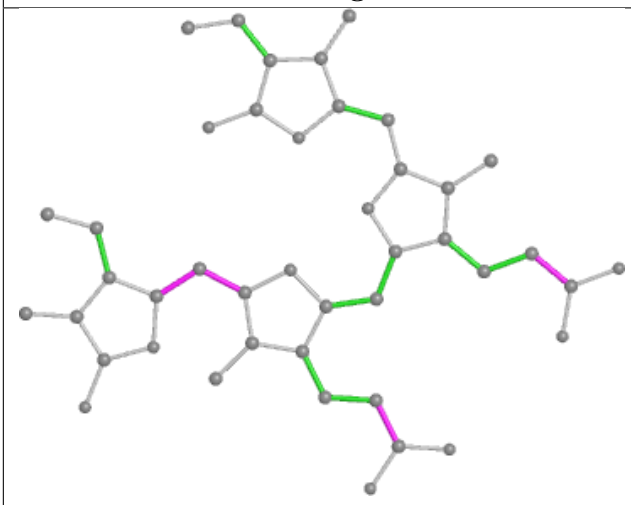
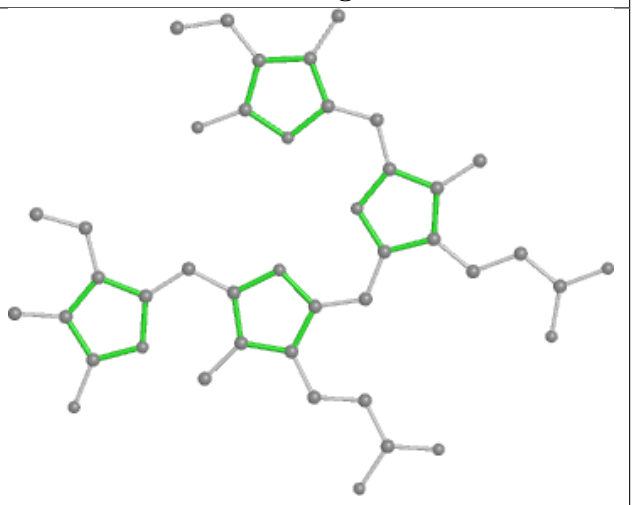
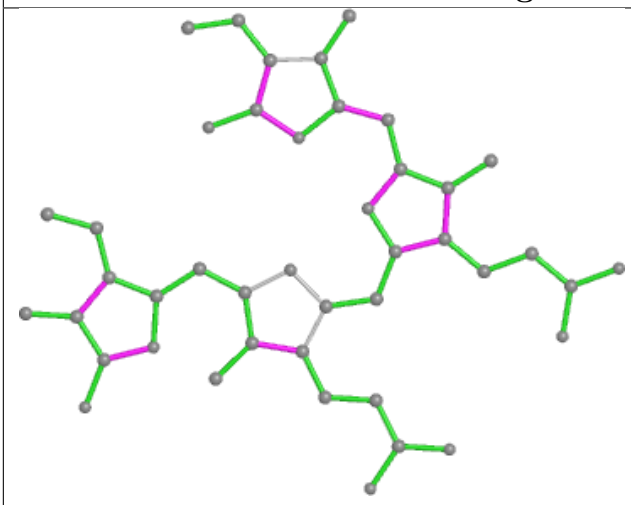


Torsions



Rings

Ligand PUB L5 203



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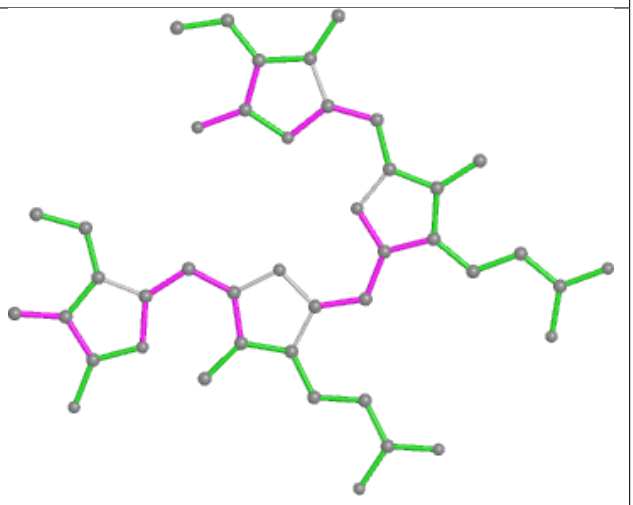

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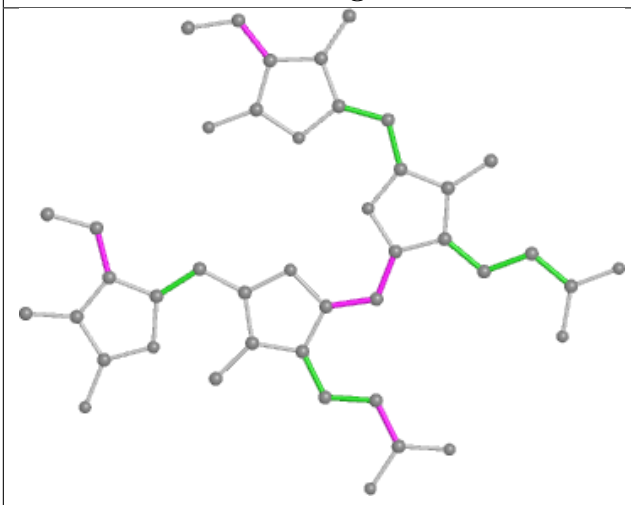

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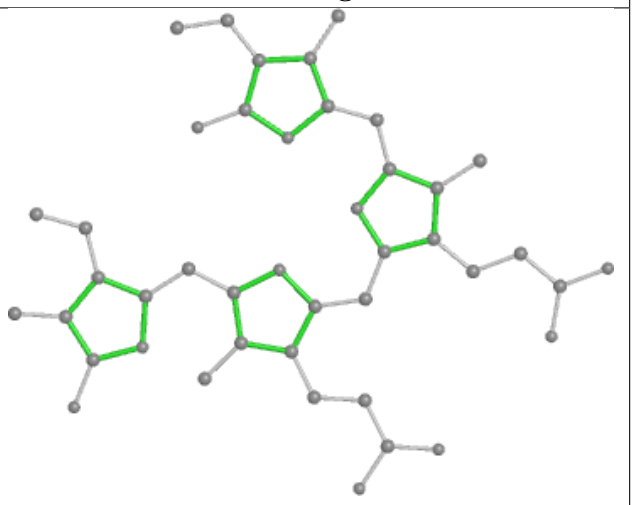
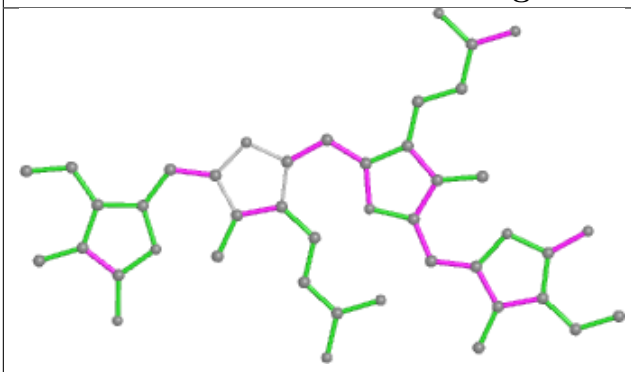


Rings

Ligand CYC X1 201



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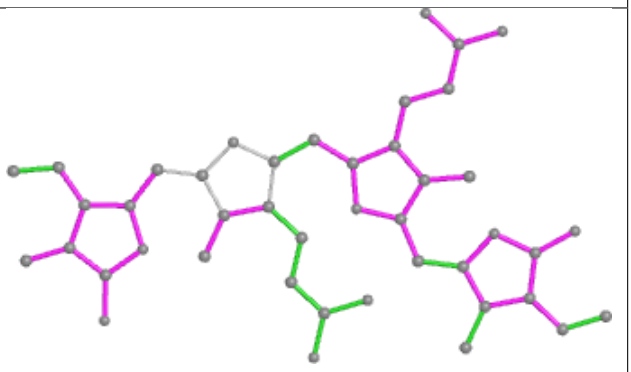

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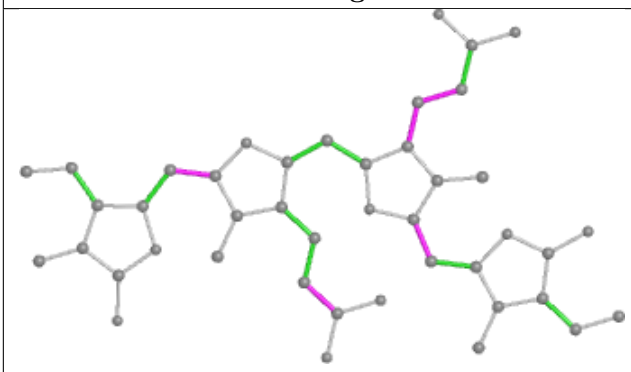

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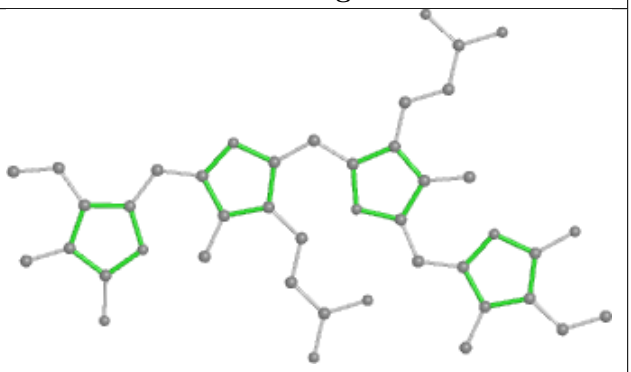

Rings

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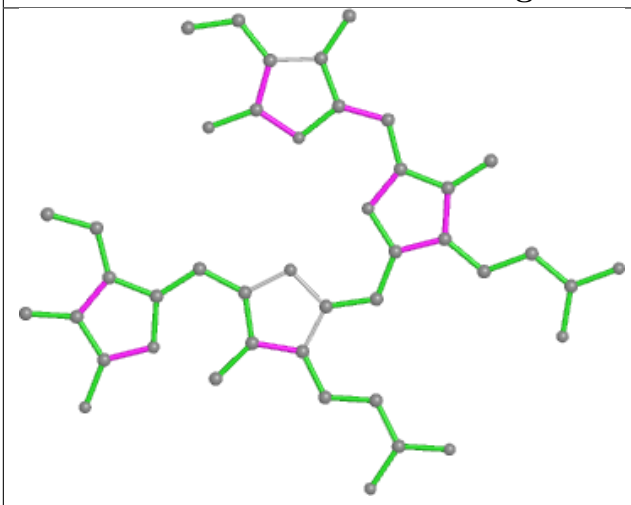

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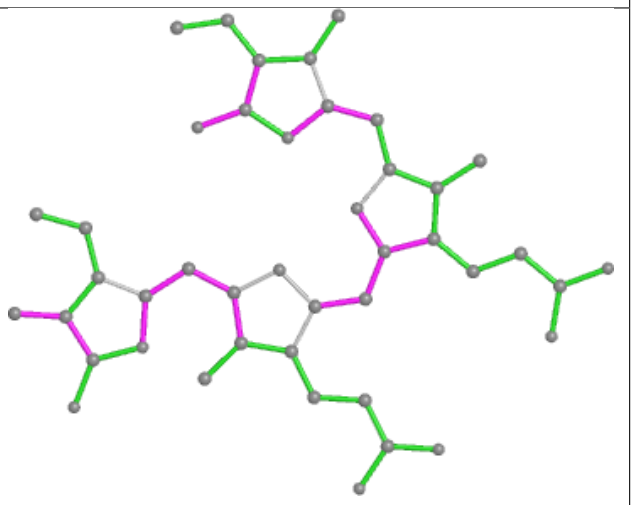

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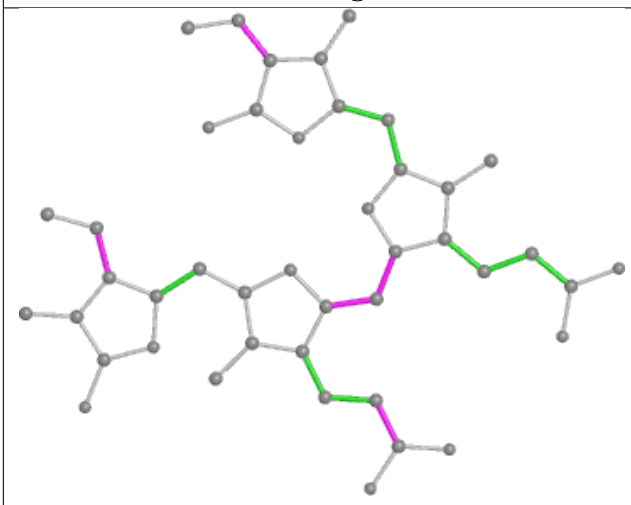

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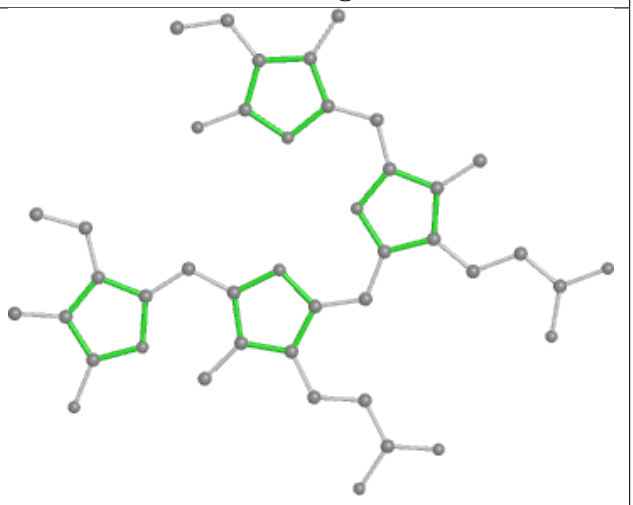
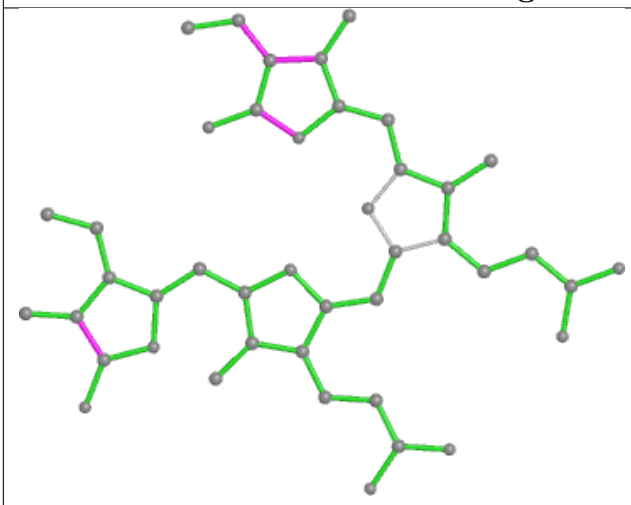


Rings

Ligand PEB Z5 303



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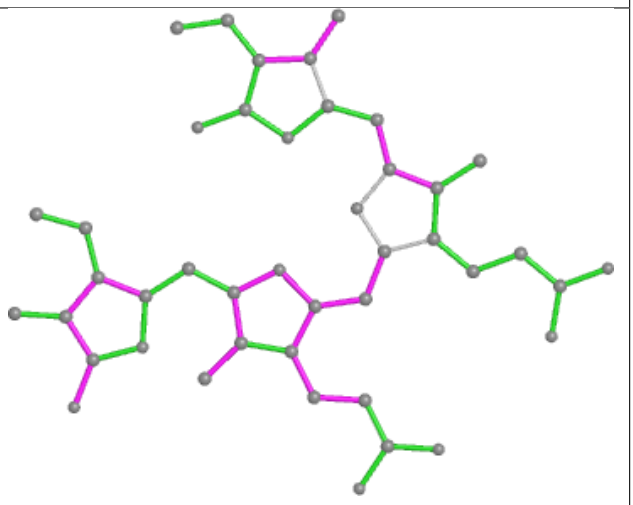

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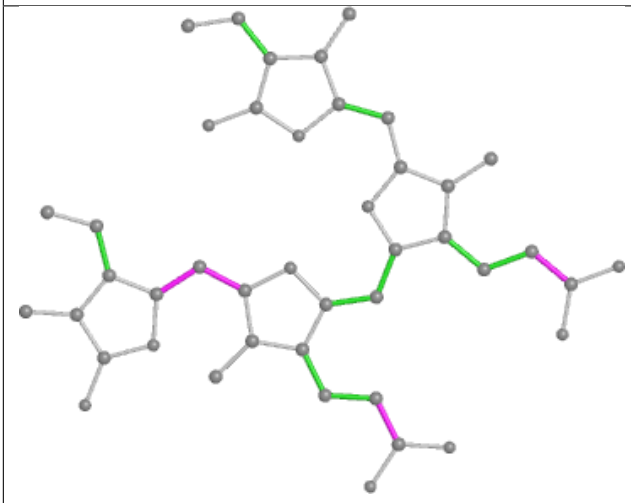

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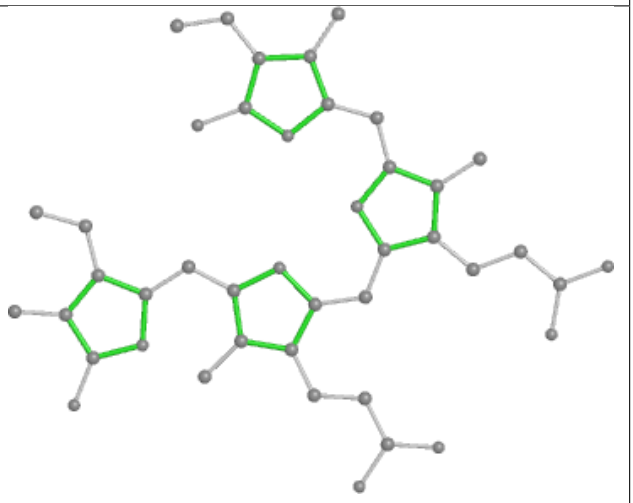

Rings

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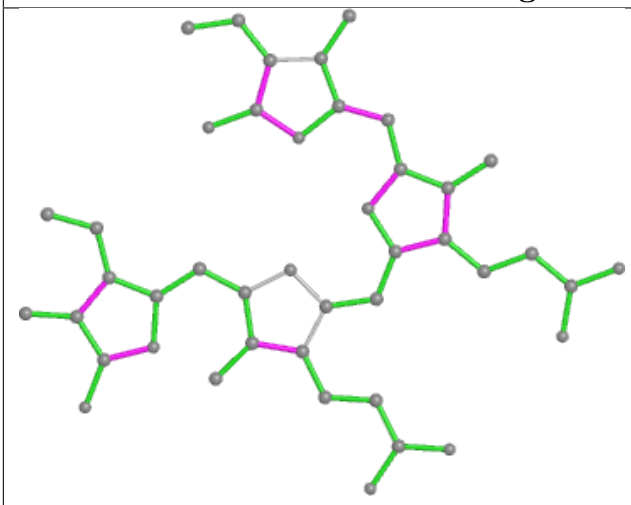

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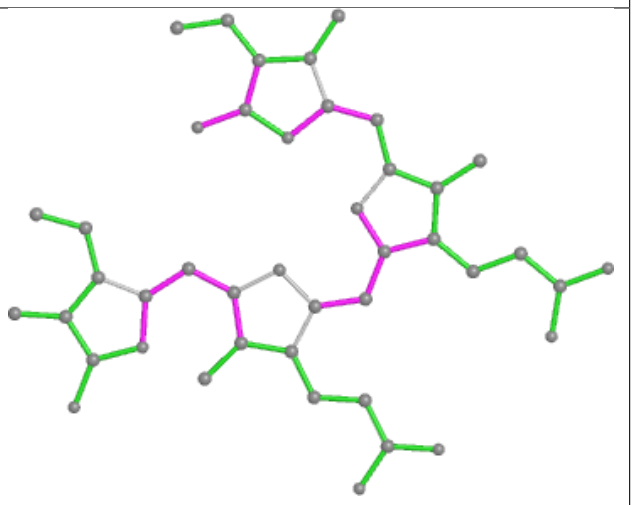

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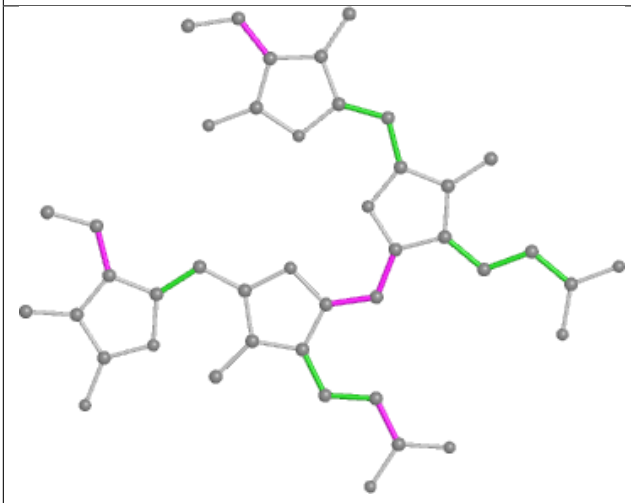

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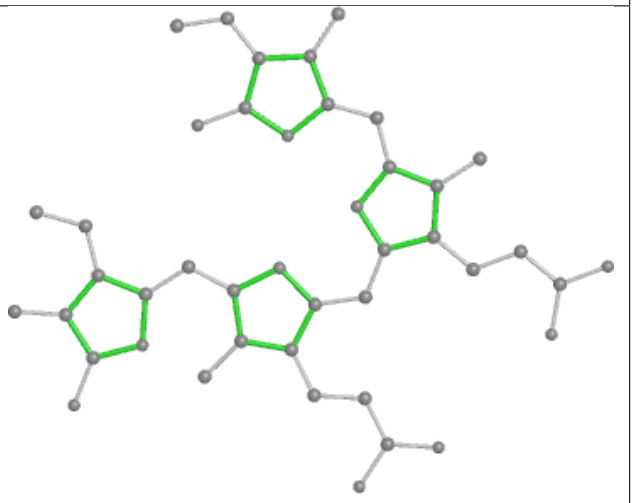
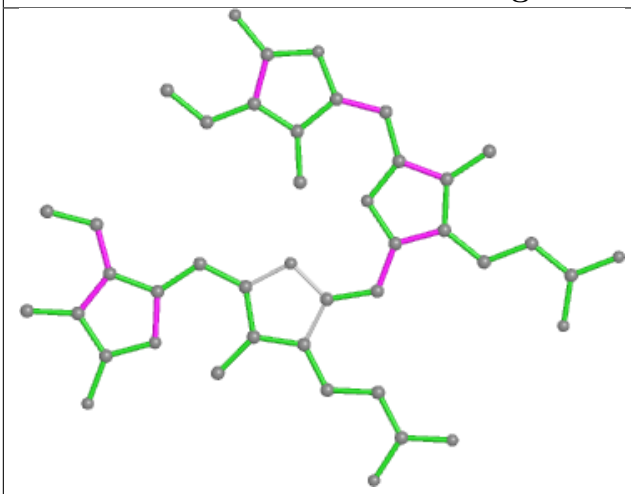


Rings

Ligand PVN dw 404



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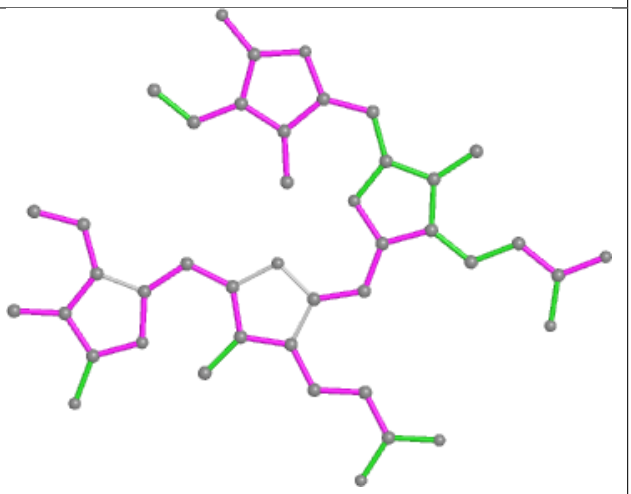

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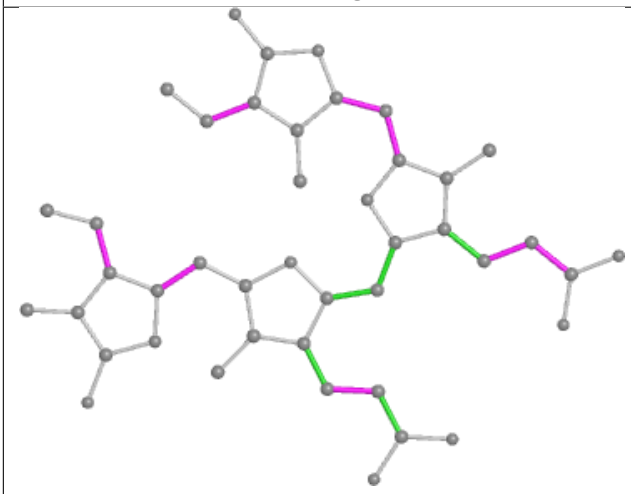

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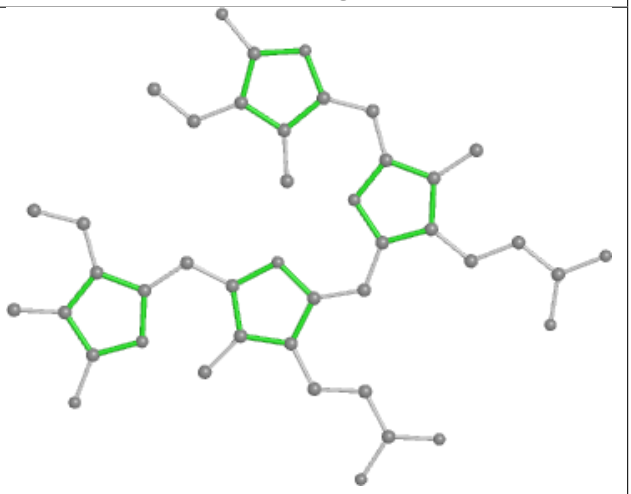
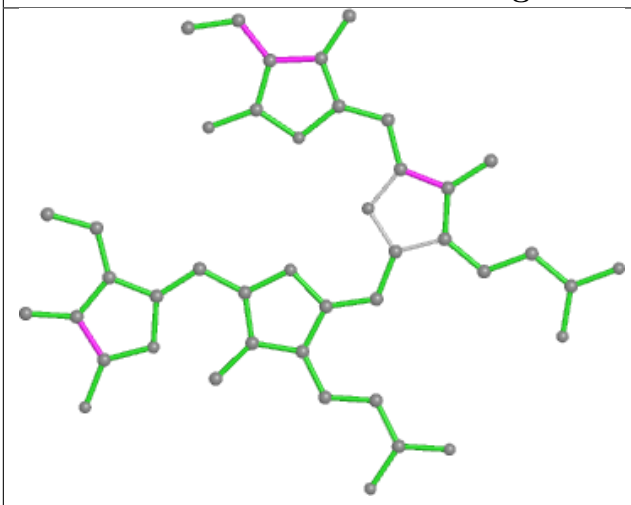


Rings

Ligand PEB iF 1002



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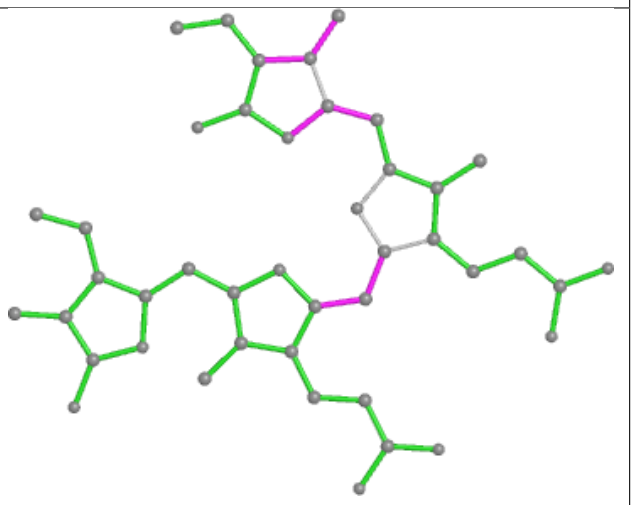

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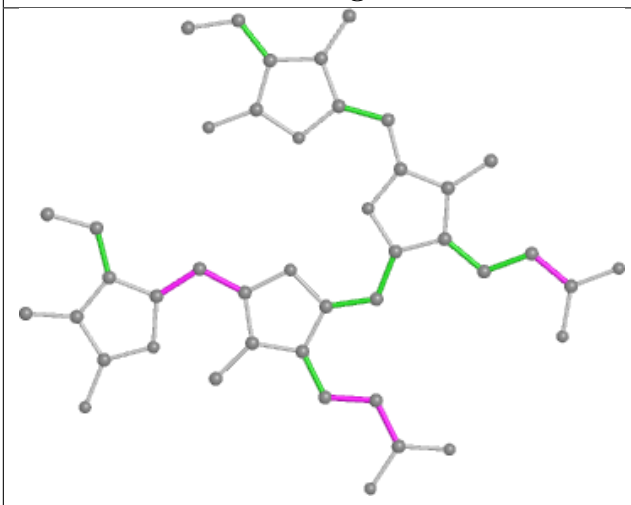

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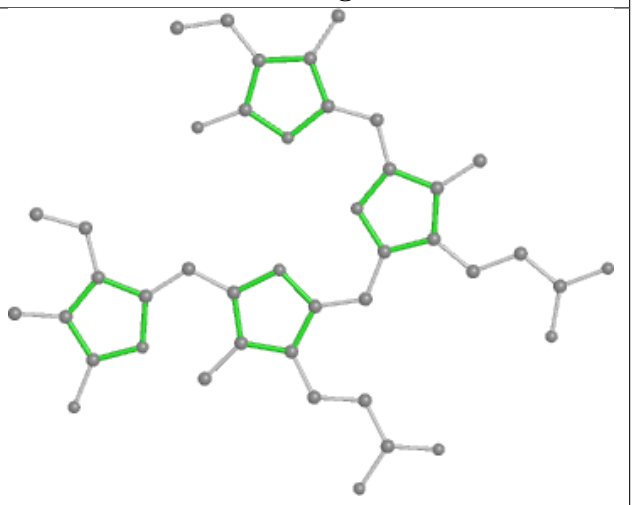
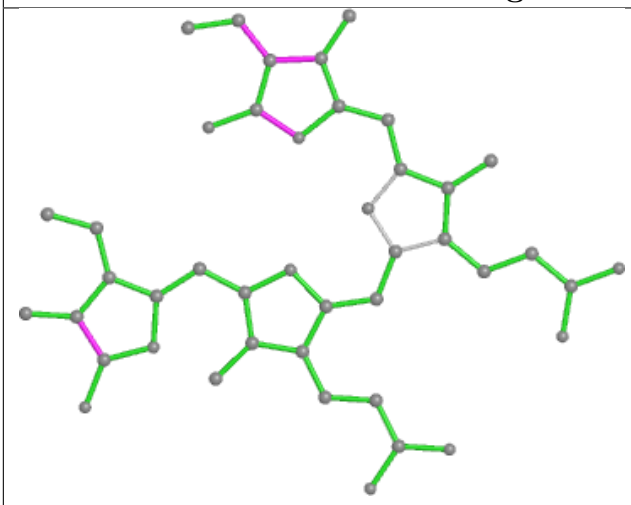


Rings

Ligand PEB Y5 1003



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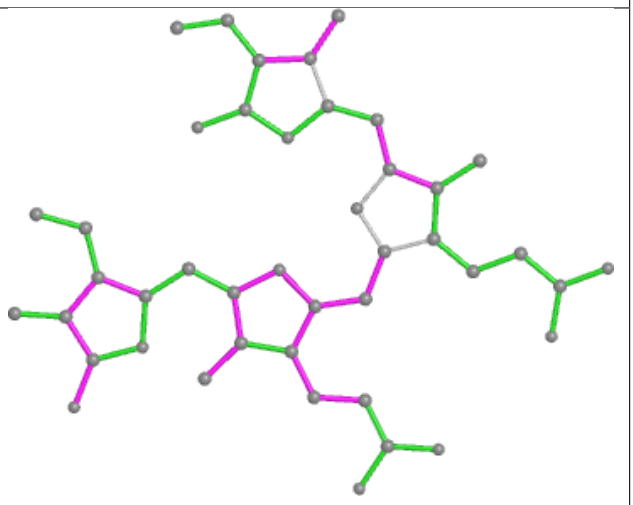

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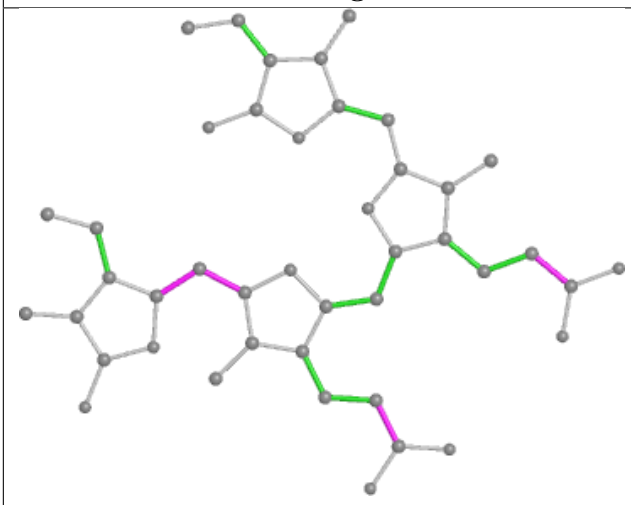

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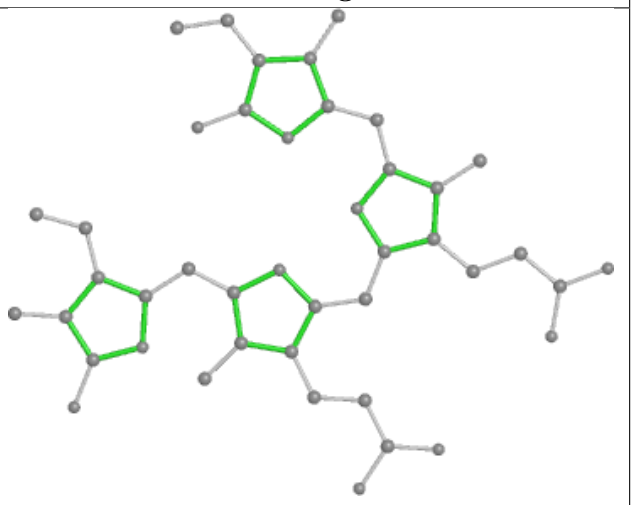
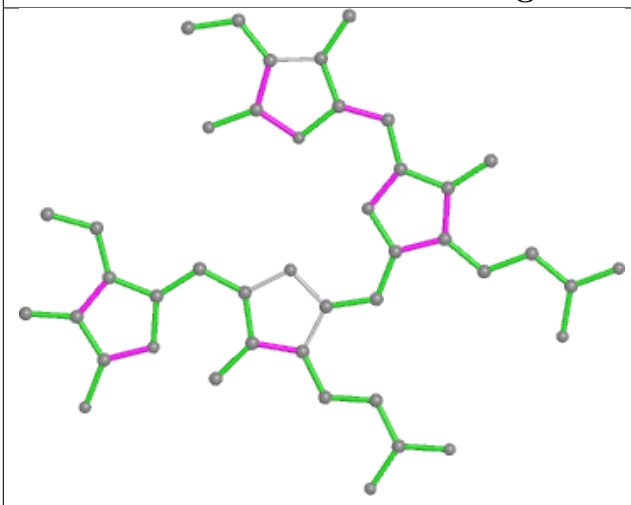


Rings

Ligand PUB p5 202



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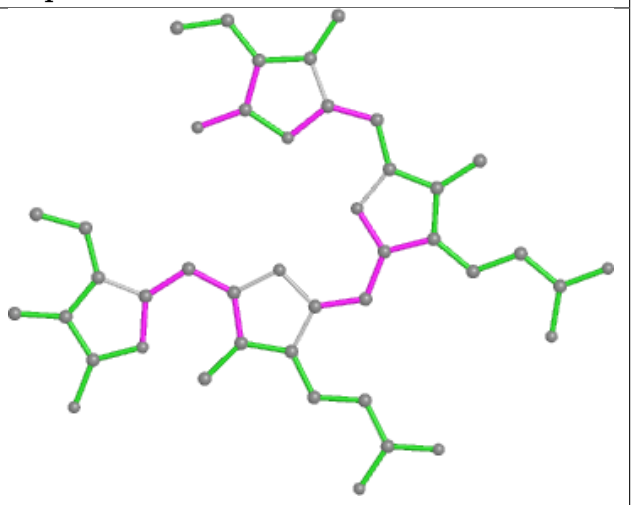

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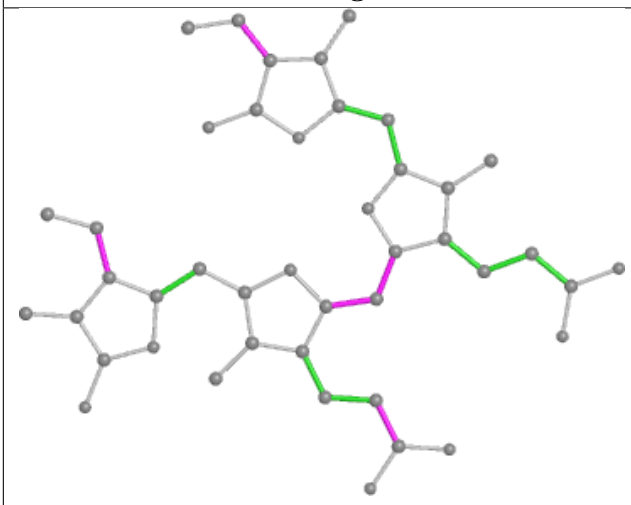

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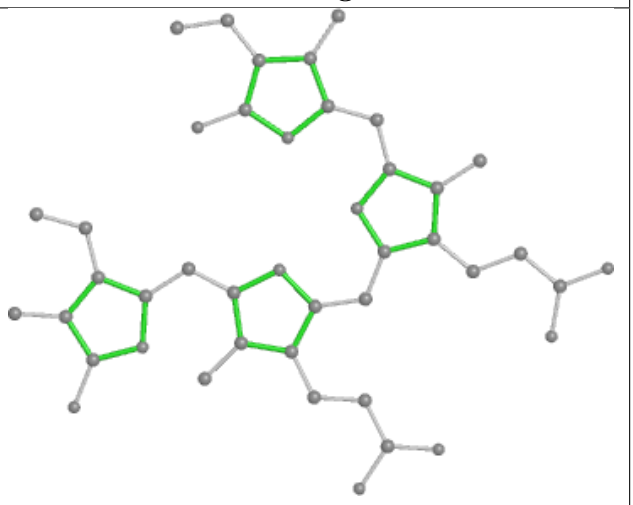
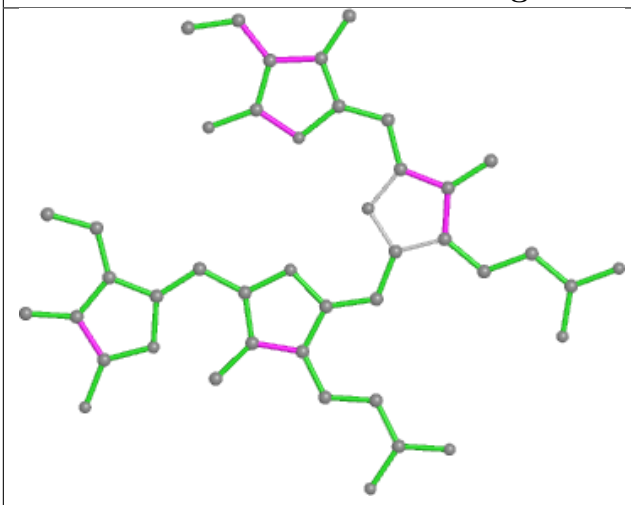


Rings

Ligand PEB 34 1001



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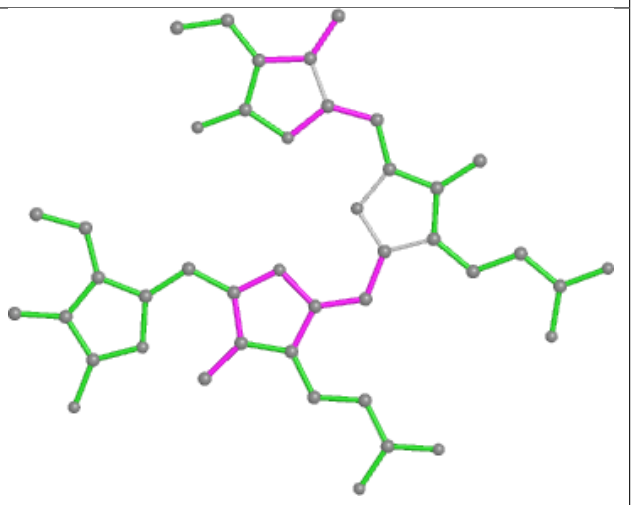

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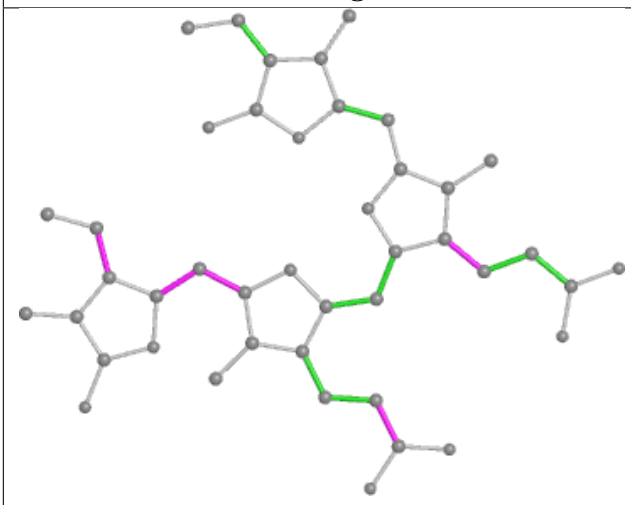

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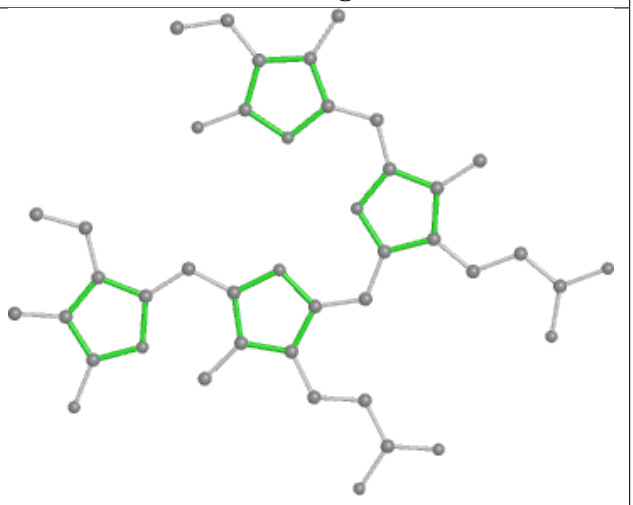
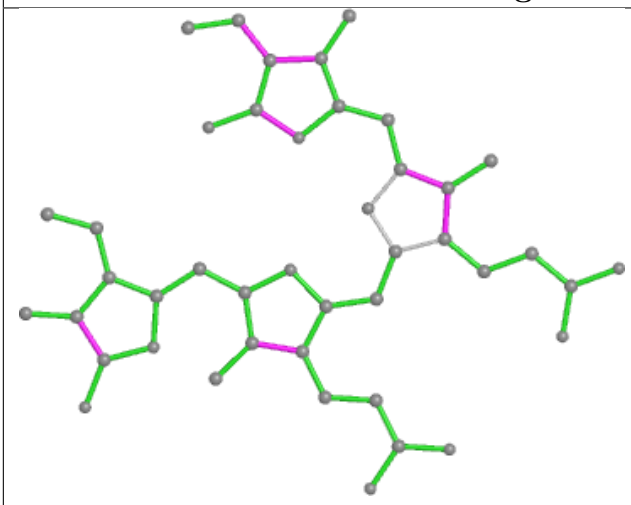


Rings

Ligand PEB N9 202



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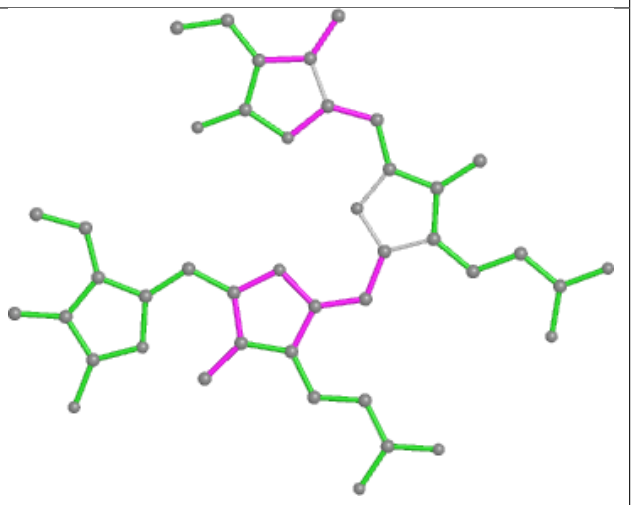

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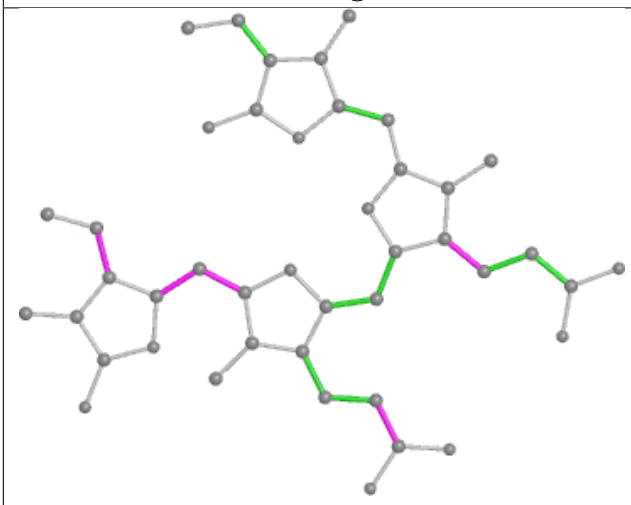

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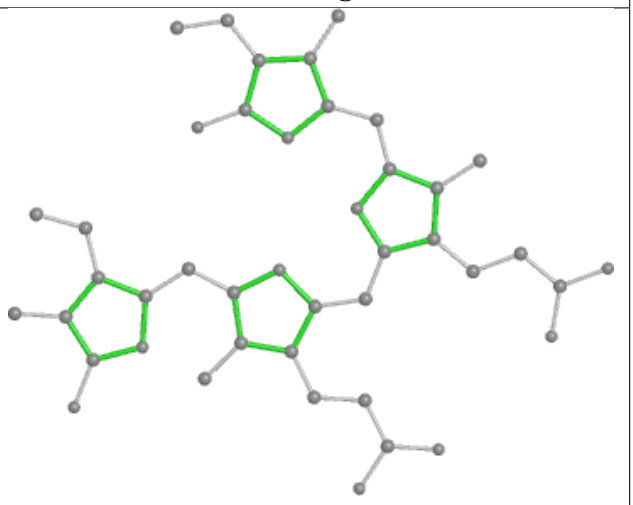
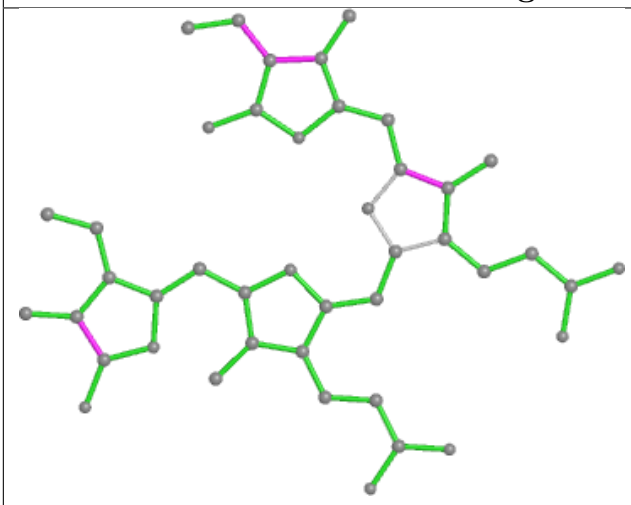


Rings

Ligand PEB hS 202



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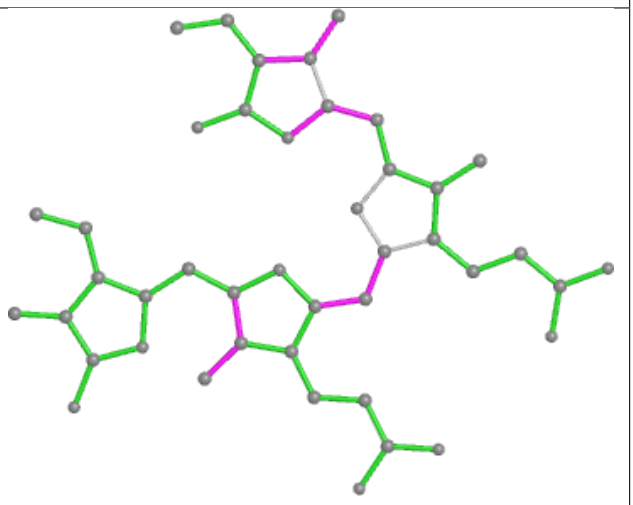

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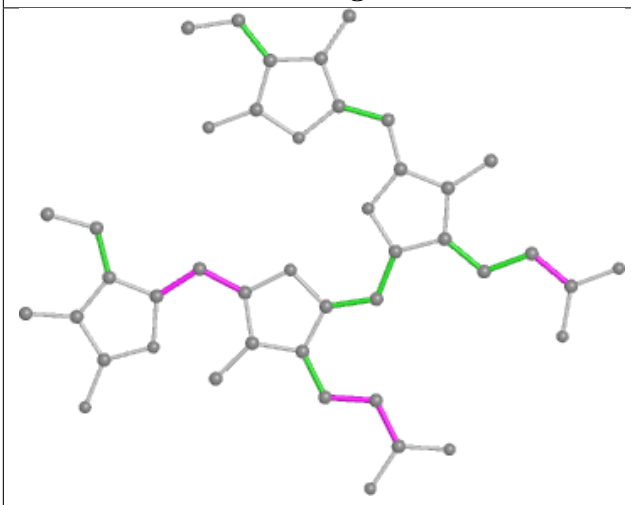

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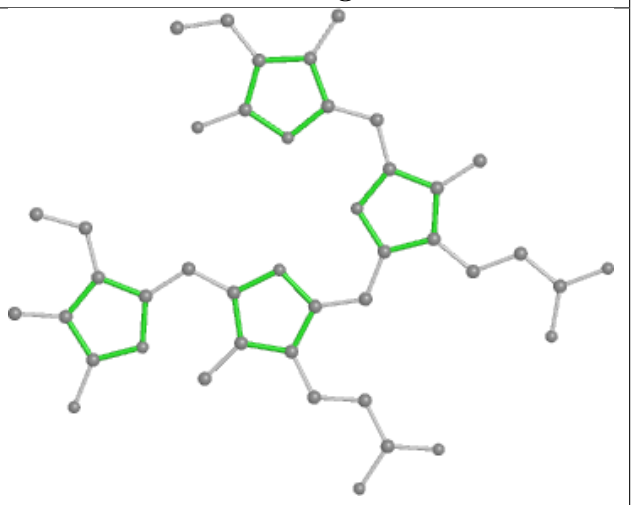
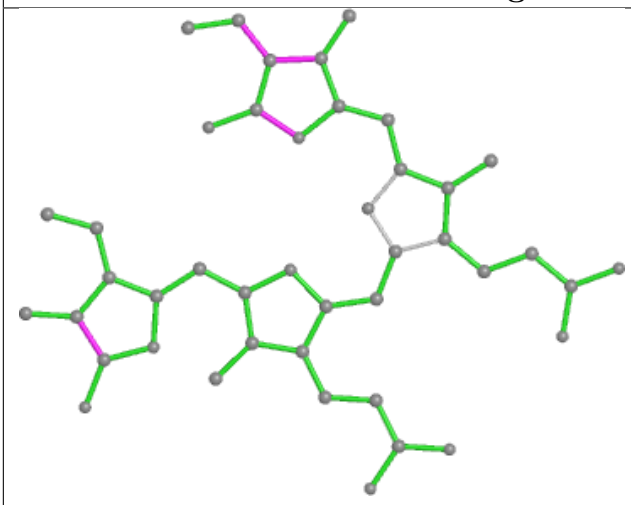
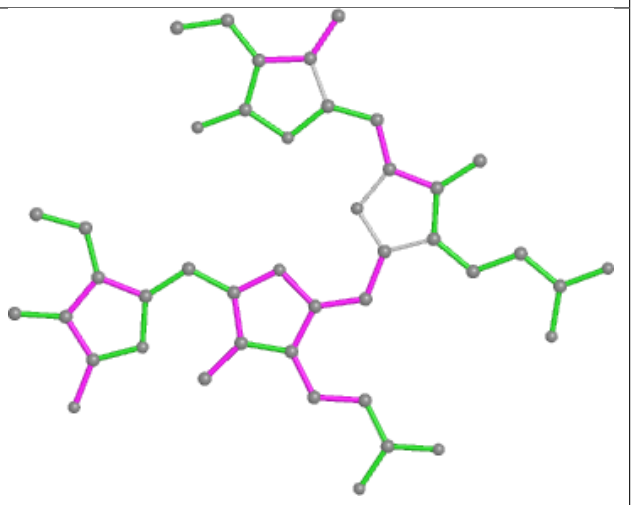


Rings

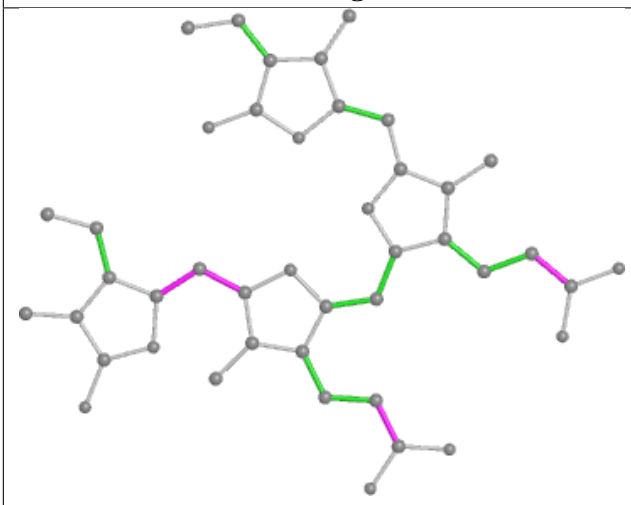
Ligand PEB dZ 1001



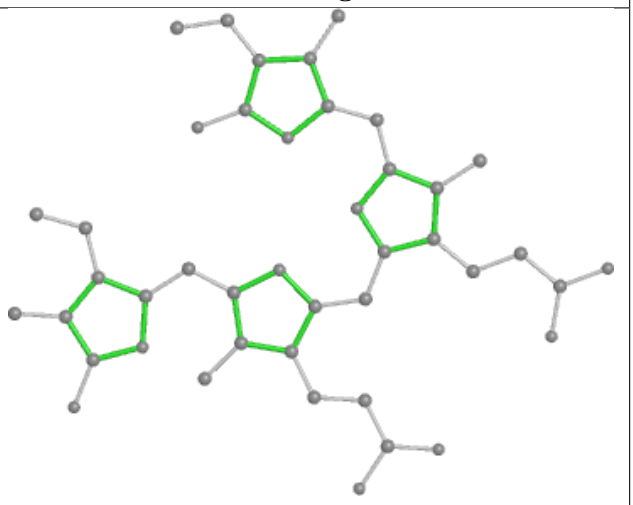
Bond lengths



Bond angles

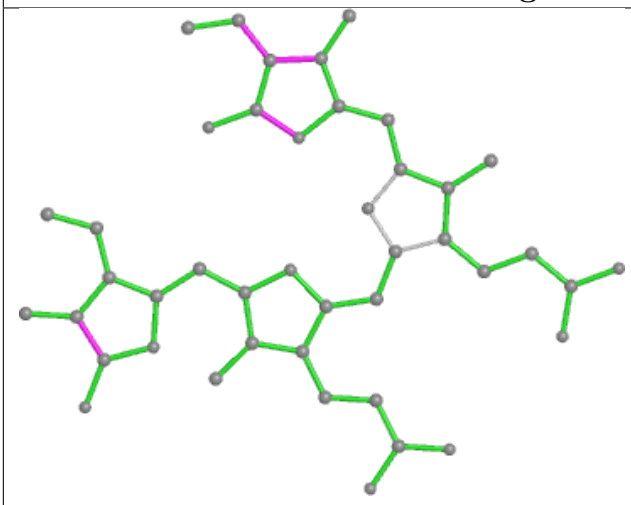


Torsions



Rings

Ligand PEB x5 201



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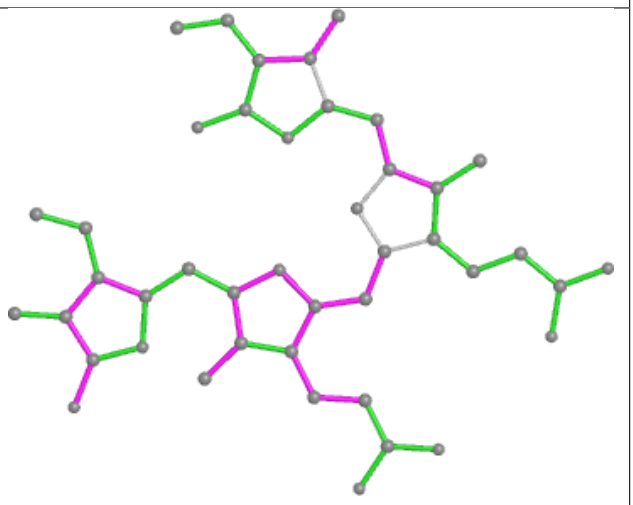

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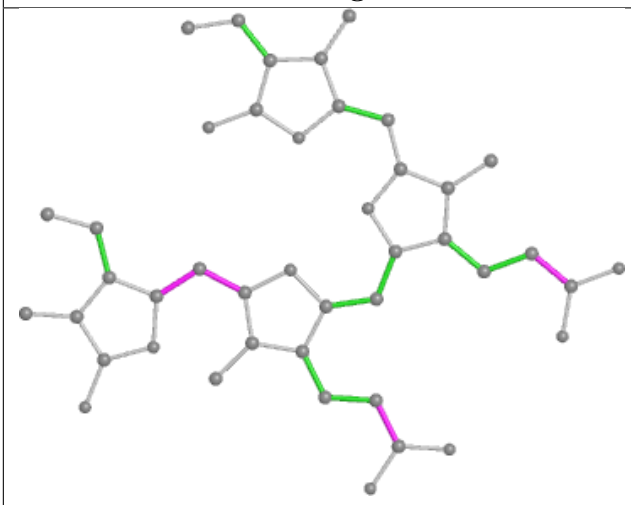

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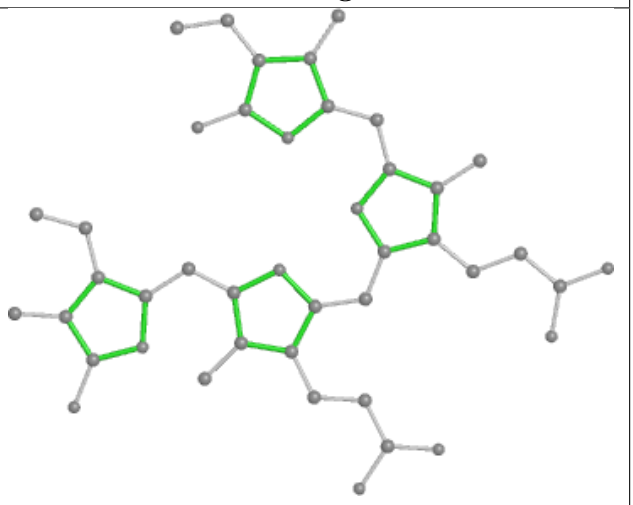
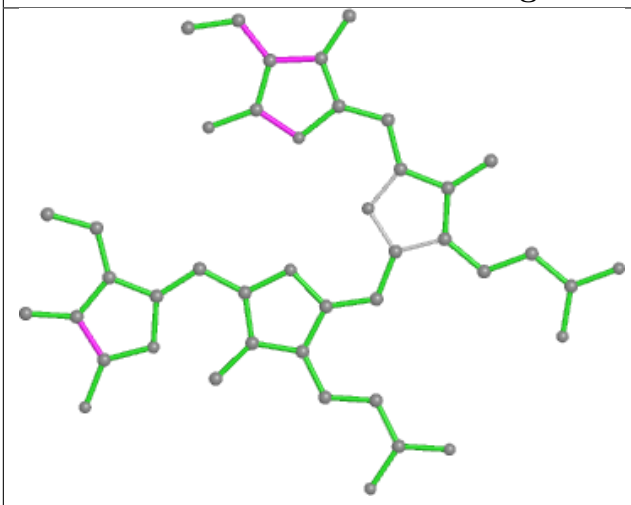


Rings

Ligand PEB cd 201



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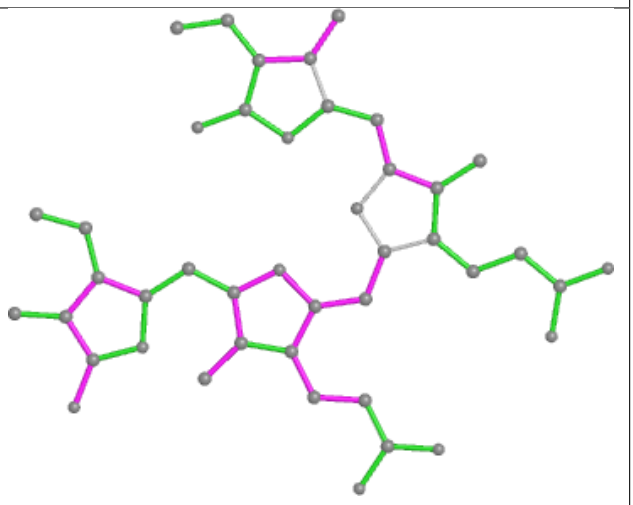
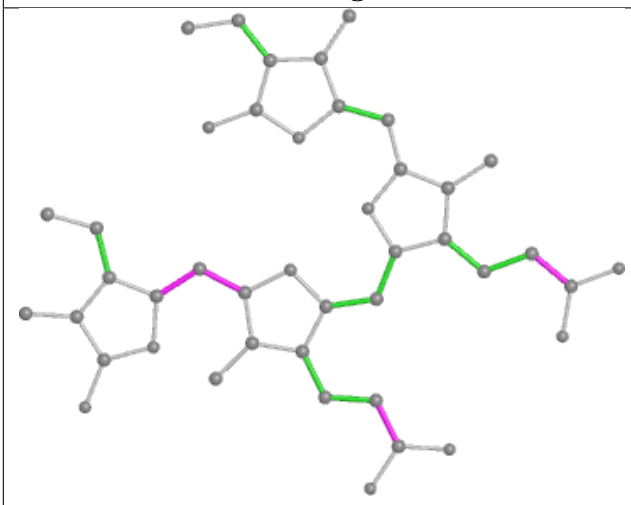


Bond angles



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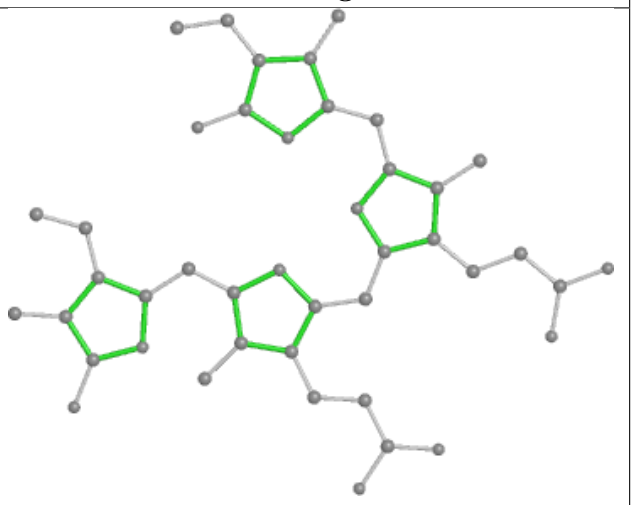
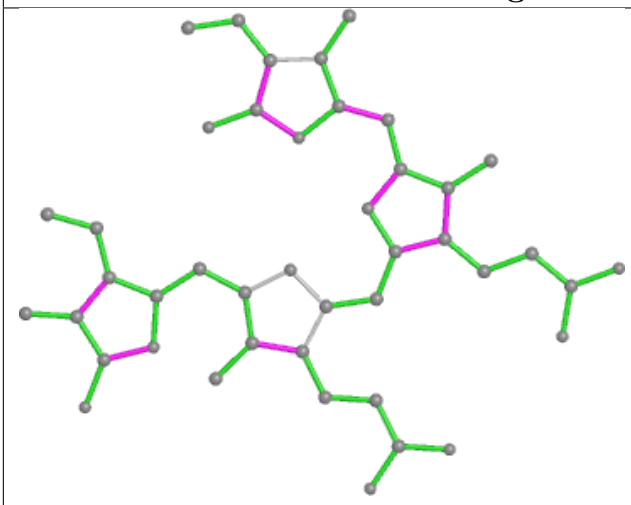


Rings

Ligand PUB kS 1003



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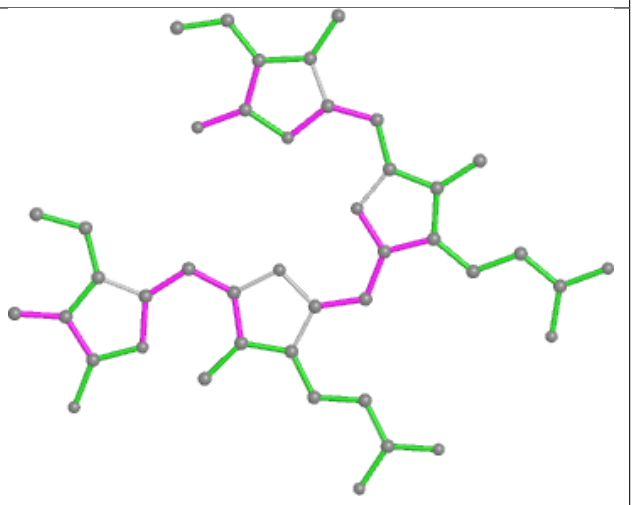

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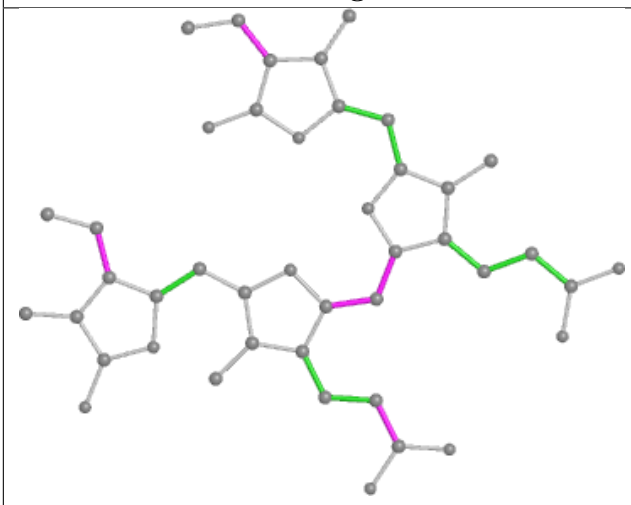

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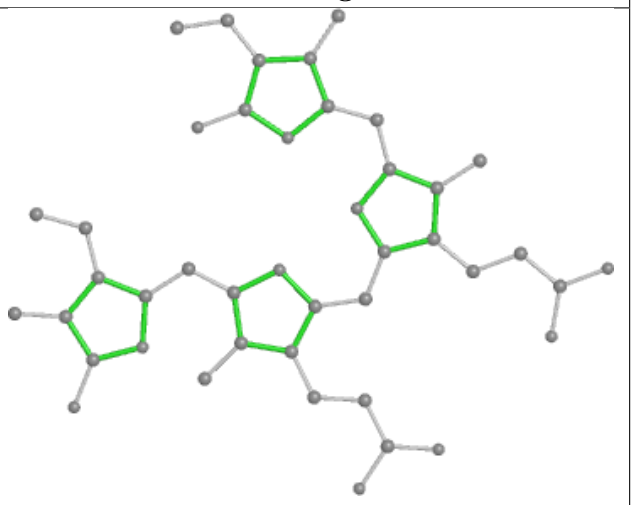
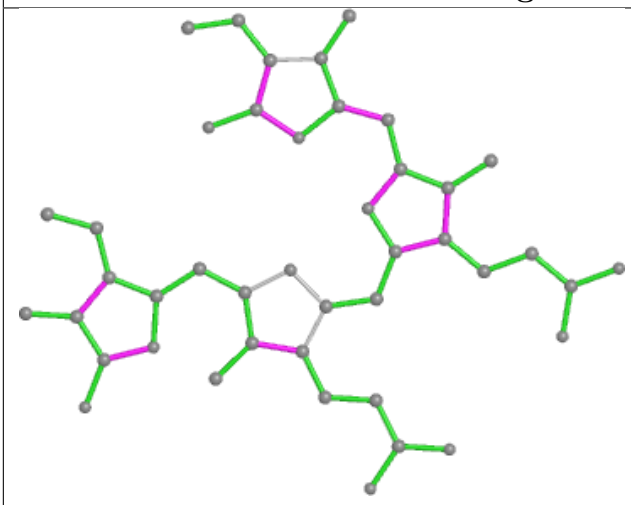


Rings

Ligand PUB b6 203



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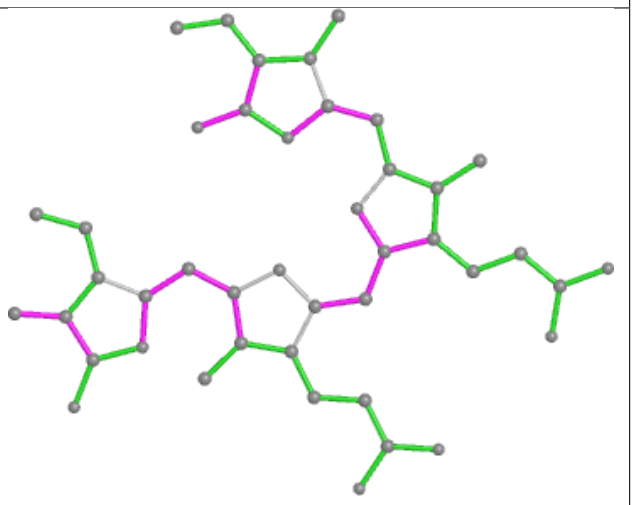

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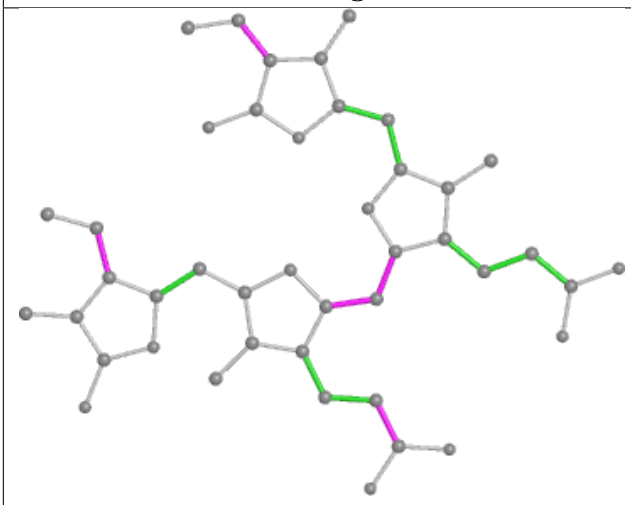

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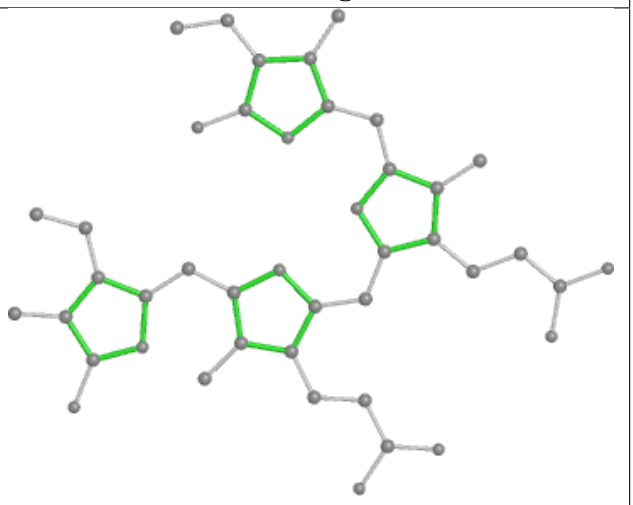
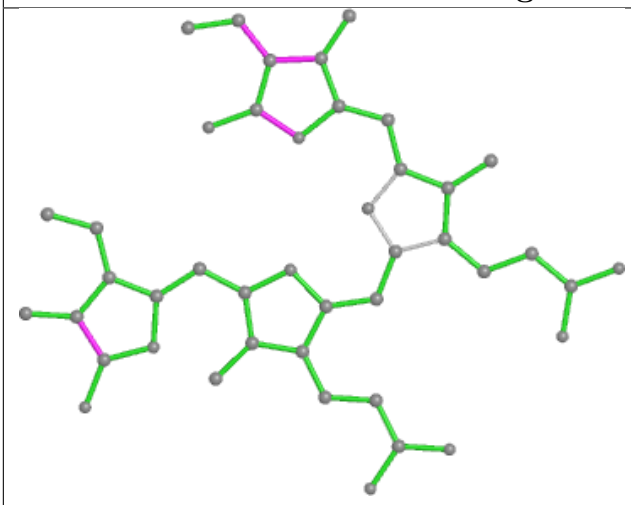


Rings

Ligand PEB cR 202



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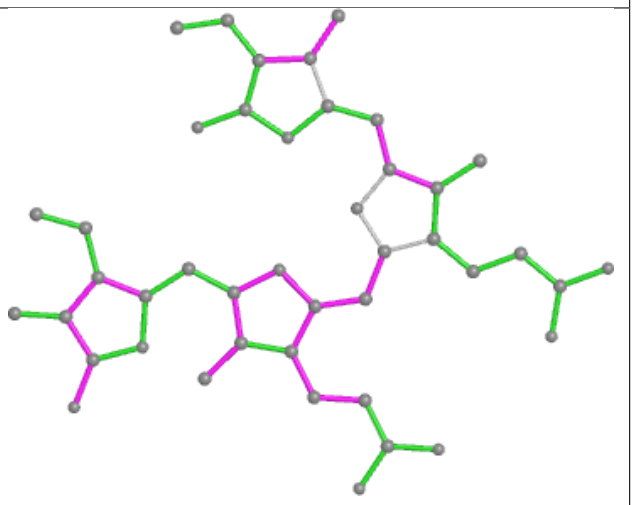
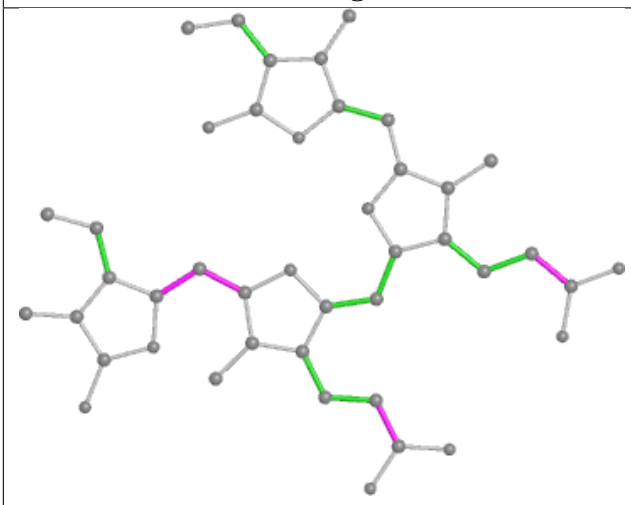


Bond angles



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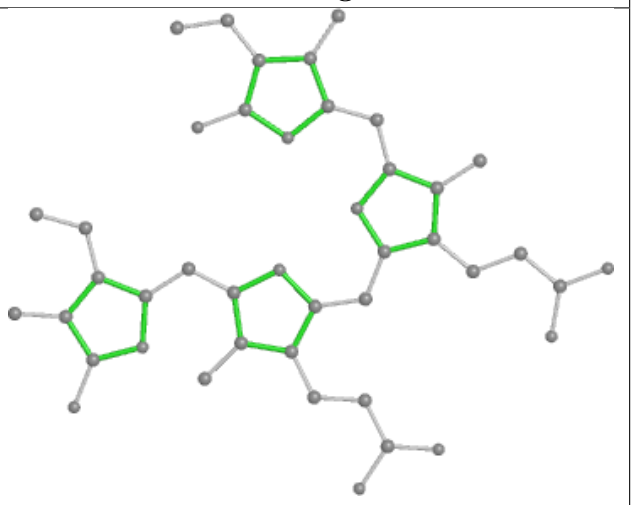

Rings

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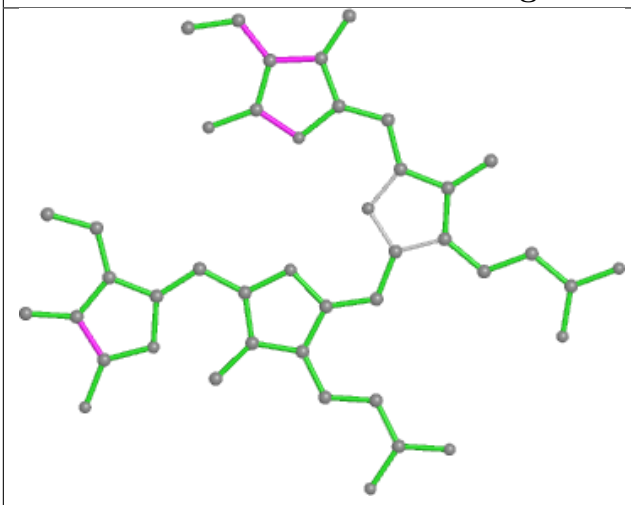

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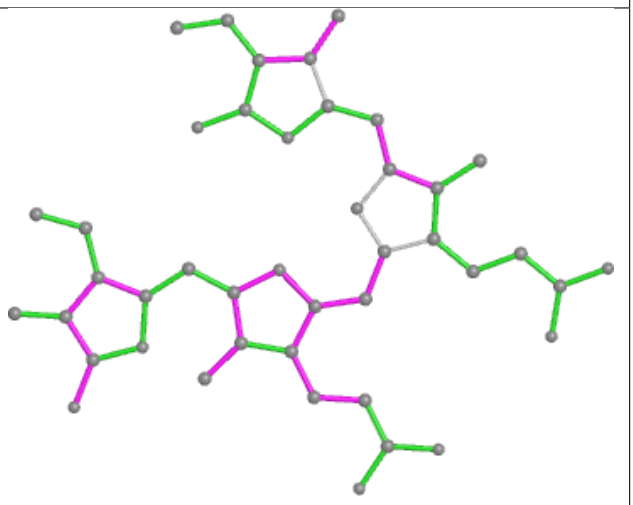
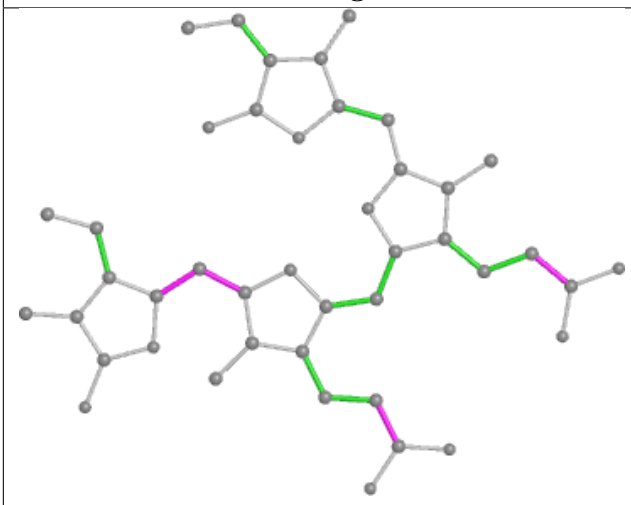


Bond angles



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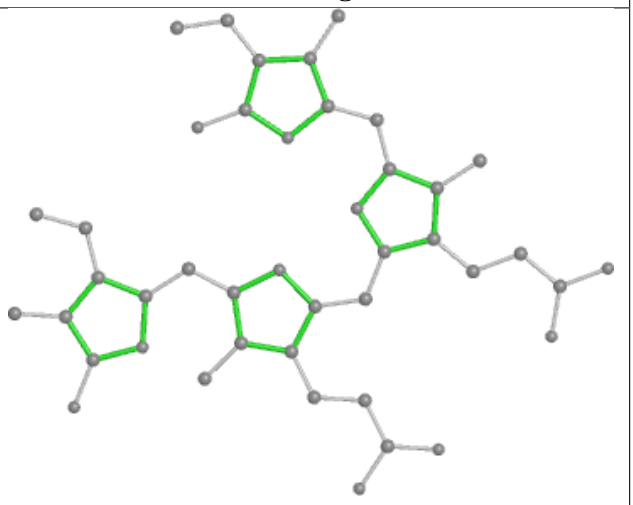
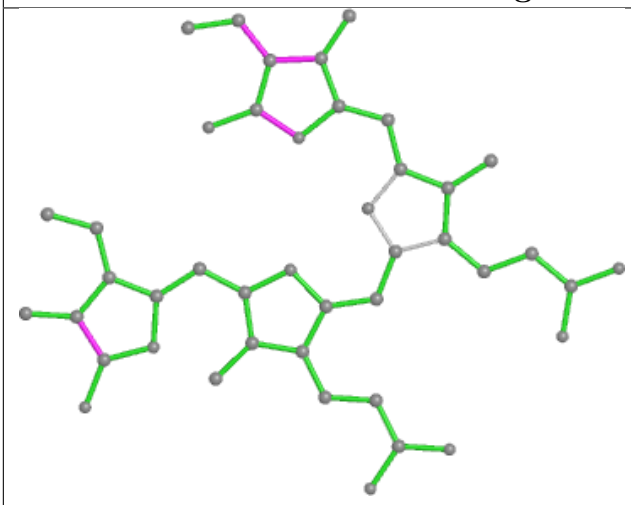


Rings

Ligand PEB bX 402



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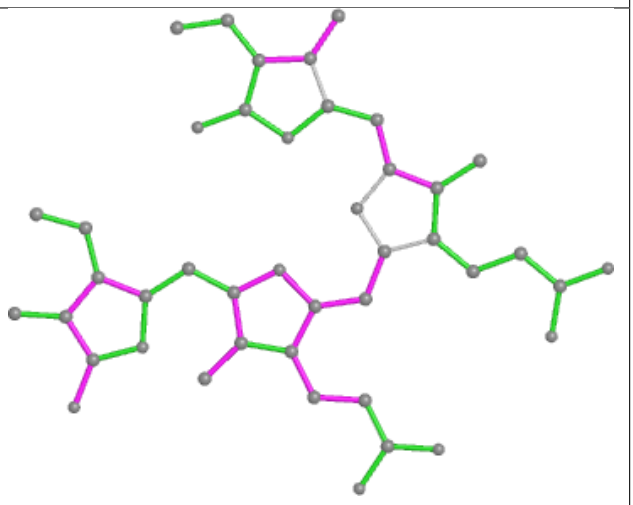

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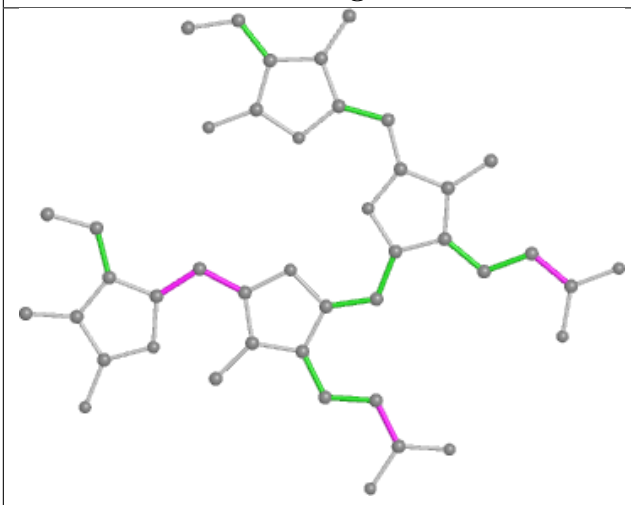

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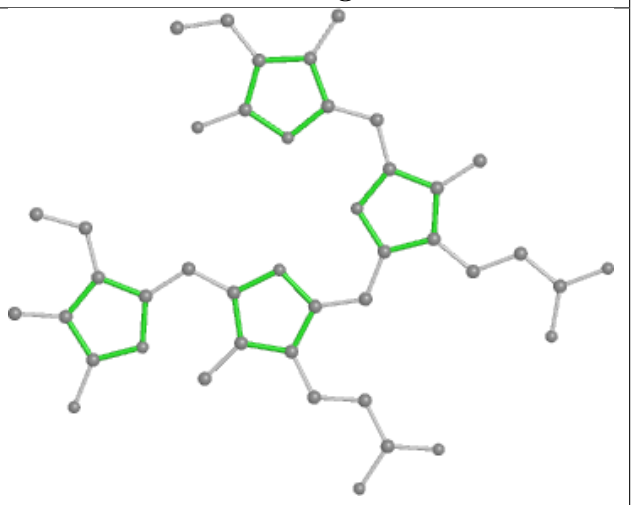
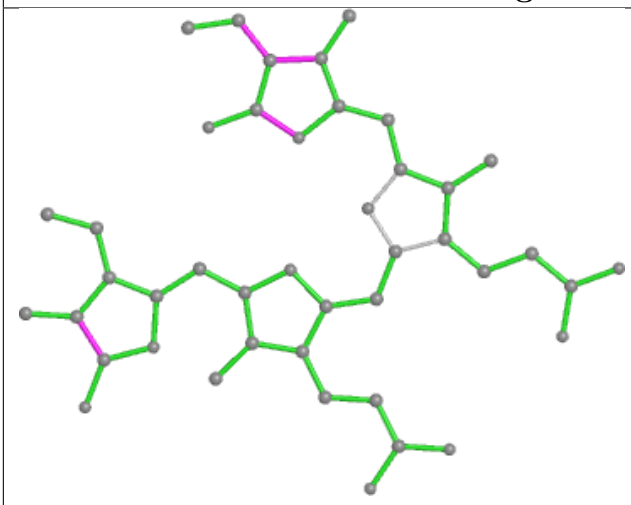


Rings

Ligand PEB eU 202



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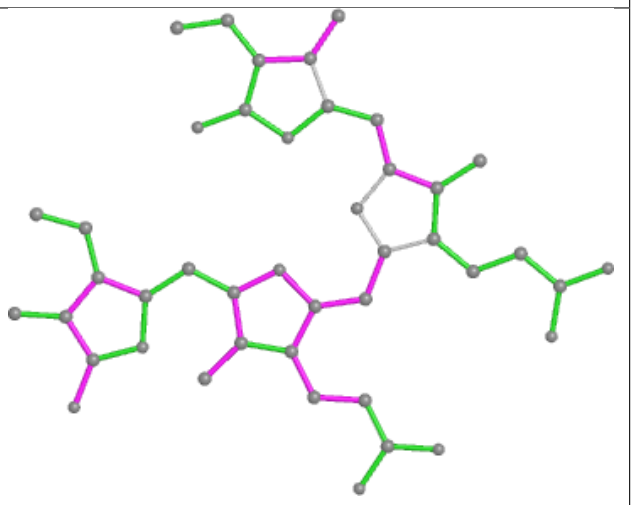

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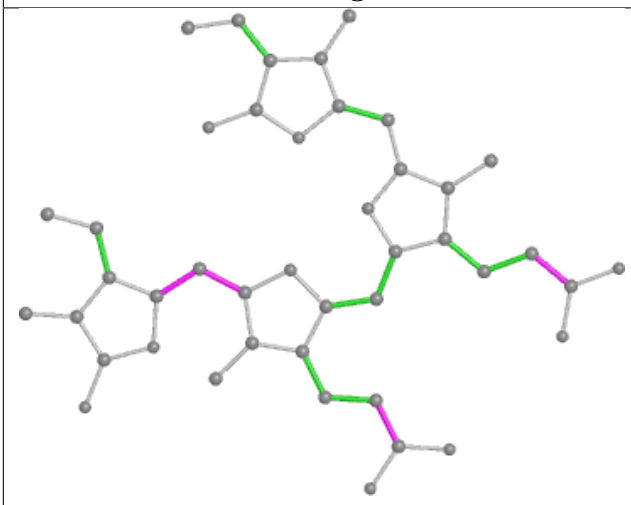

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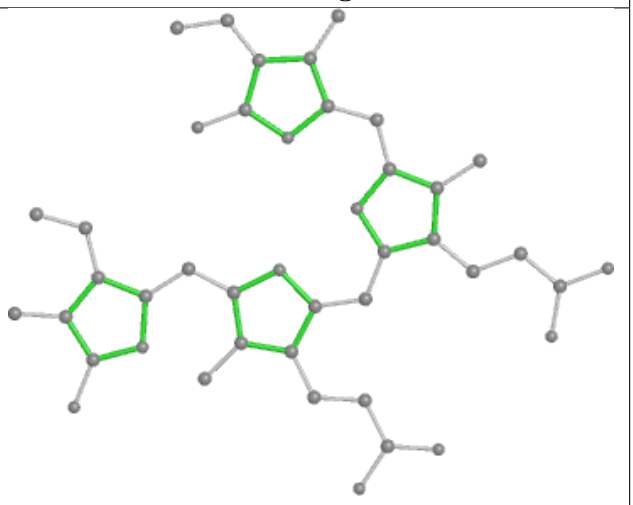
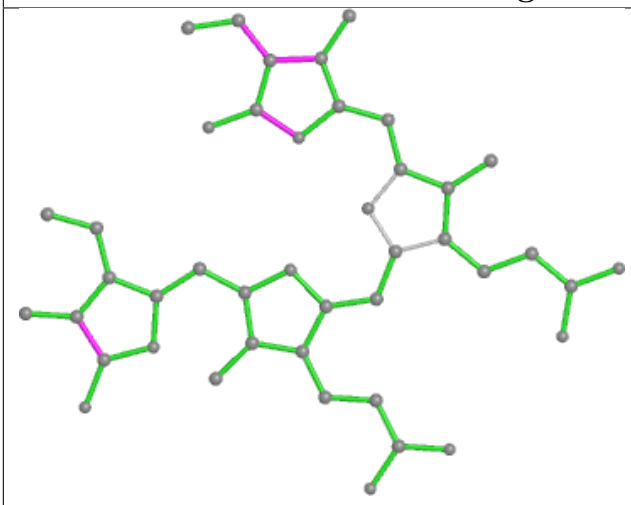


Rings

Ligand PEB F6 201



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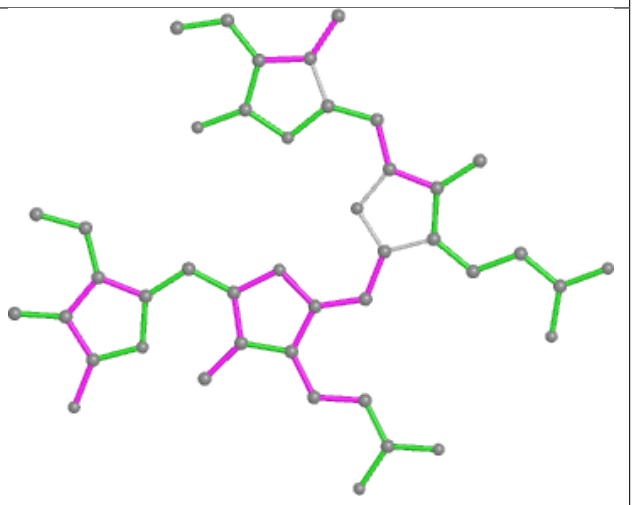

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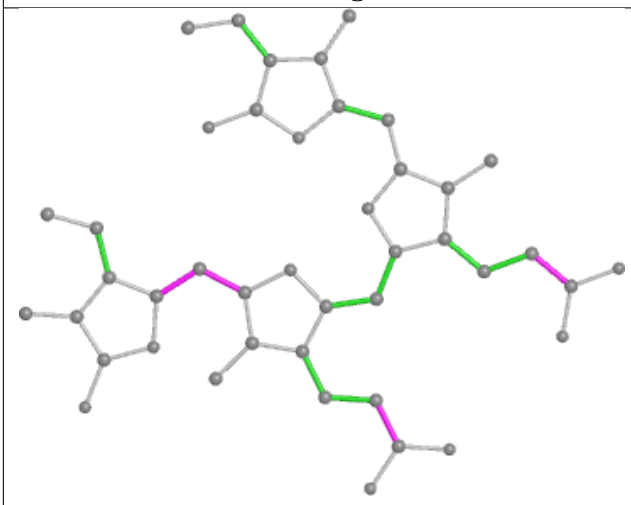

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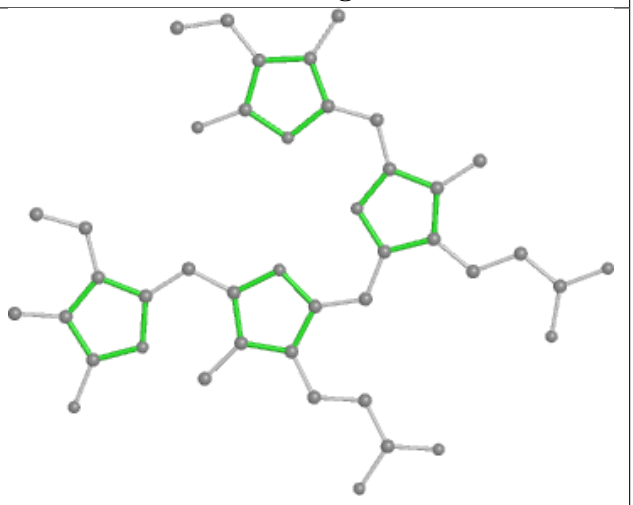
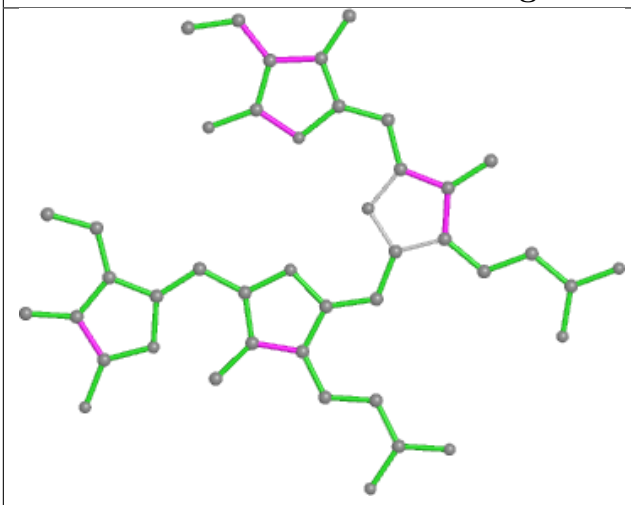


Rings

Ligand PEB J6 202



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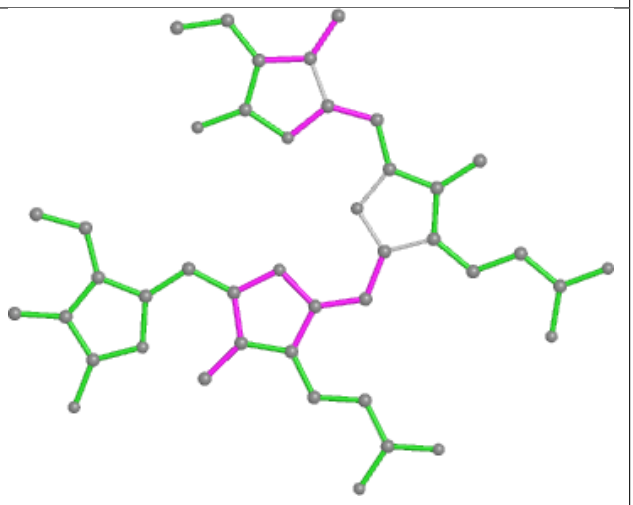

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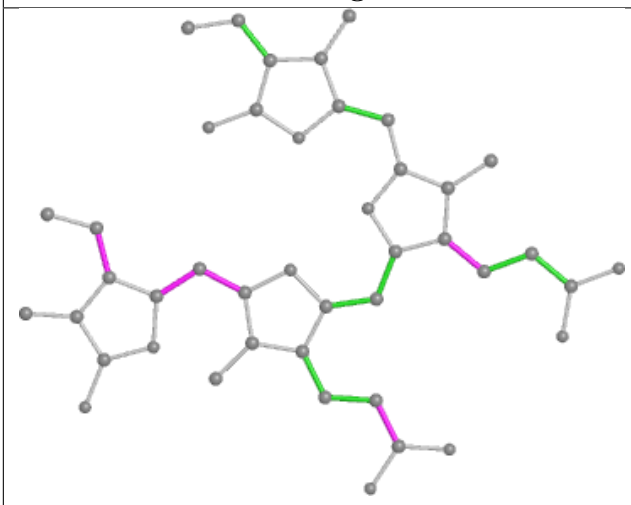

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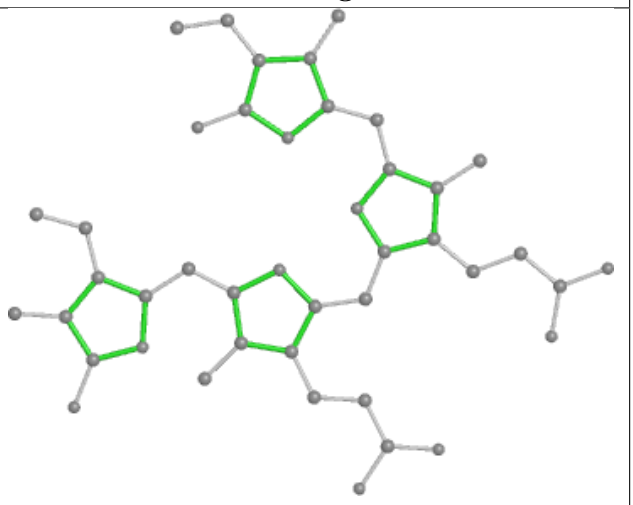
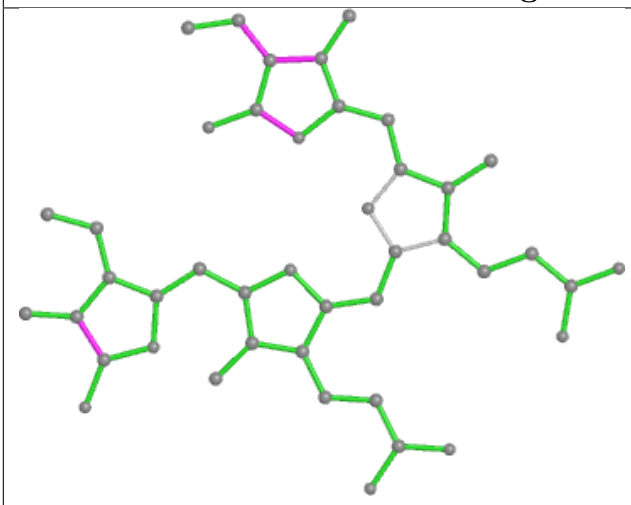


Rings

Ligand PEB dr 202



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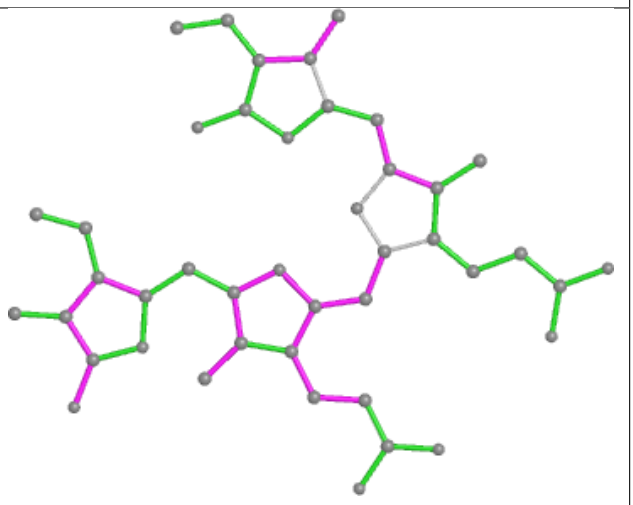

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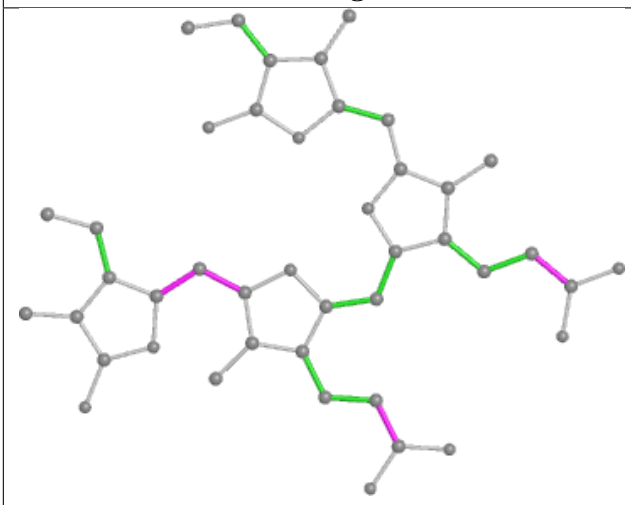

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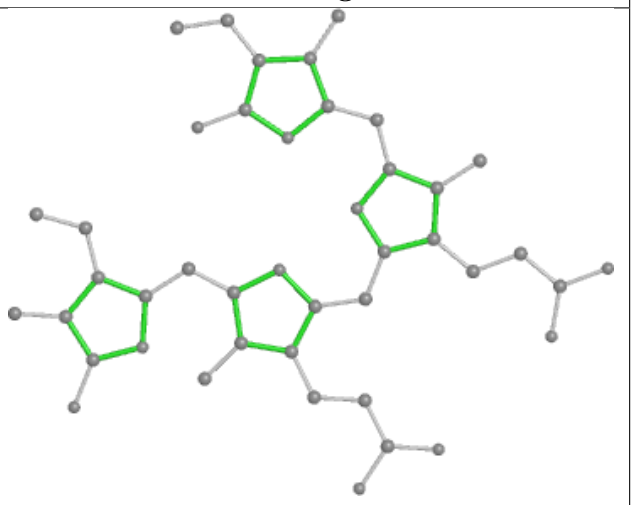
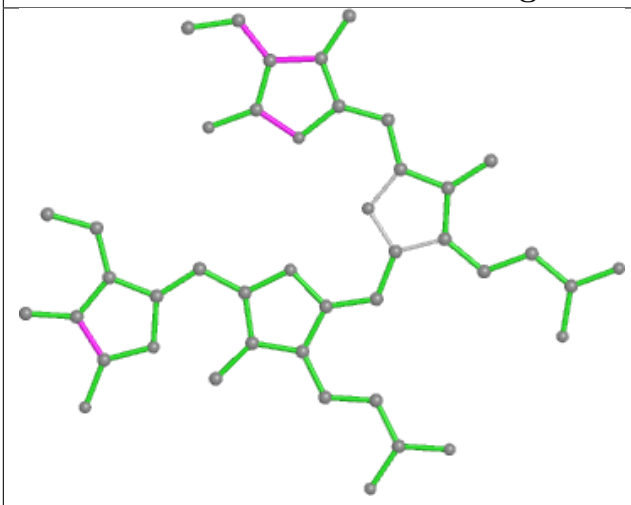


Rings

Ligand PEB x2 201



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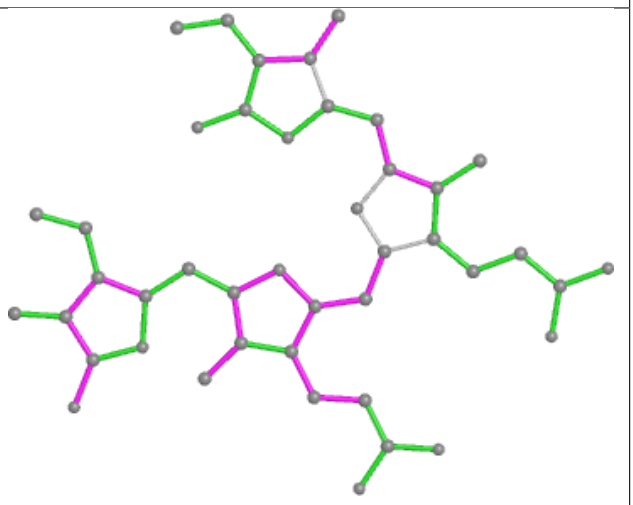
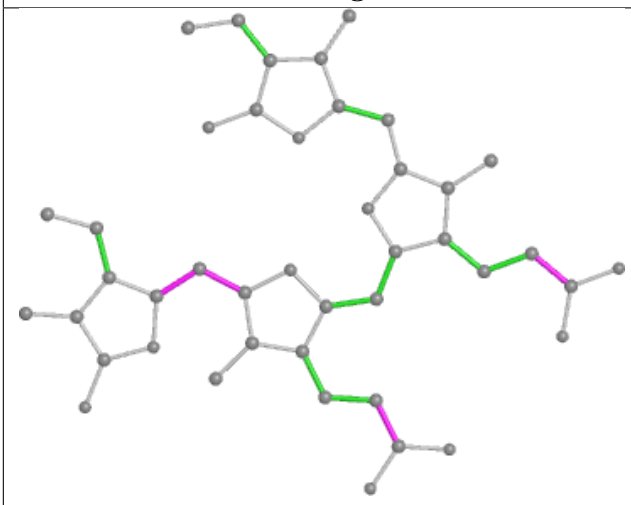


Bond angles



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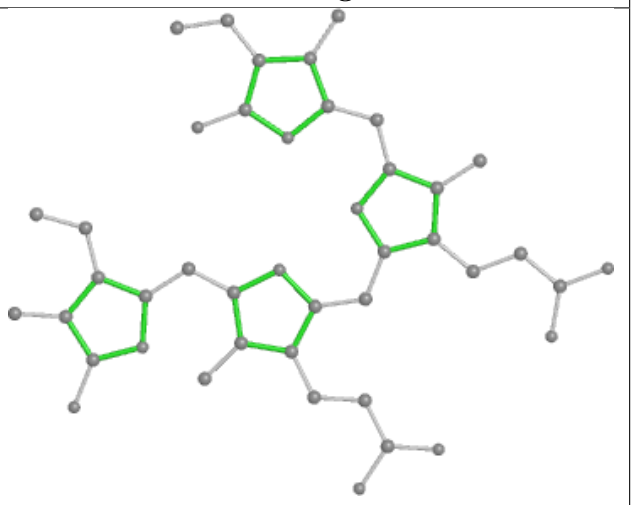
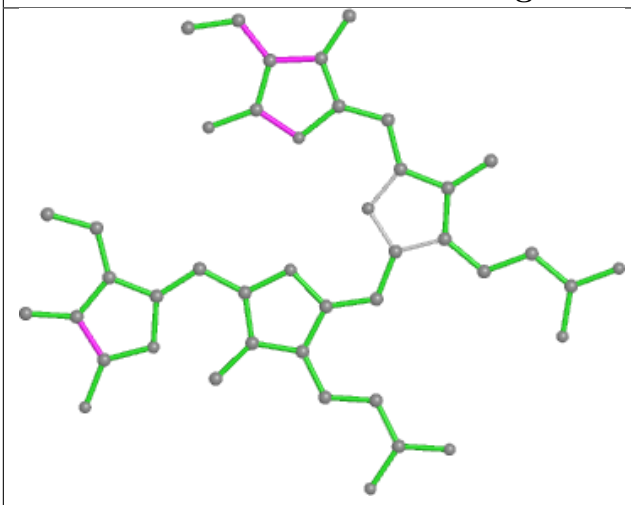


Rings

Ligand PEB O6 202



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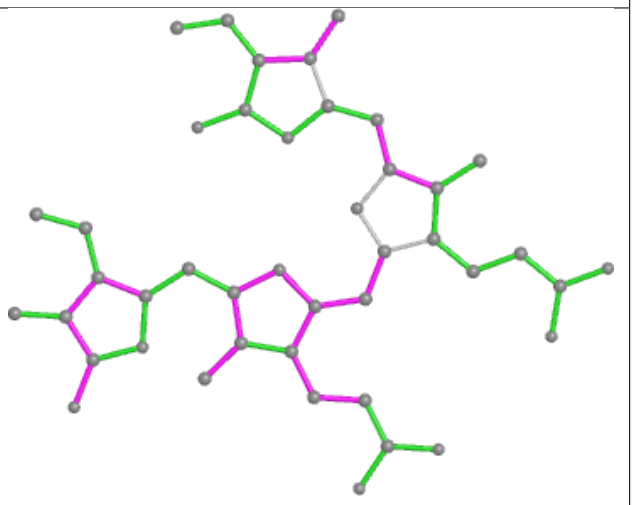
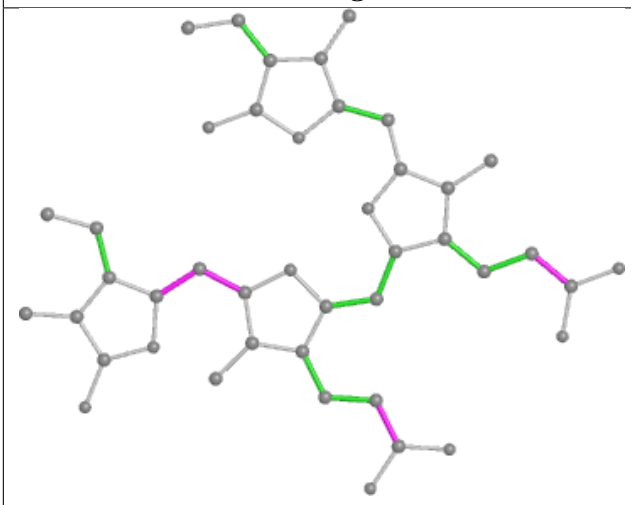
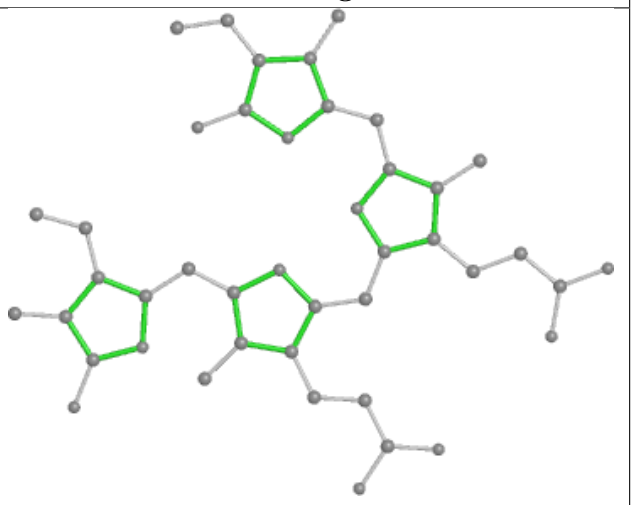


Bond angles

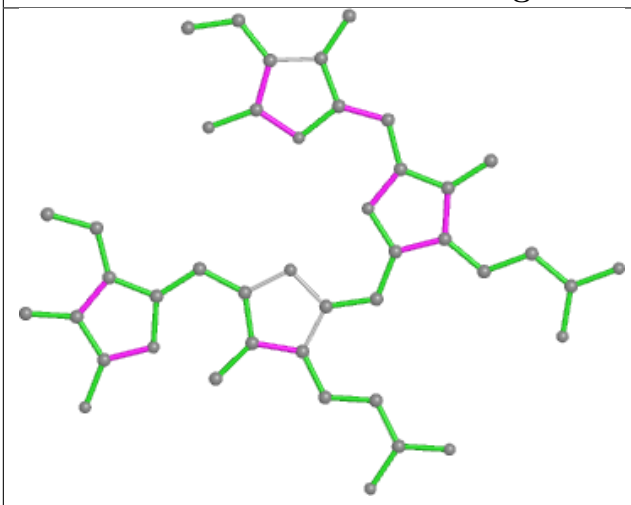


Torsions



Rings

Ligand PUB D2 304



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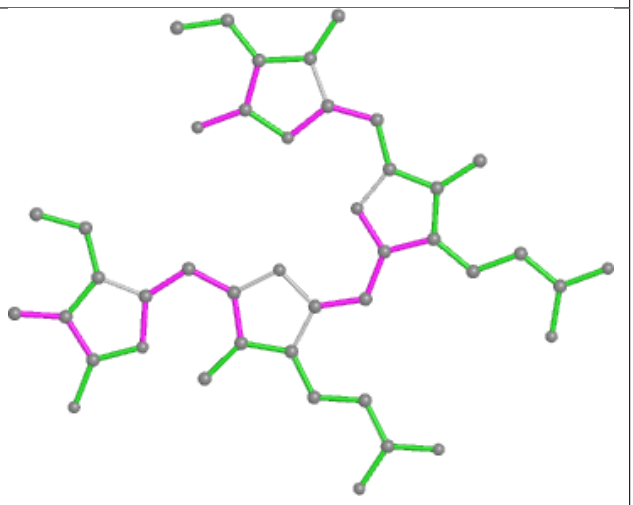

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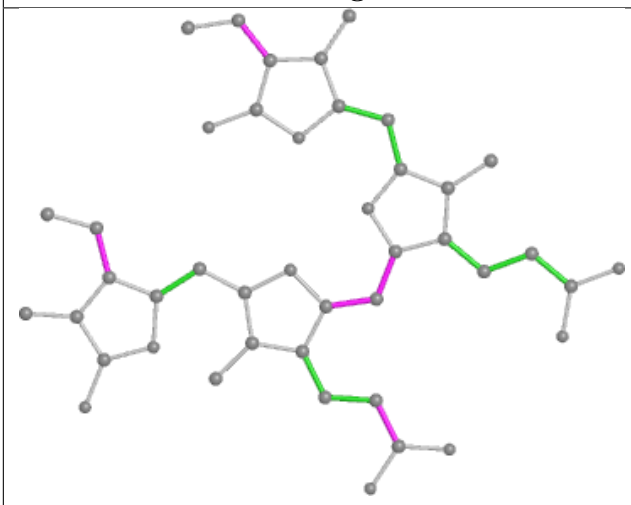

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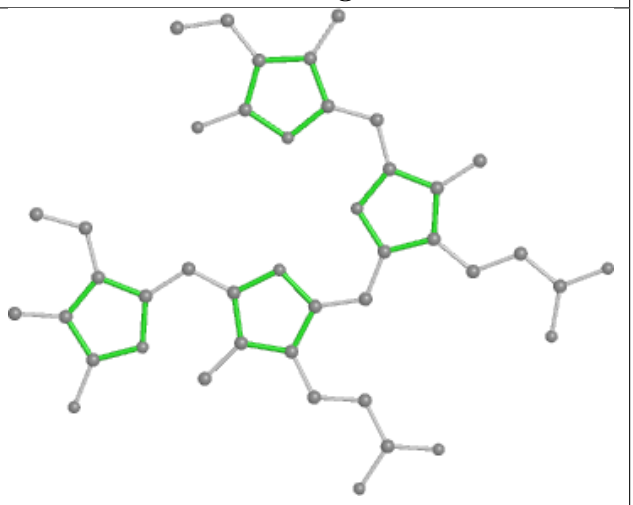
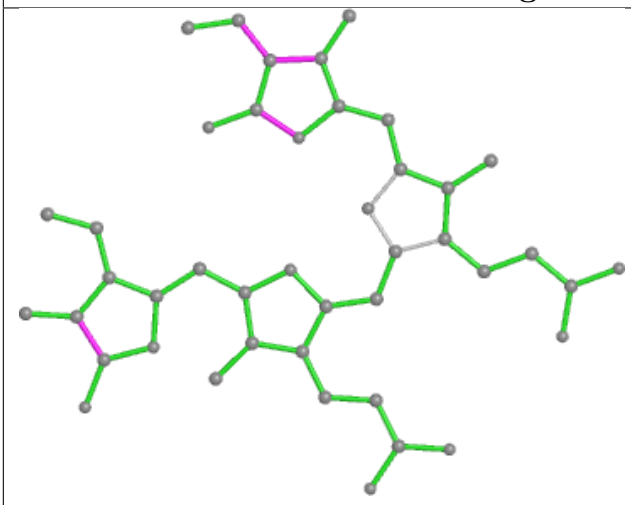


Rings

Ligand PEB J4 202



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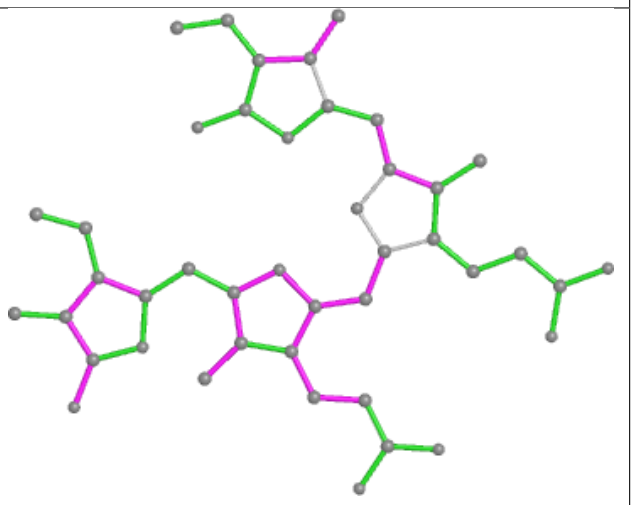

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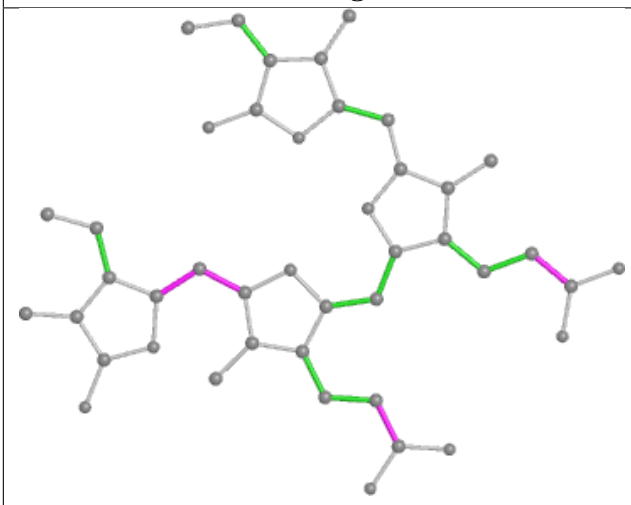

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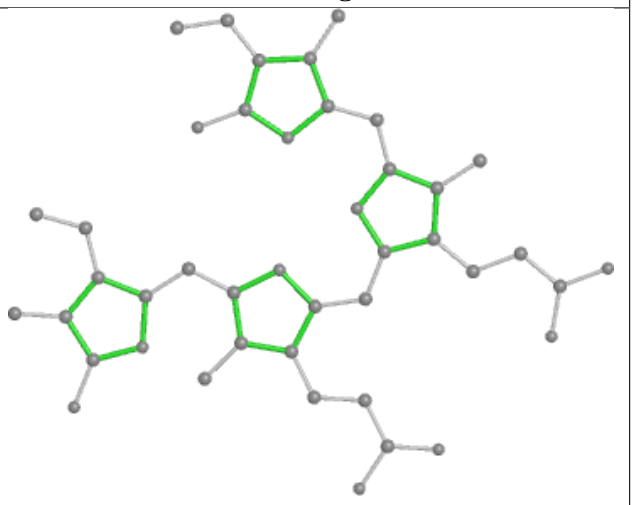
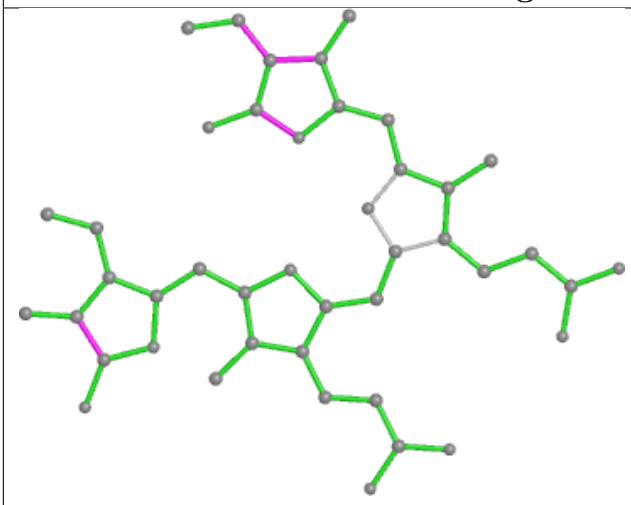


Rings

Ligand PEB cX 202



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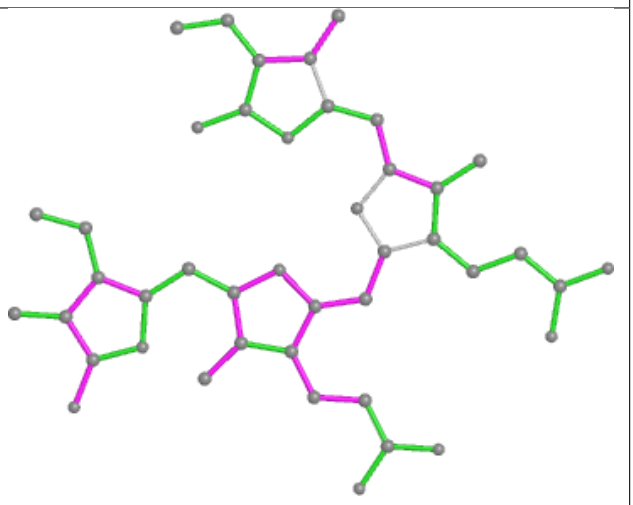
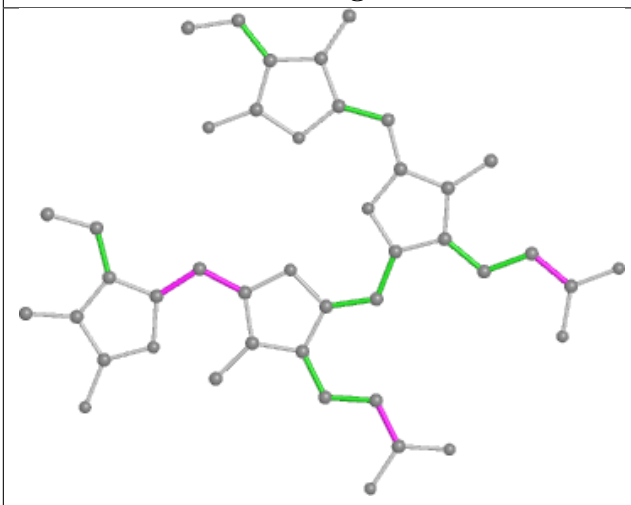


Bond angles



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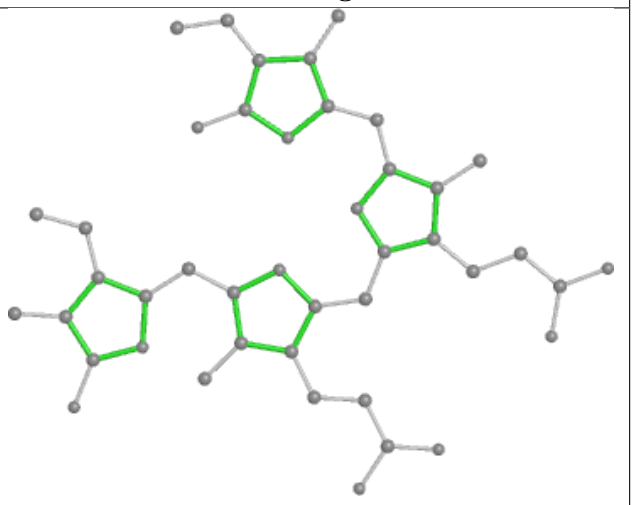
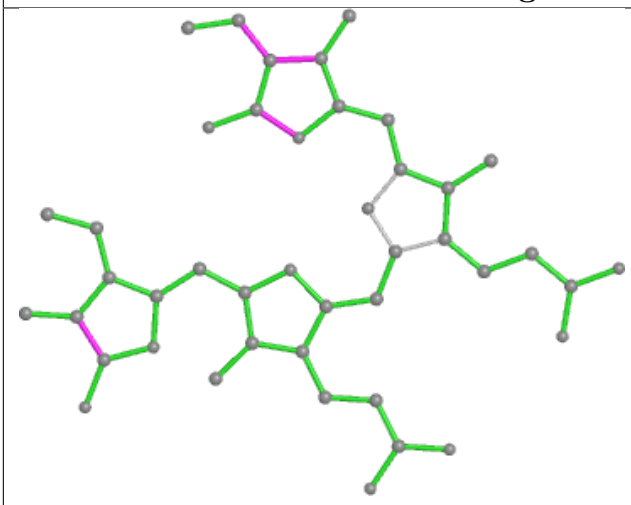


Rings

Ligand PEB n3 201



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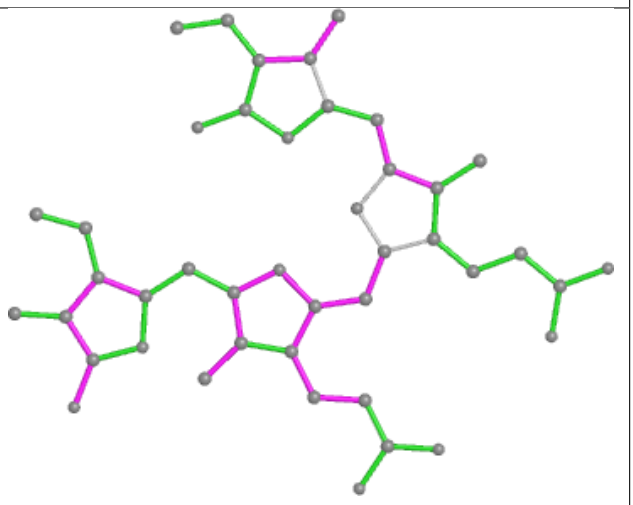

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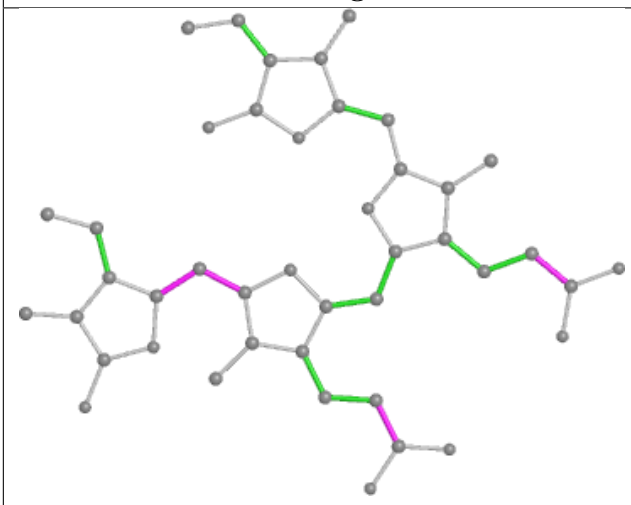

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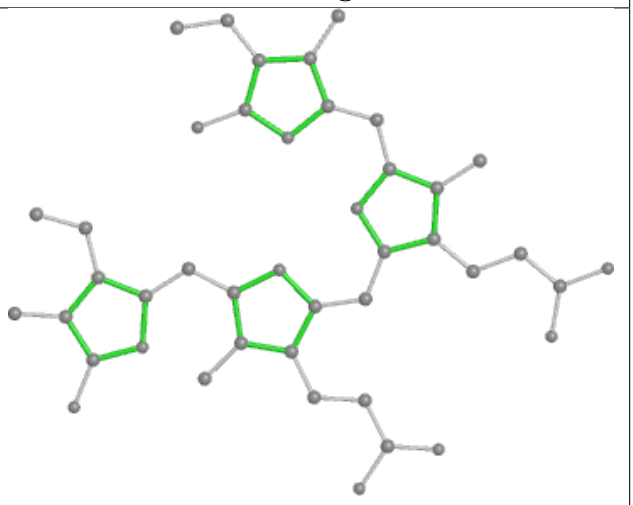

Rings

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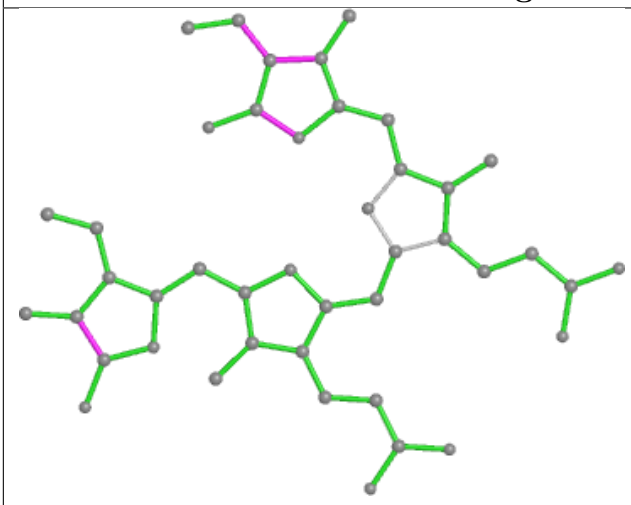

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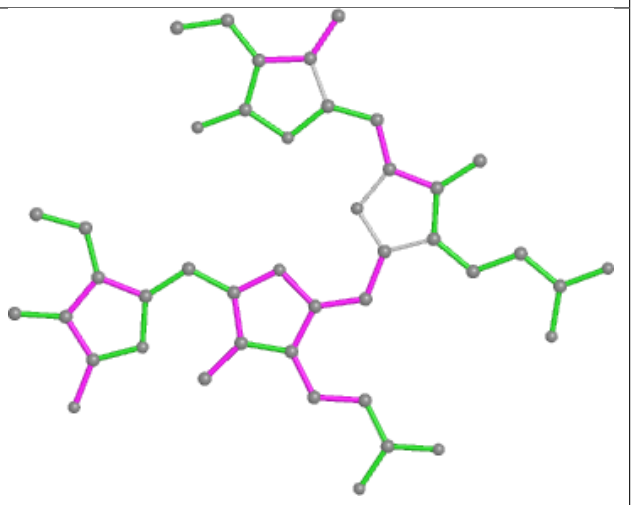

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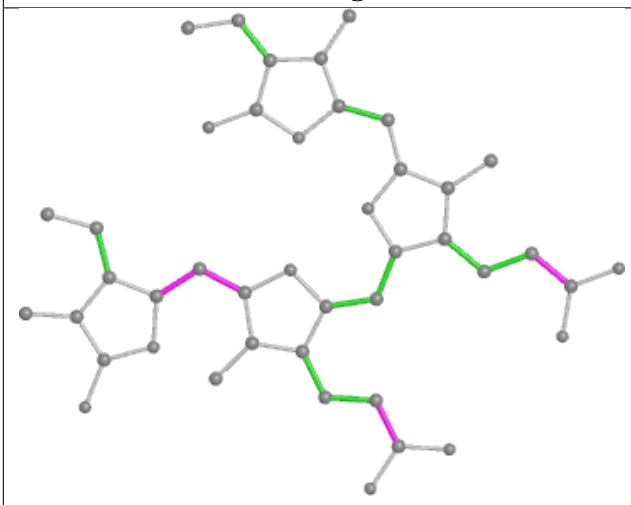

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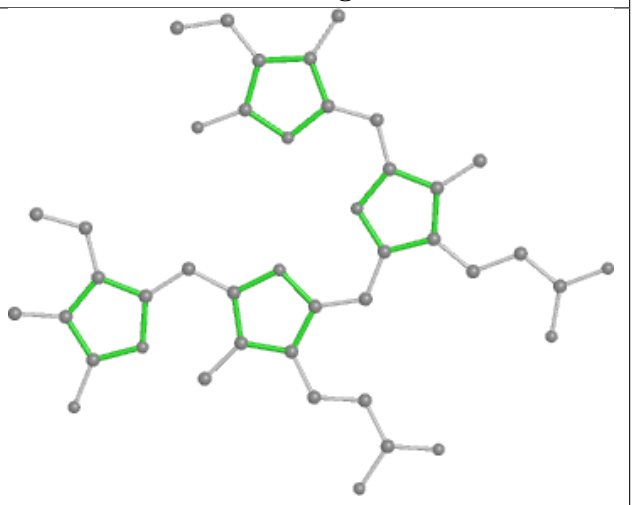
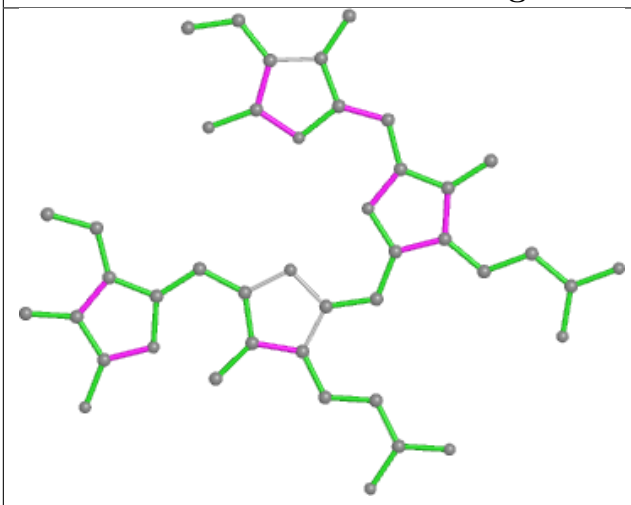


Rings

Ligand PUB 34 1005



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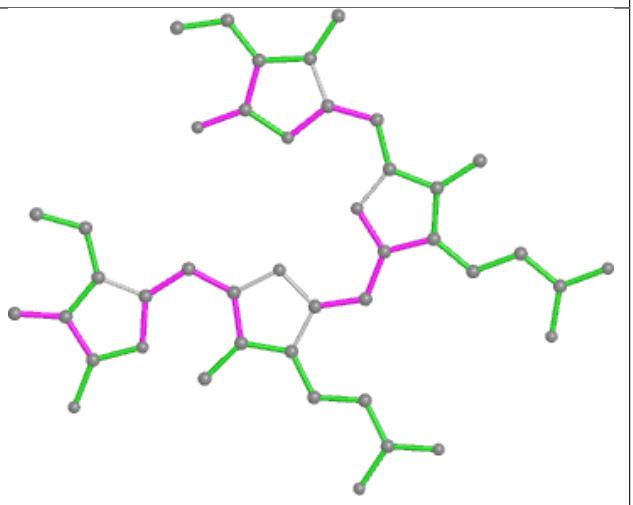

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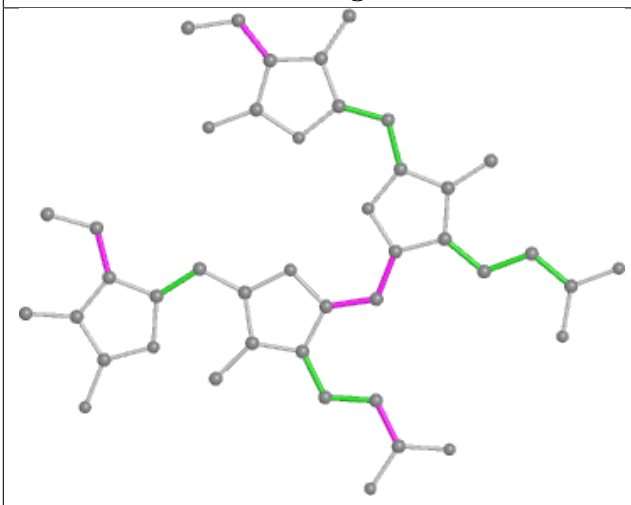

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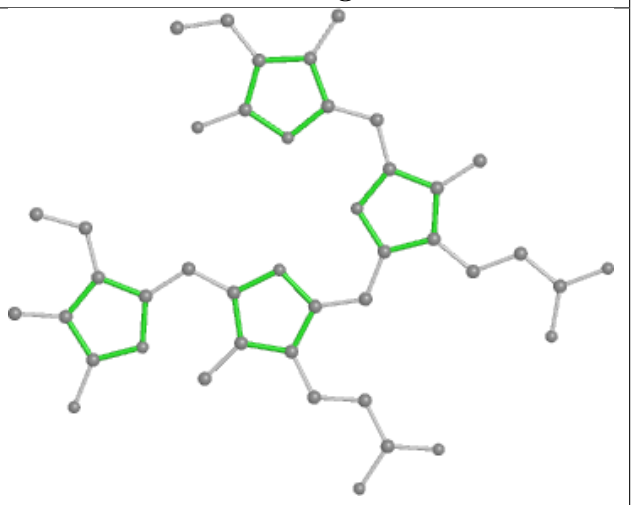

Rings

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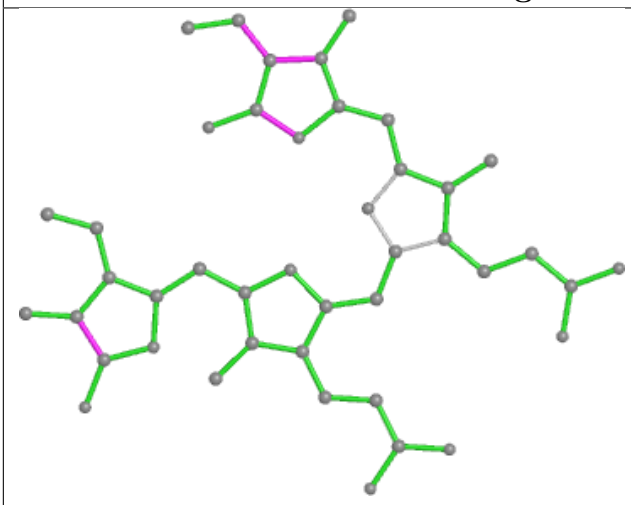

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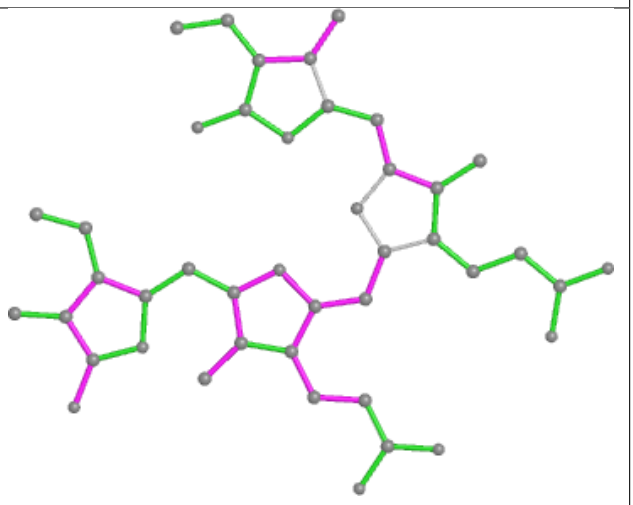

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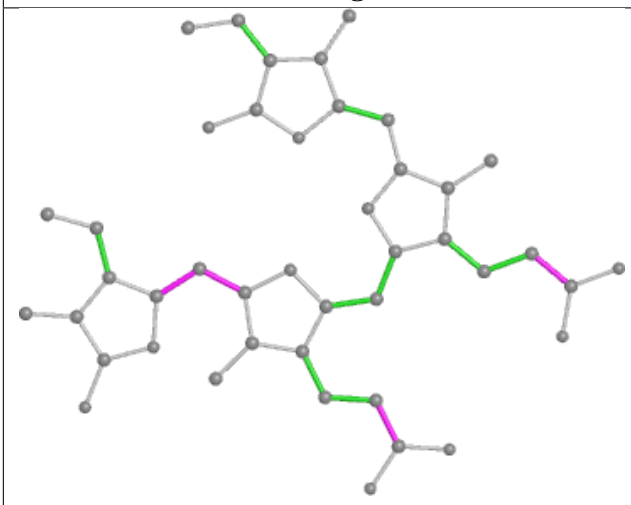

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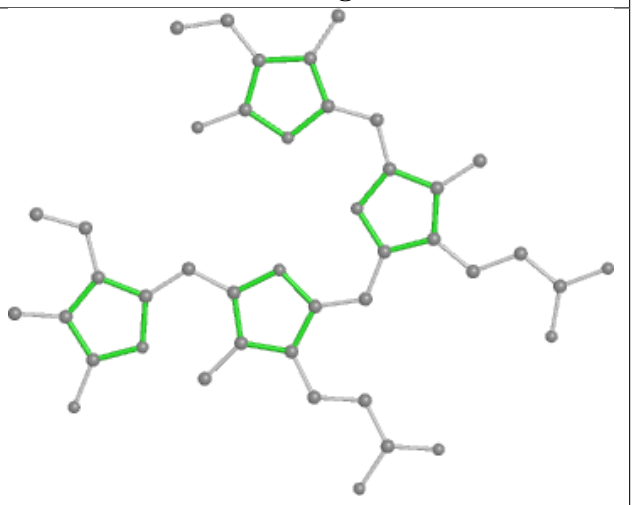

Rings

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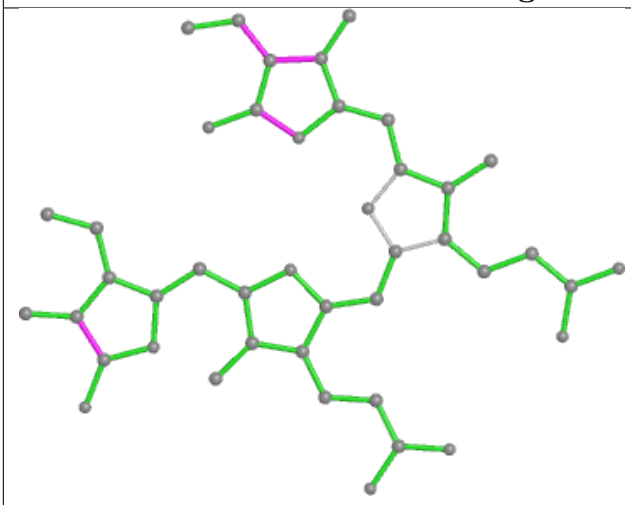

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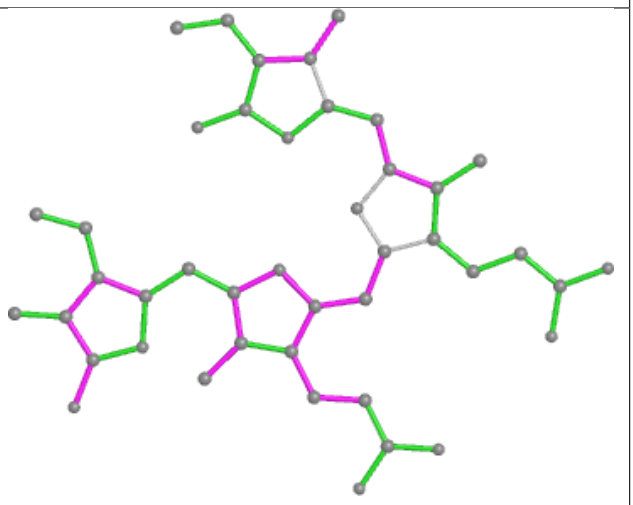

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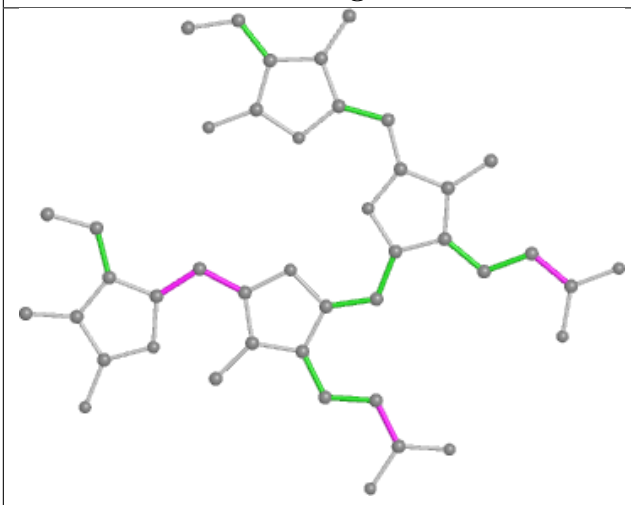

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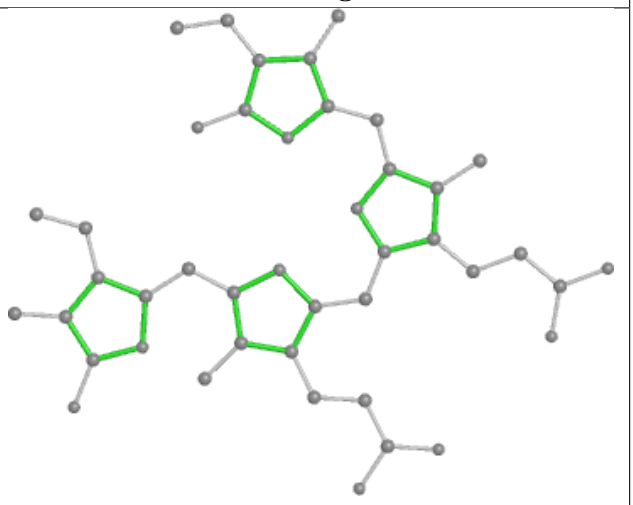

Rings

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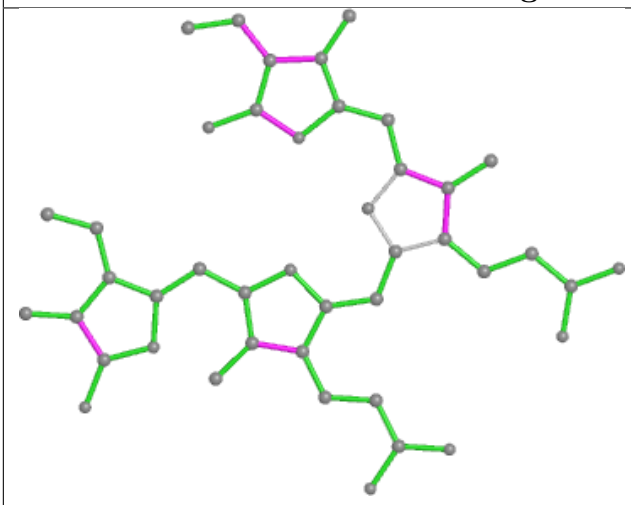

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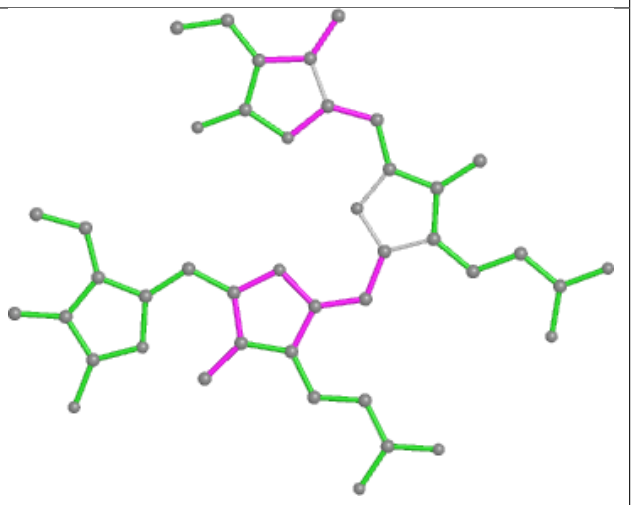

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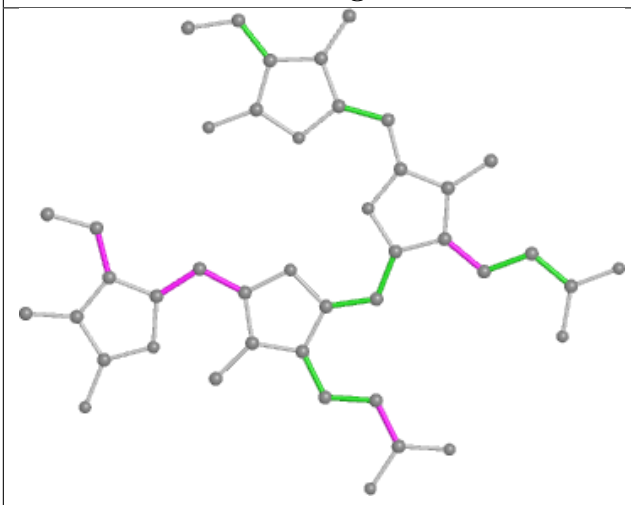

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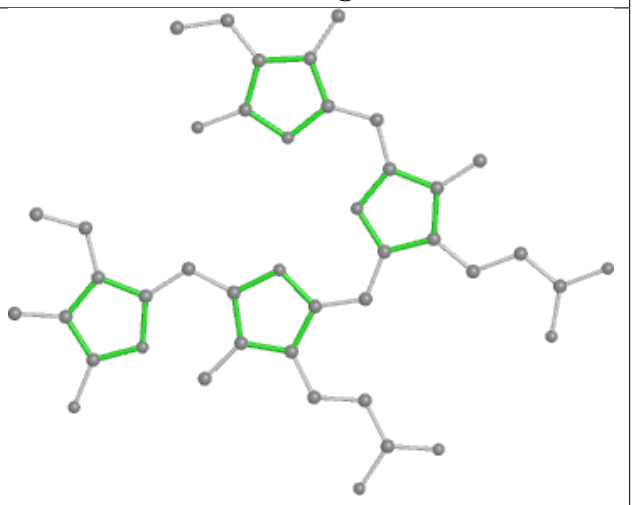
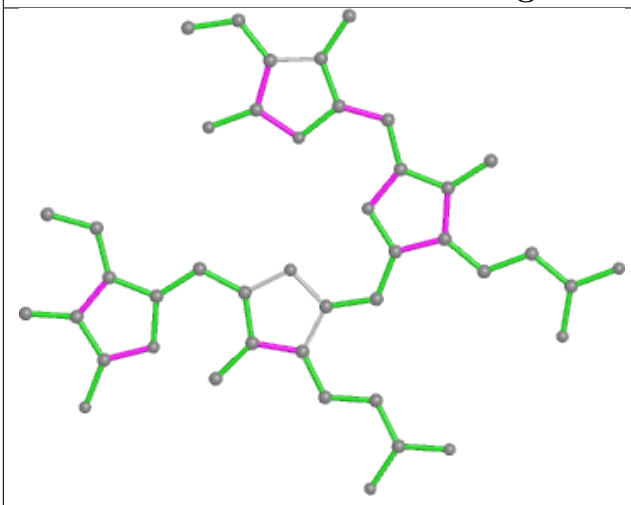


Rings

Ligand PUB gx 203



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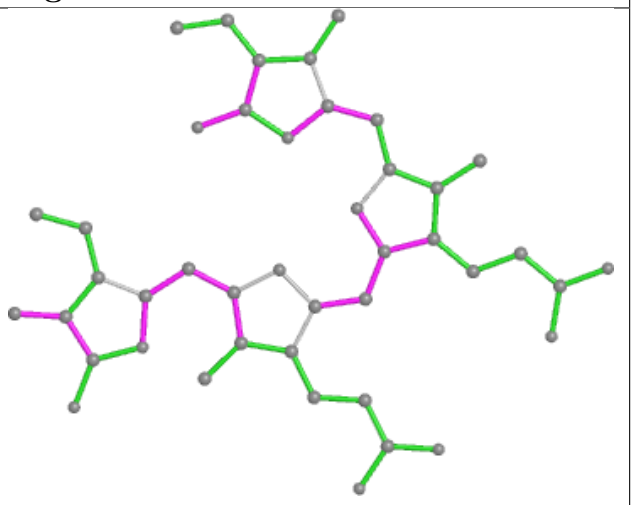

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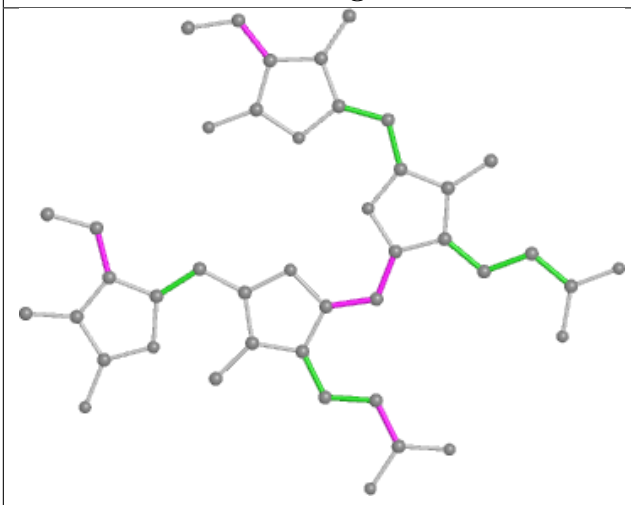

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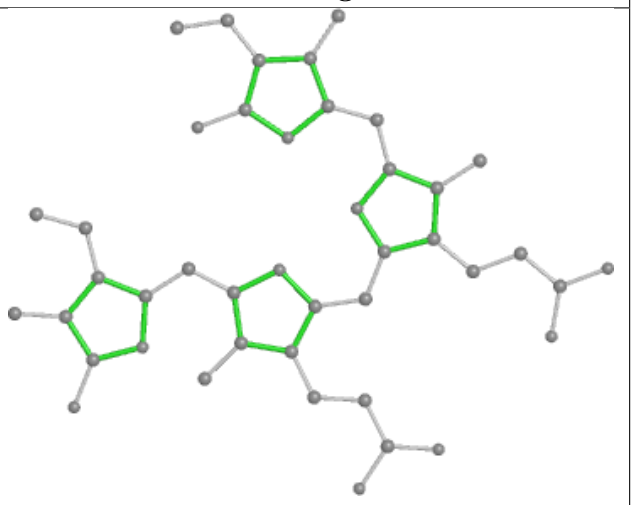
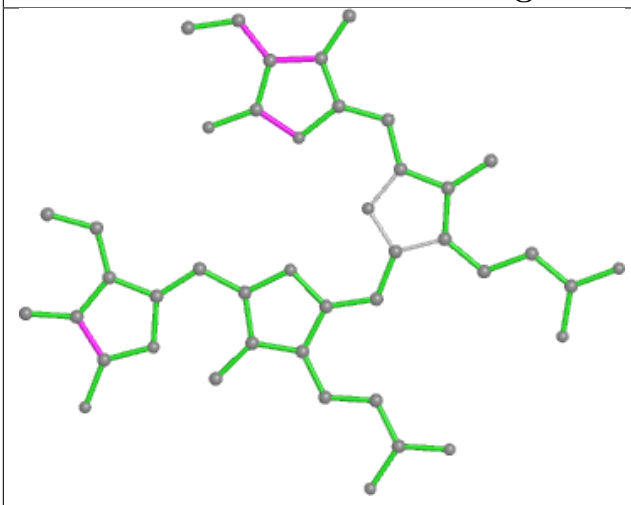


Rings

Ligand PEB O8 201



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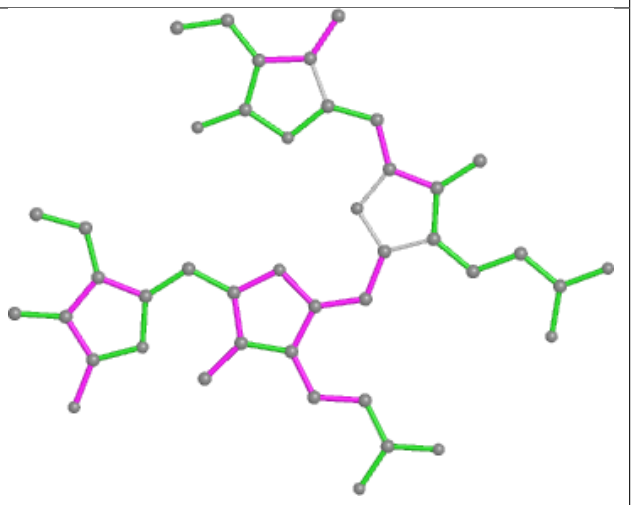

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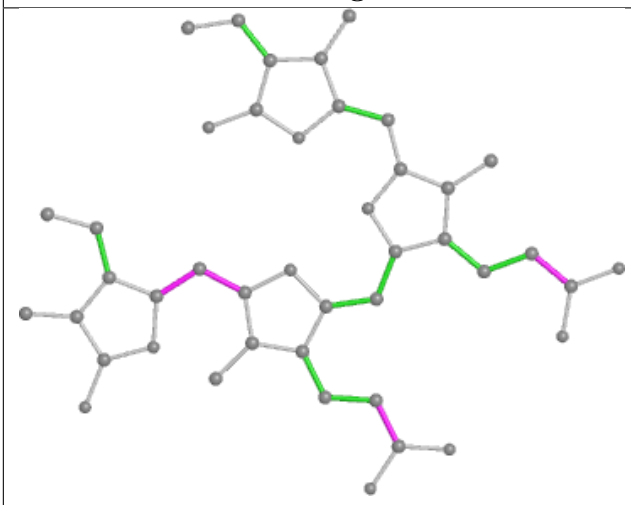

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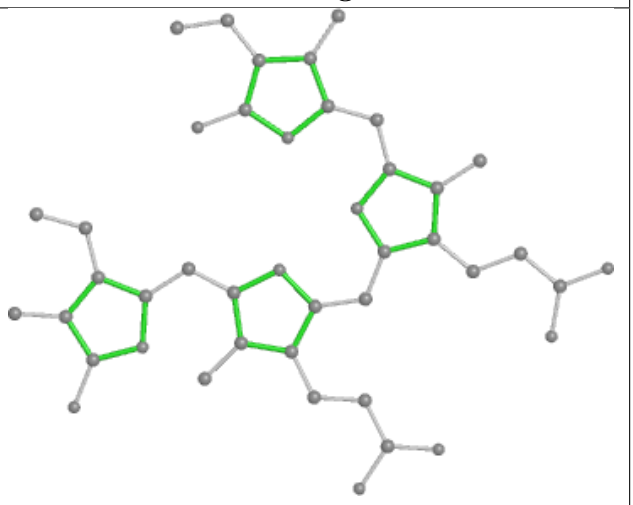

Rings

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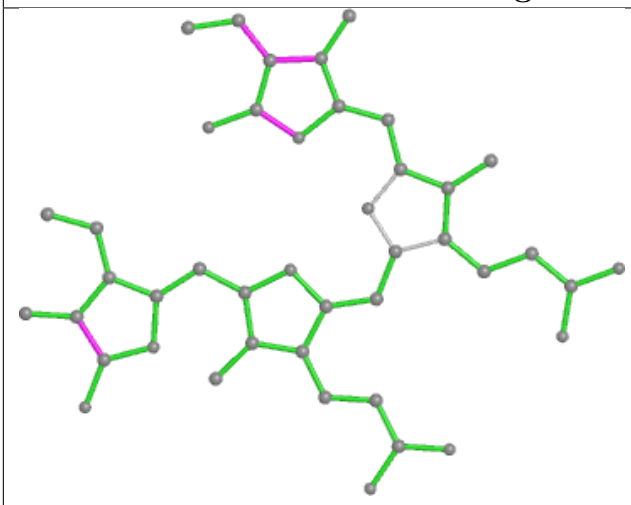

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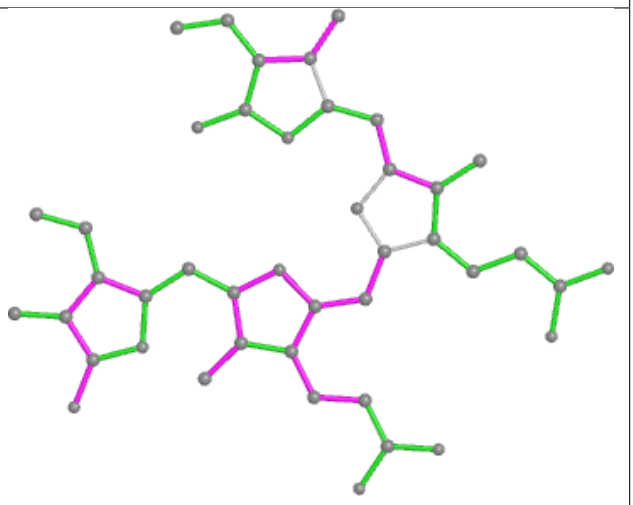

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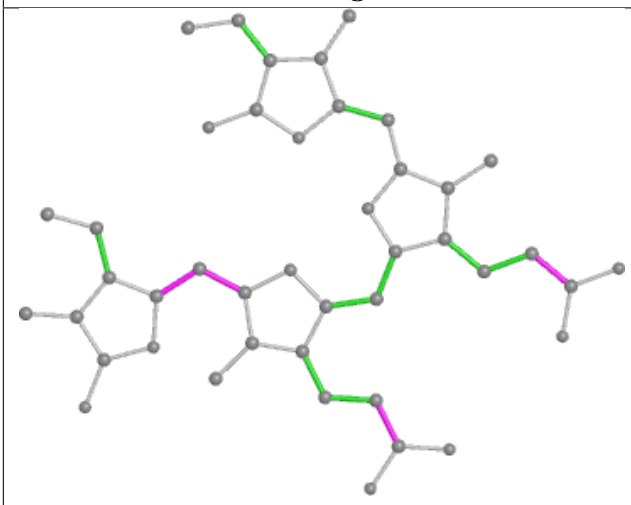

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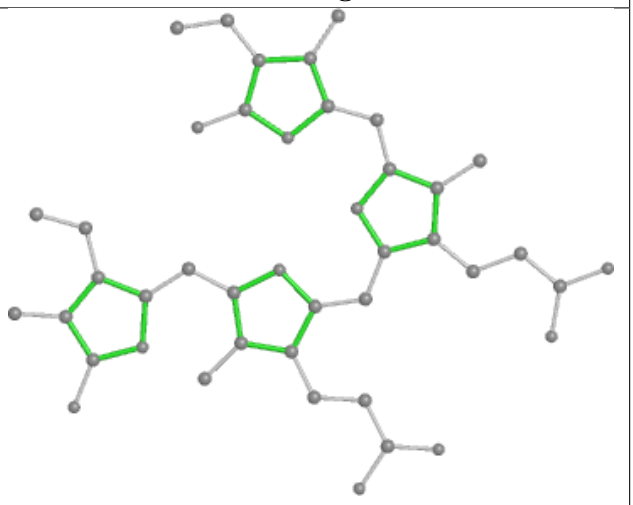
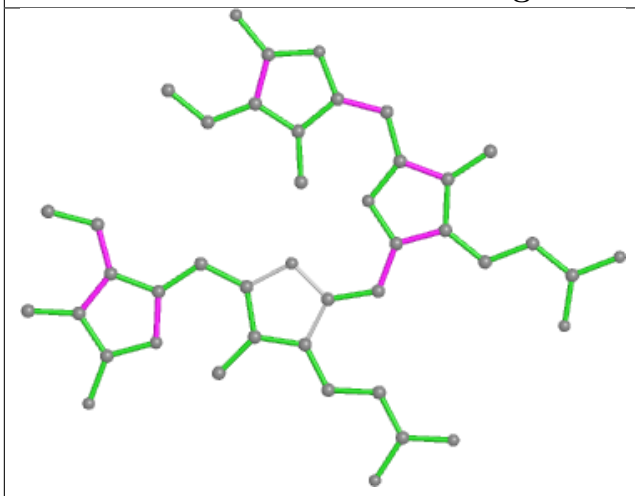


Rings

Ligand PVN Y9 303



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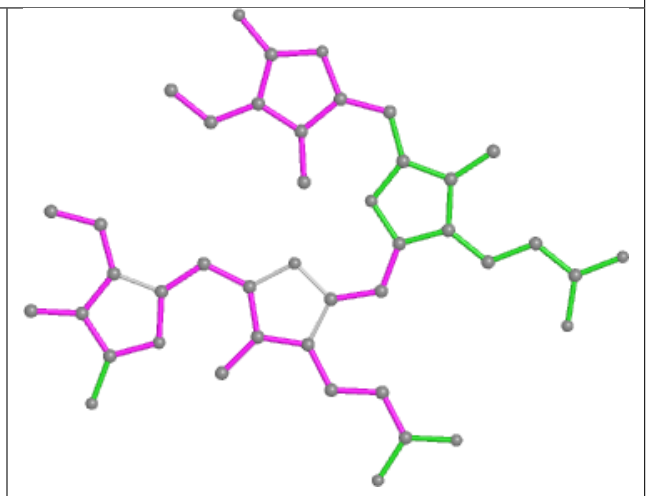
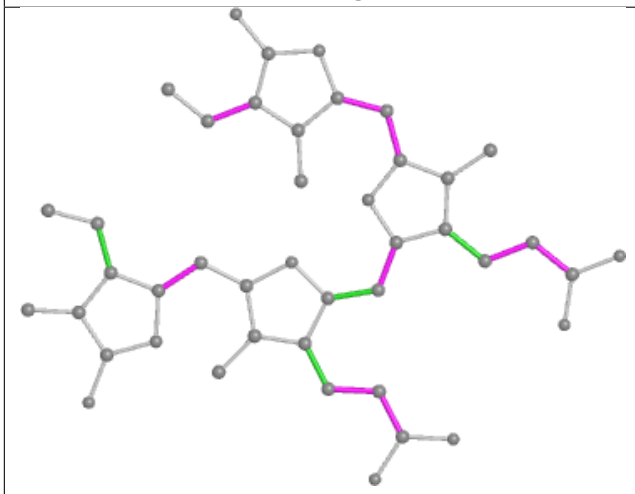
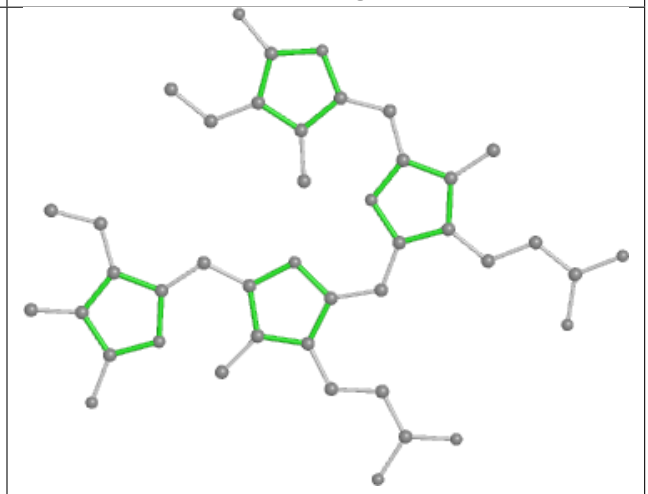


Bond angles

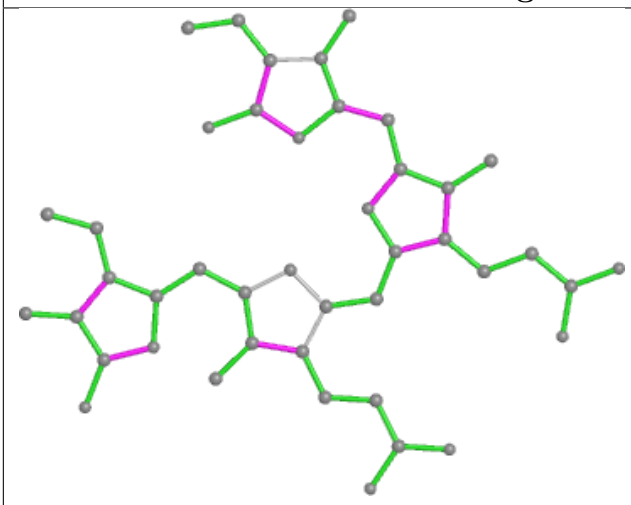


Torsions



Rings

Ligand PUB p3 203



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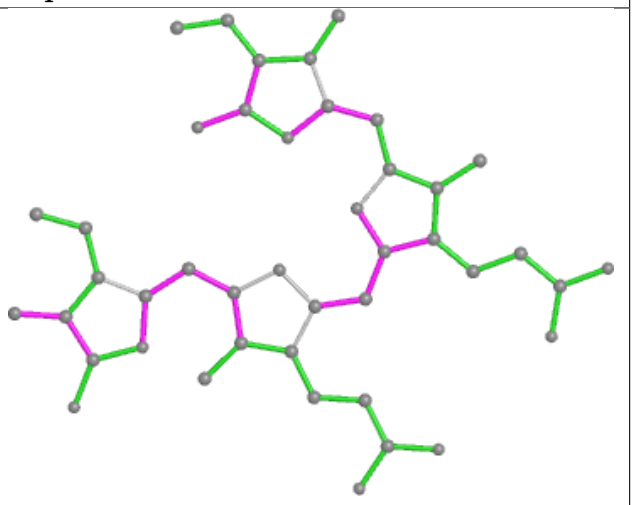

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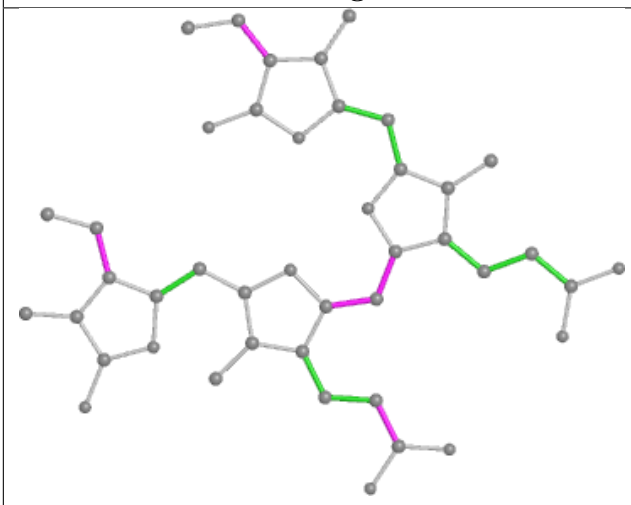

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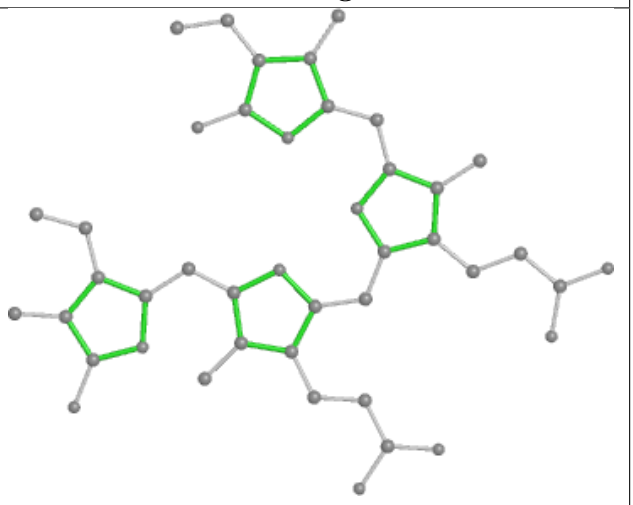
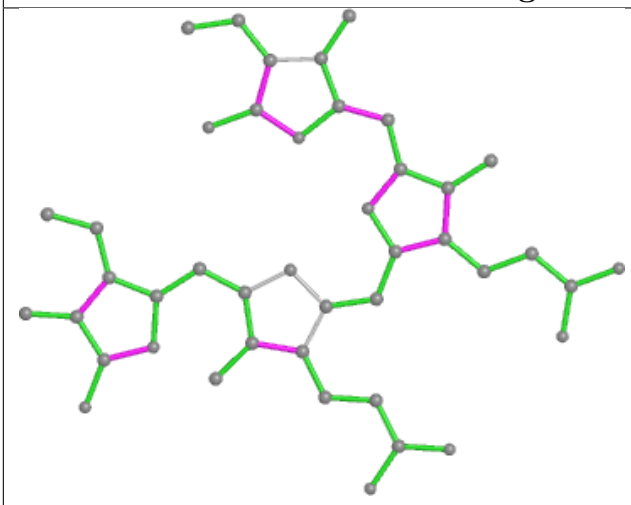


Rings

Ligand PUB cJ 203



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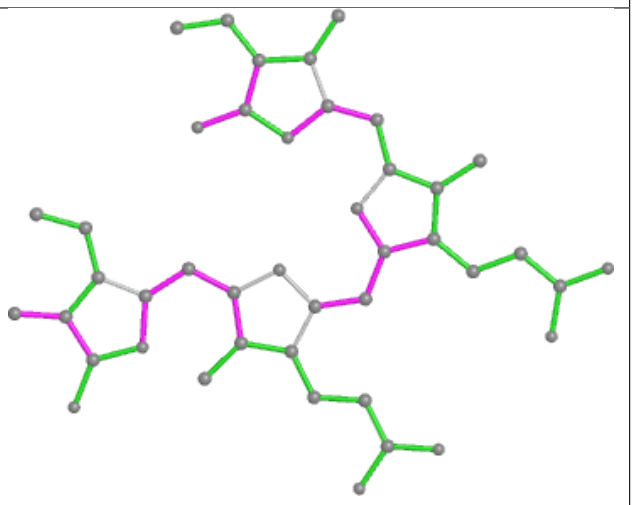

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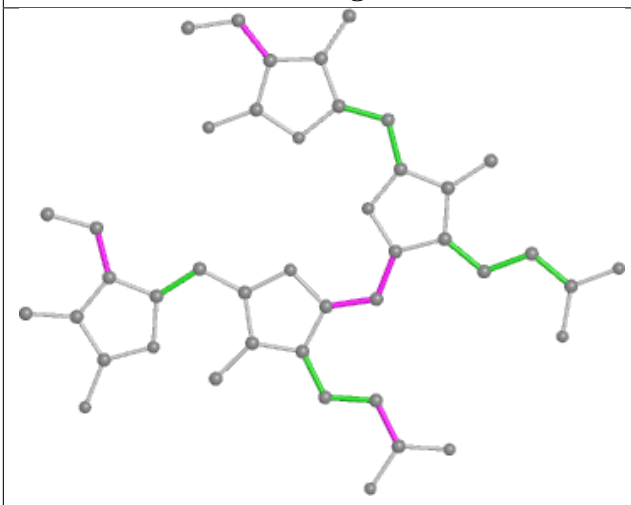

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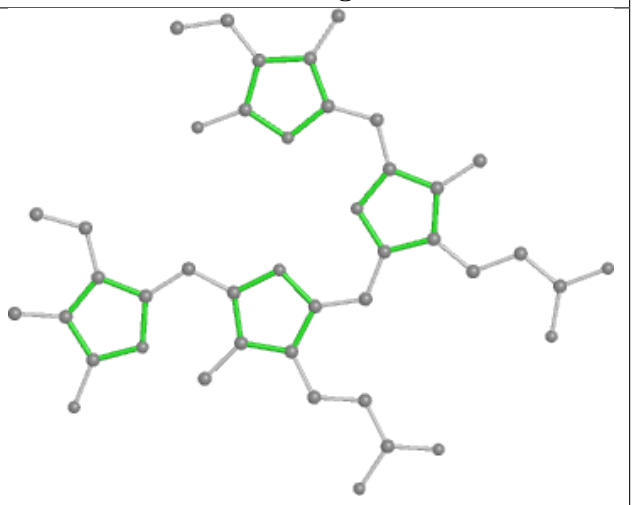
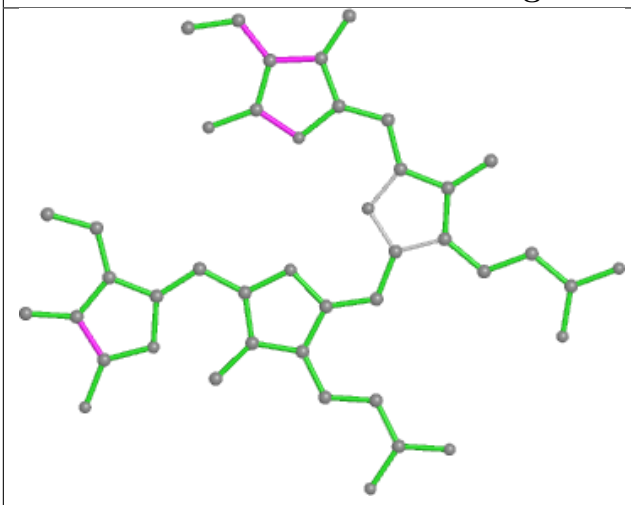


Rings

Ligand PEB lq 201



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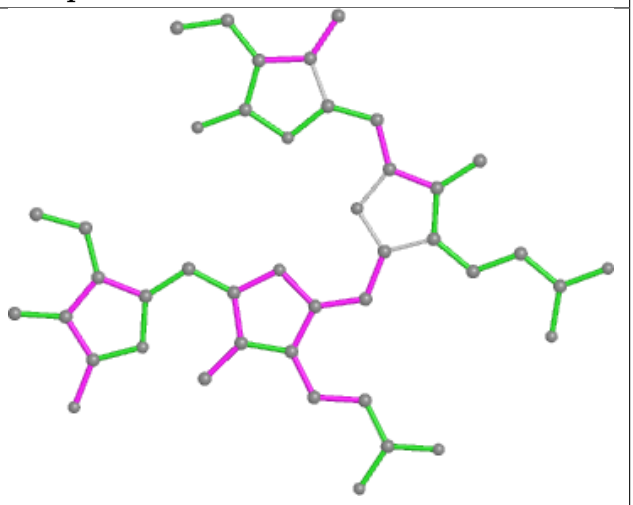

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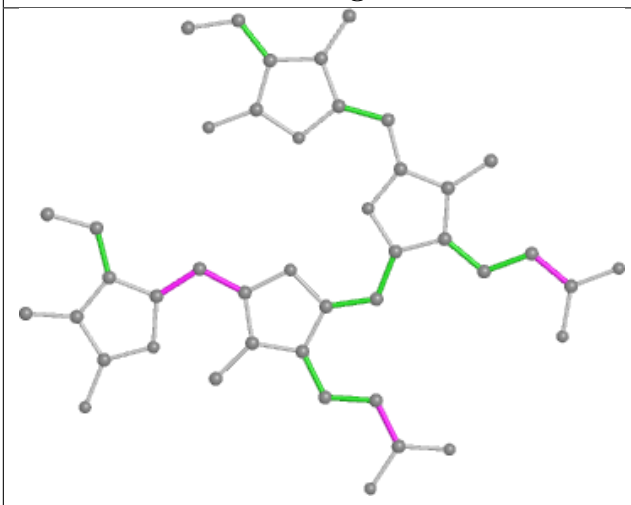

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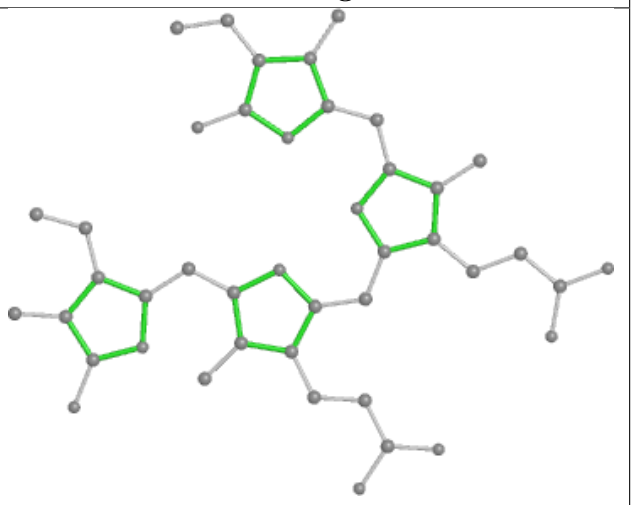
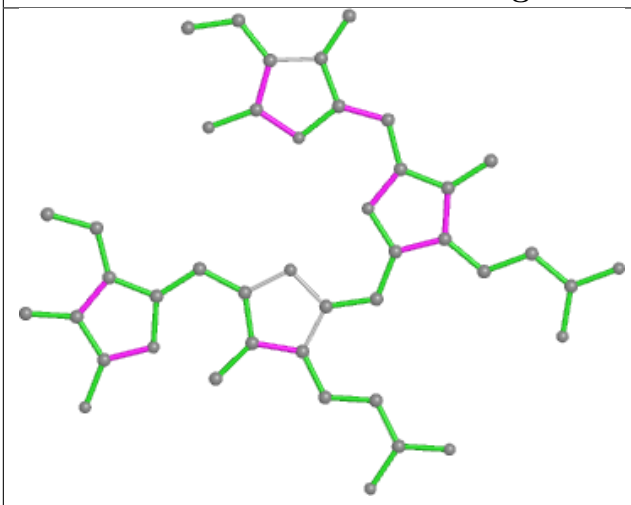


Rings

Ligand PUB dD 203



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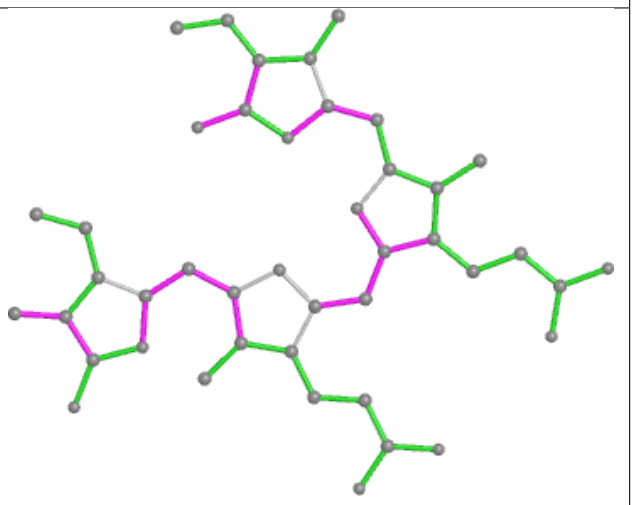

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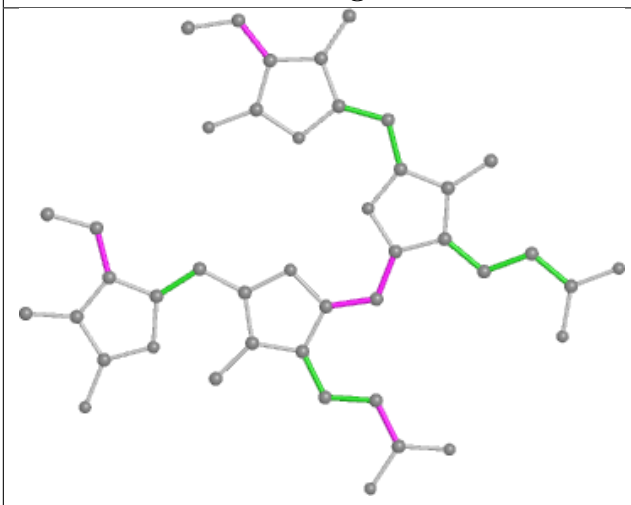

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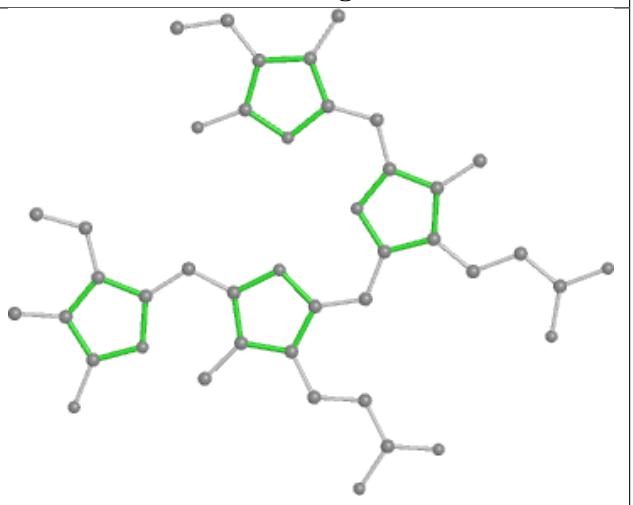
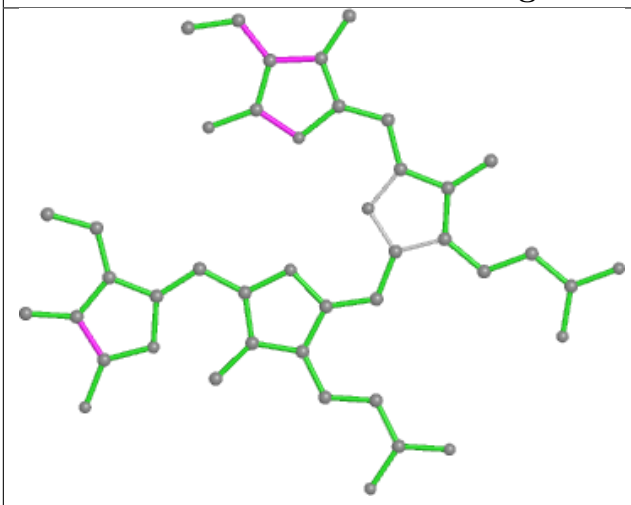


Rings

Ligand PEB h5 201



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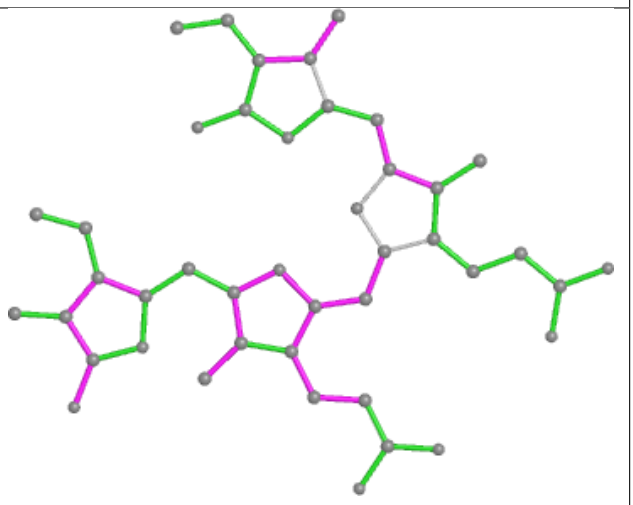

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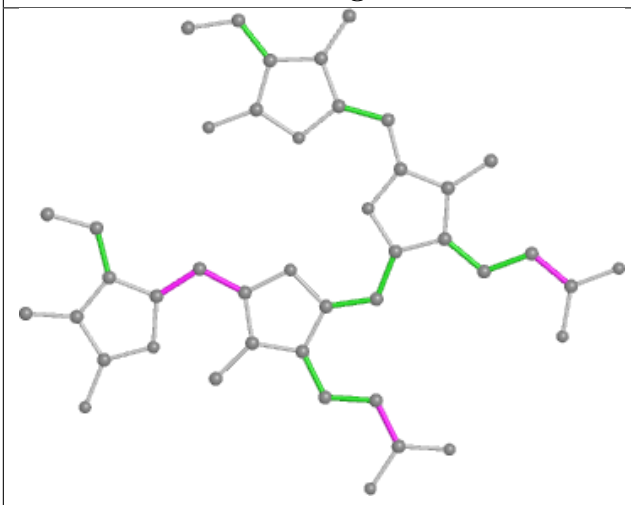

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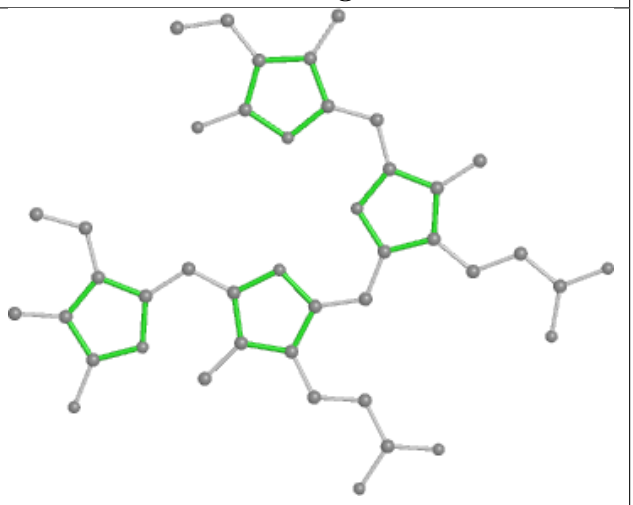

Rings

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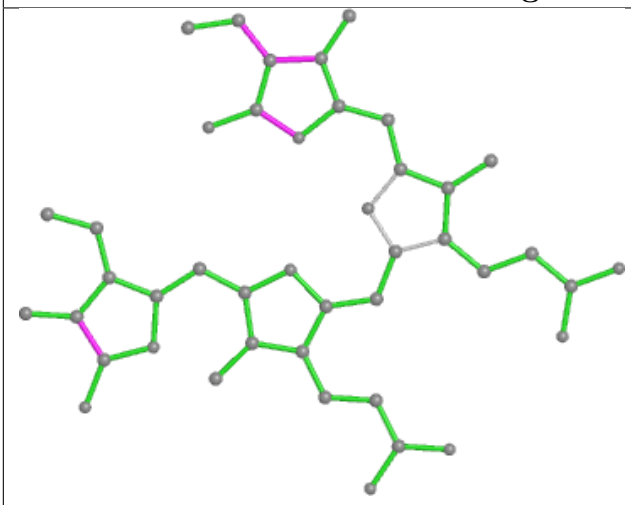

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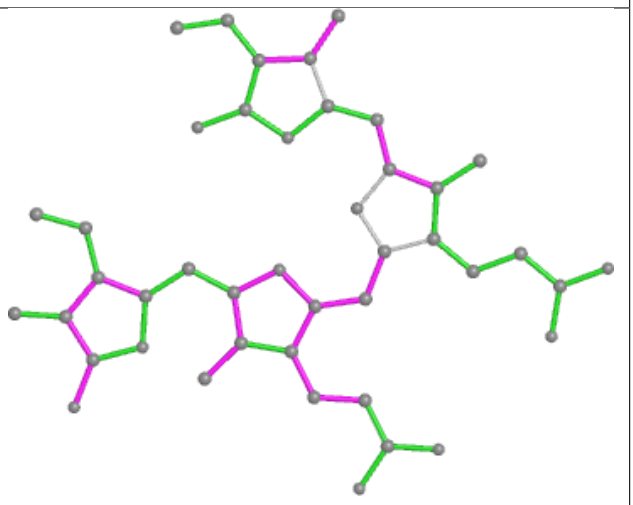

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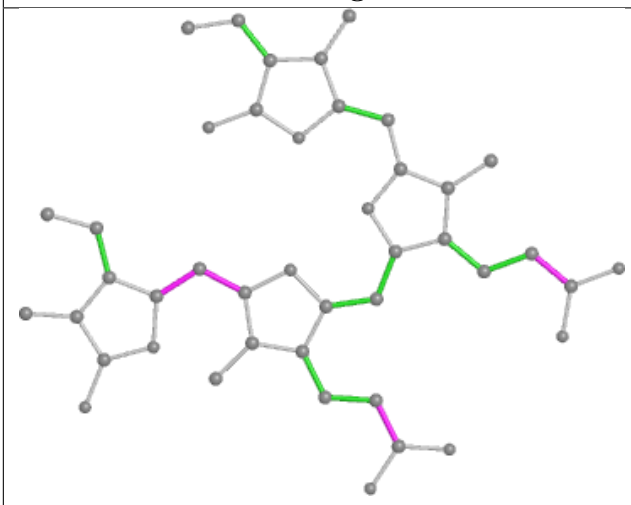

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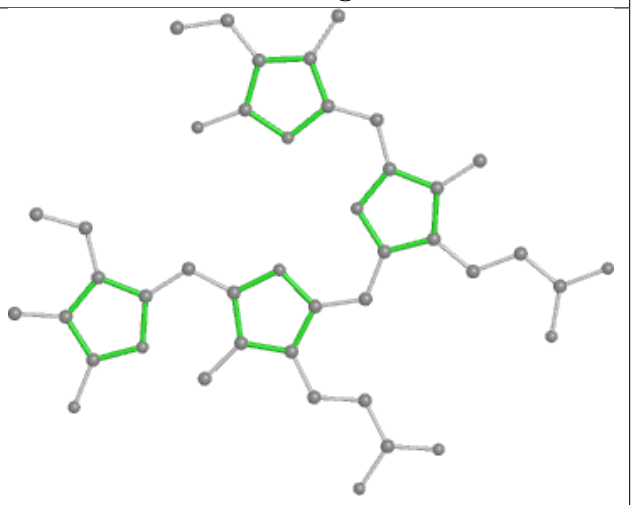
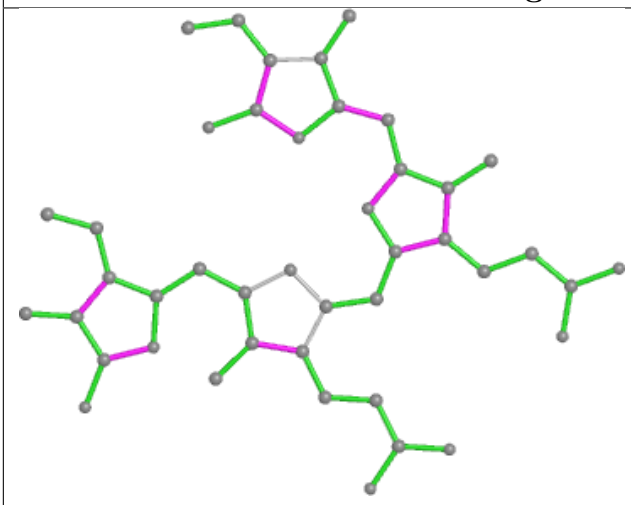


Rings

Ligand PUB lf 203



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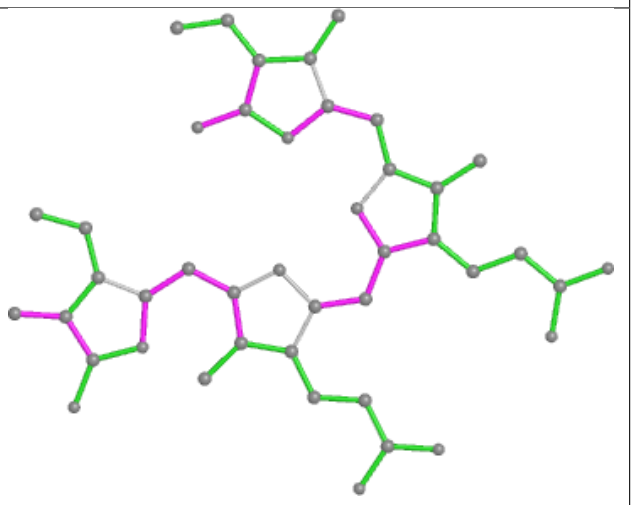

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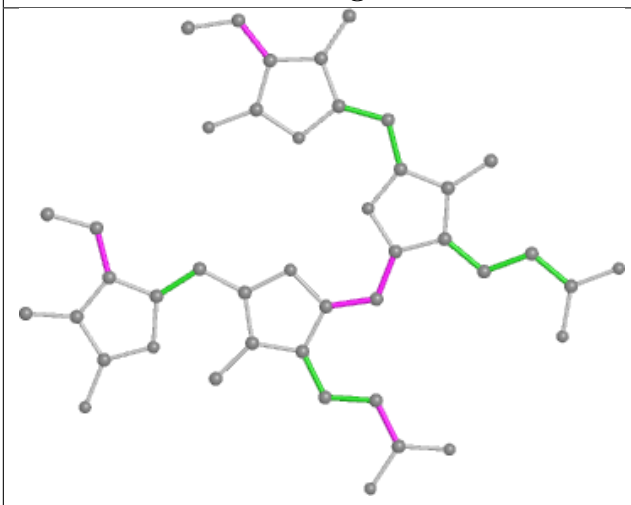

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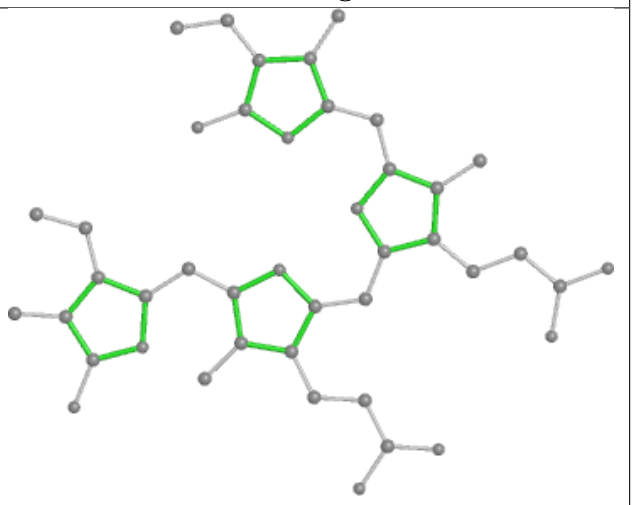
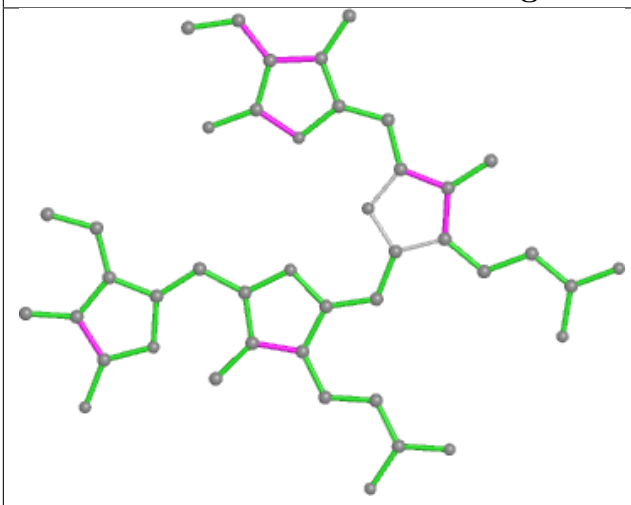


Rings

Ligand PEB e4 202



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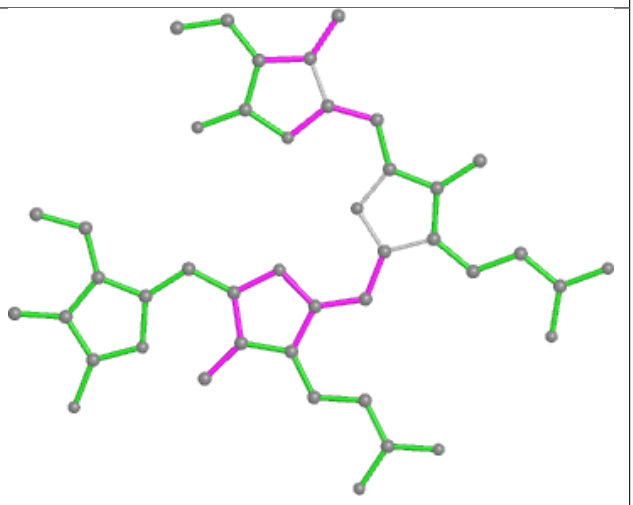

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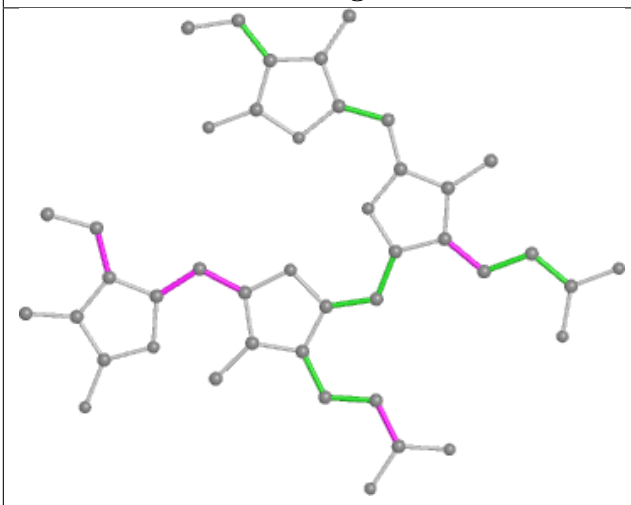

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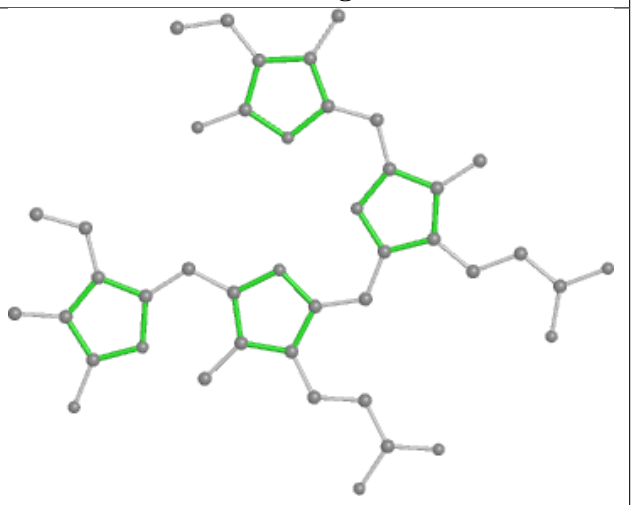
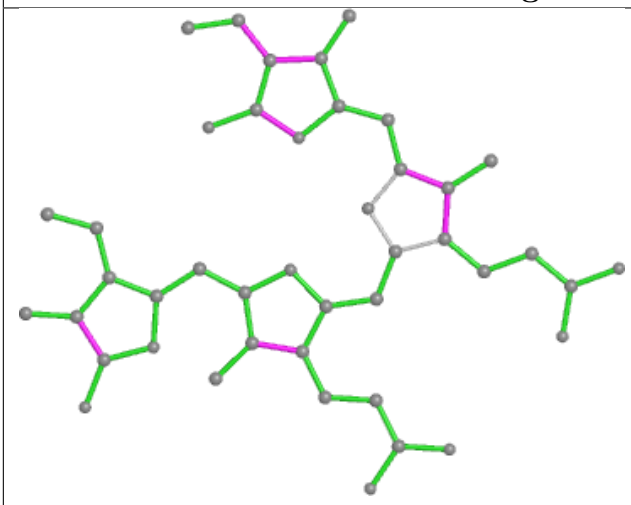


Rings

Ligand PEB t5 202



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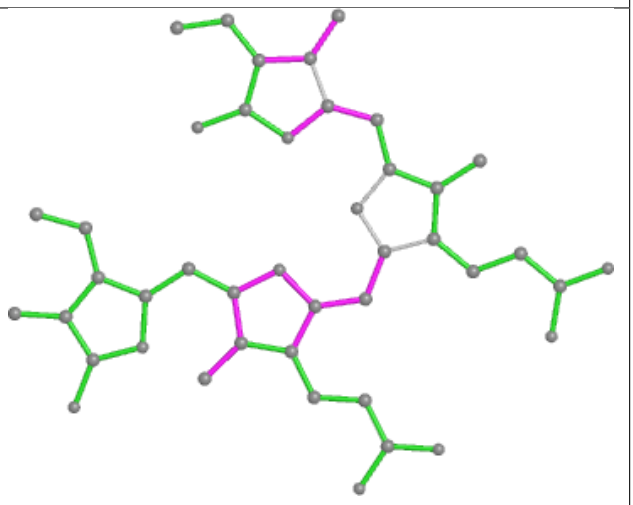

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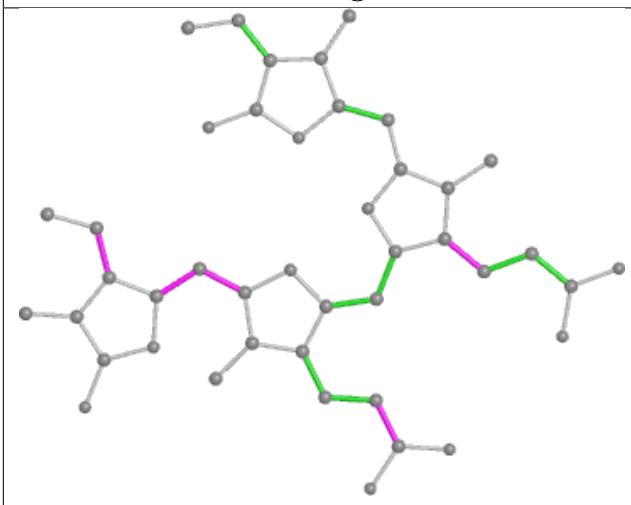

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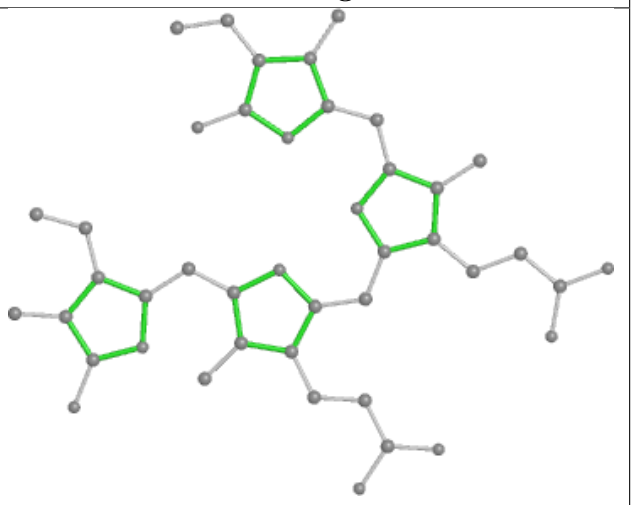
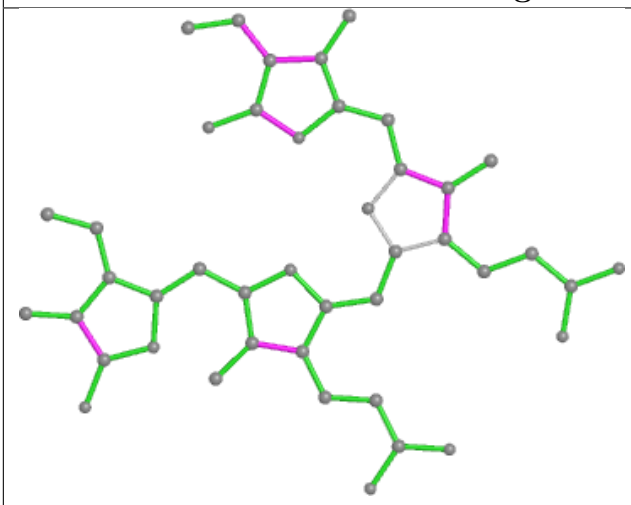


Rings

Ligand PEB bD 202



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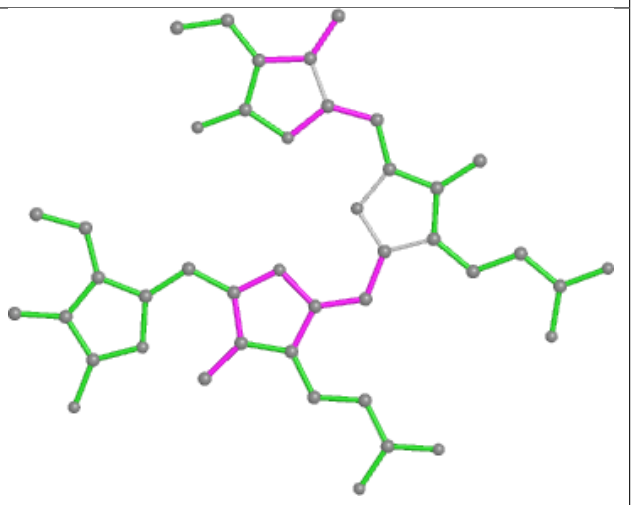

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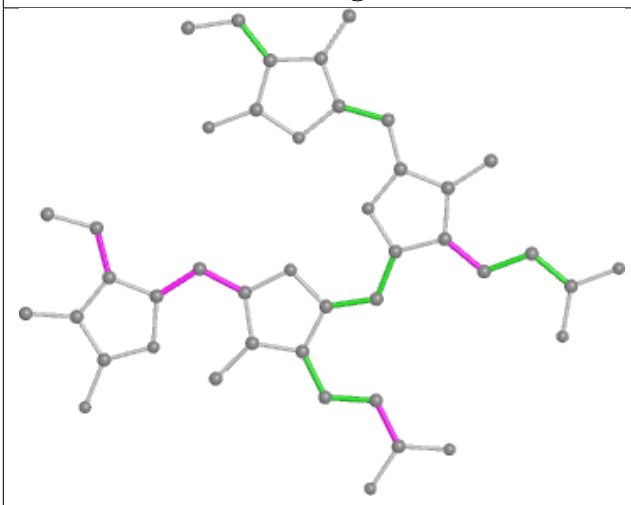

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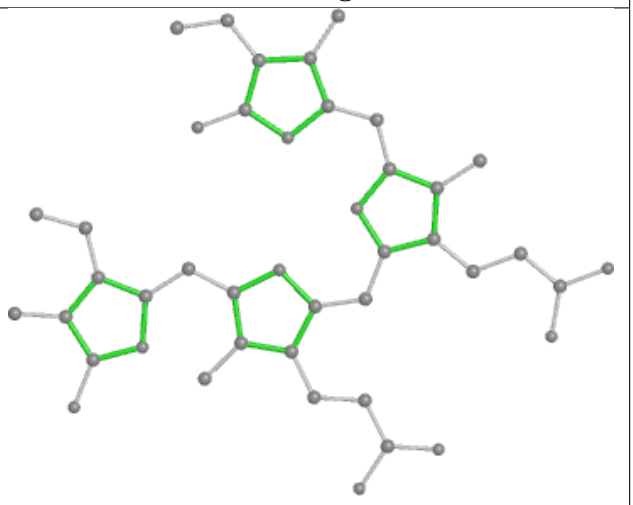
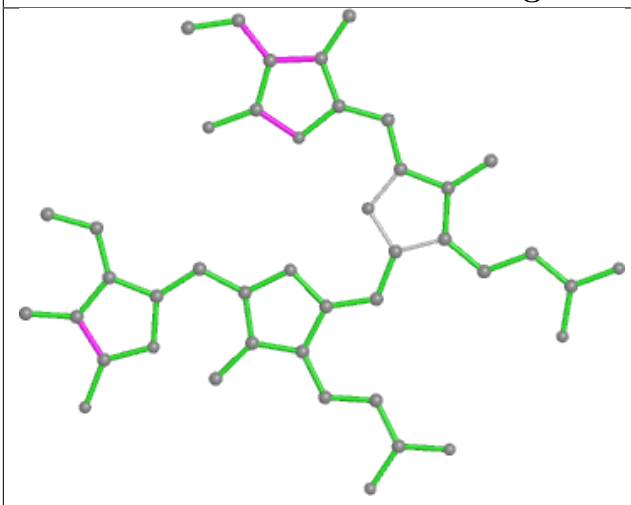


Rings

Ligand PEB f6 201



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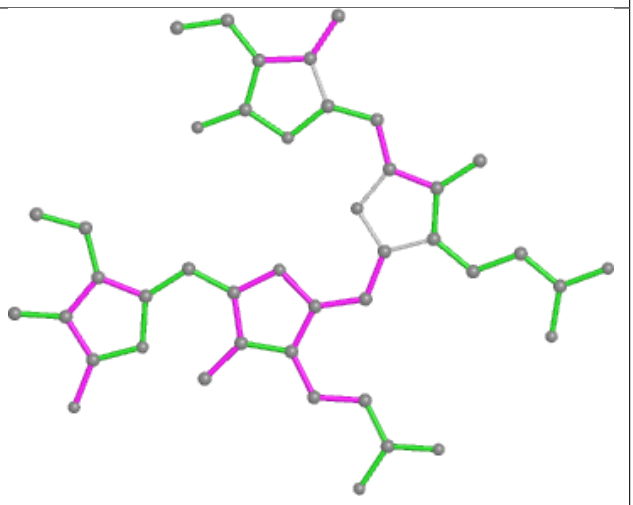
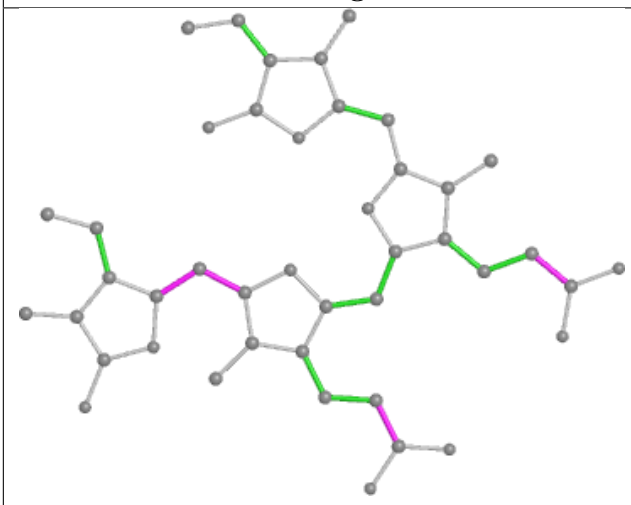


Bond angles



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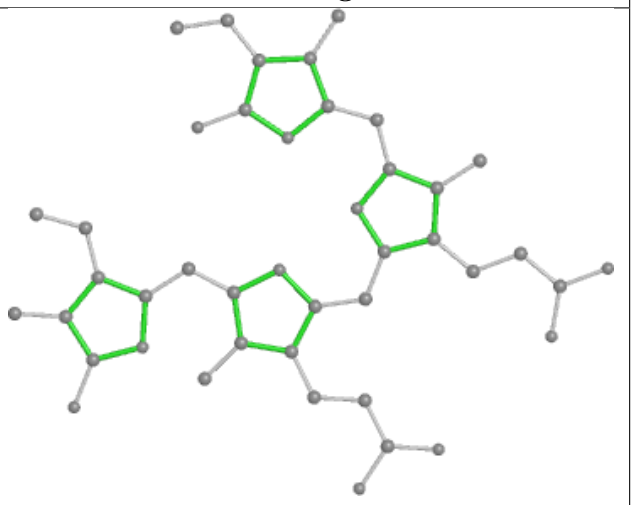
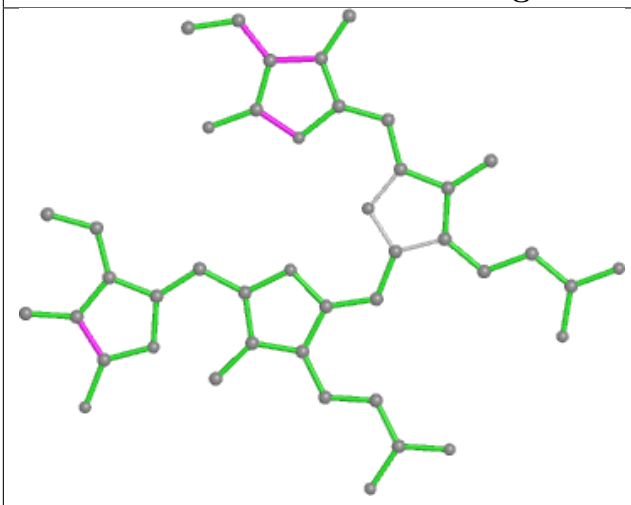


Rings

Ligand PEB dm 202



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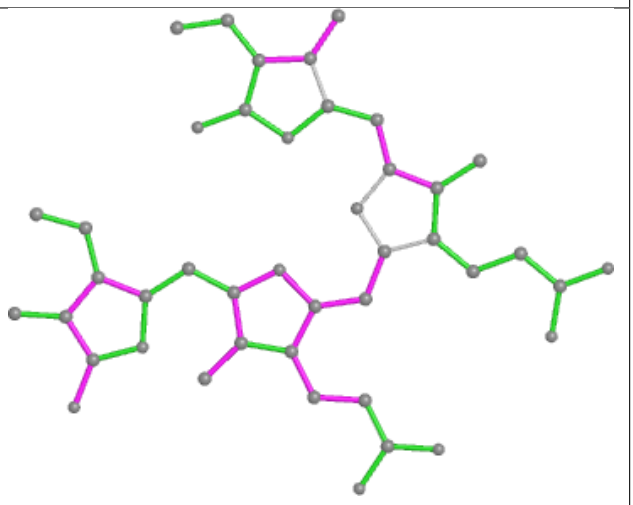

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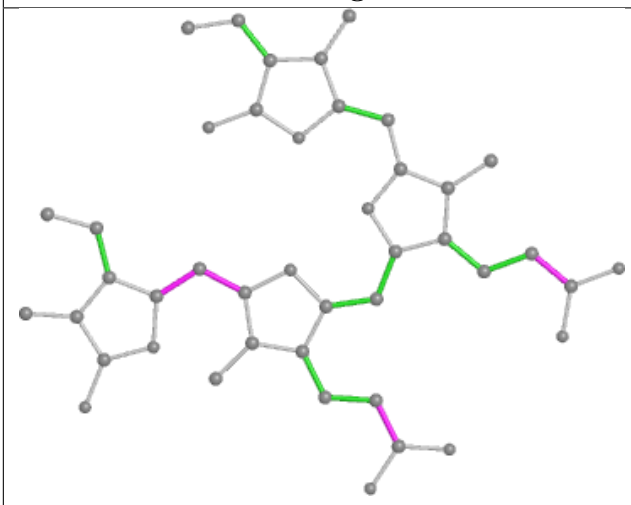

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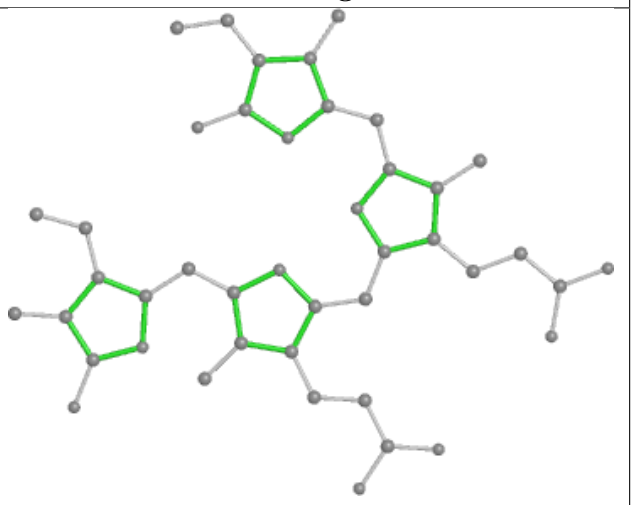
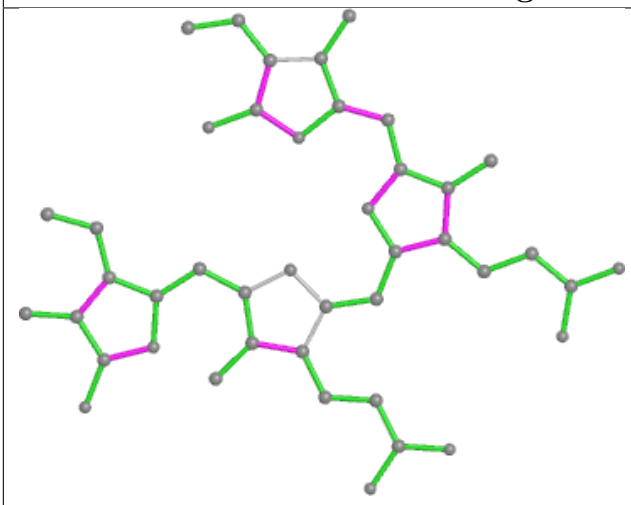


Rings

Ligand PUB bo 202



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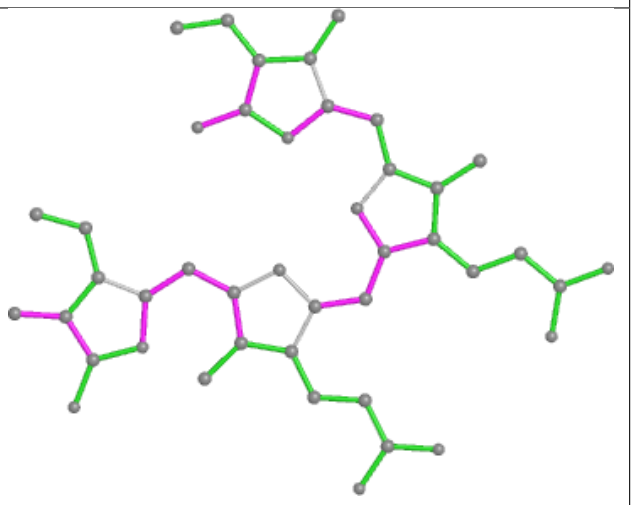
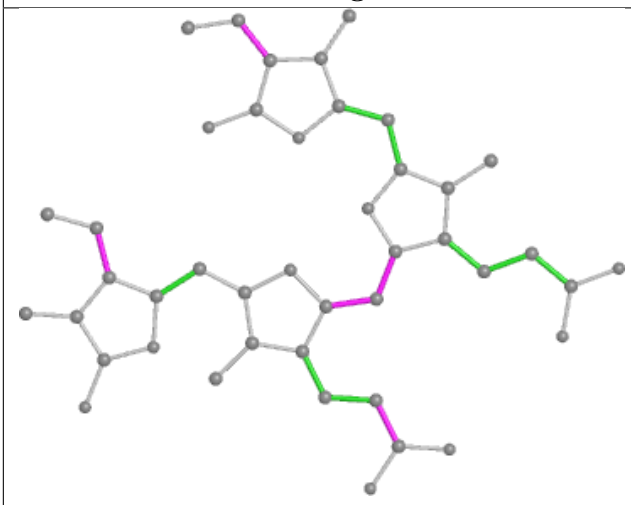


Bond angles



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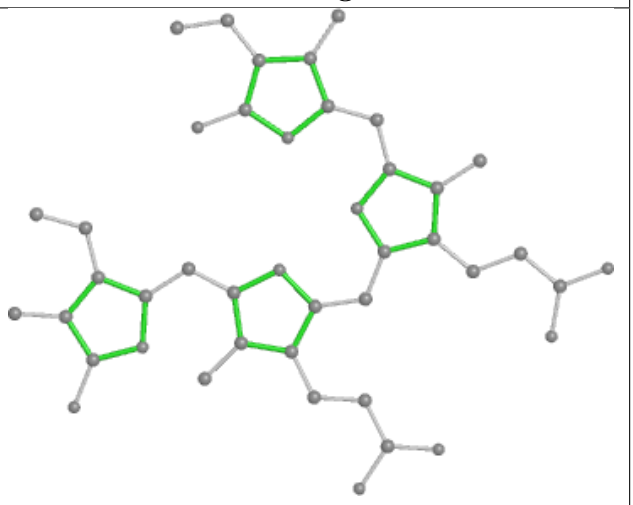
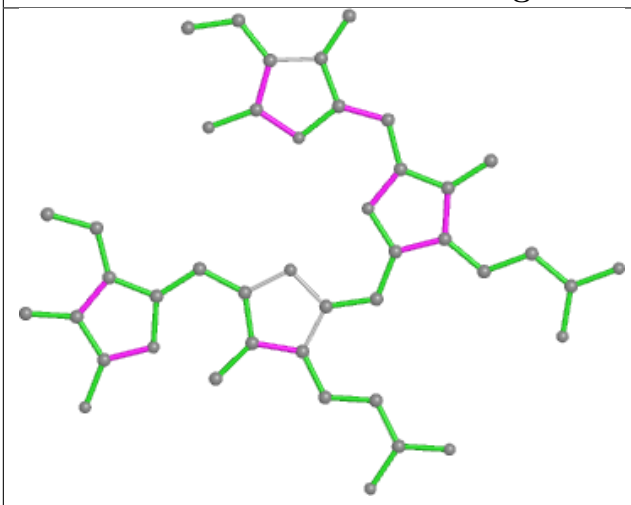


Rings

Ligand PUB dB 202



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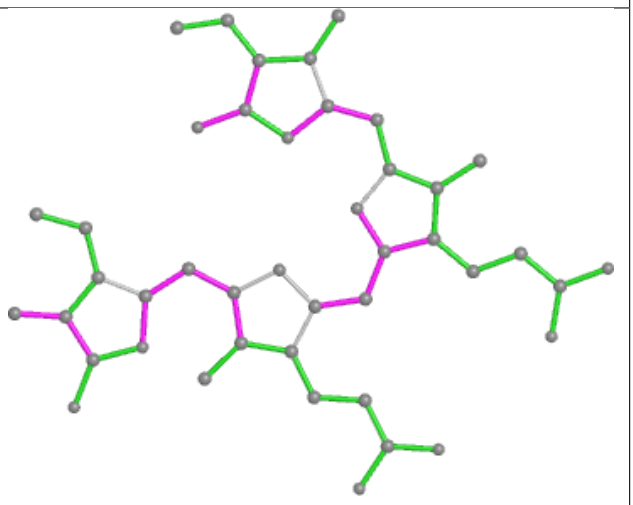

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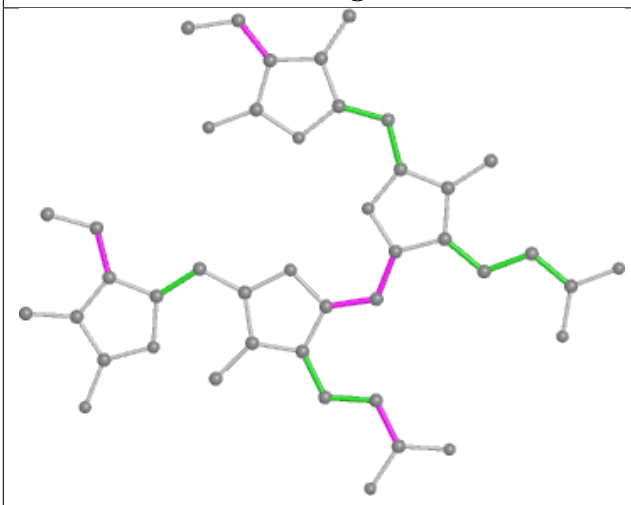
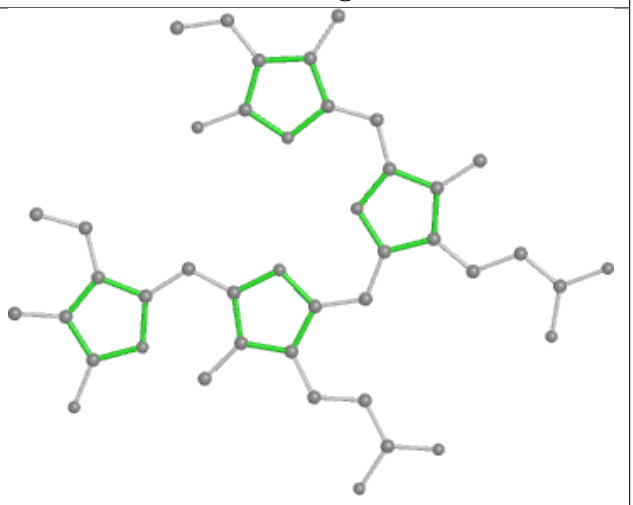
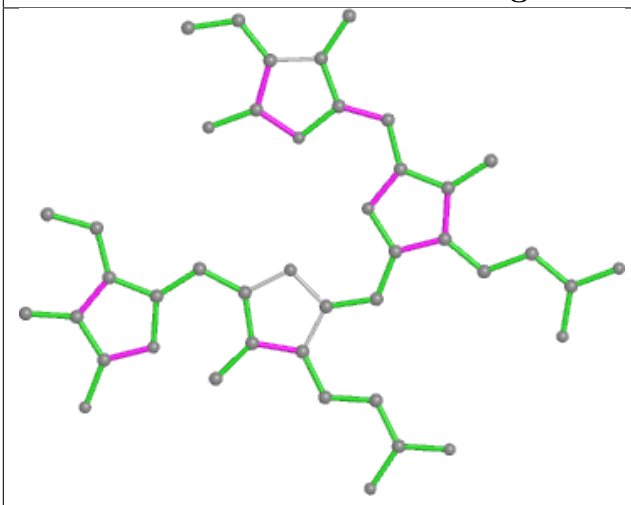


Torsions



Rings

Ligand PUB jL 1003



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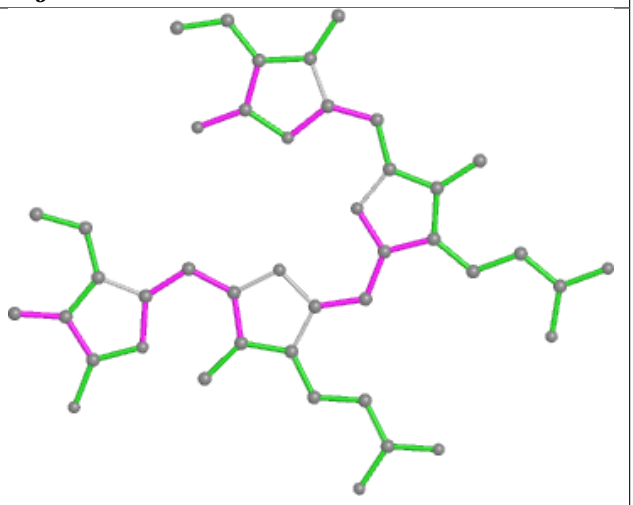

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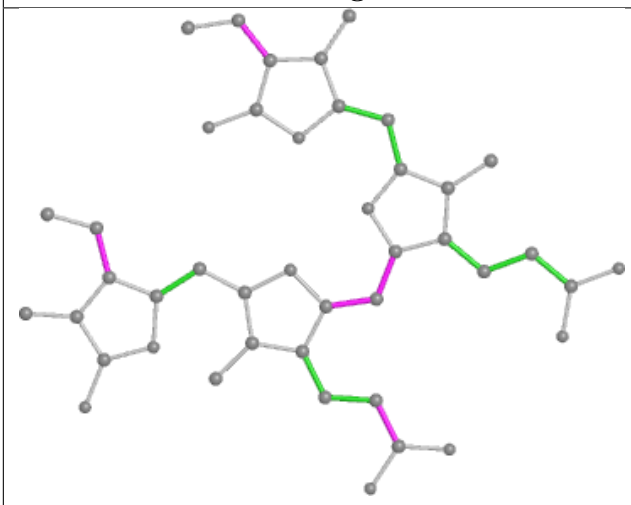

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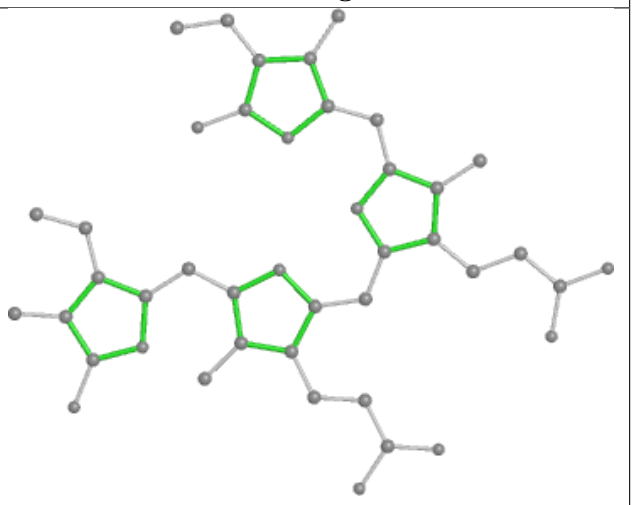
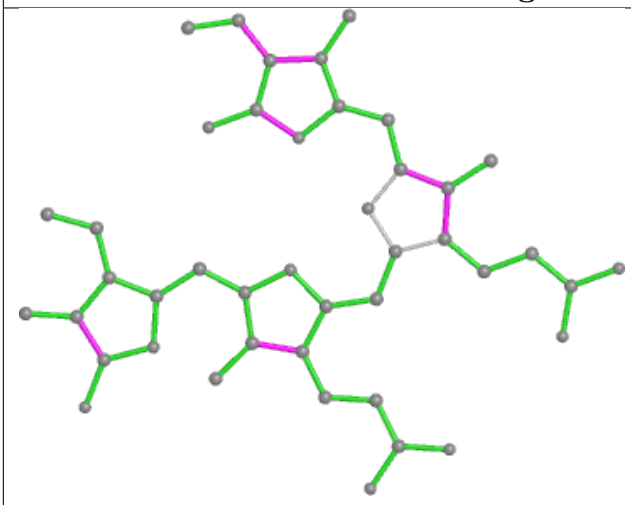


Rings

Ligand PEB L3 202



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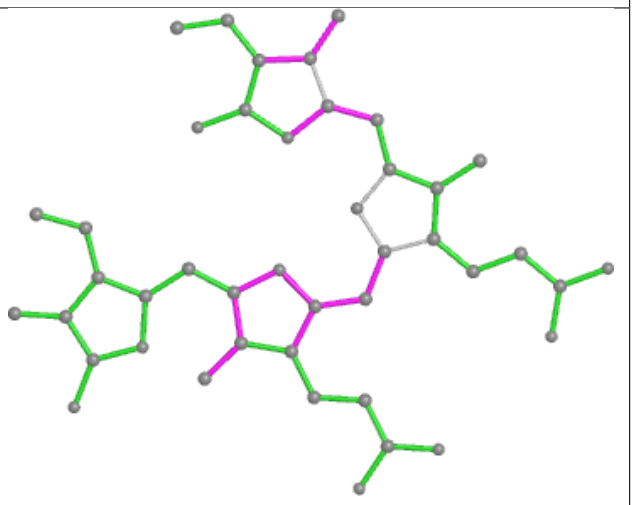

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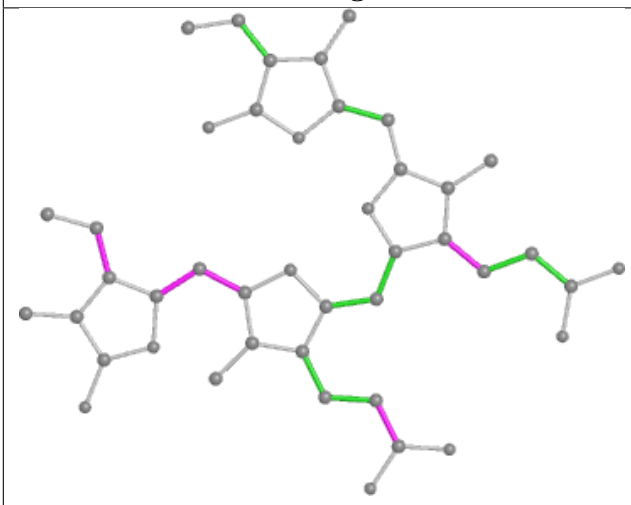

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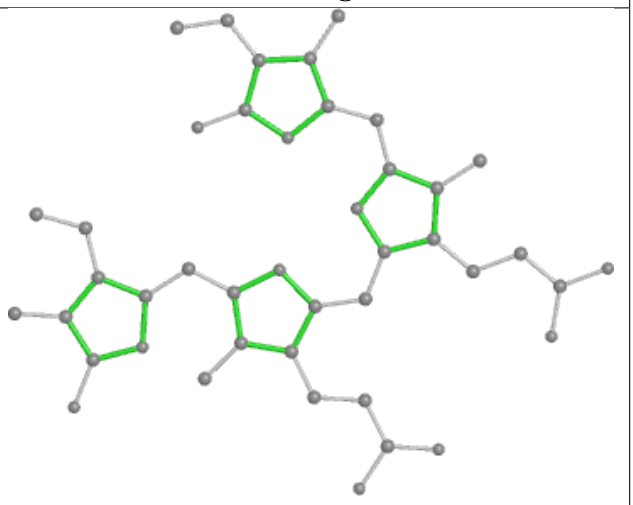
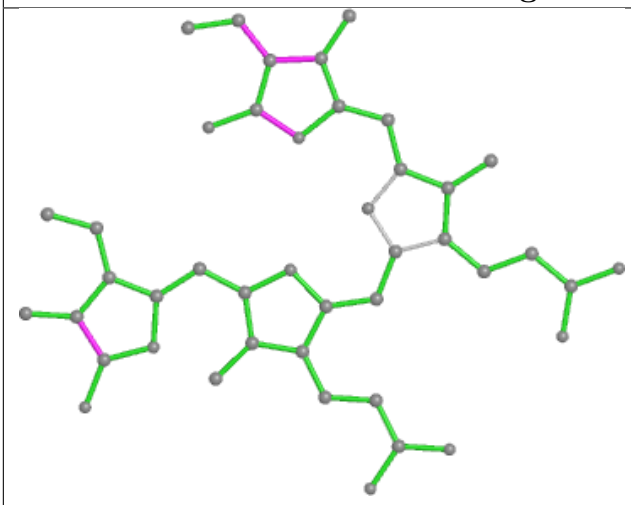


Rings

Ligand PEB cu 201



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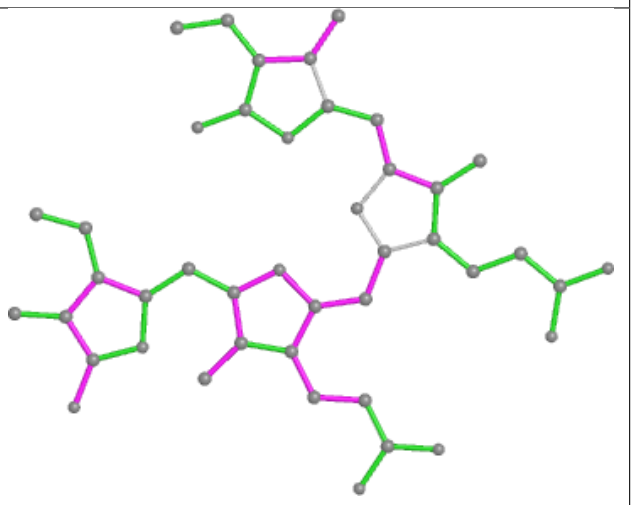

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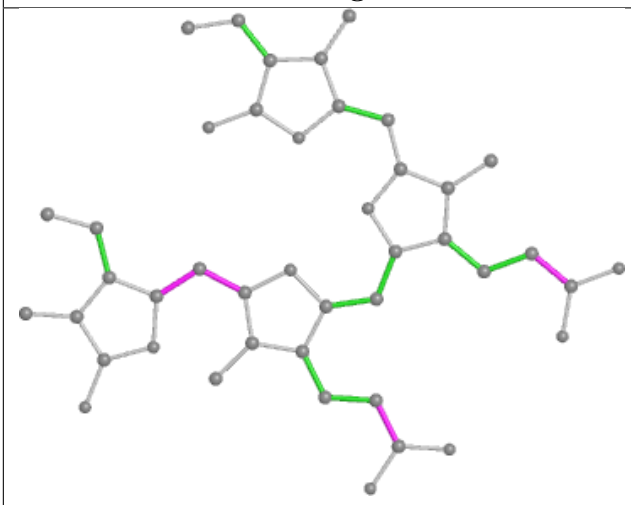

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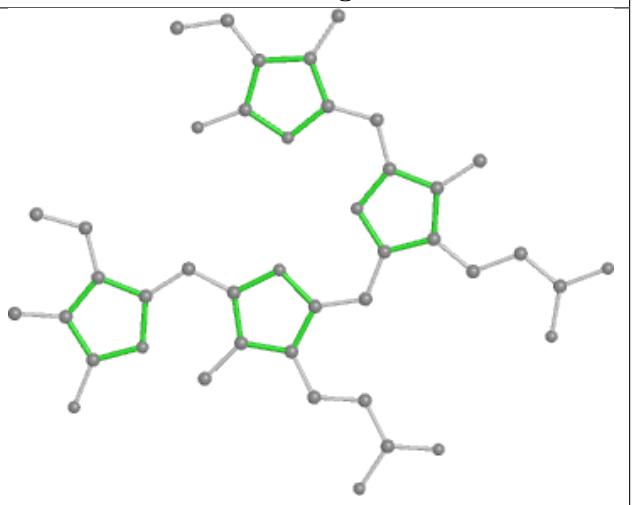

Rings

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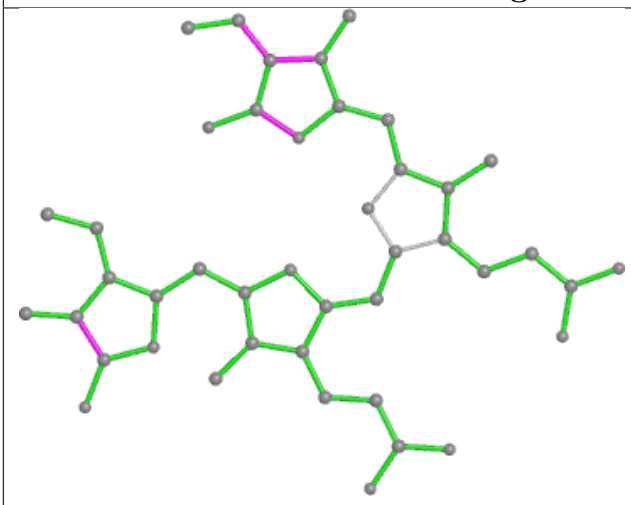

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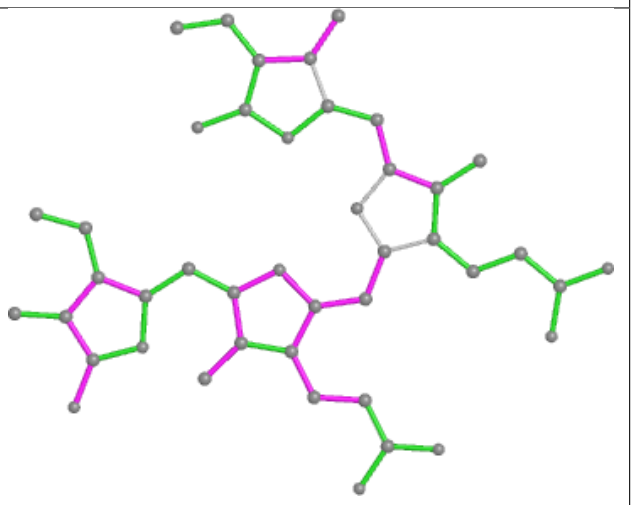

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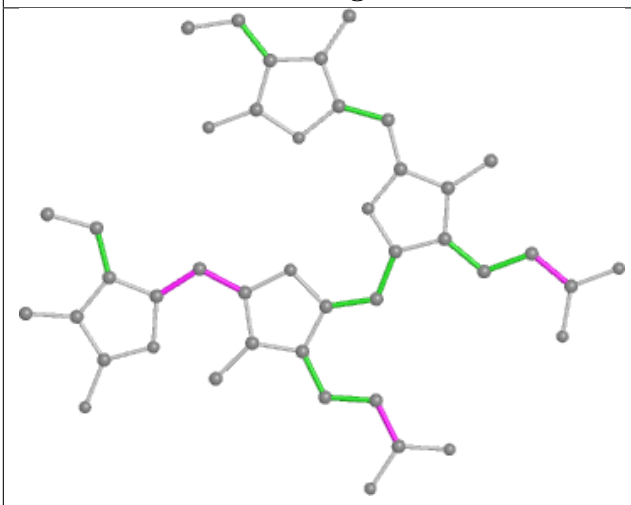

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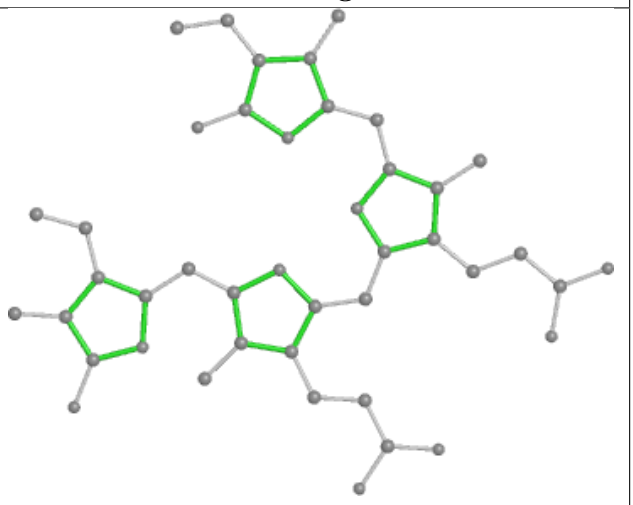

Rings

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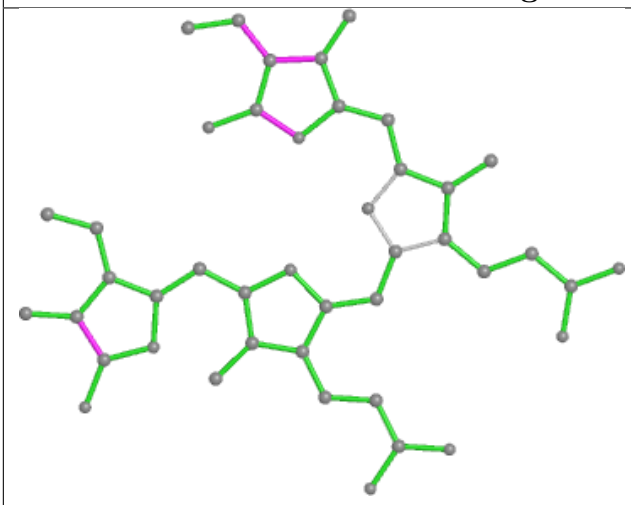

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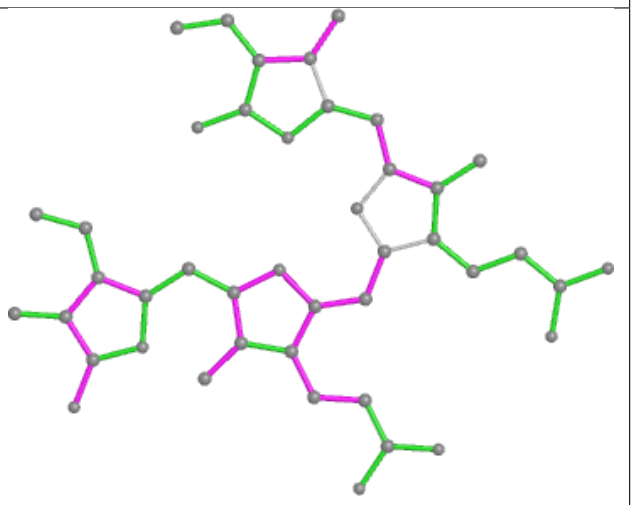

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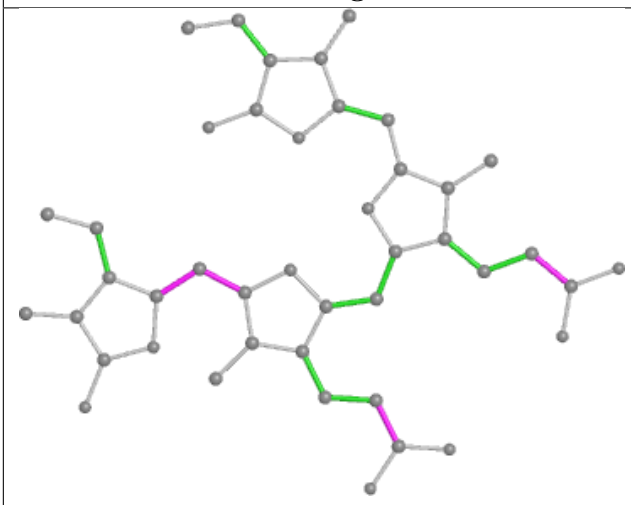

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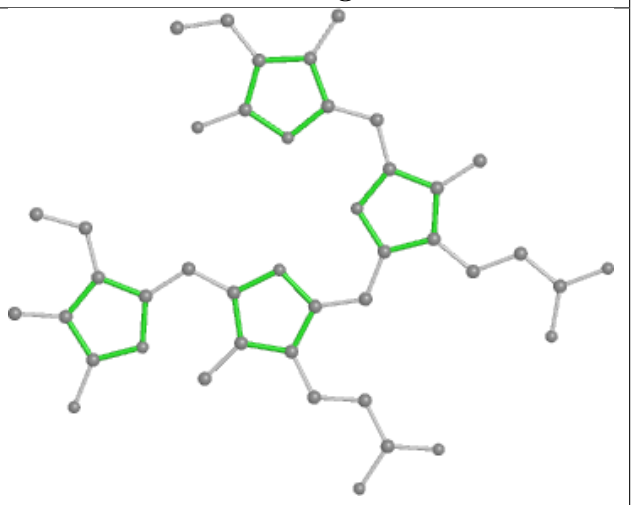

Rings

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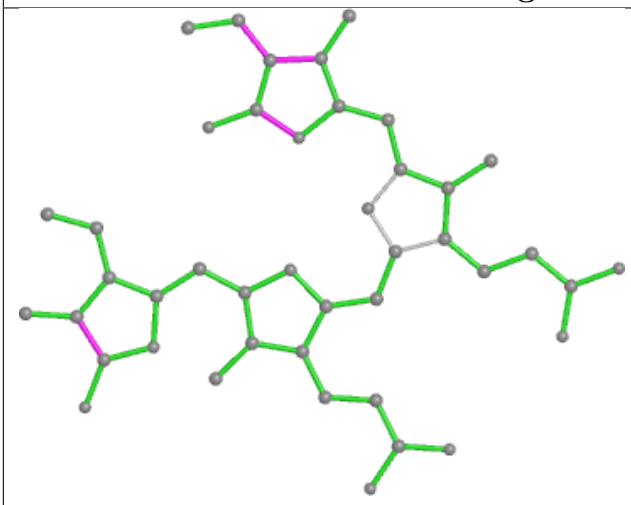

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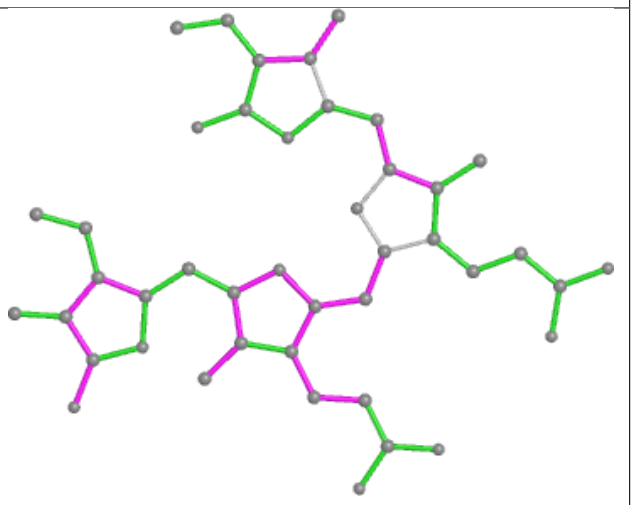

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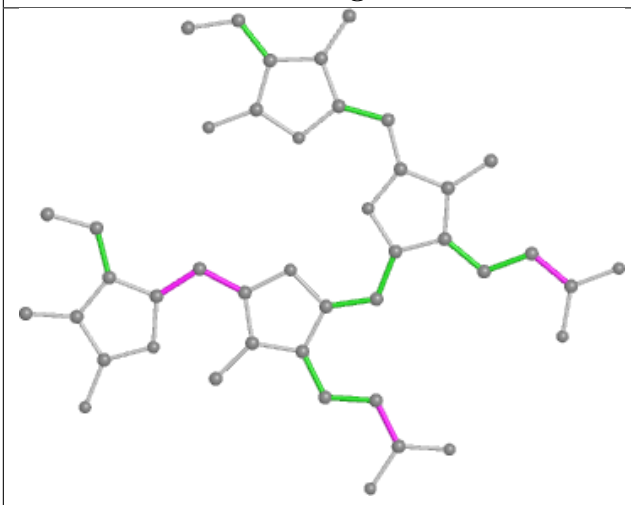

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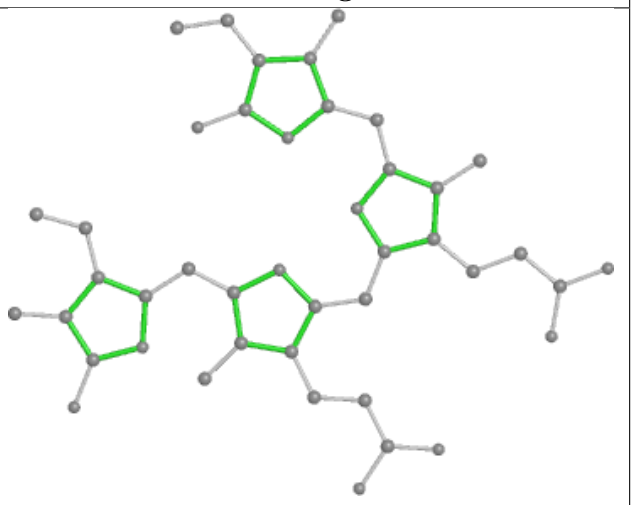

Rings

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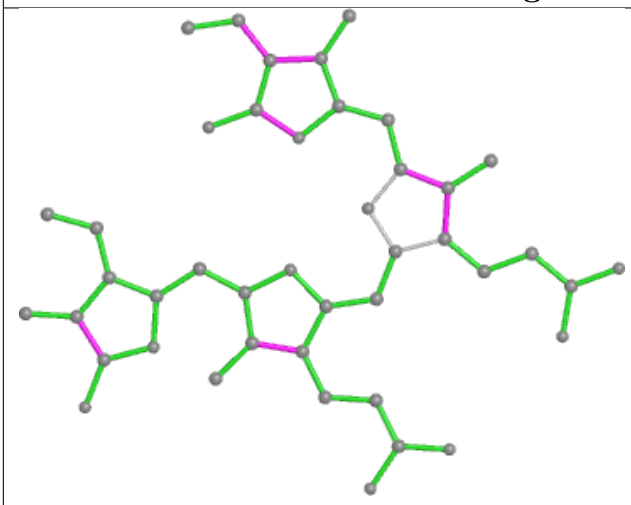

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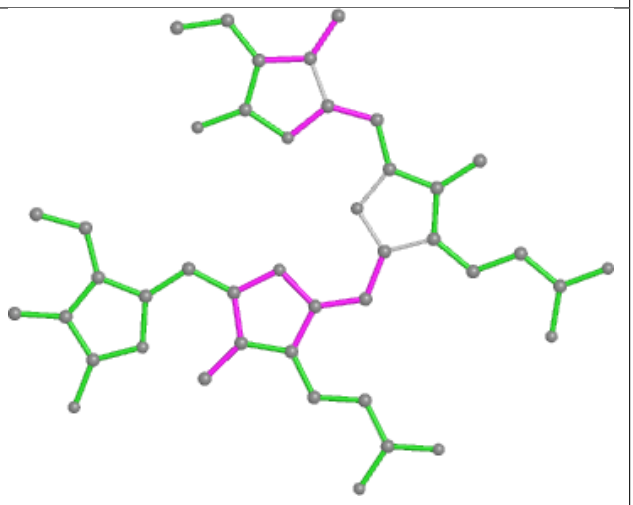

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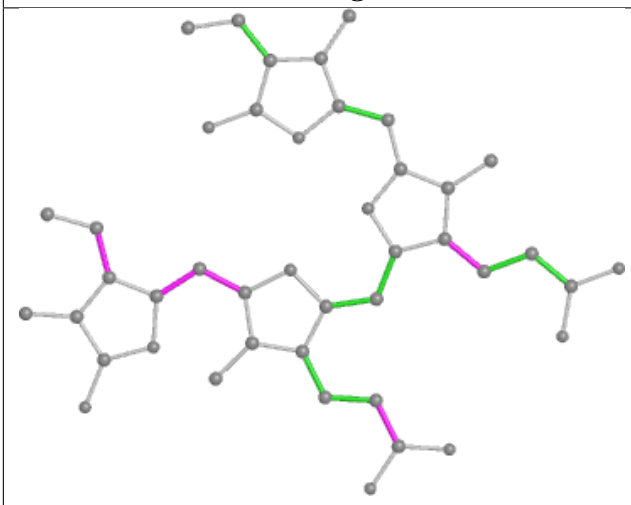

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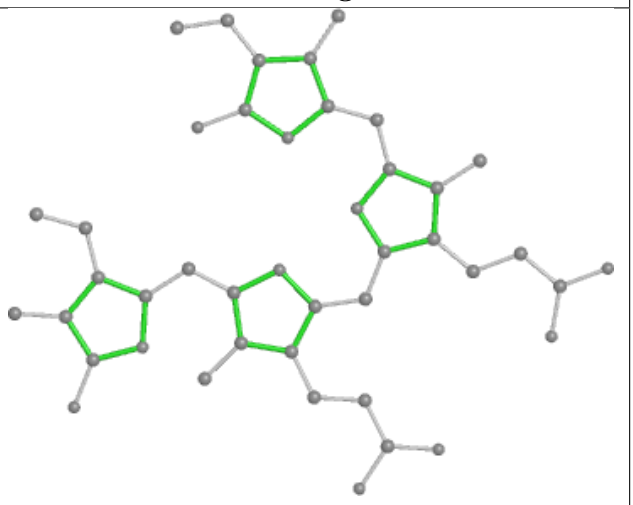

Rings

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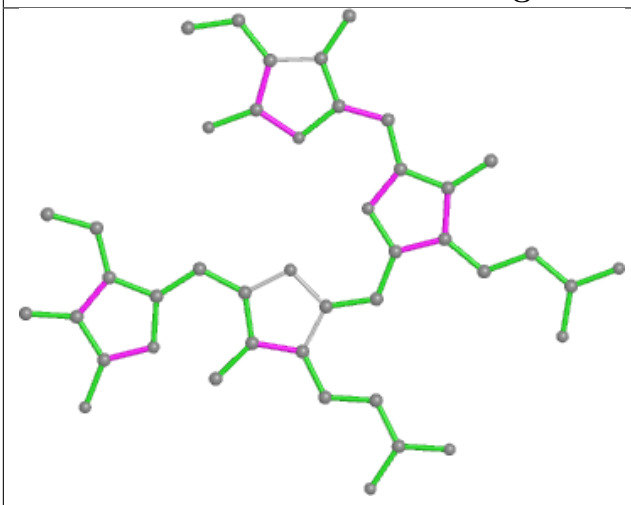

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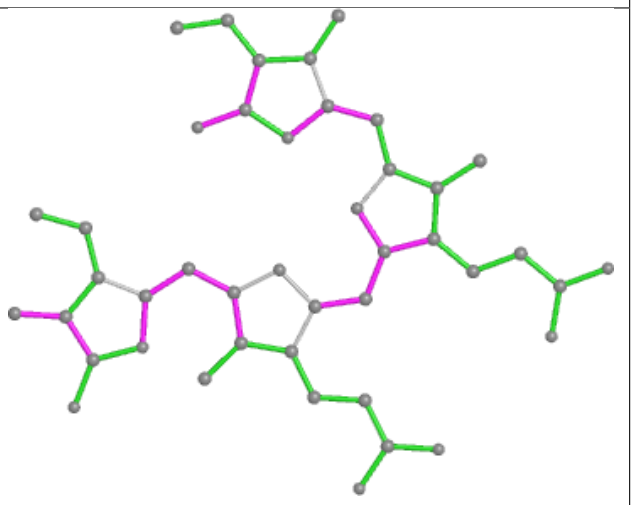

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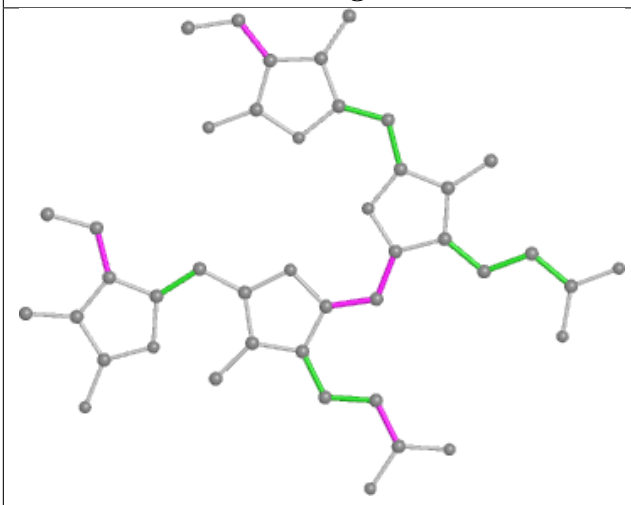

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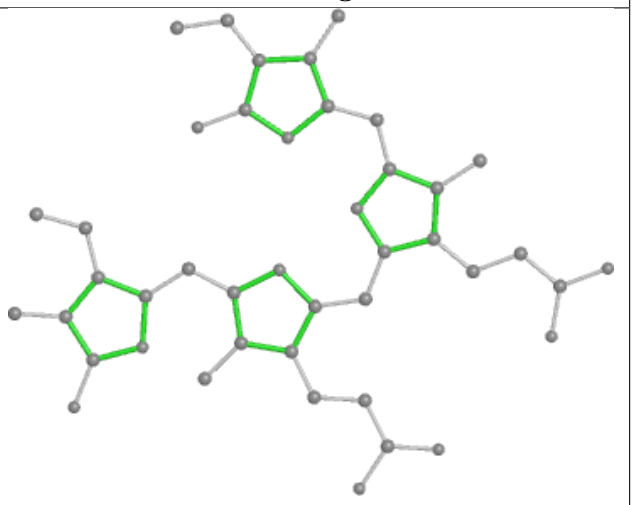

Rings

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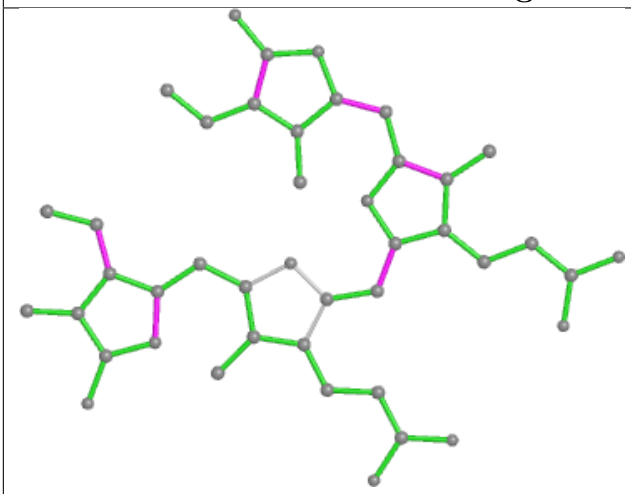

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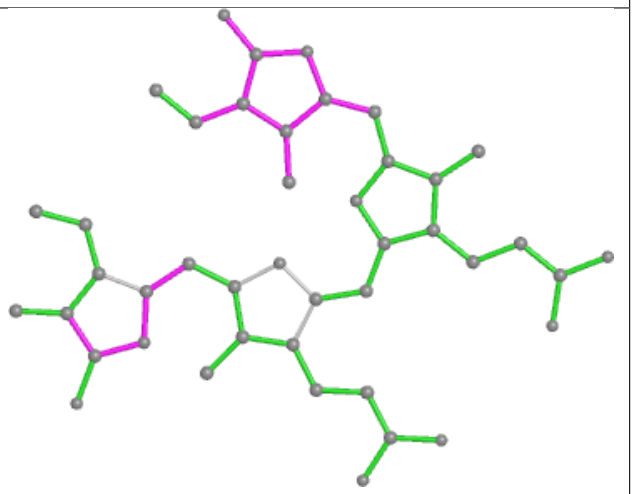

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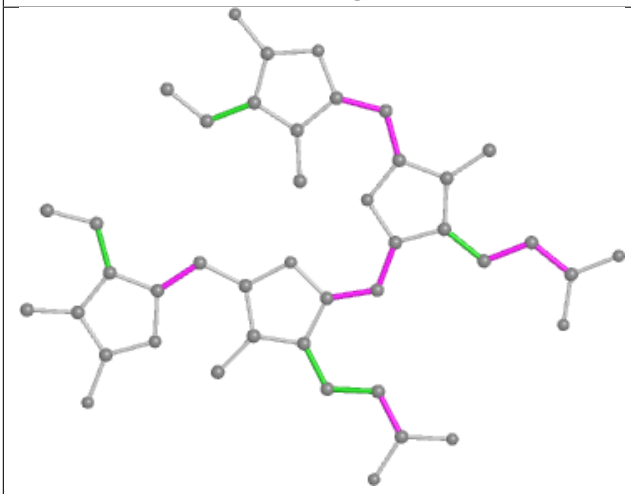

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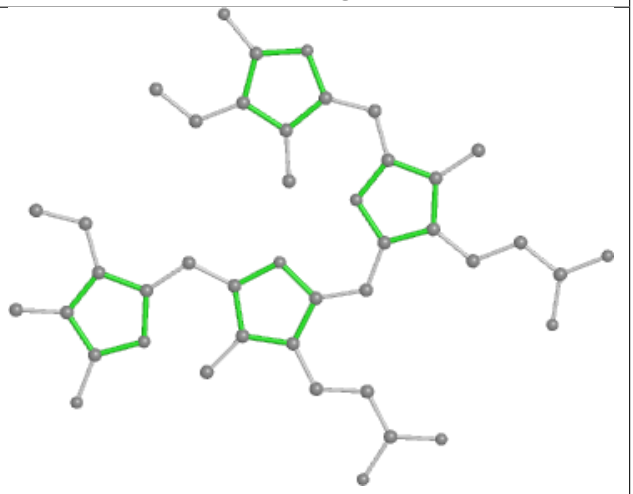
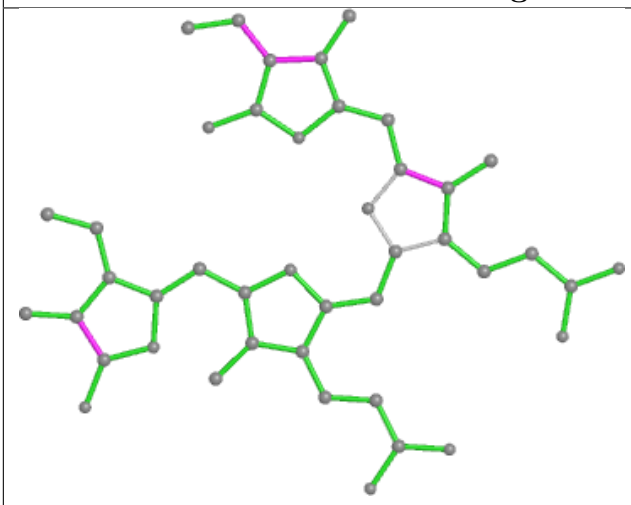


Rings

Ligand PEB y5 1002



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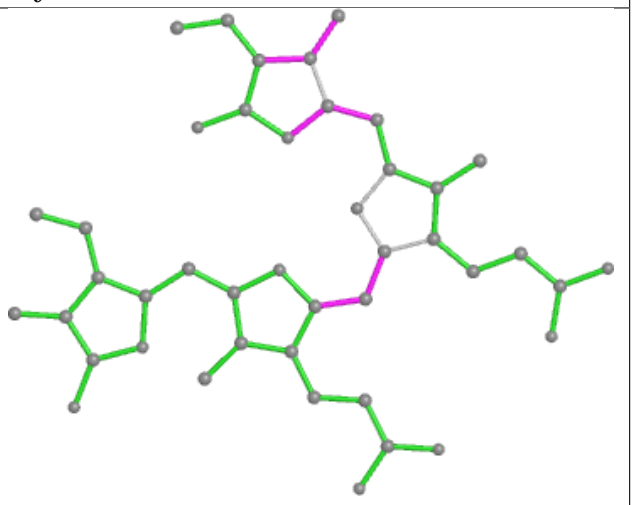

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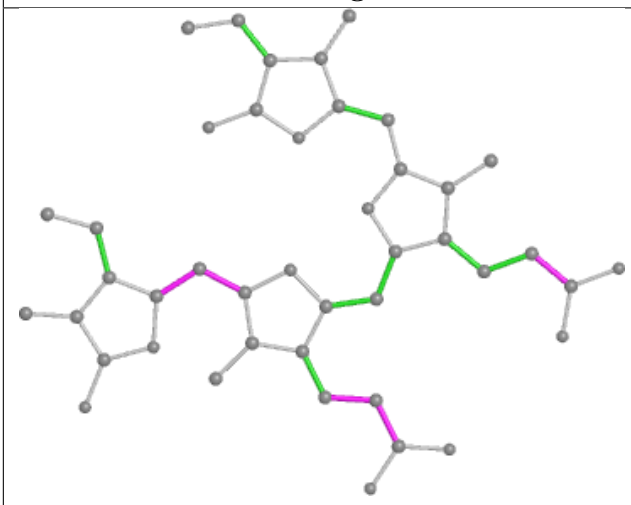

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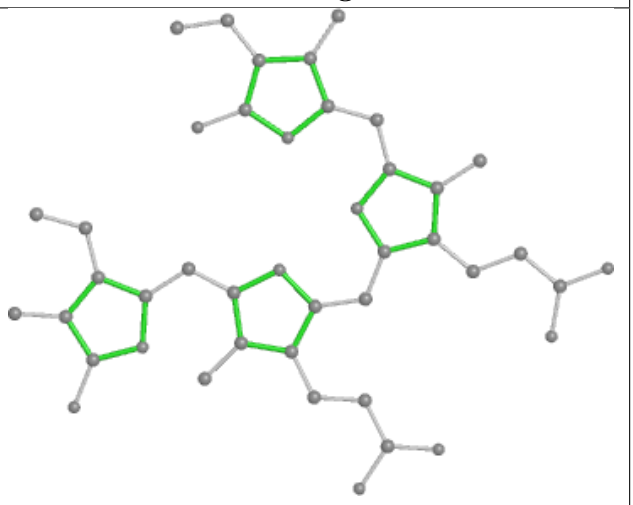
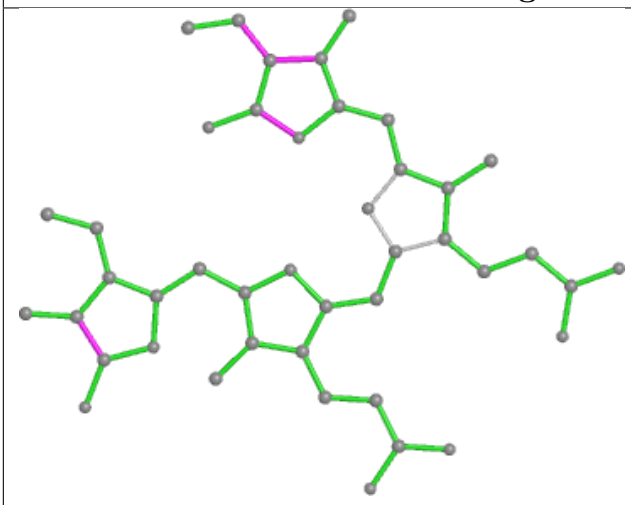


Rings

Ligand PEB S8 401



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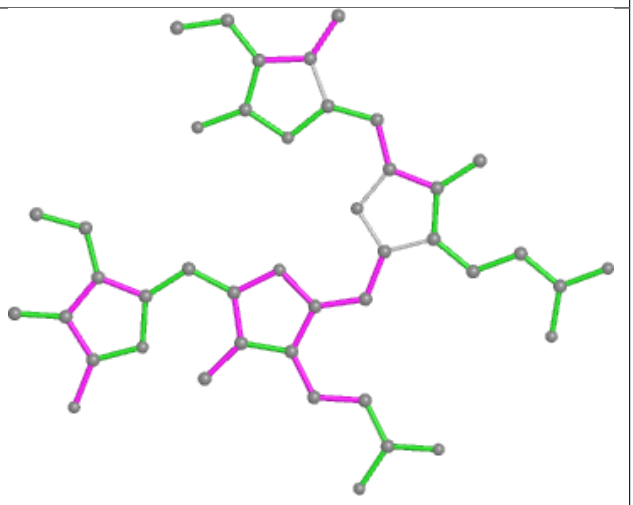
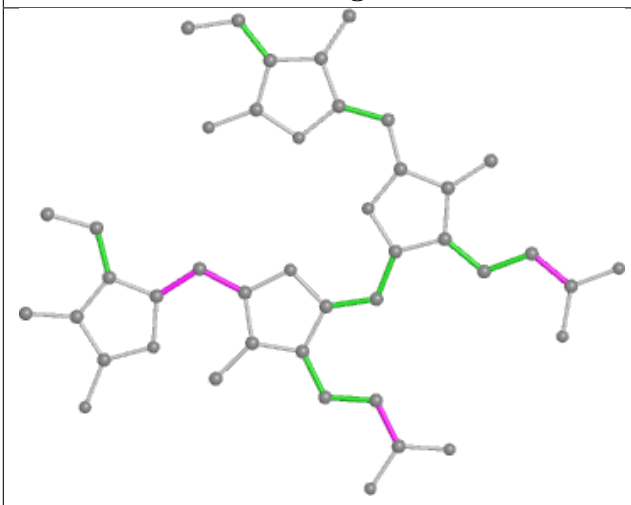


Bond angles



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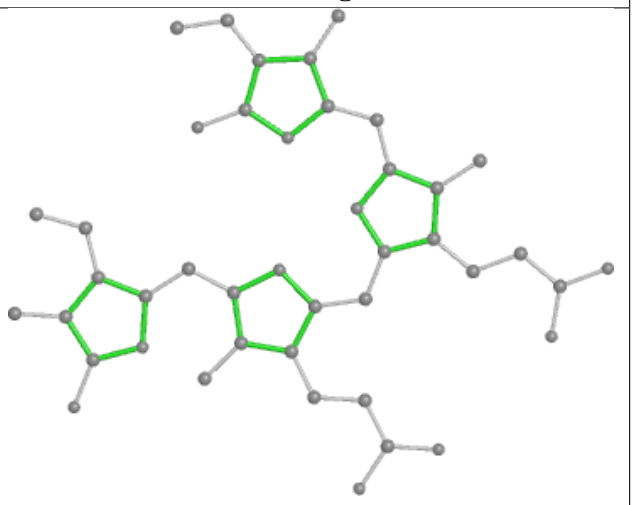
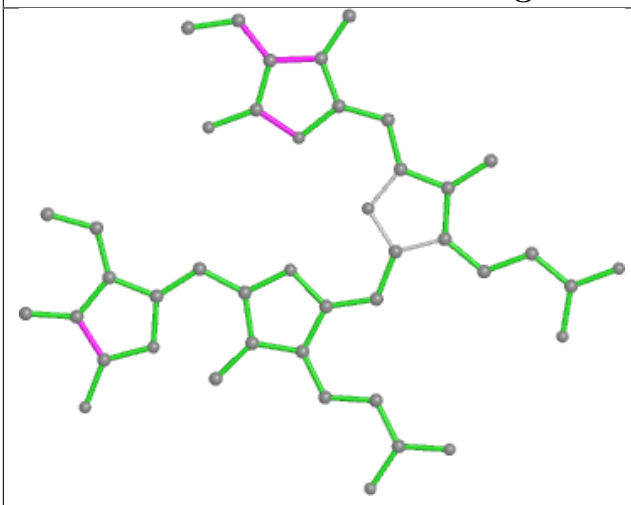


Rings

Ligand PEB N7 201



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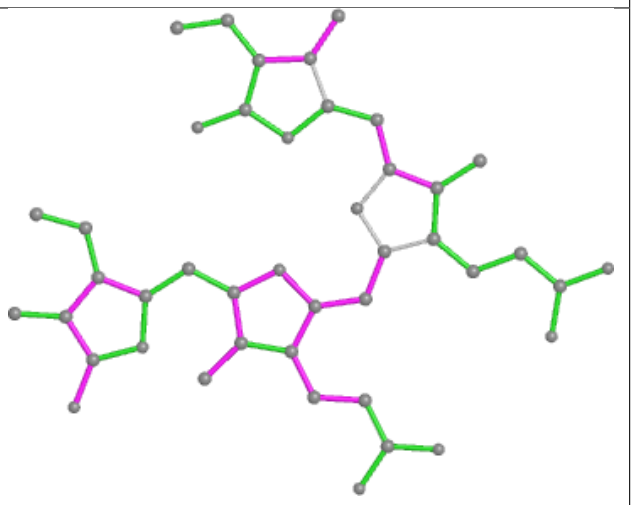

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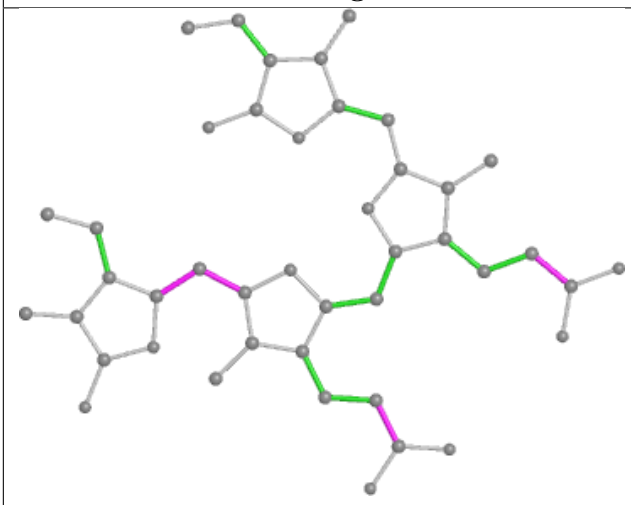

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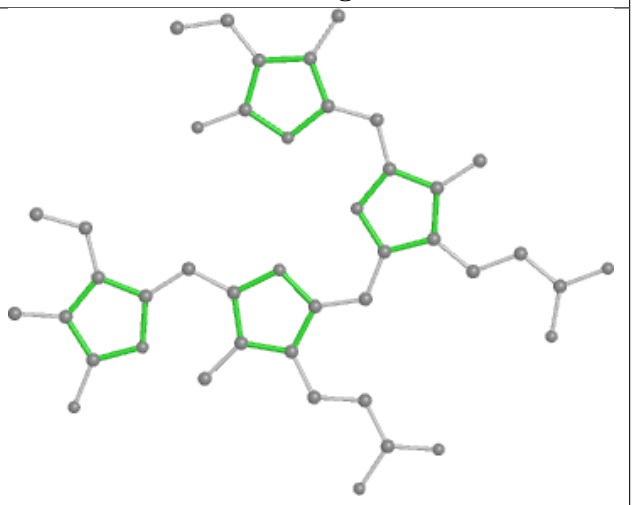
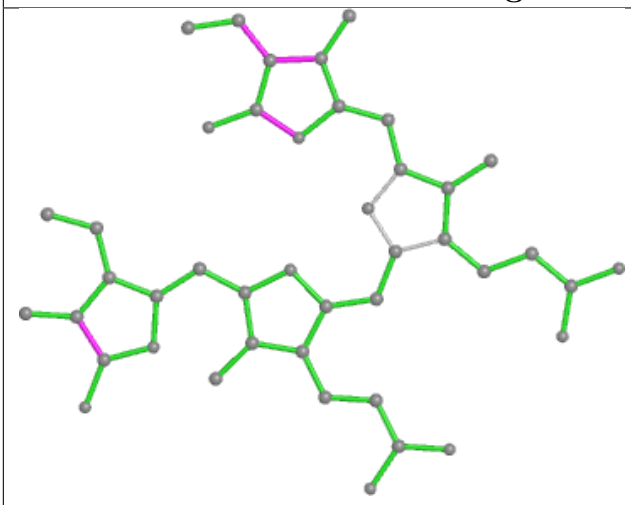


Rings

Ligand PEB bY 1003



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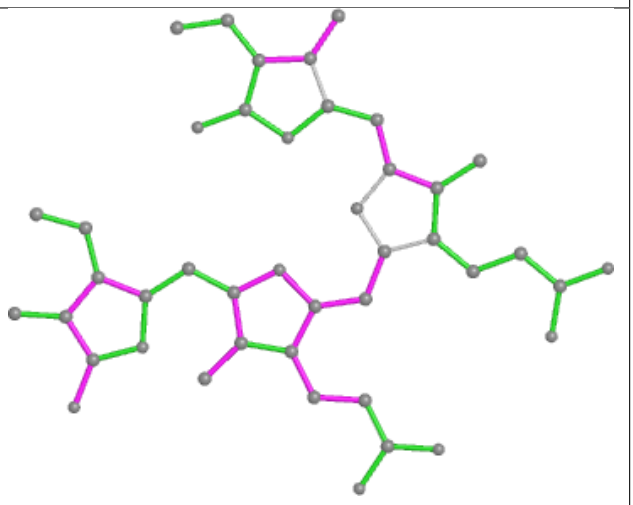
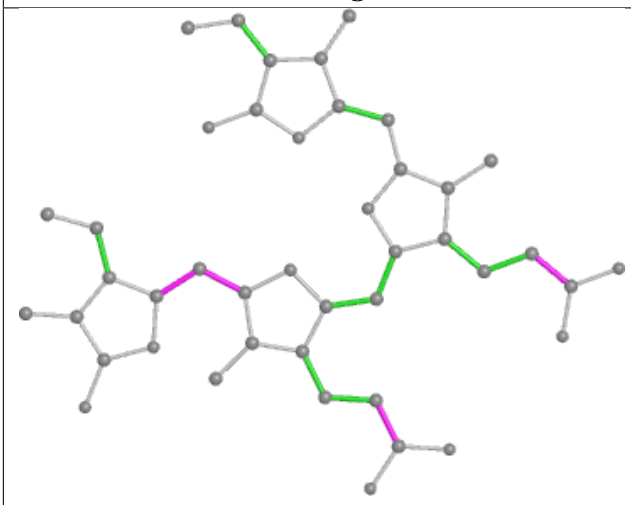
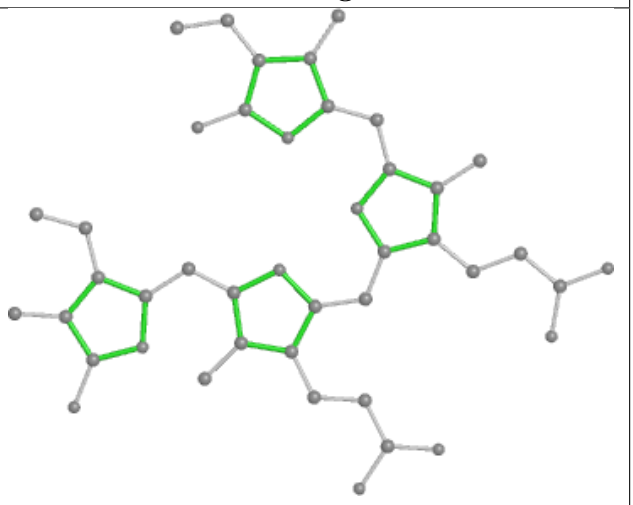


Bond angles

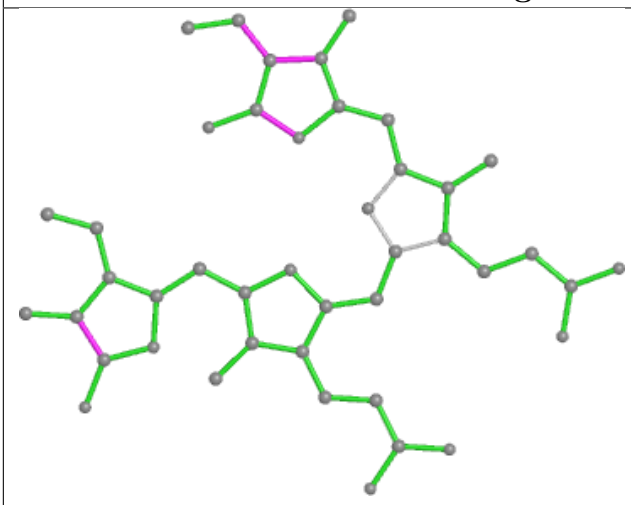


Torsions



Rings

Ligand PEB dY 201



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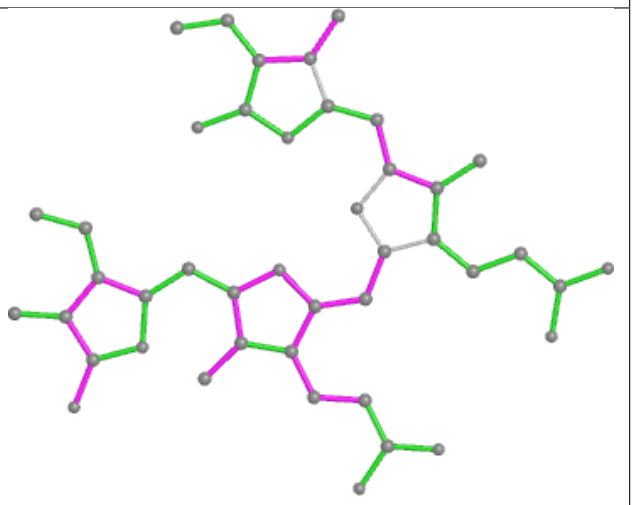

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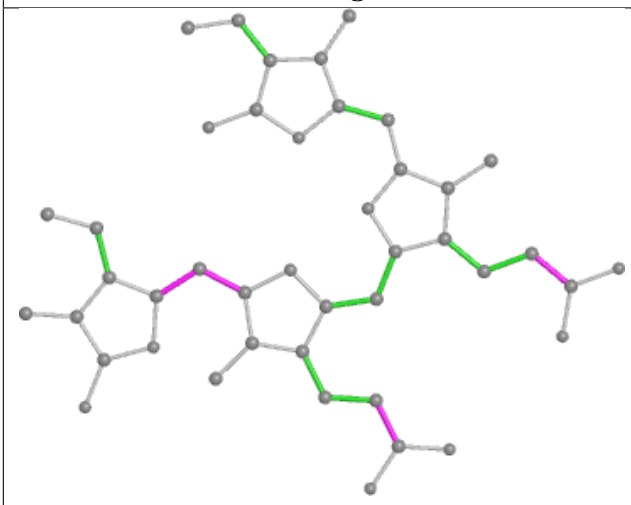

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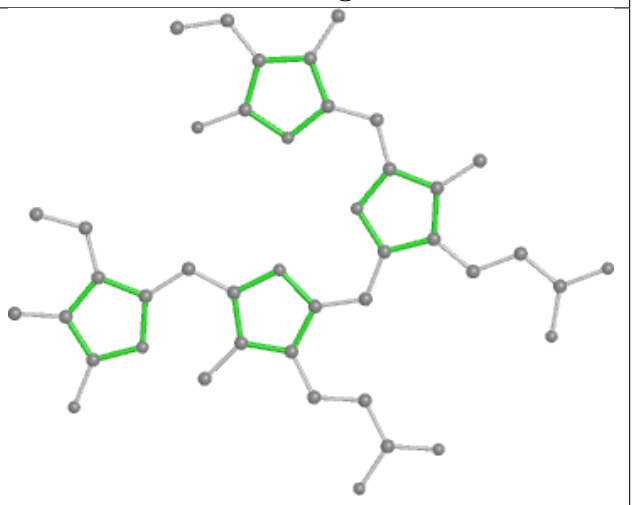
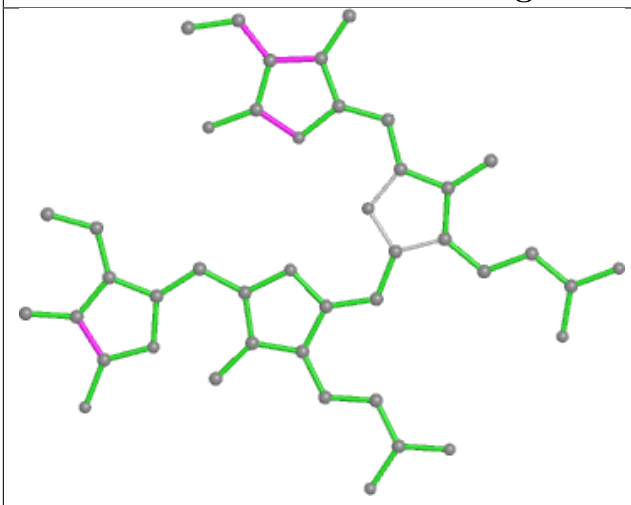


Rings

Ligand PEB V3 201



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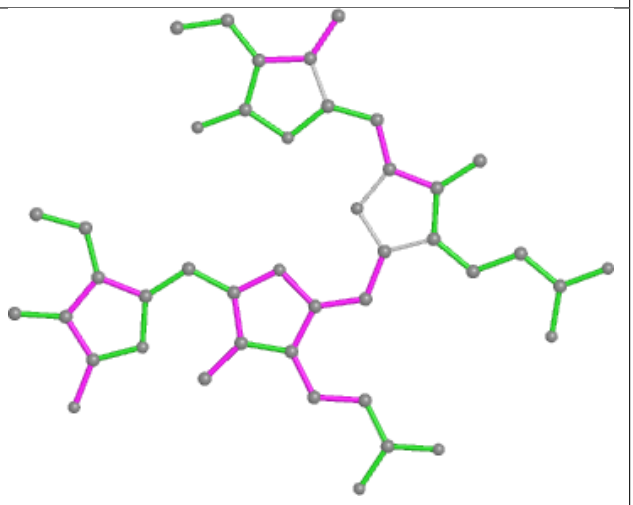

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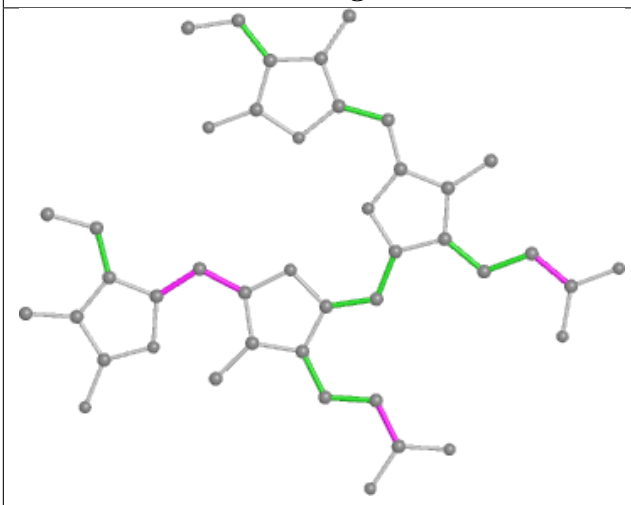

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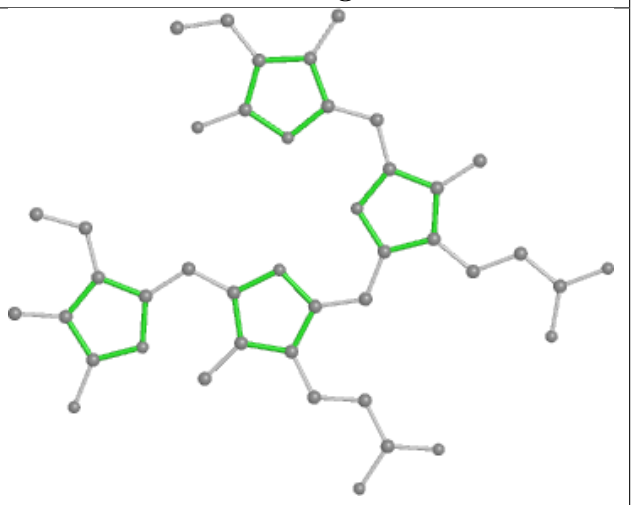

Rings

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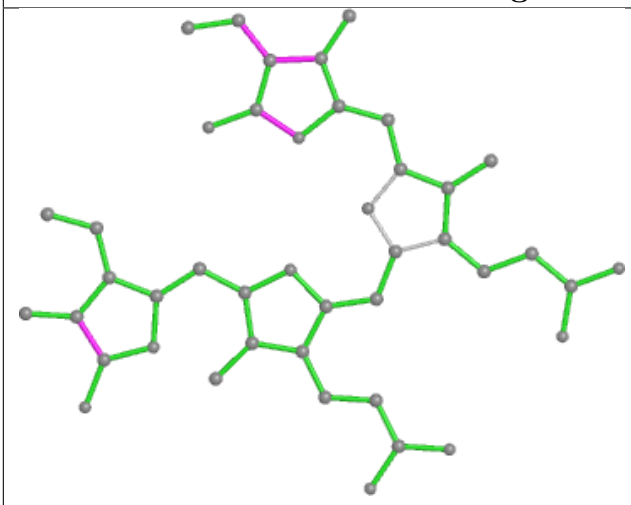

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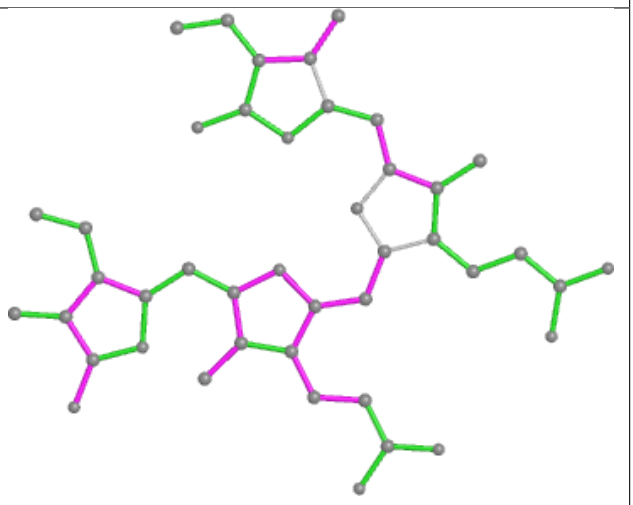
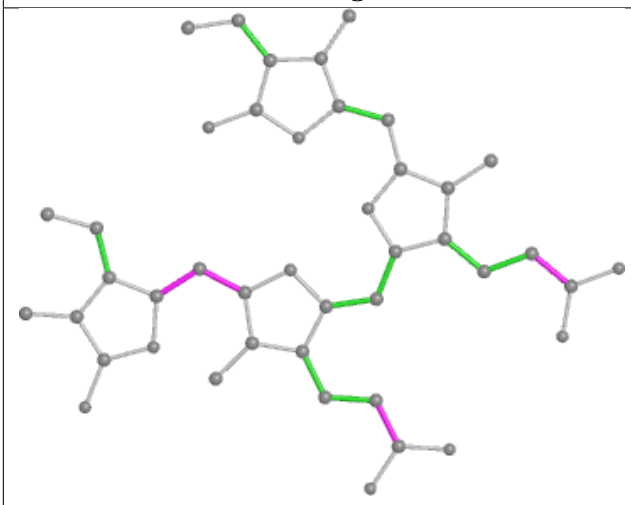


Bond angles



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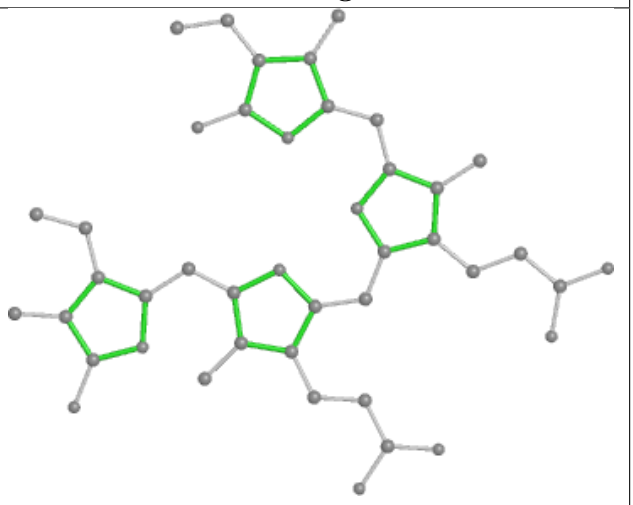
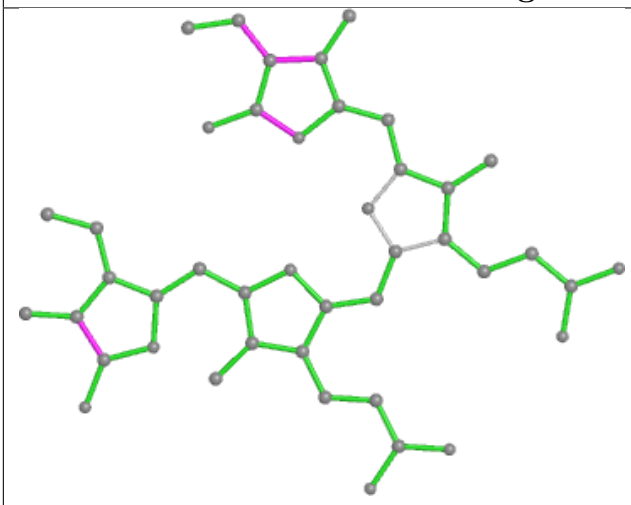


Rings

Ligand PEB bq 202



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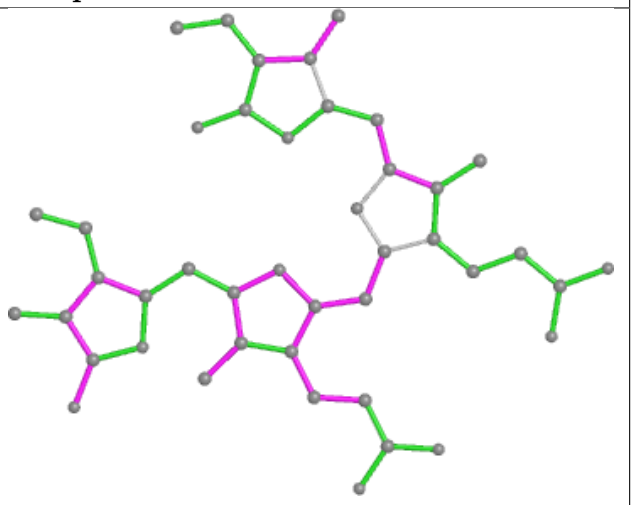

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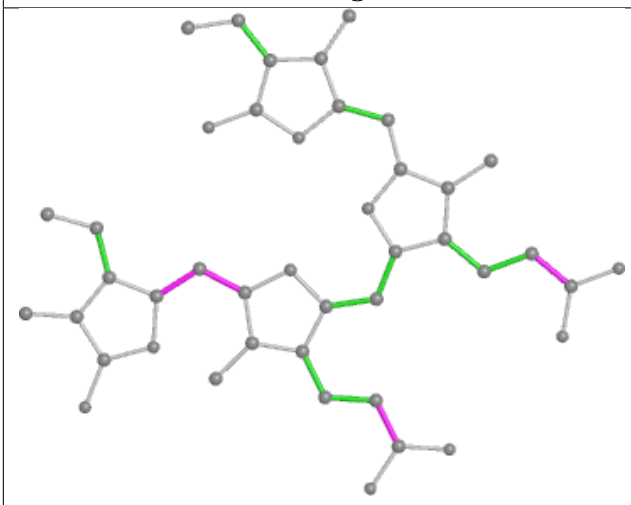

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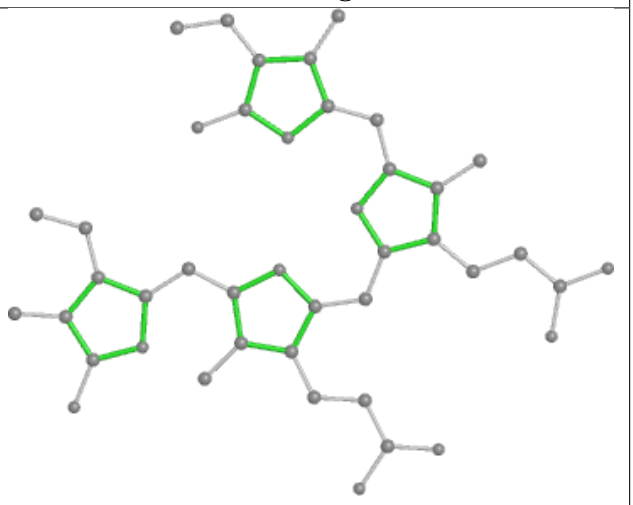

Rings

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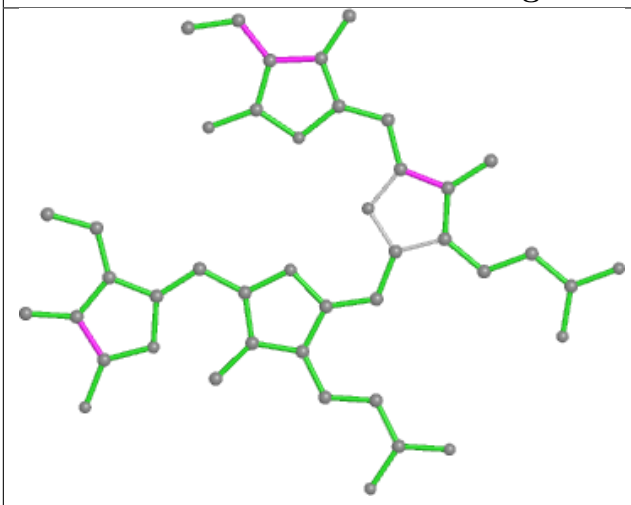

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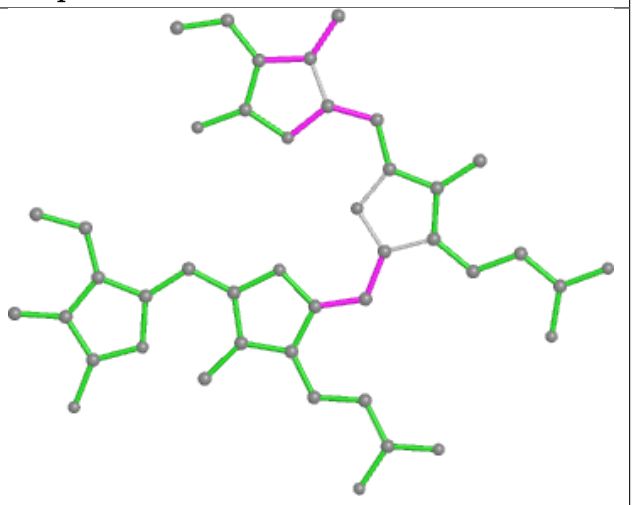

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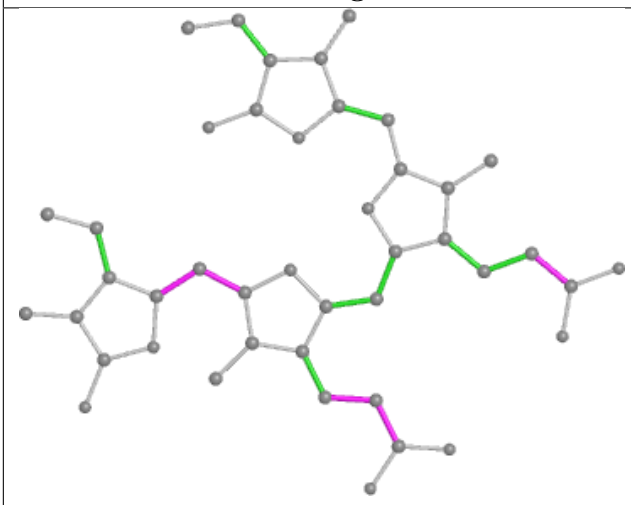

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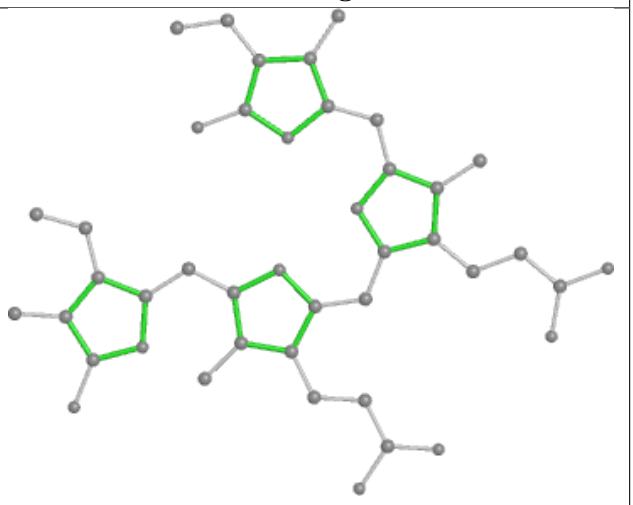

Rings

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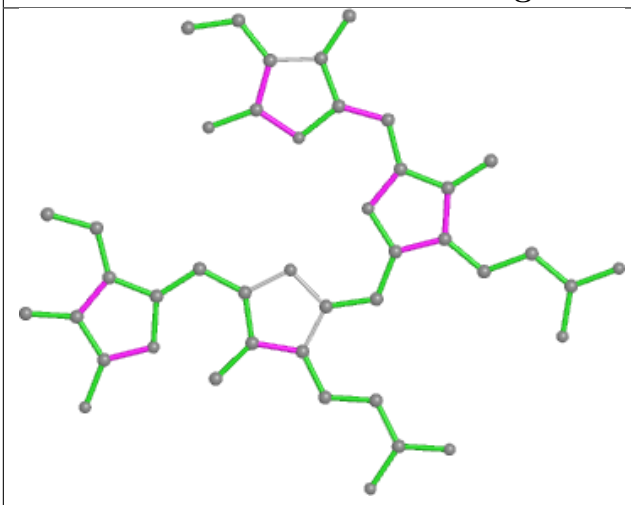

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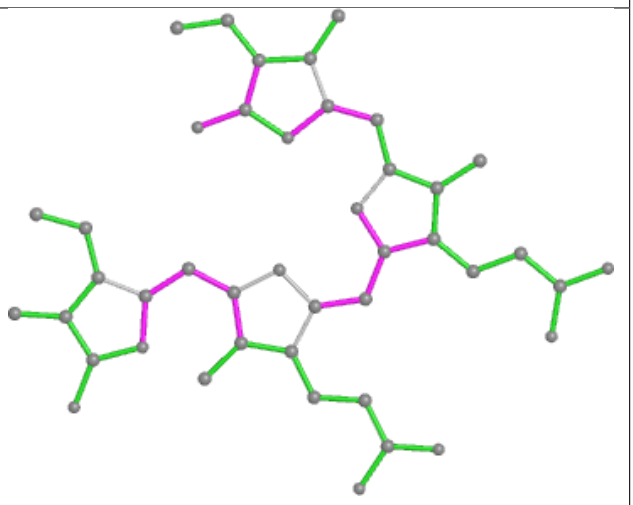

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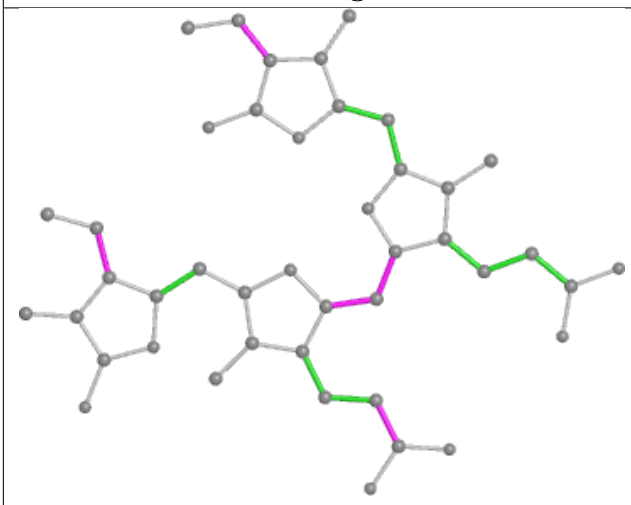

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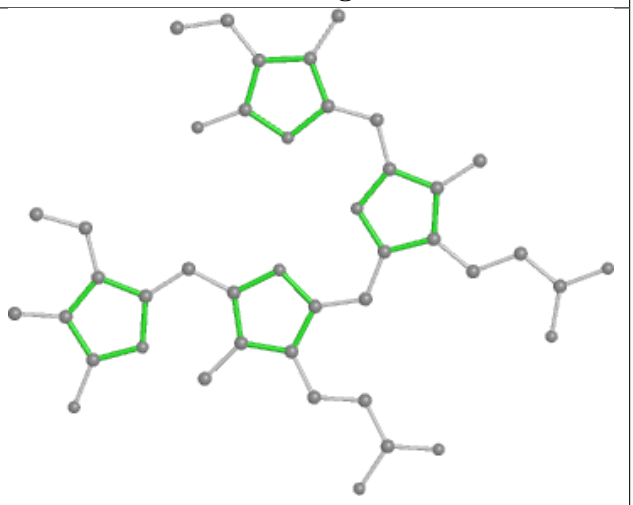

Rings

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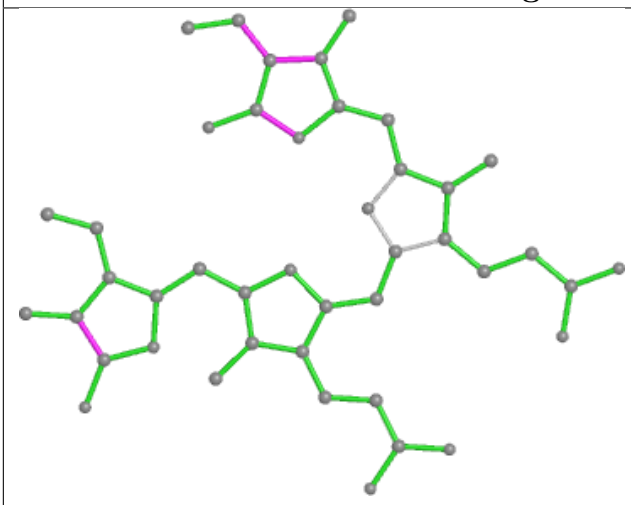

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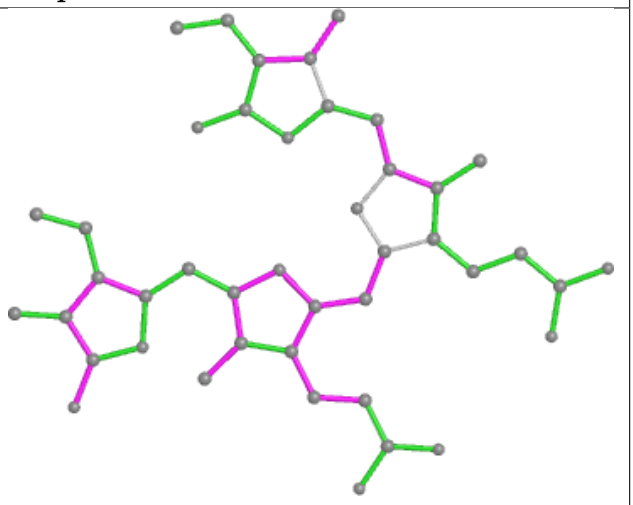

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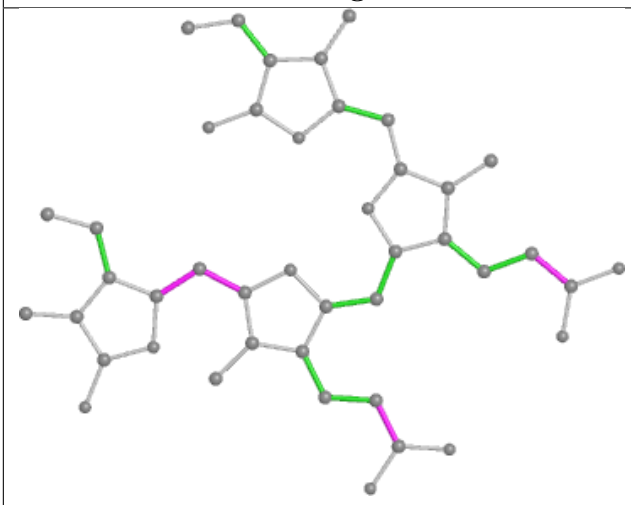

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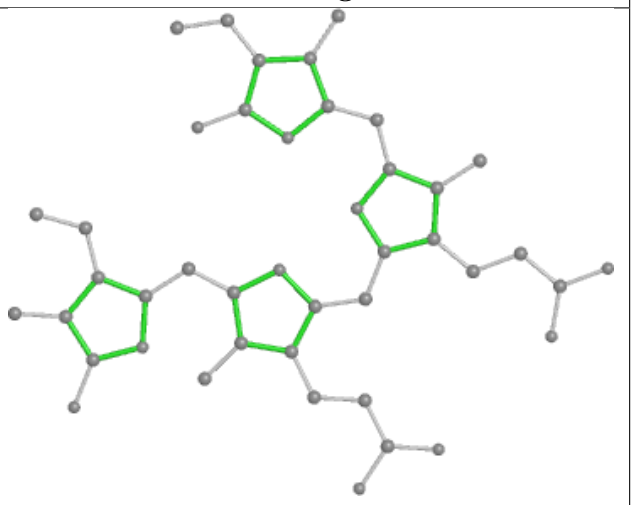

Rings

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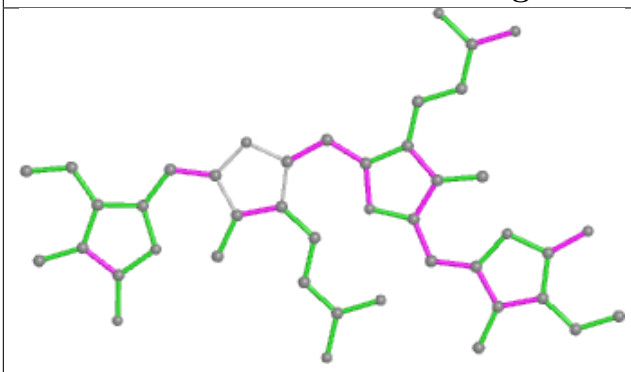

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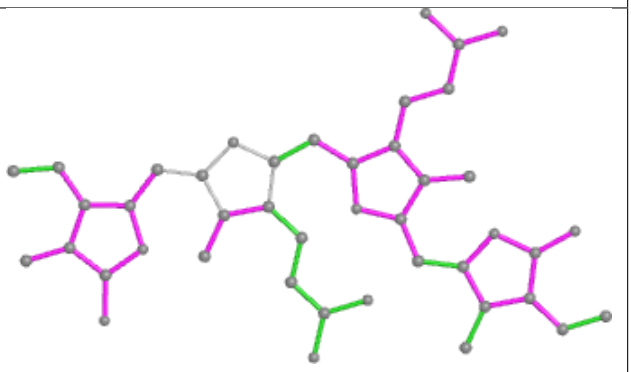

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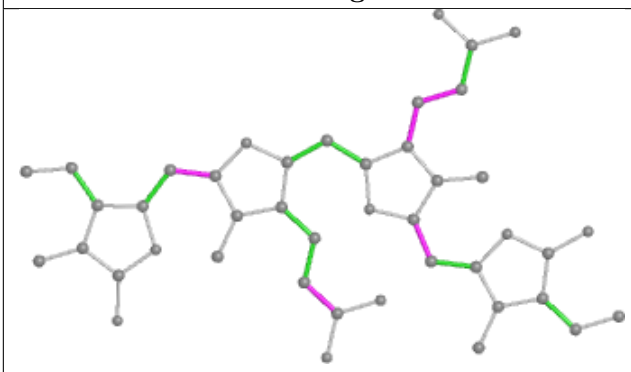

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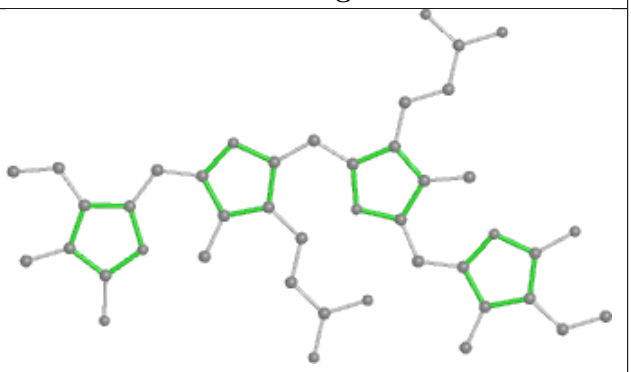

Rings

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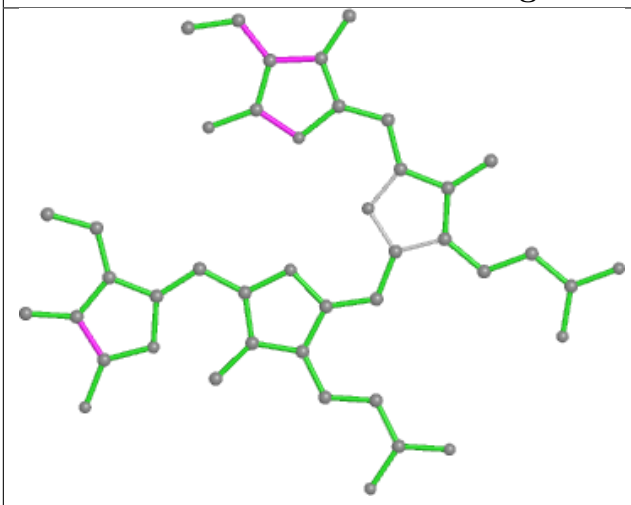

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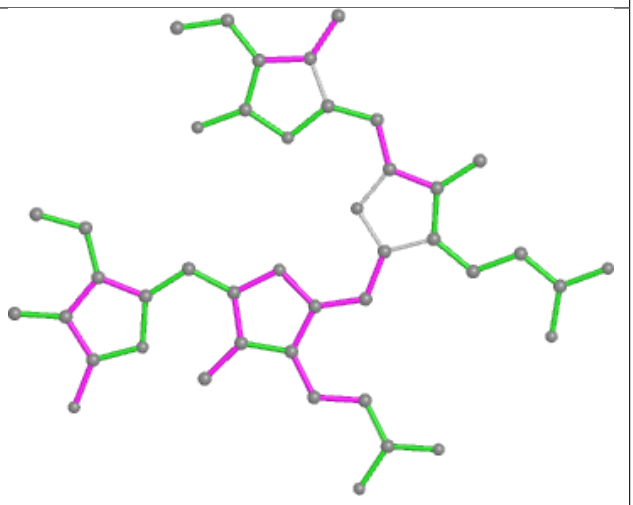

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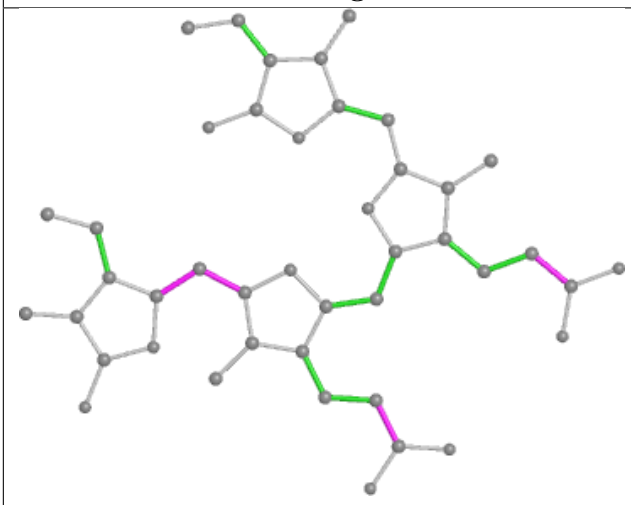

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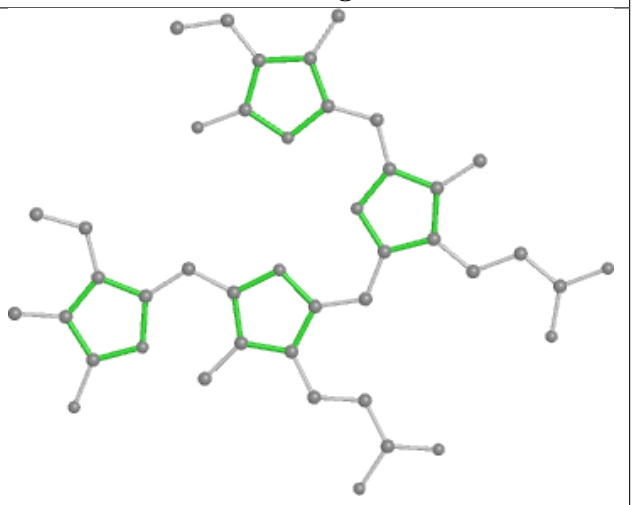
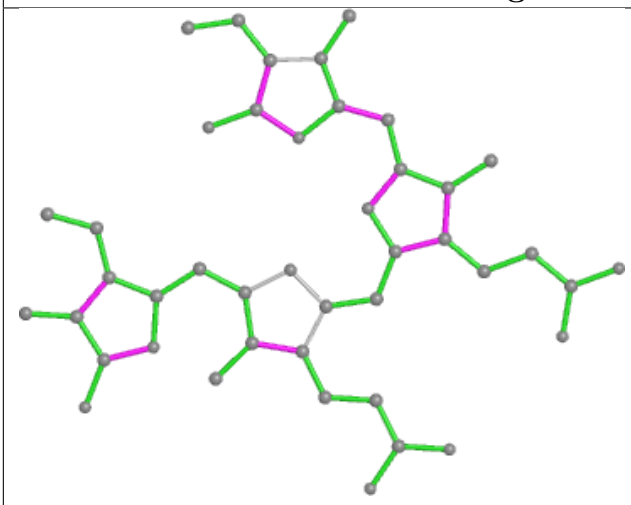


Rings

Ligand PUB jO 1003



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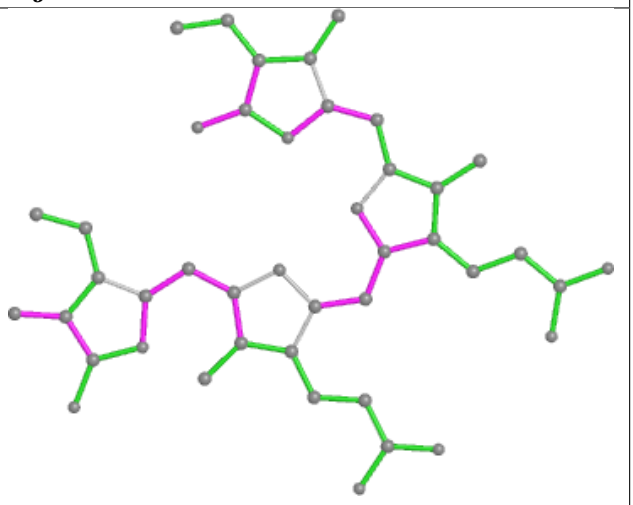

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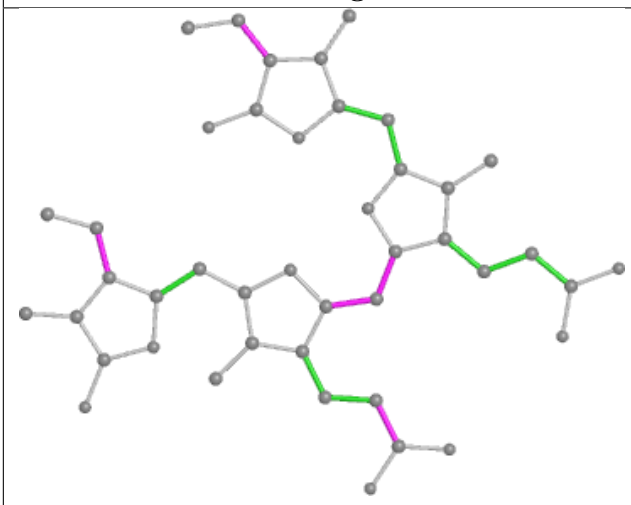

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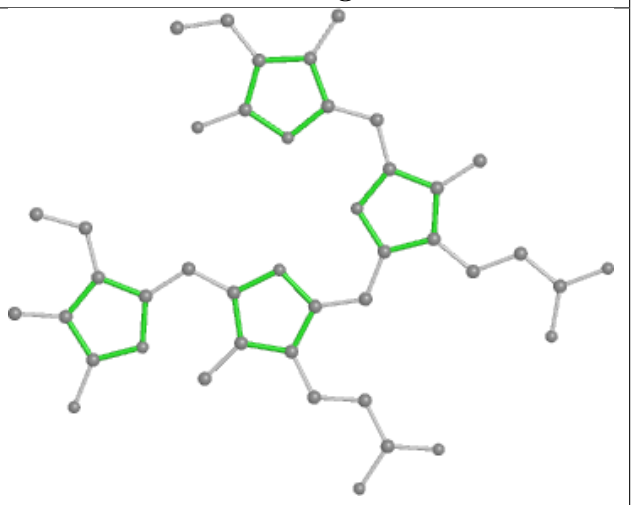

Rings

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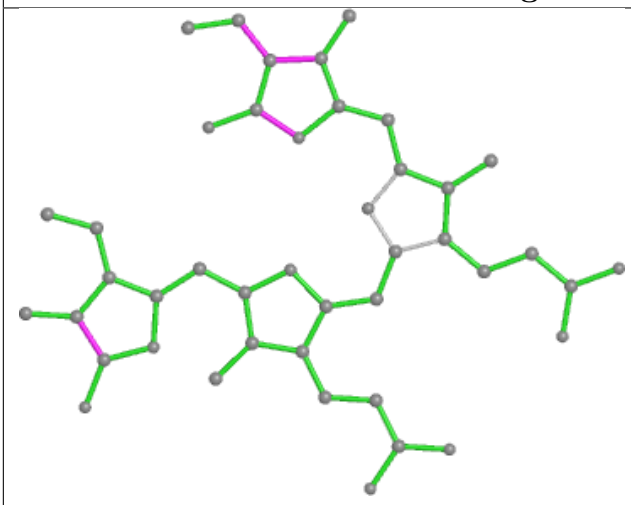

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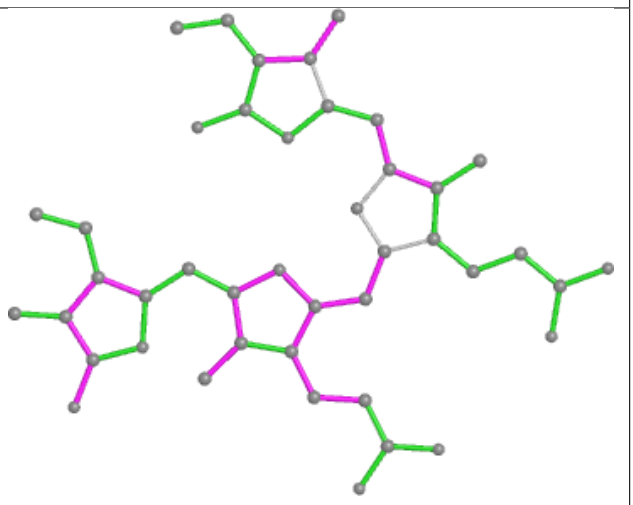

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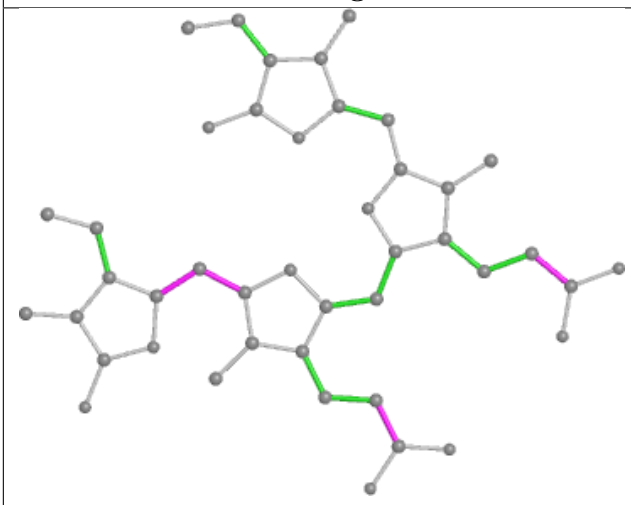

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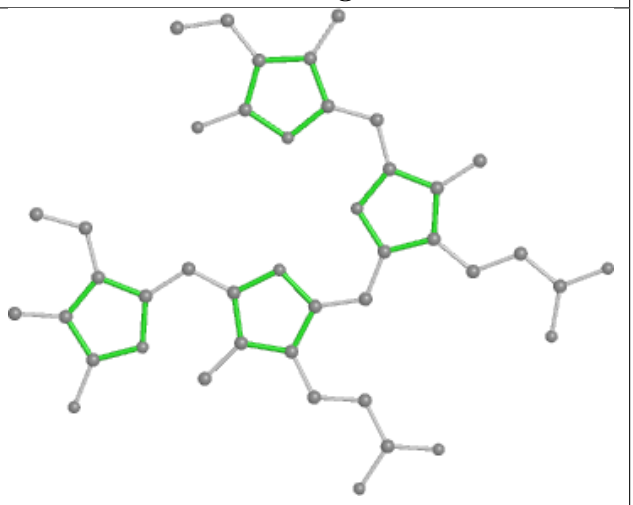
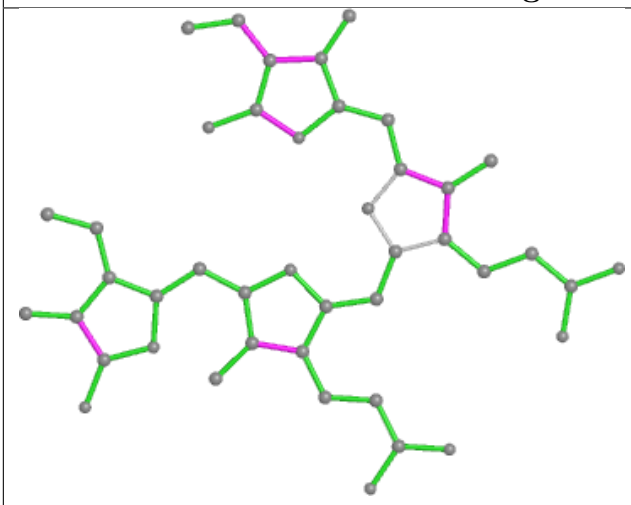


Rings

Ligand PEB et 202



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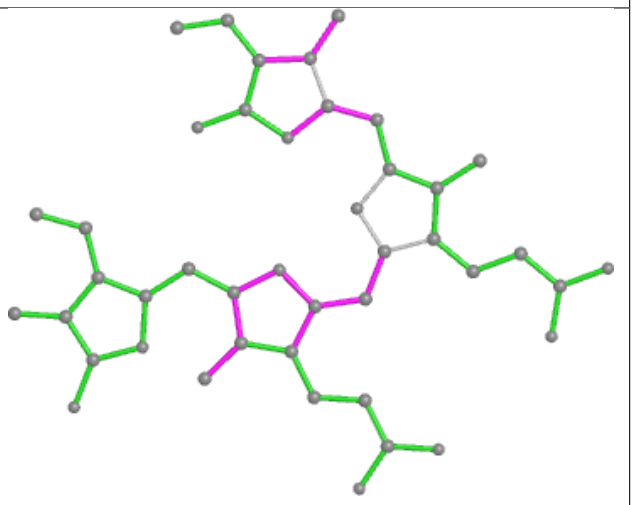

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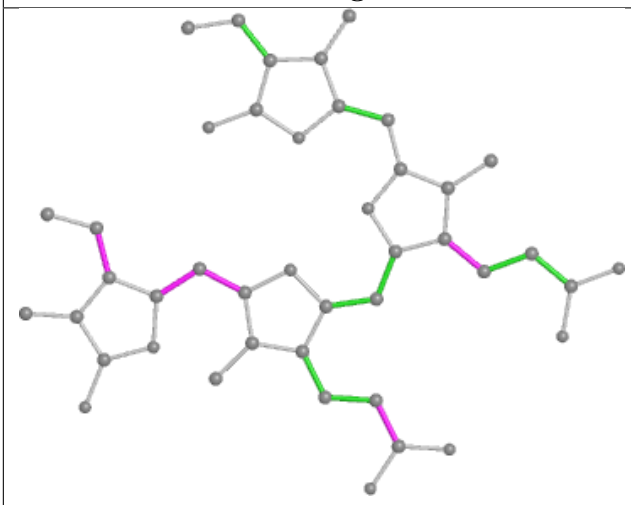

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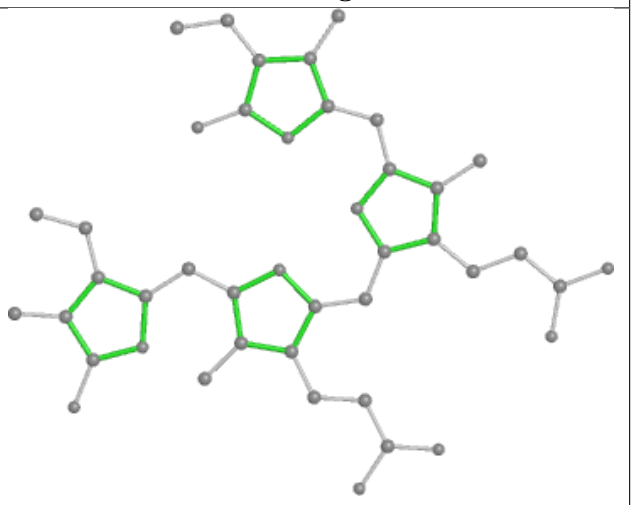
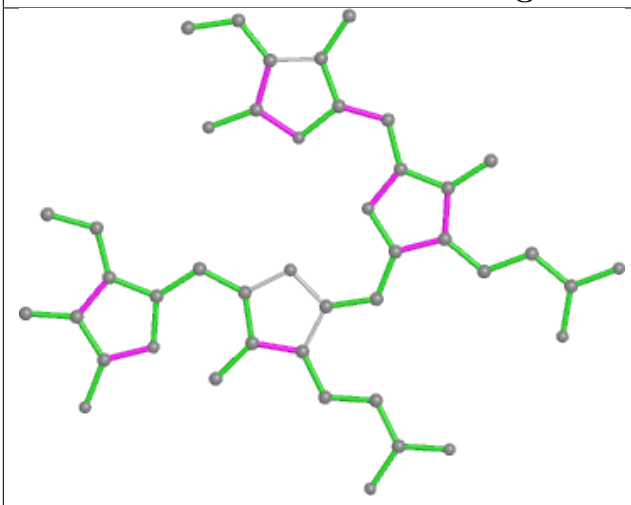


Rings

Ligand PUB aZ 304



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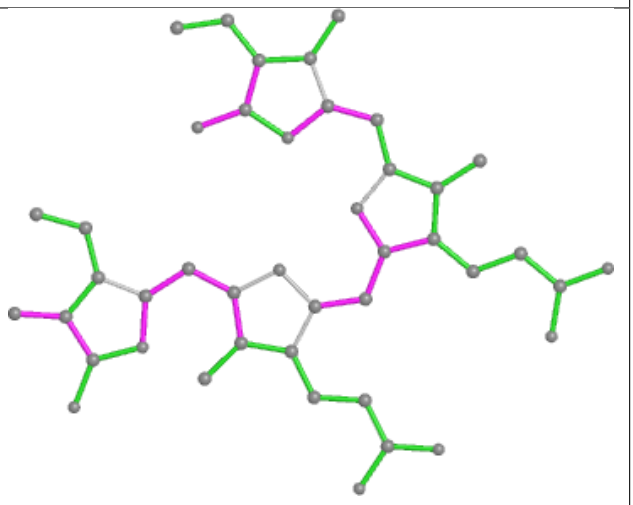
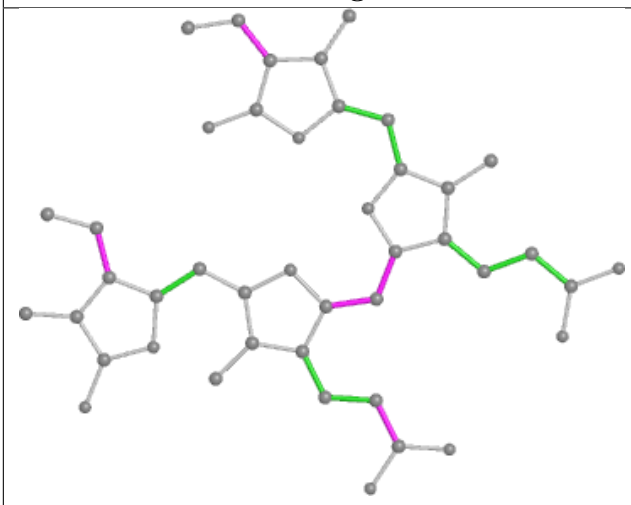
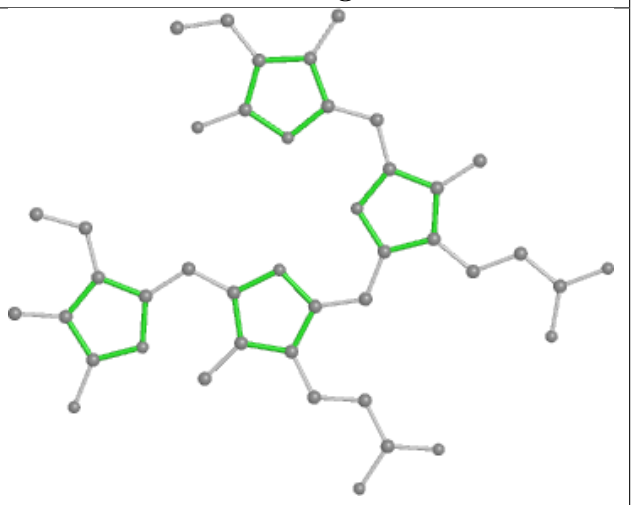


Bond angles

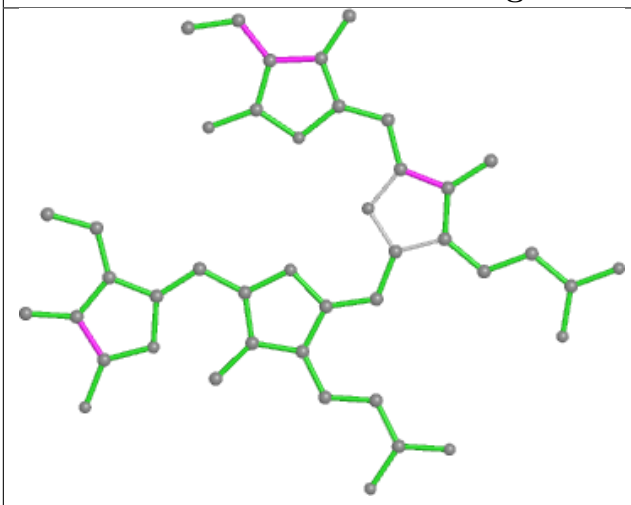


Torsions



Rings

Ligand PEB Y5 1002



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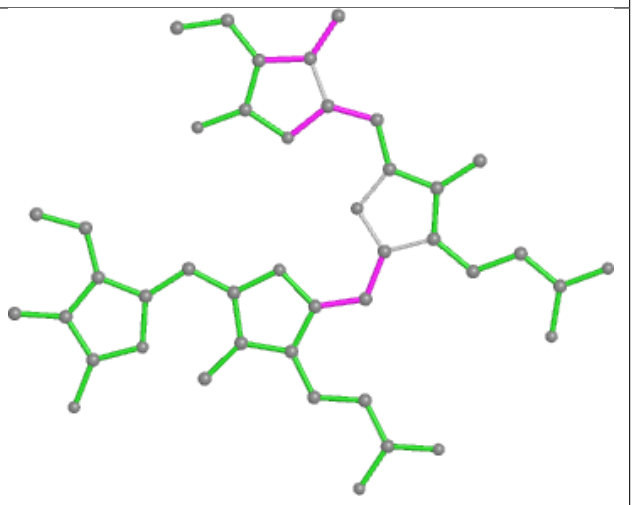
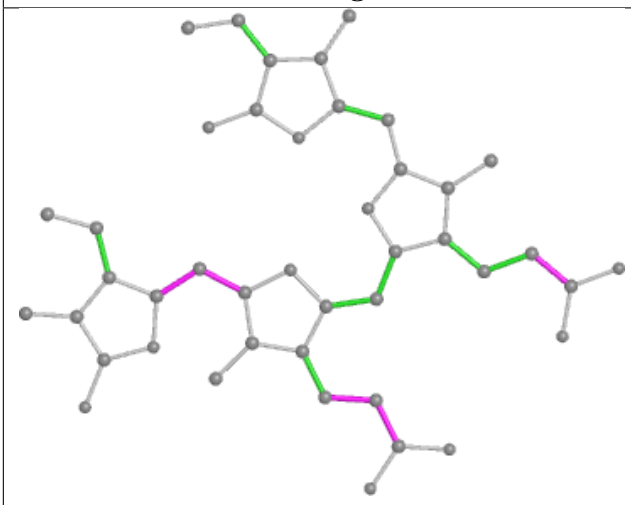


Bond angles



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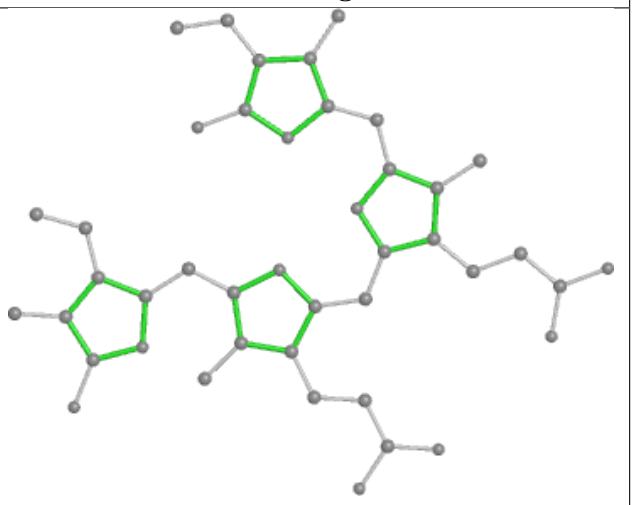
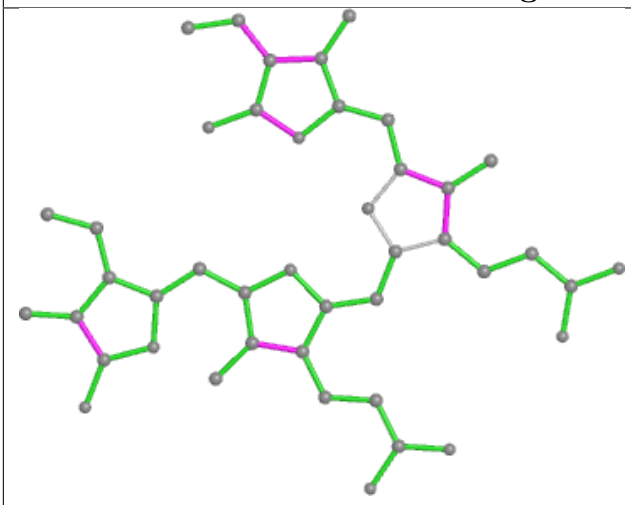


Rings

Ligand PEB av 202



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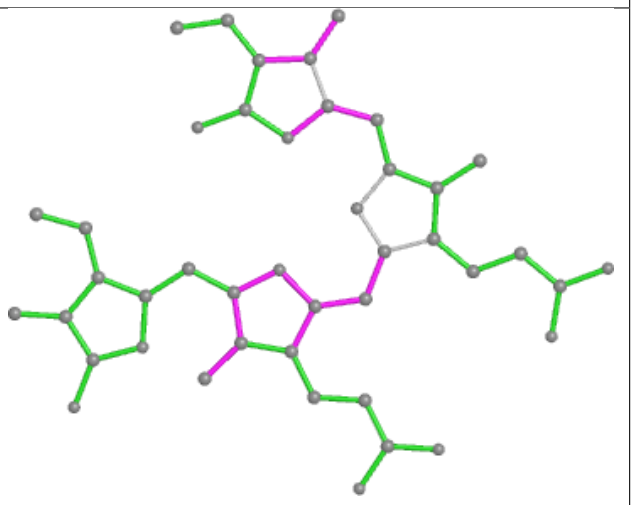

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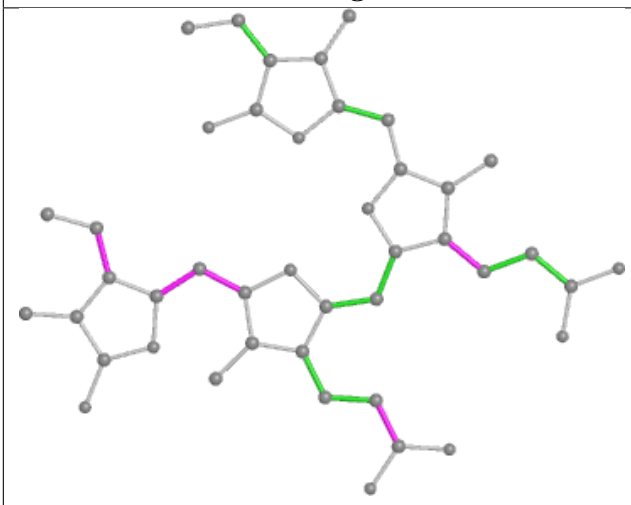

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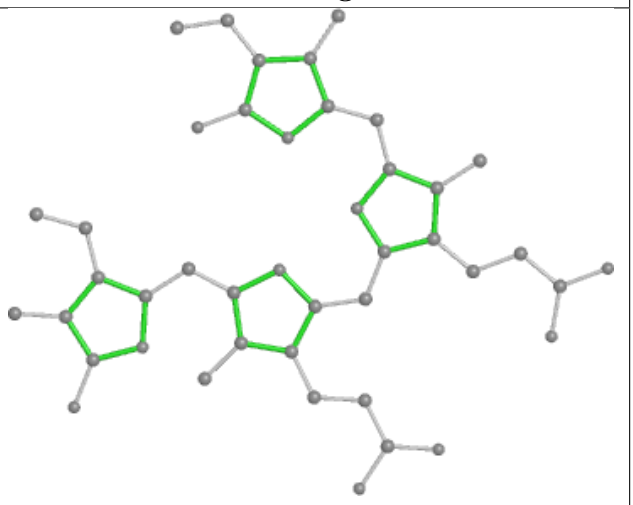
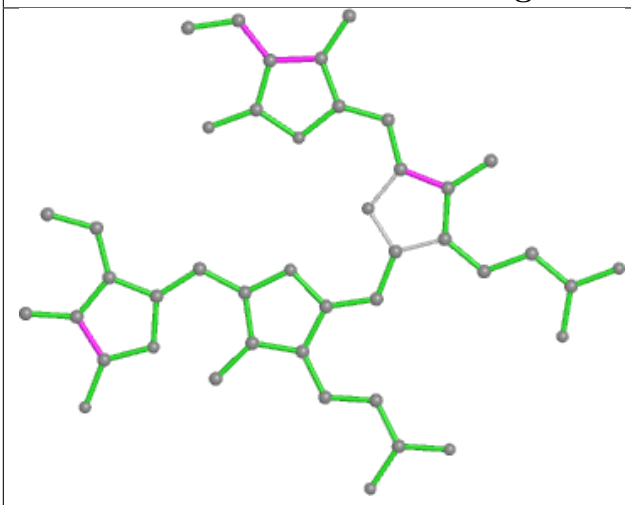


Rings

Ligand PEB G3 202



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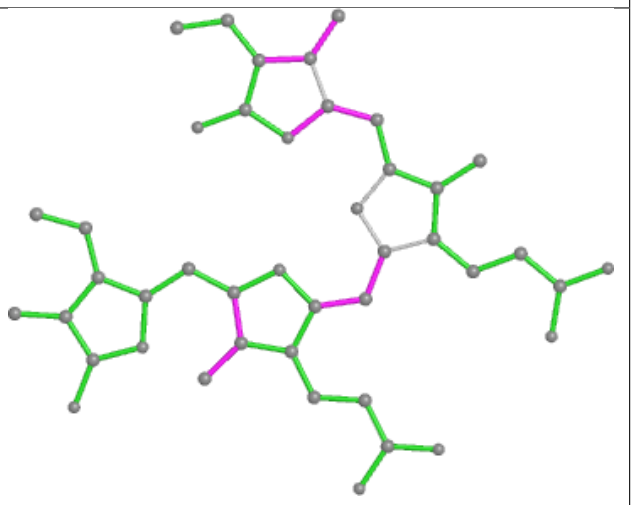

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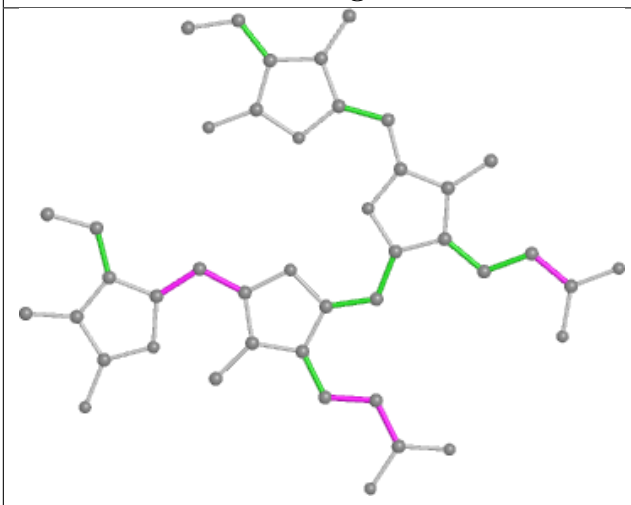

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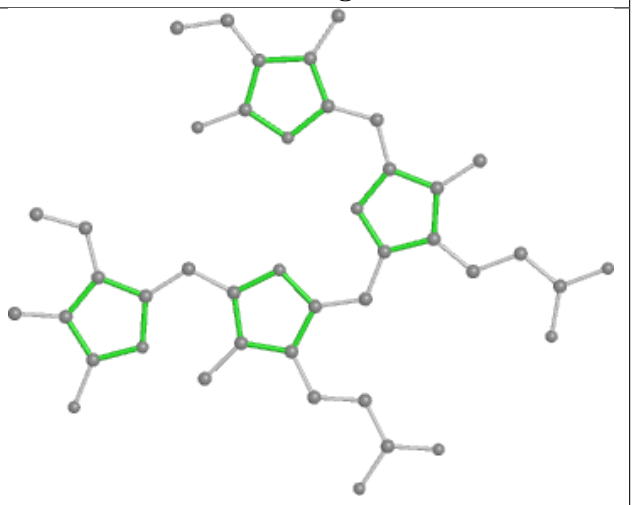
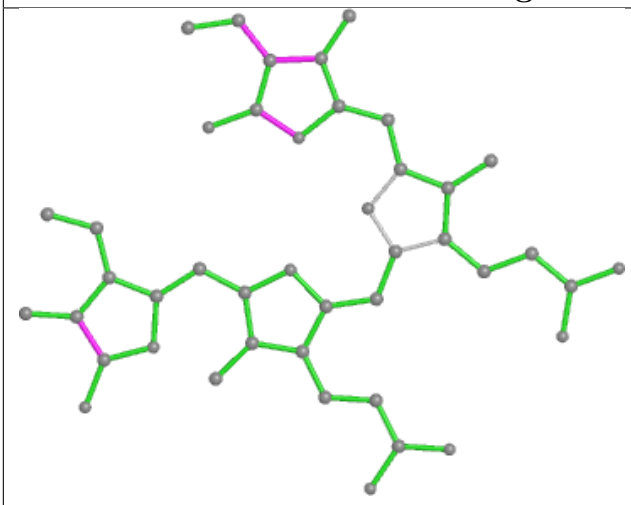


Rings

Ligand PEB Y4 202



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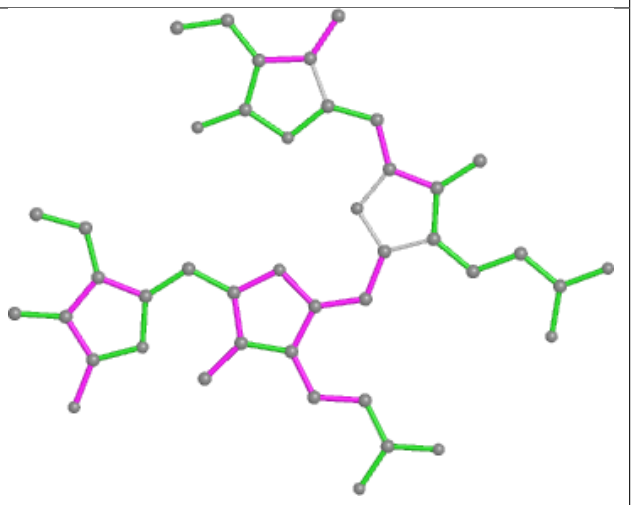

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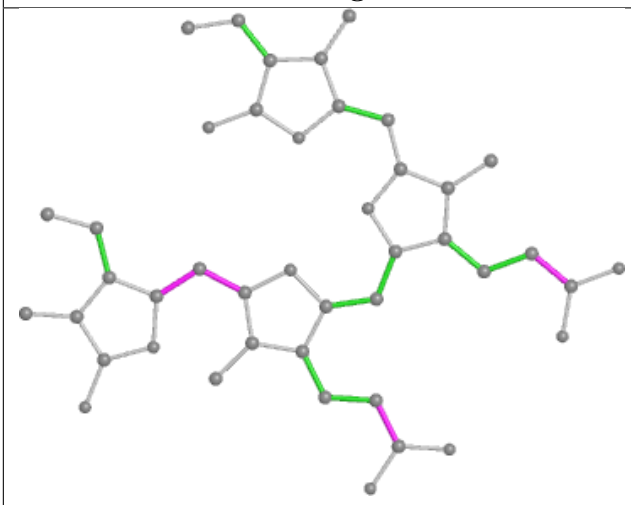

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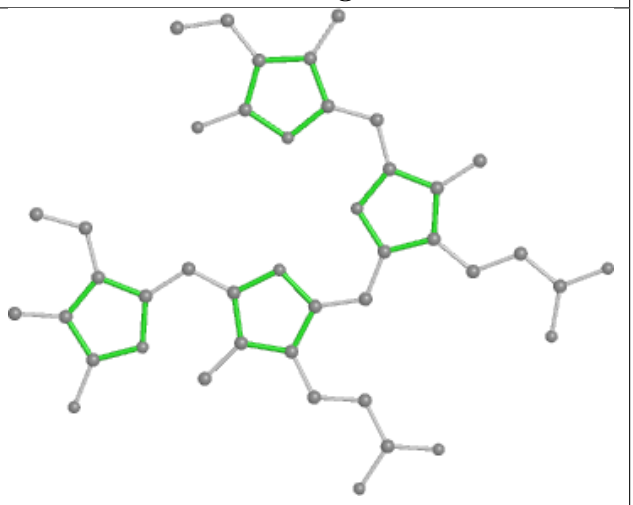

Rings

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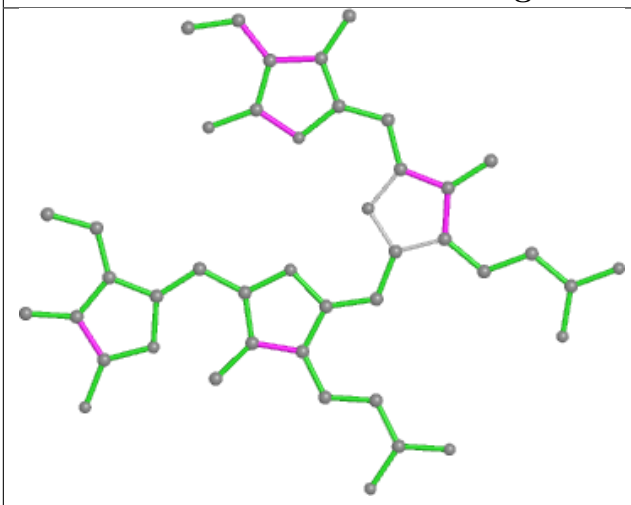

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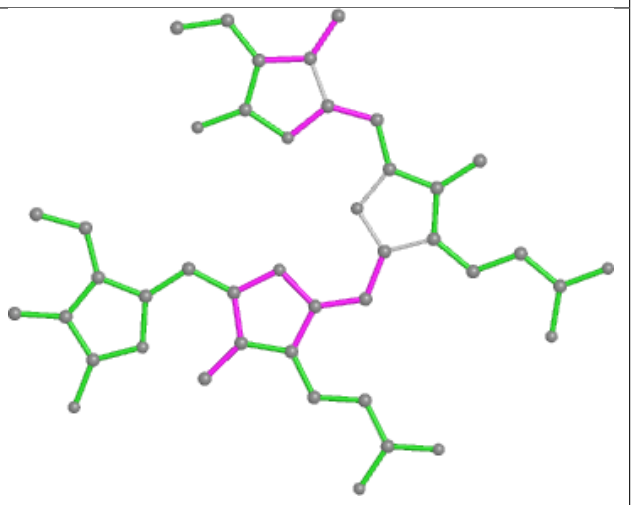

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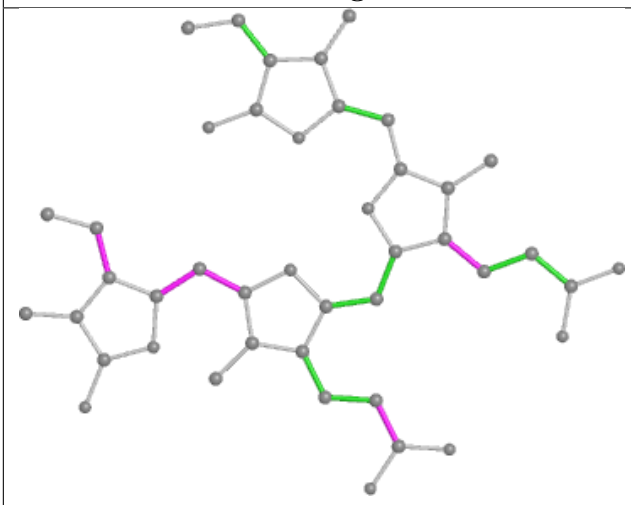

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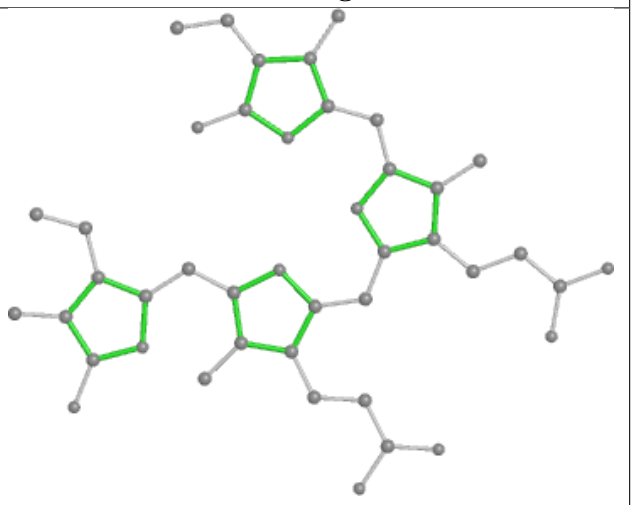
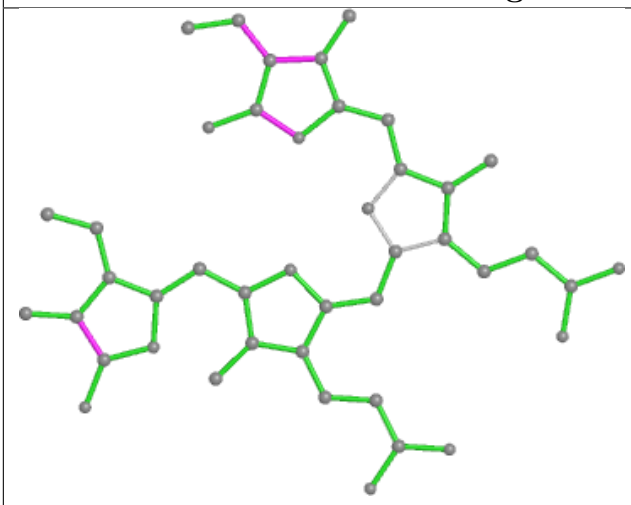


Rings

Ligand PEB kR 1001



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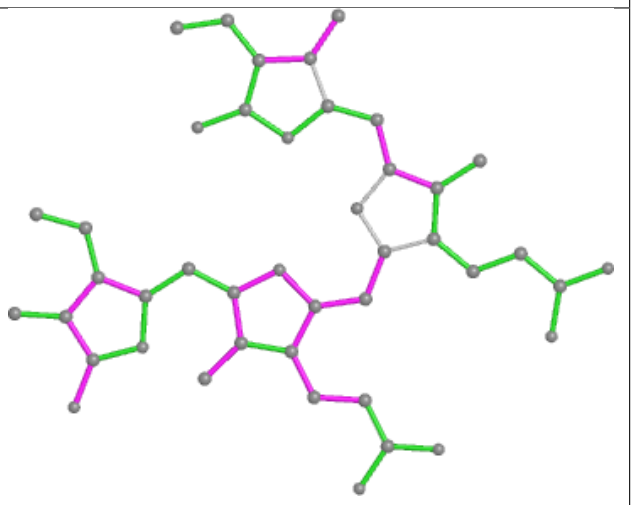

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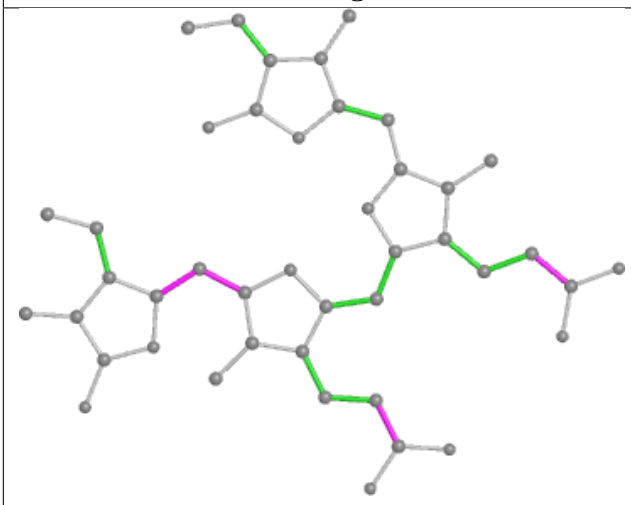

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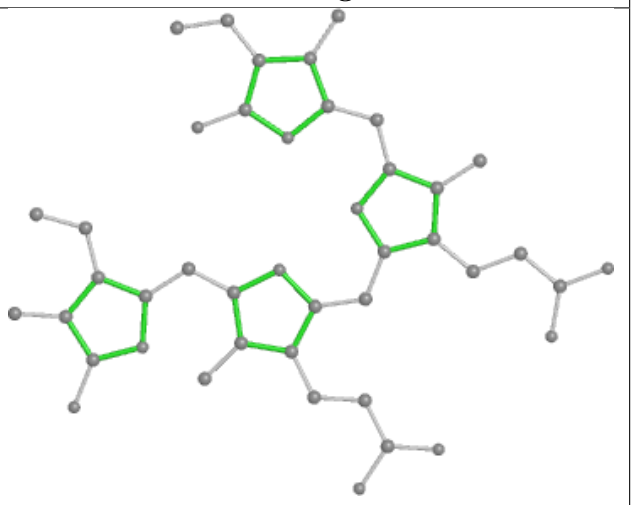

Rings

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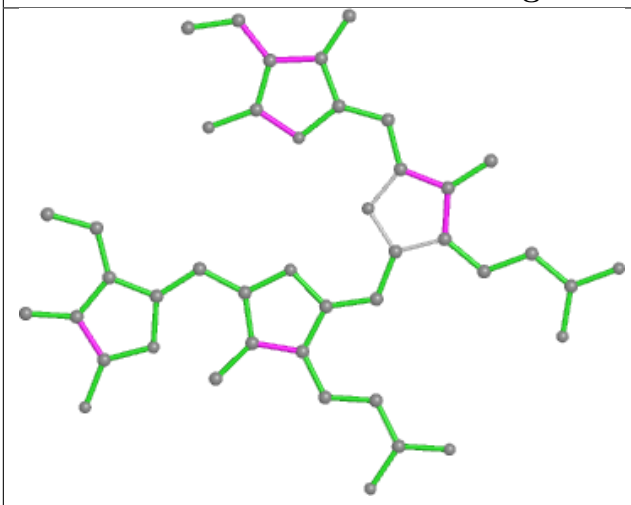

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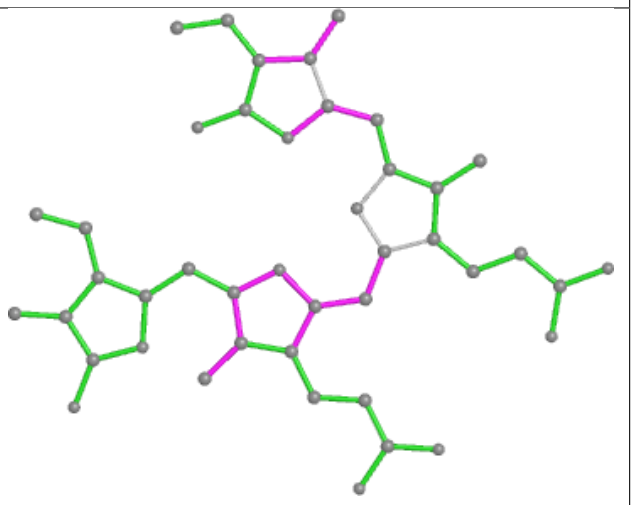

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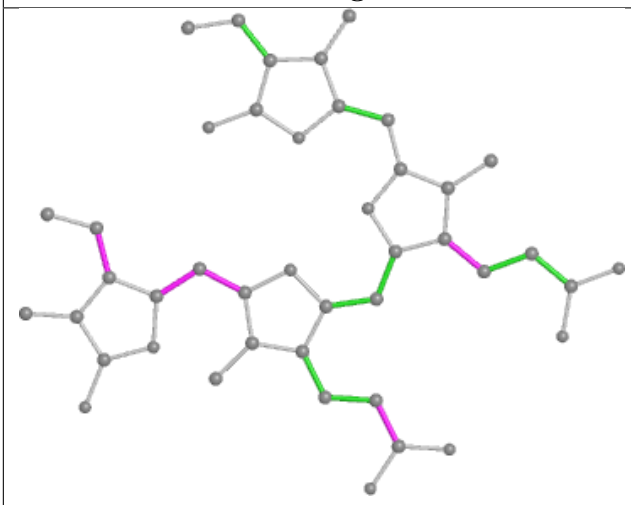

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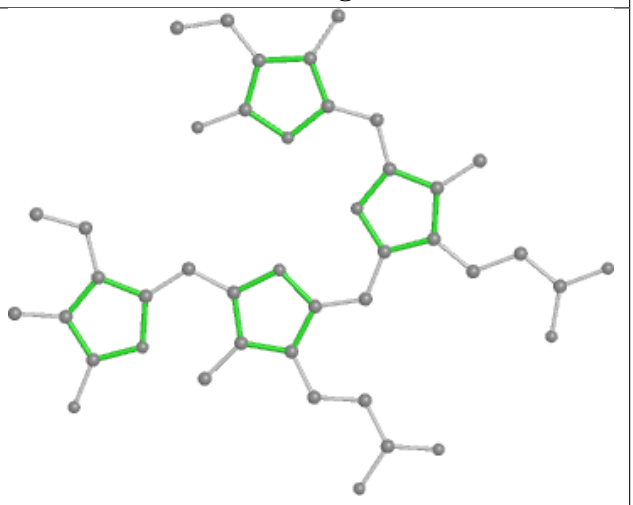
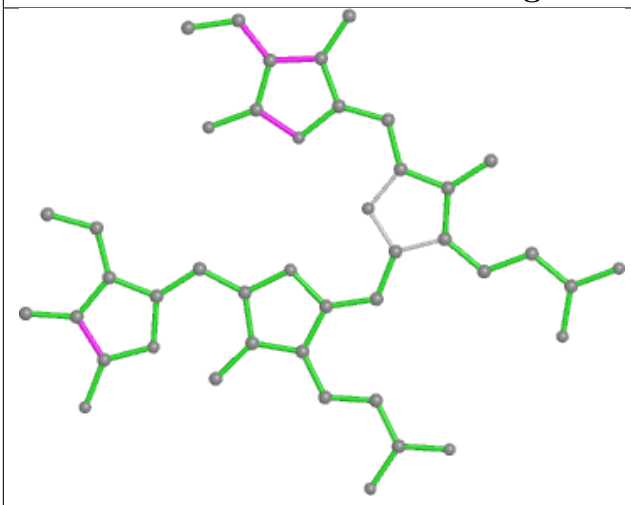


Rings

Ligand PEB j8 202



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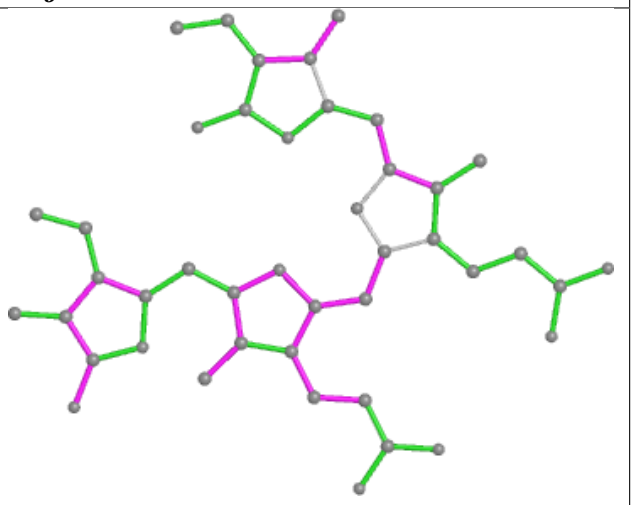

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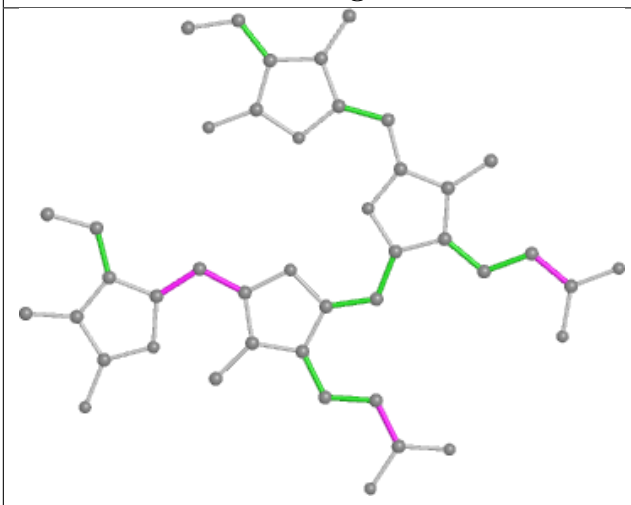

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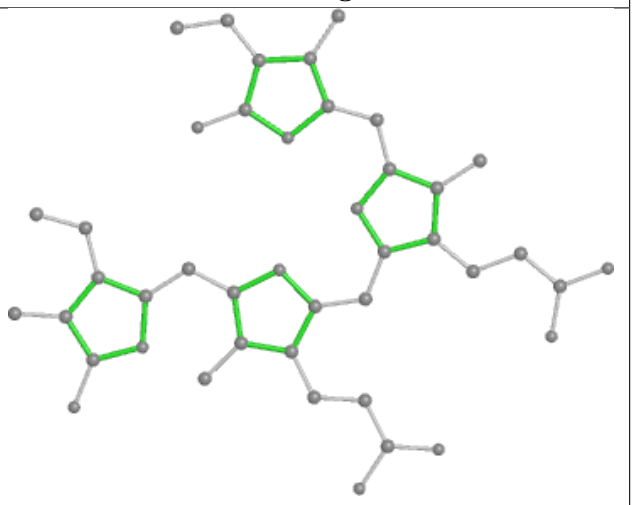
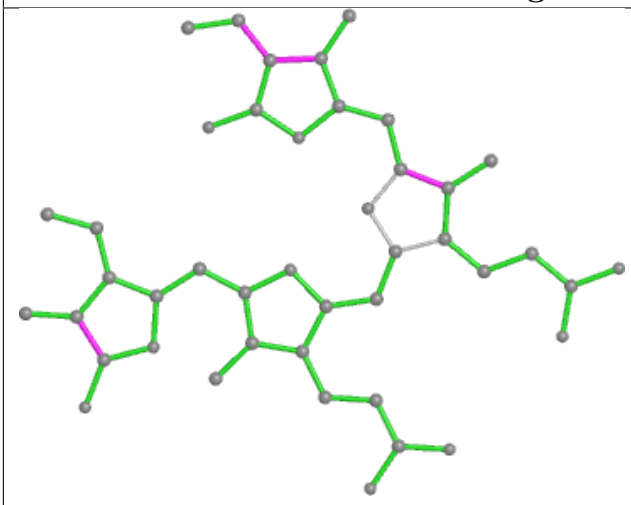


Rings

Ligand PEB lj 201



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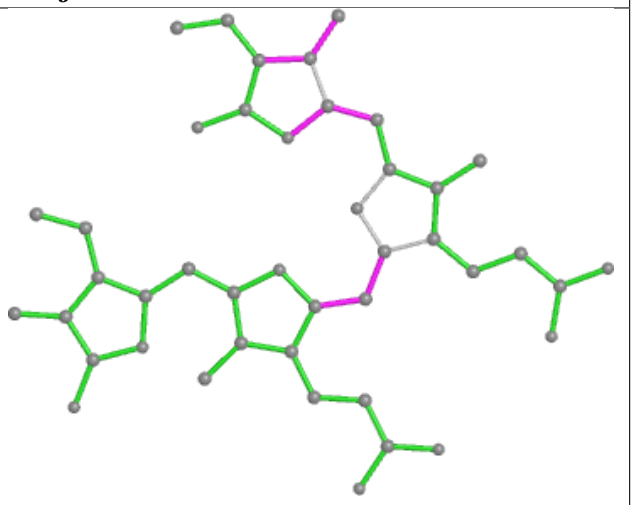

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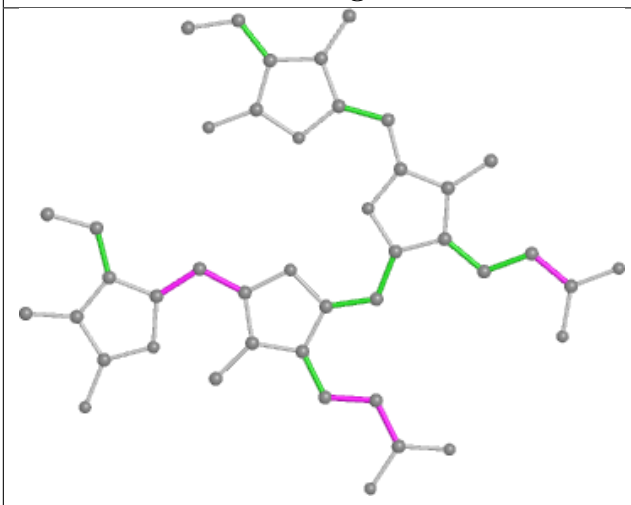

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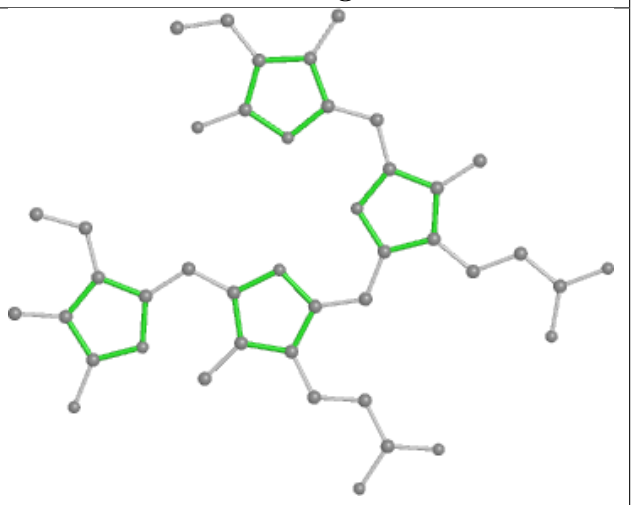
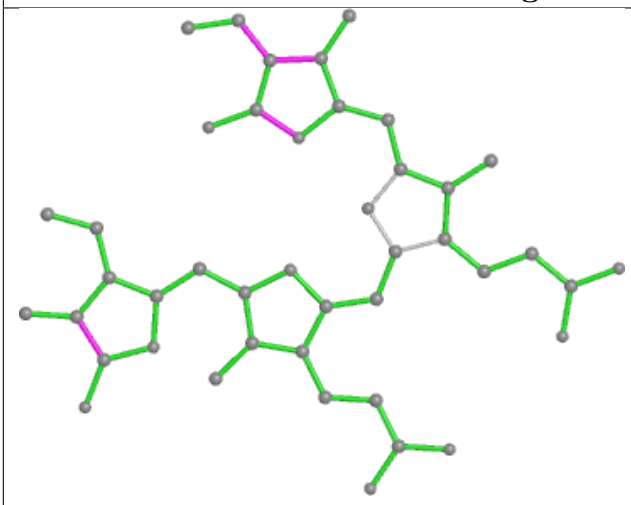


Rings

Ligand PEB r2 201



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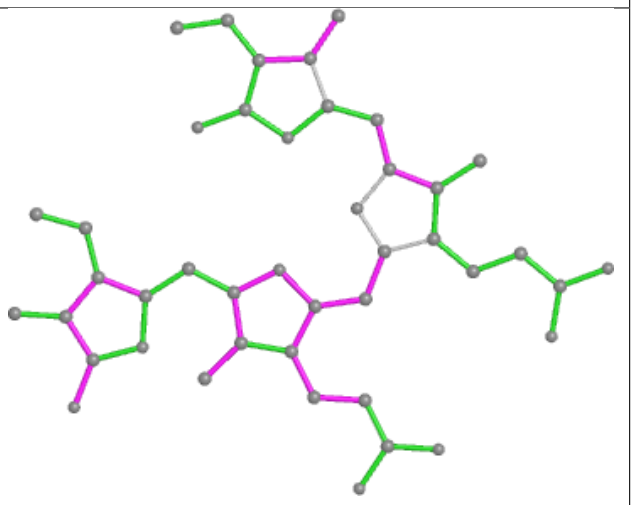

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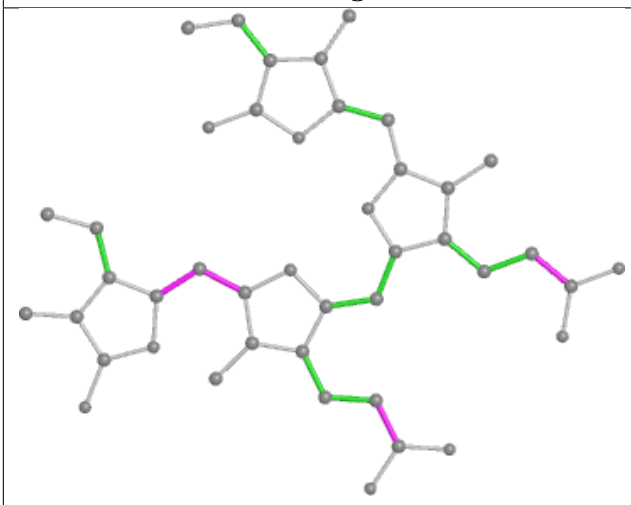

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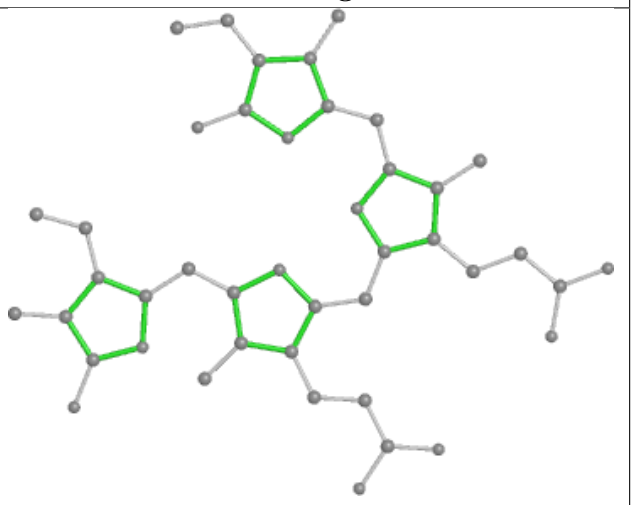
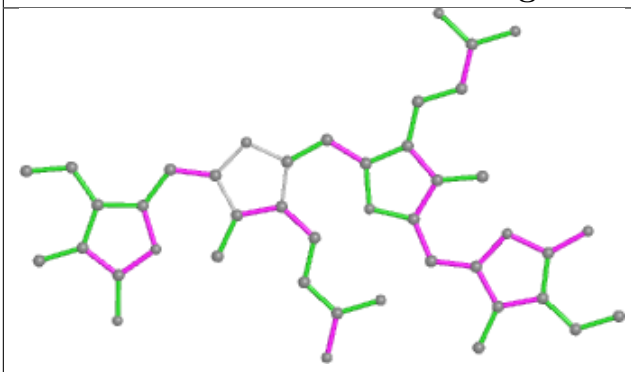


Rings

Ligand CYC r1 201



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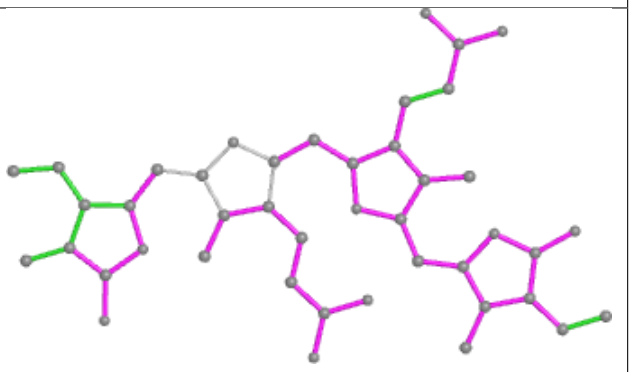

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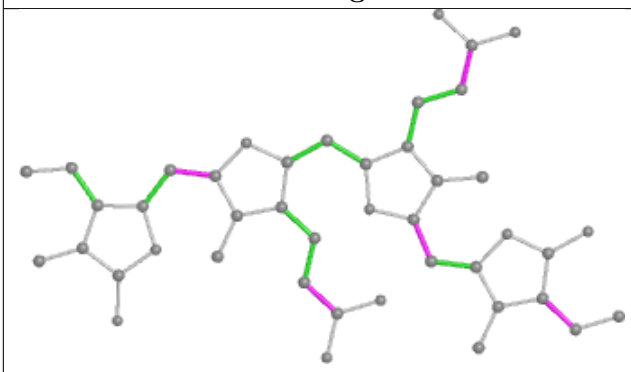

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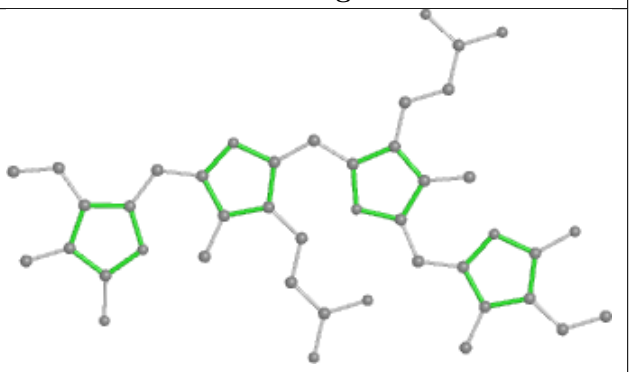
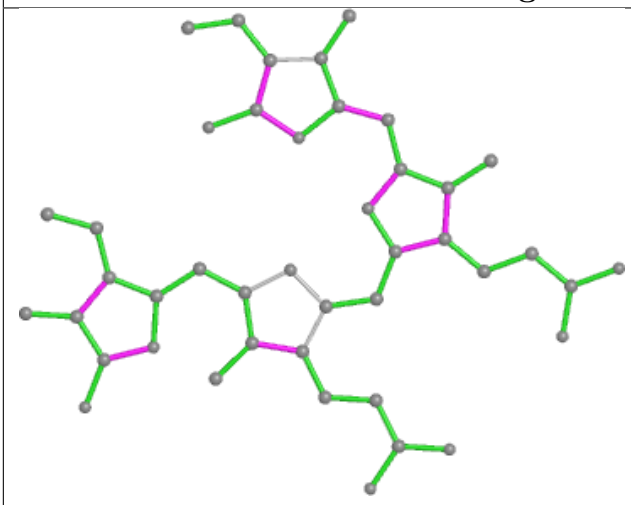


Rings

Ligand PUB dt 203



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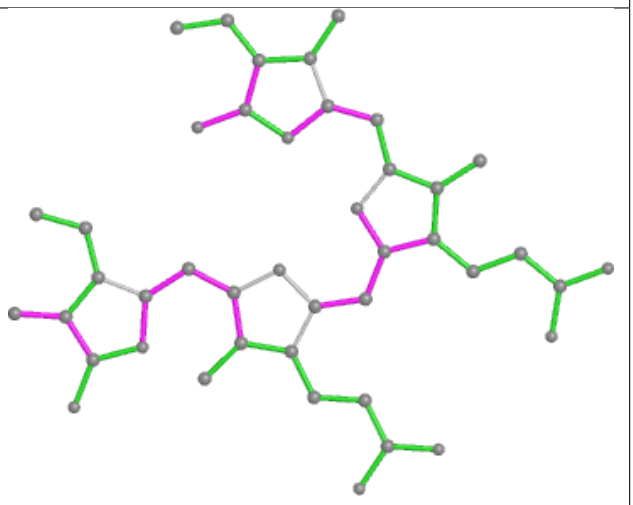
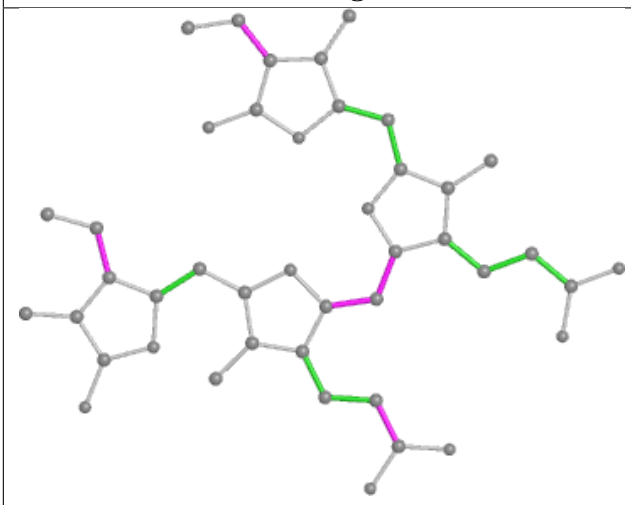


Bond angles



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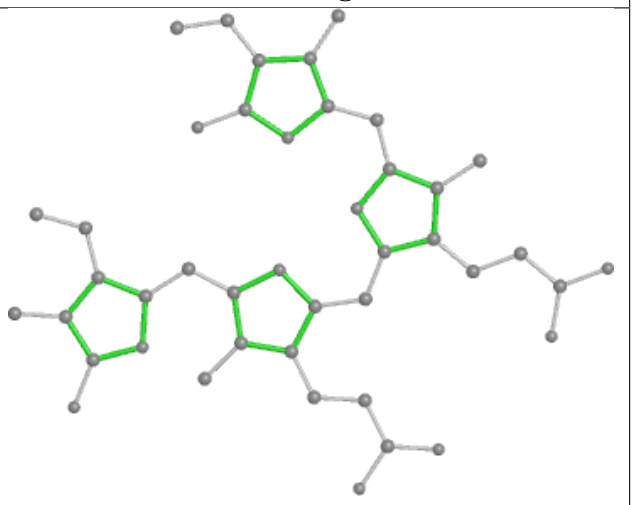
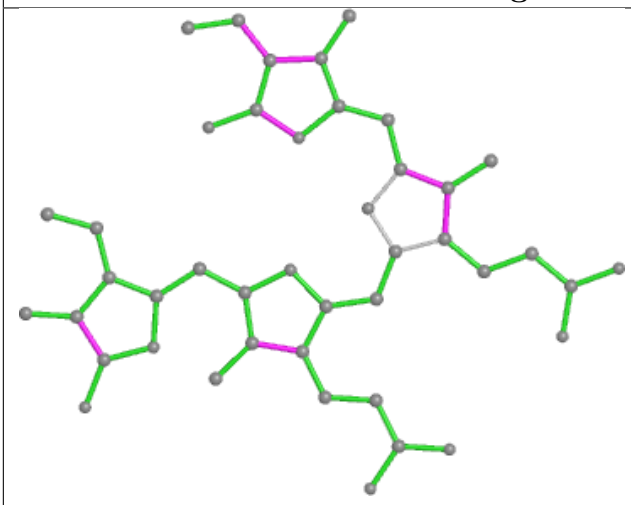


Rings

Ligand PEB W3 203



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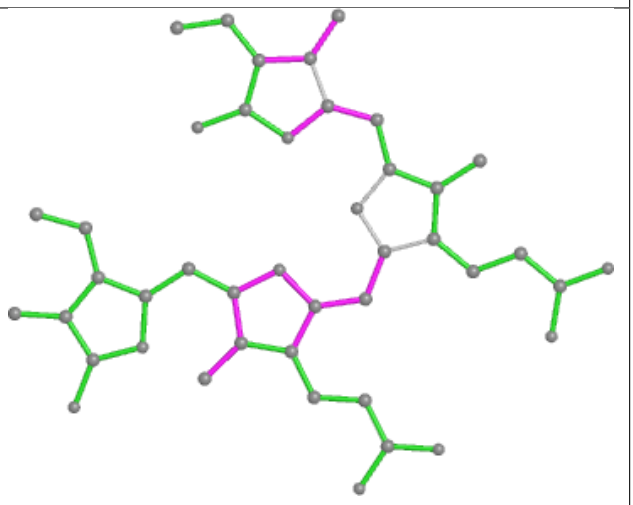
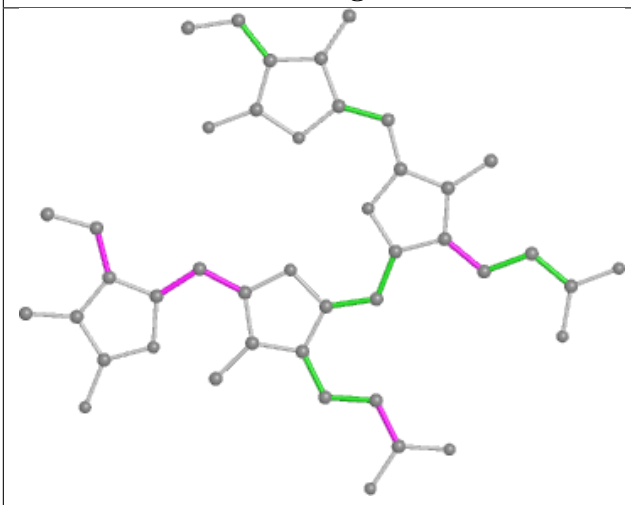


Bond angles



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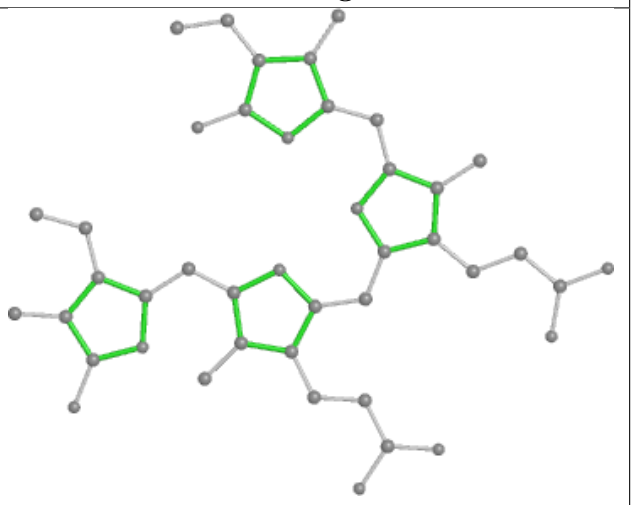
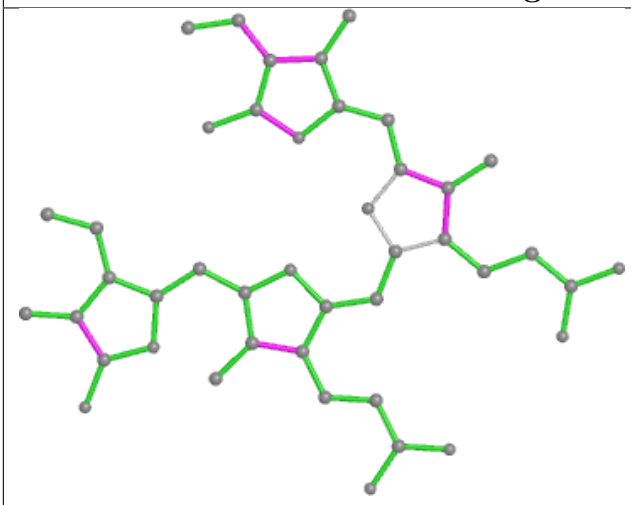


Rings

Ligand PEB lo 203



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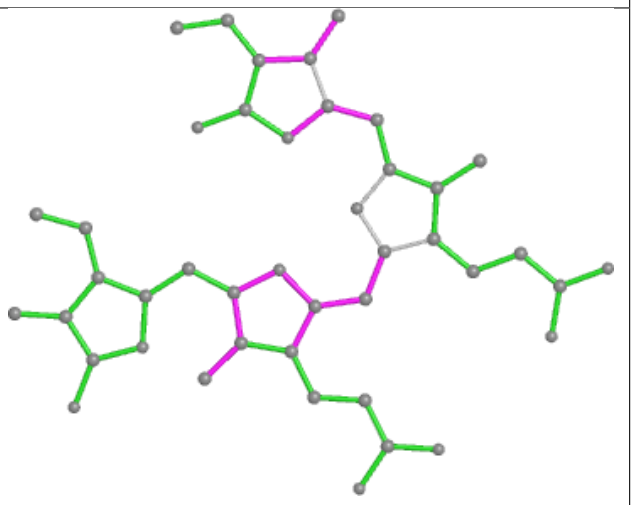

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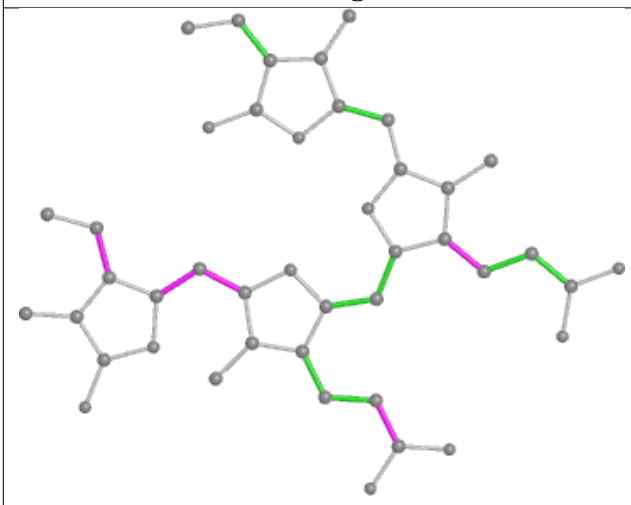
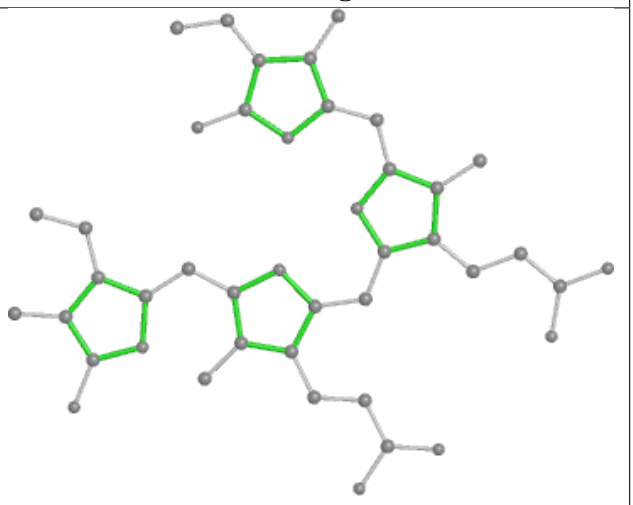
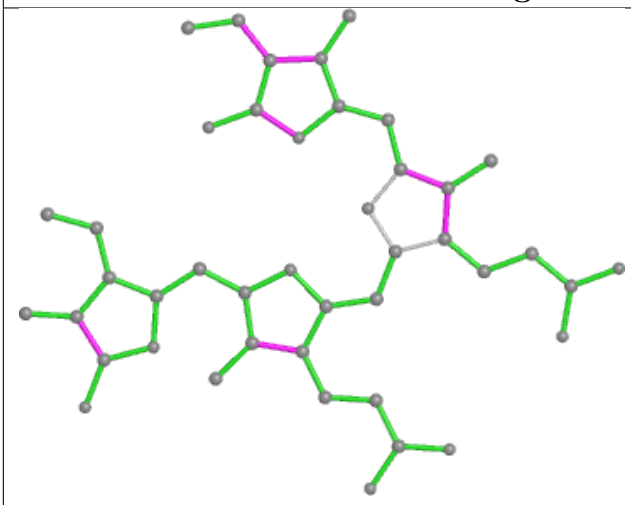


Torsions



Rings

Ligand PEB bH 202



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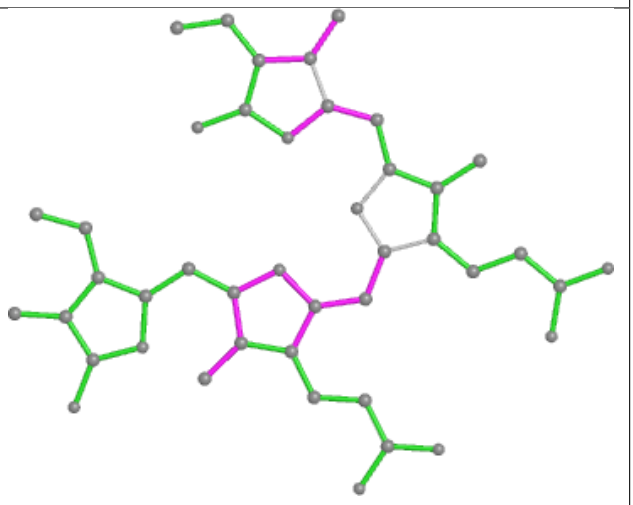

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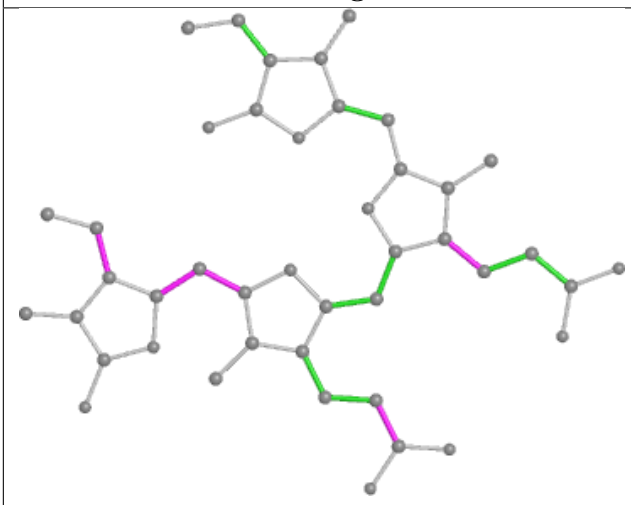

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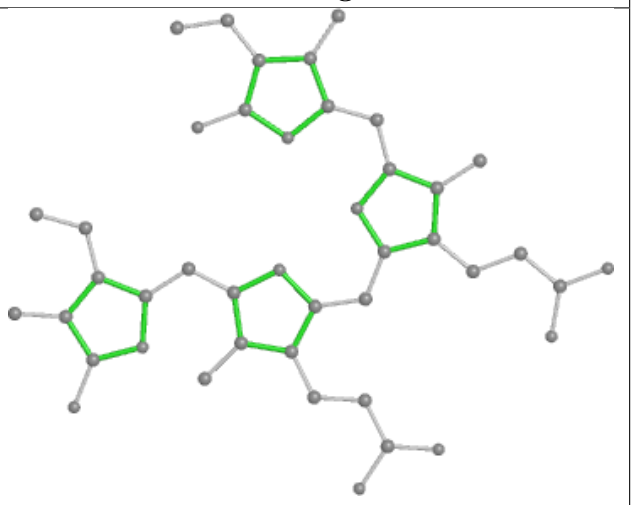
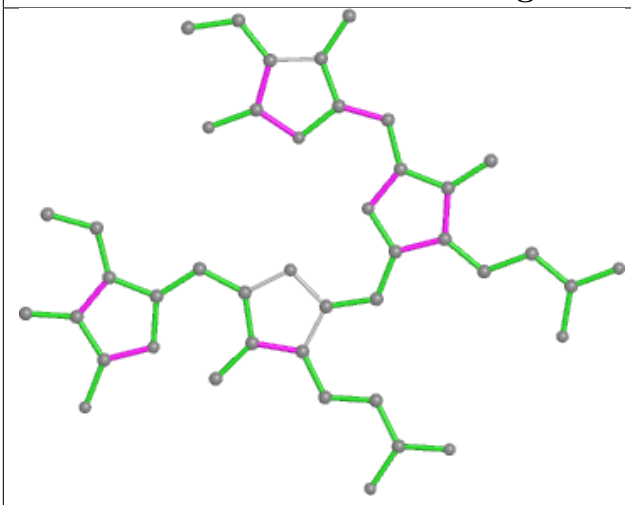


Rings

Ligand PUB b9 406



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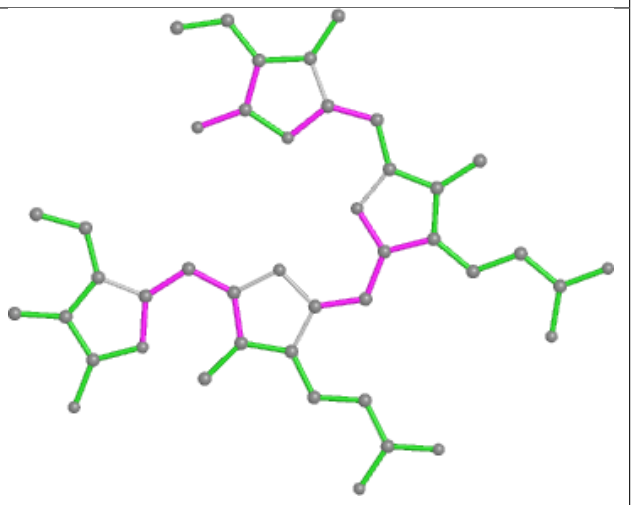

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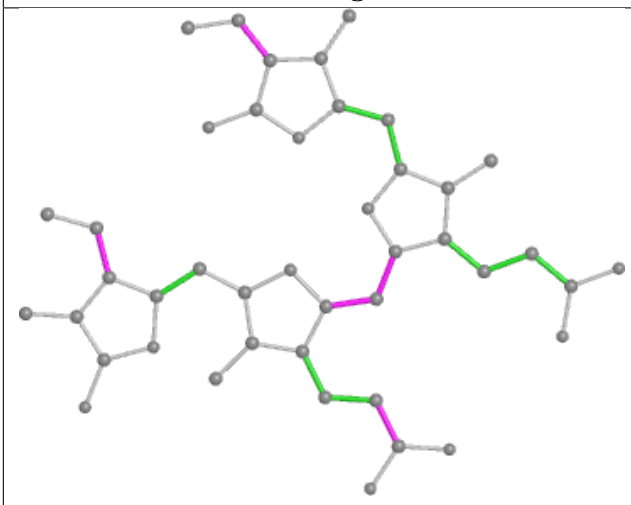

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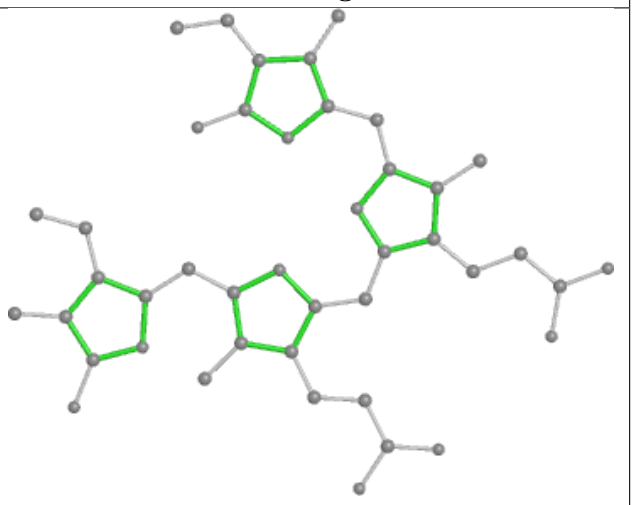

Rings

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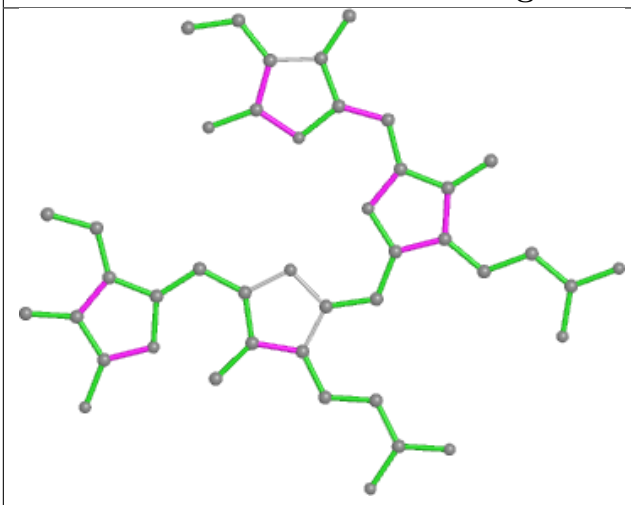

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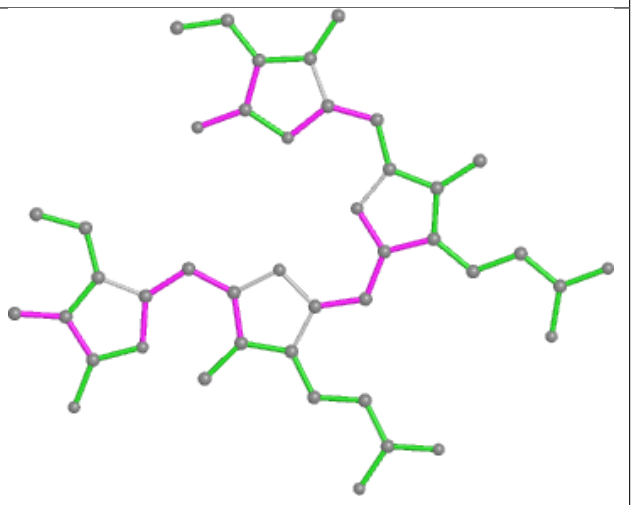

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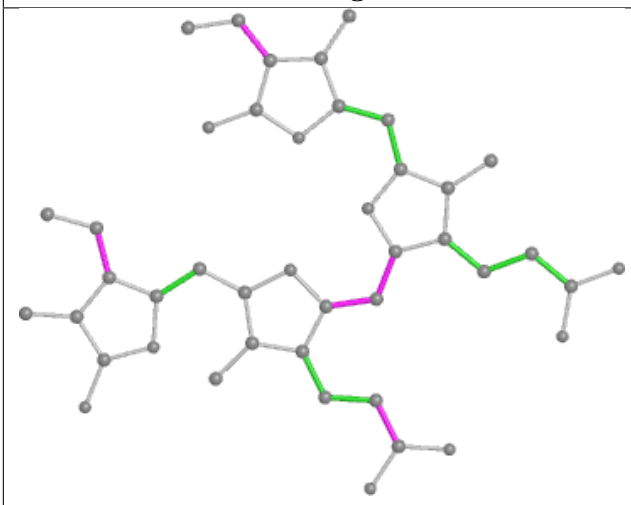

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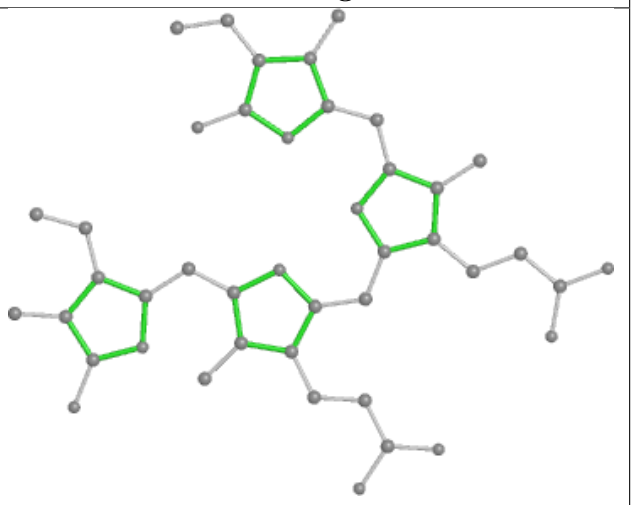

Rings

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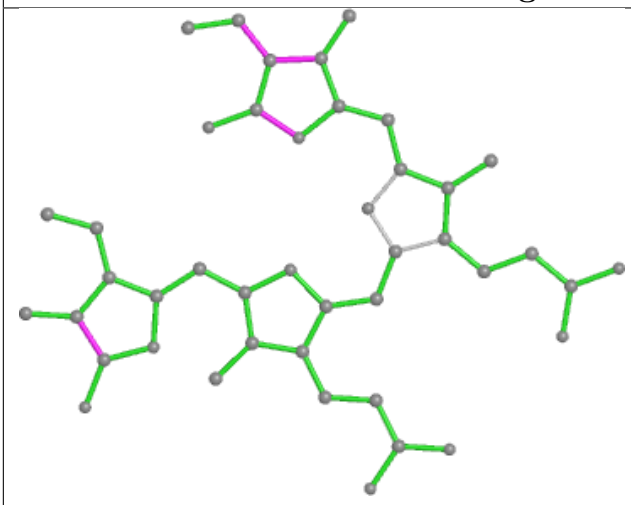

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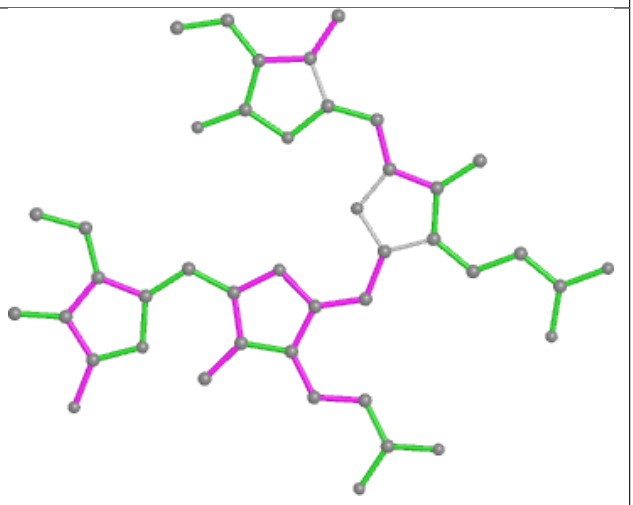

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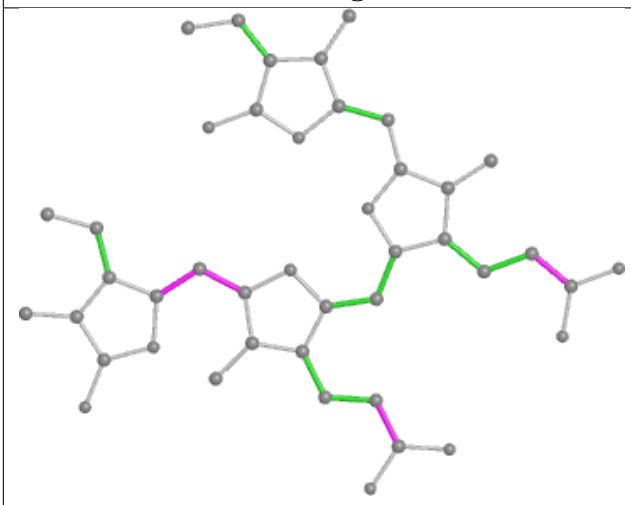

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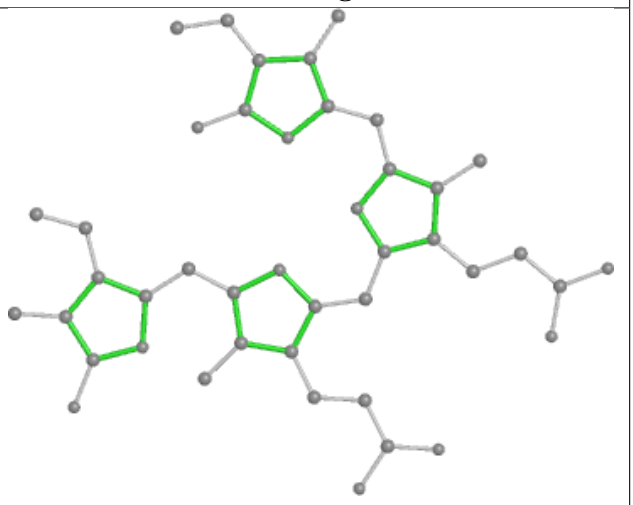

Rings

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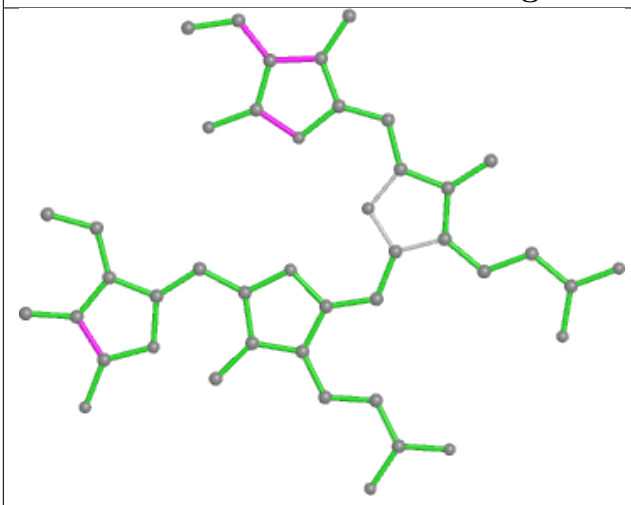

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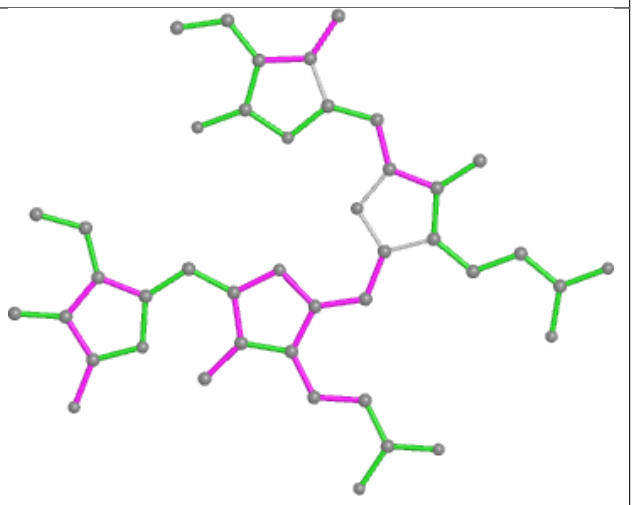

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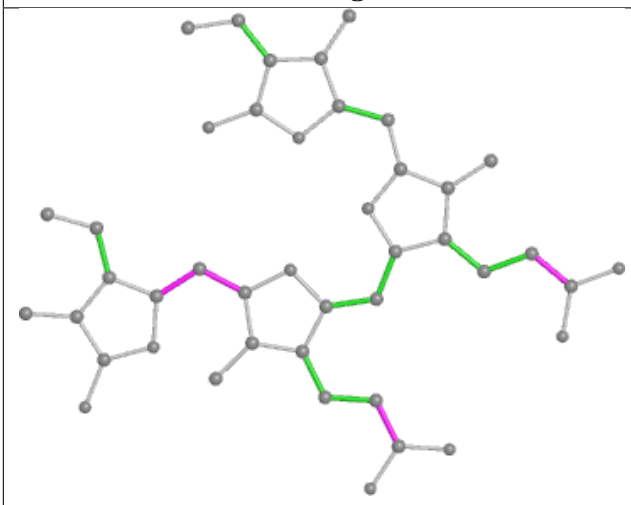

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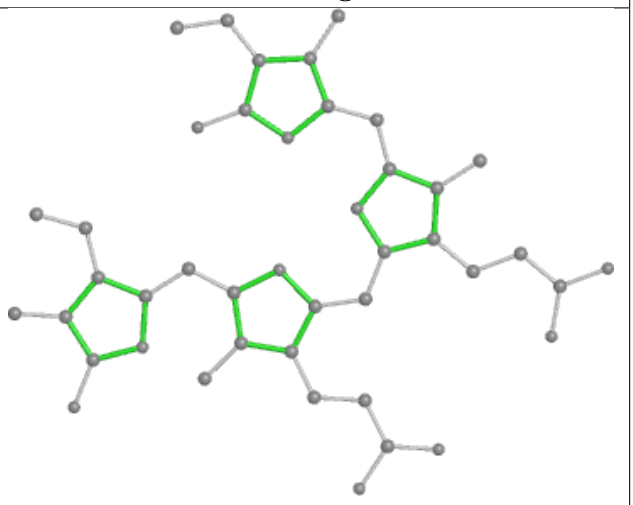

Rings

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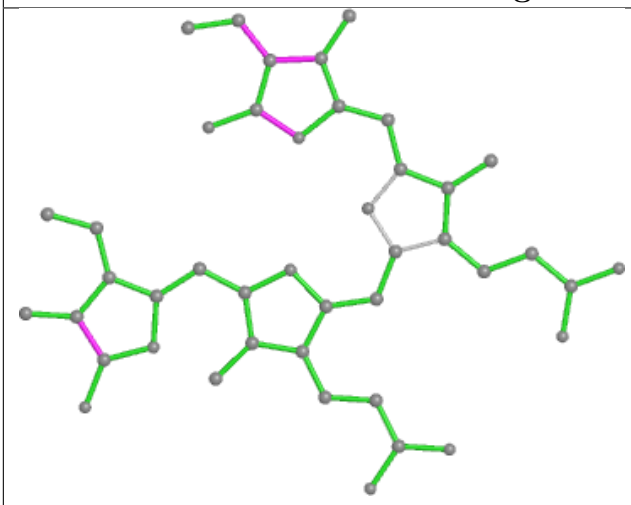

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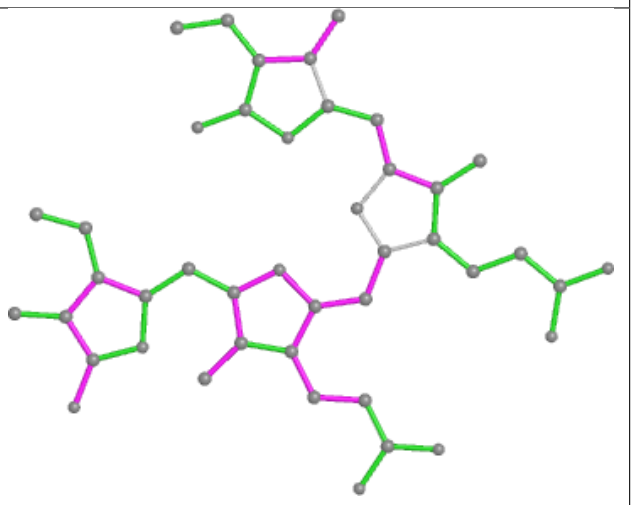

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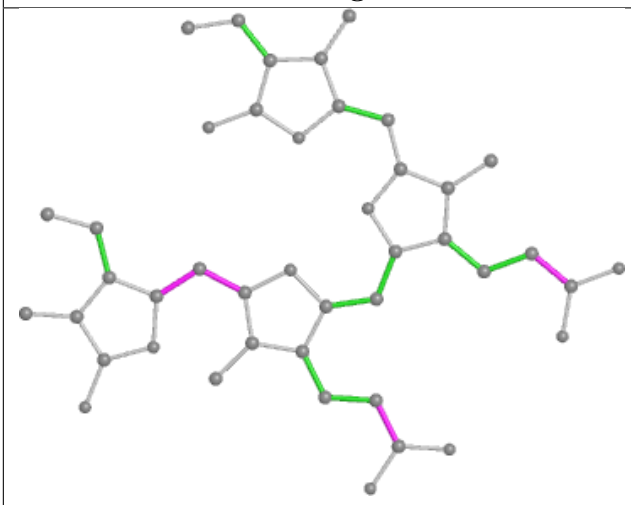

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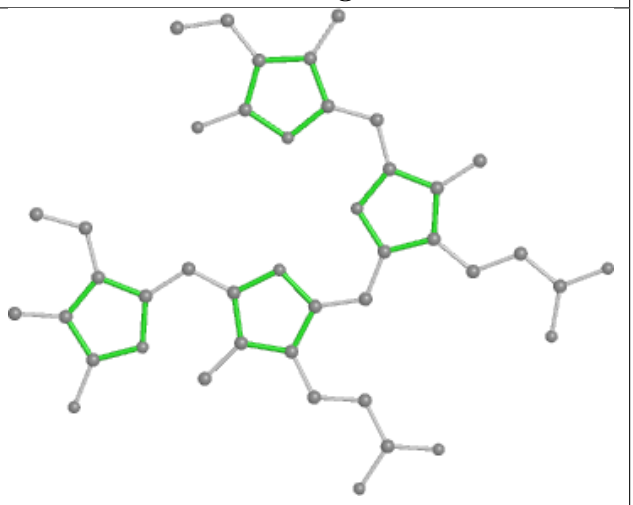

Rings

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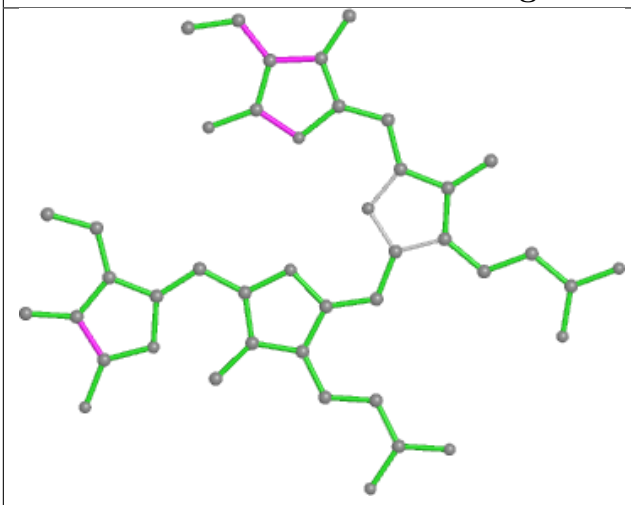

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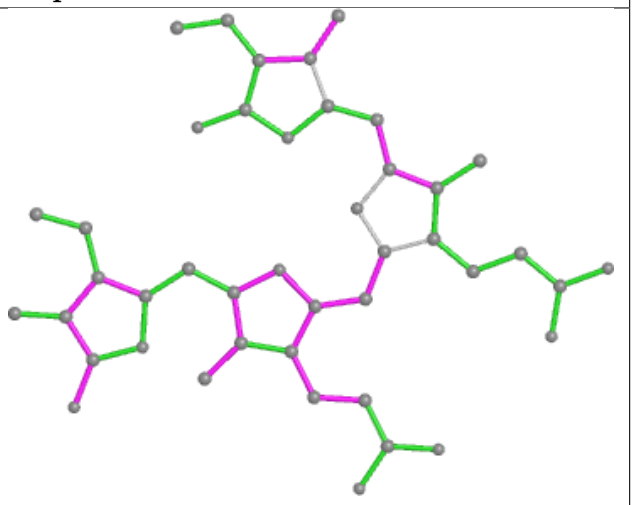

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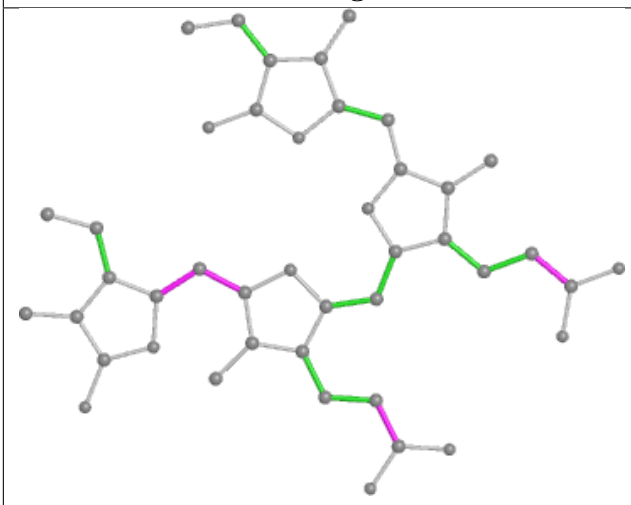

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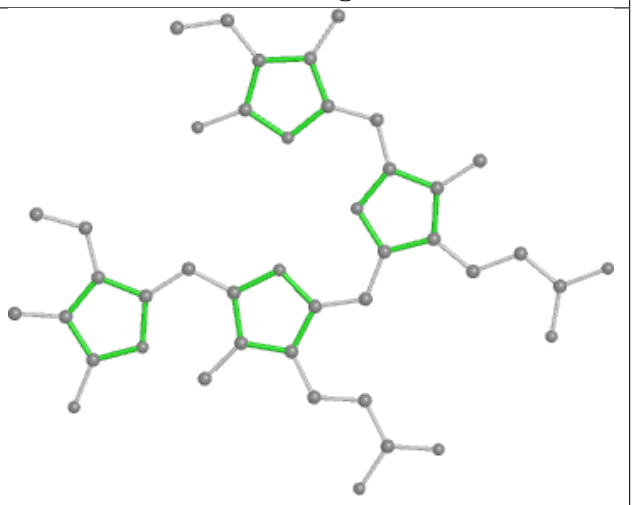

Rings

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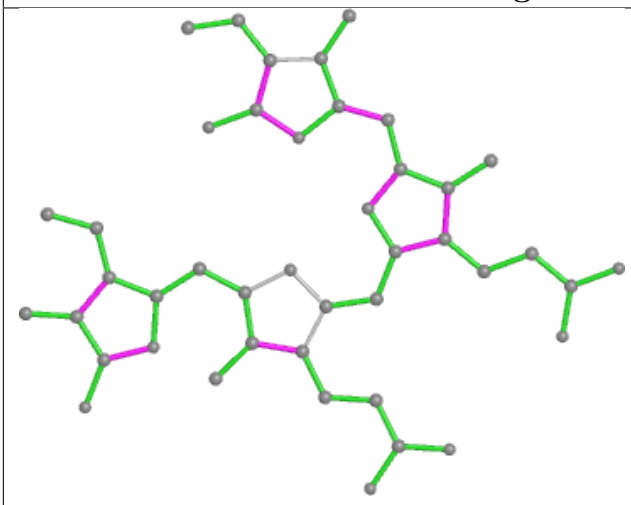

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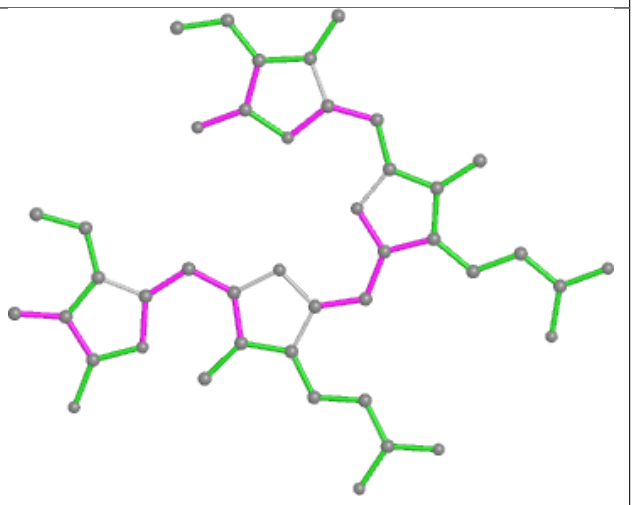

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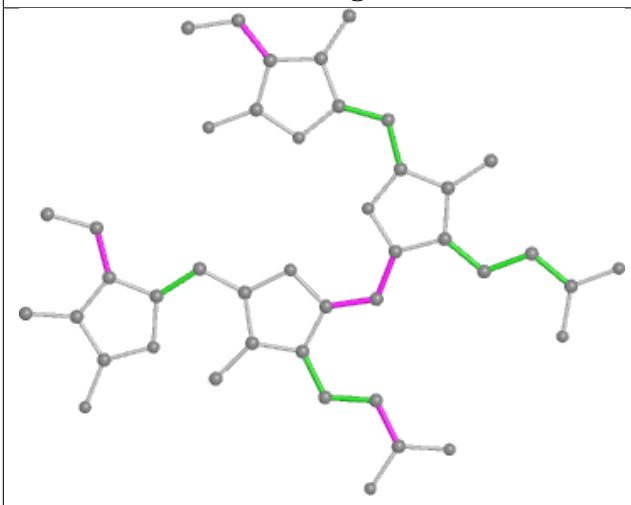

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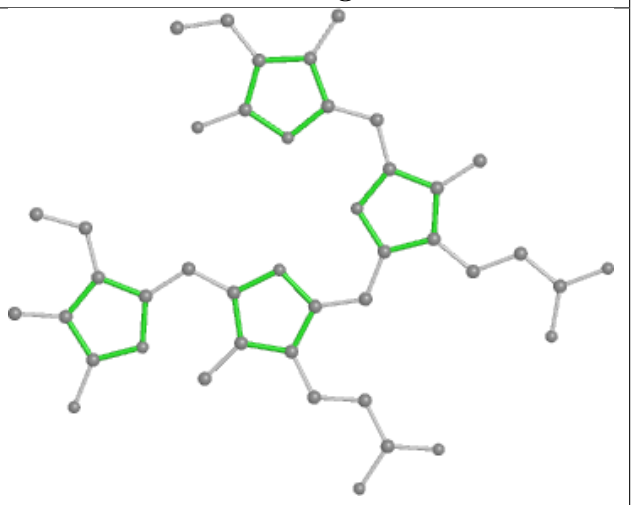
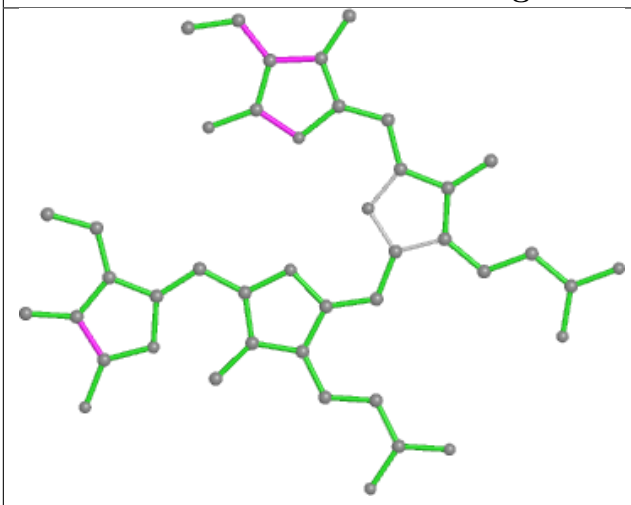


Rings

Ligand PEB jL 1001



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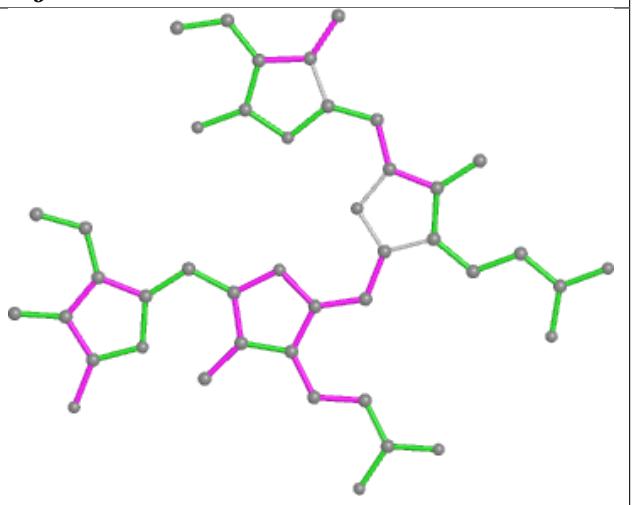

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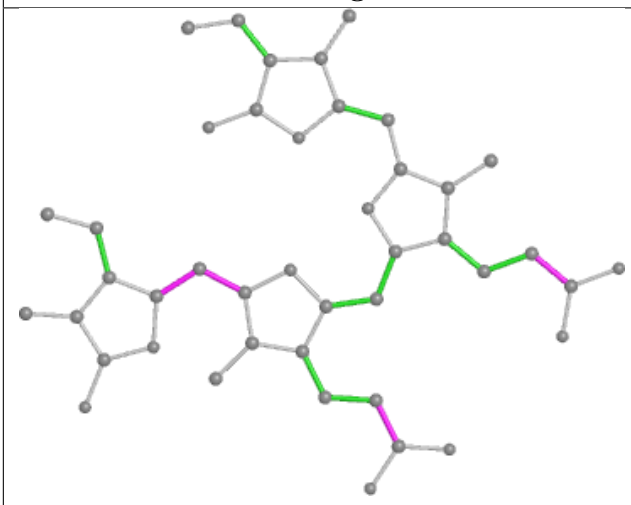

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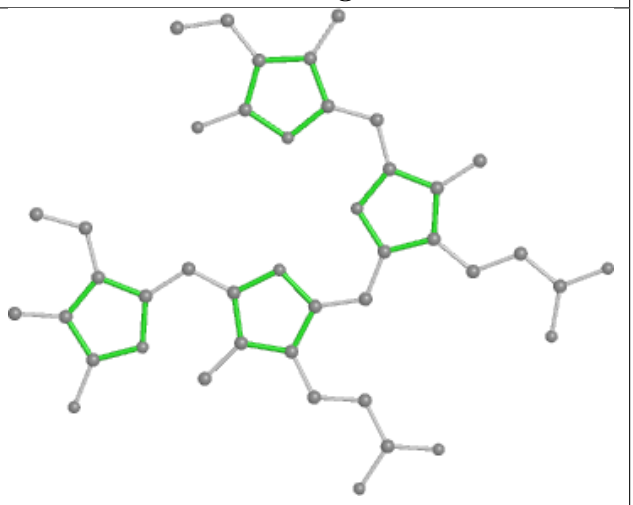
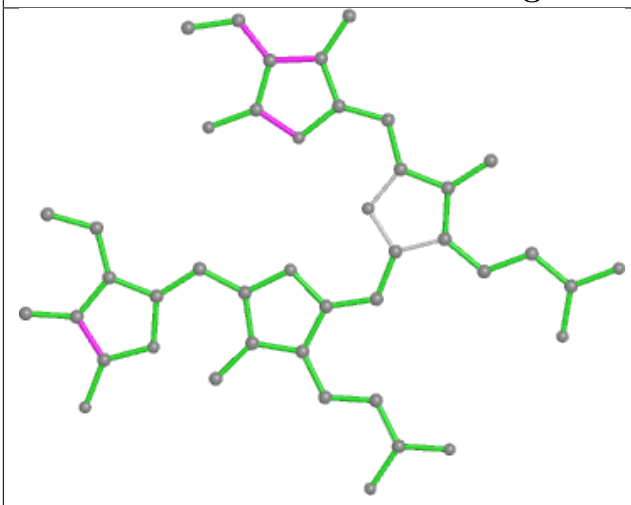


Rings

Ligand PEB j5 202



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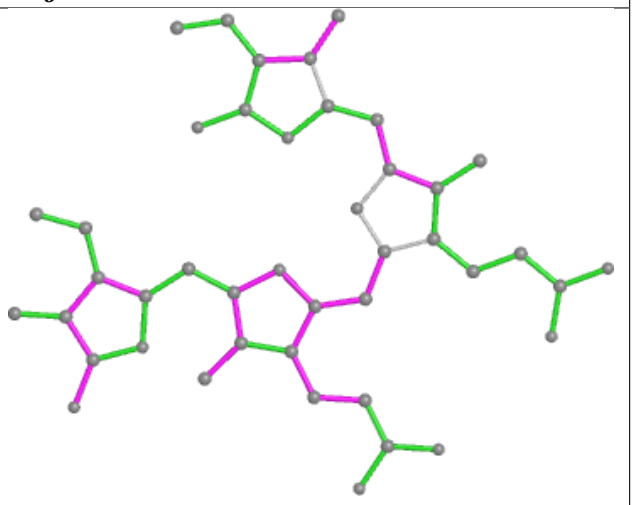

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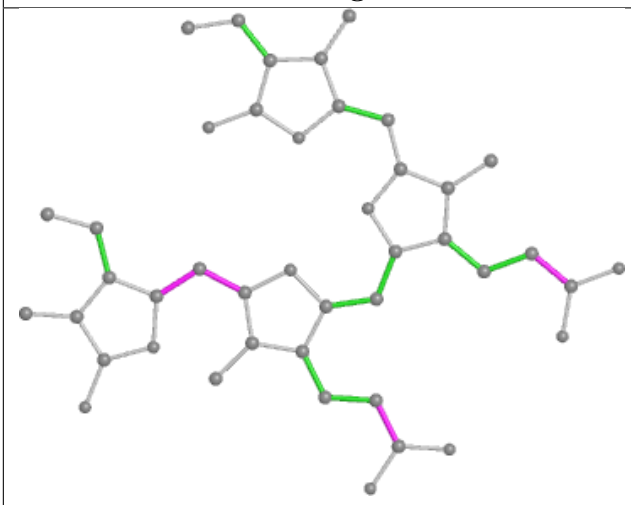

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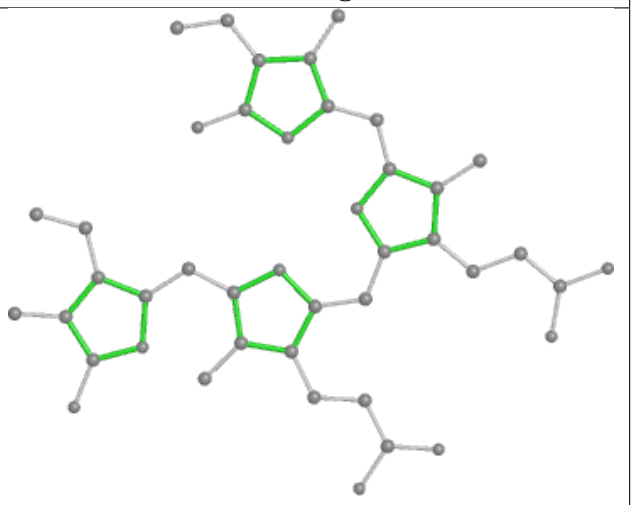

Rings

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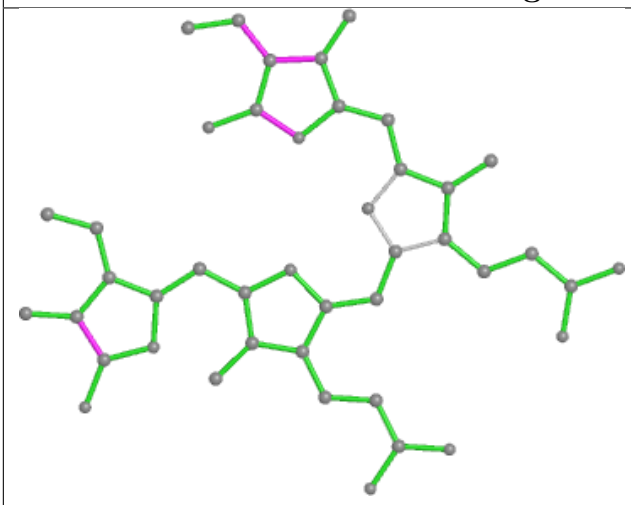

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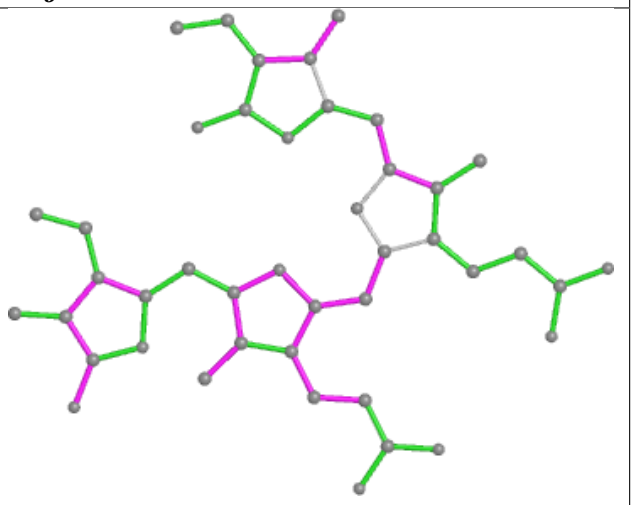

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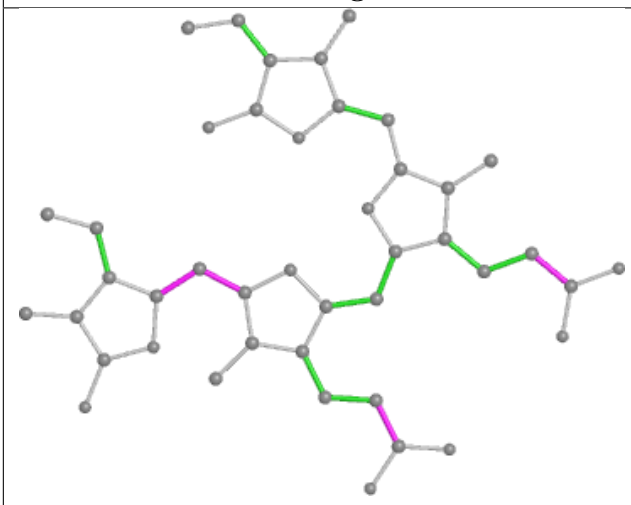

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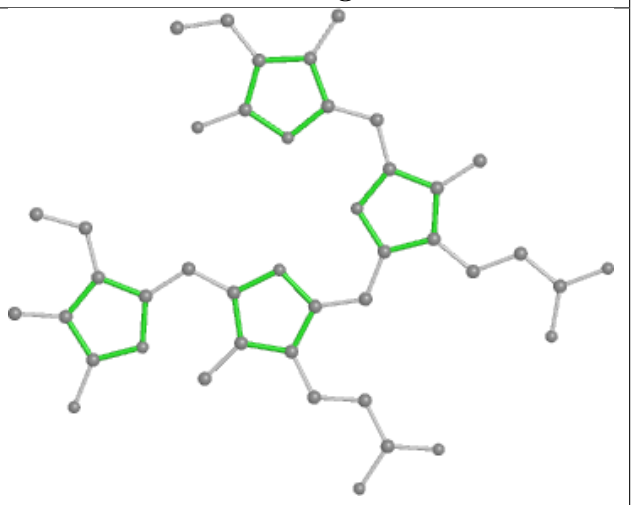
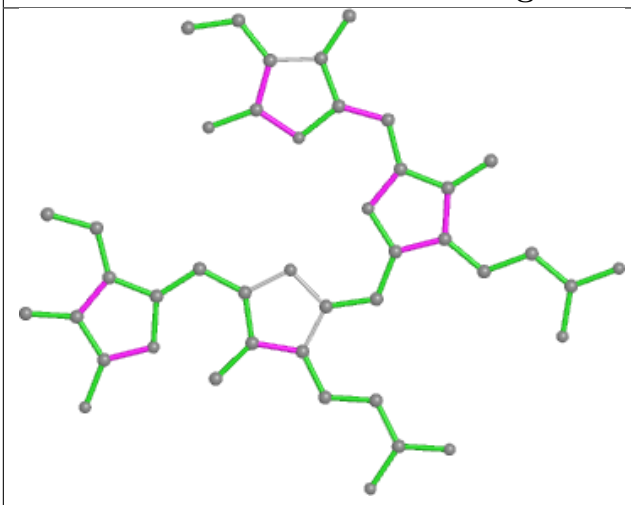


Rings

Ligand PUB d9 305



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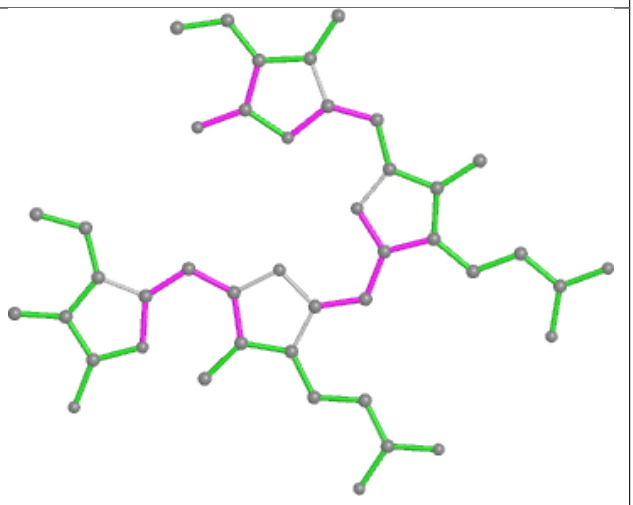

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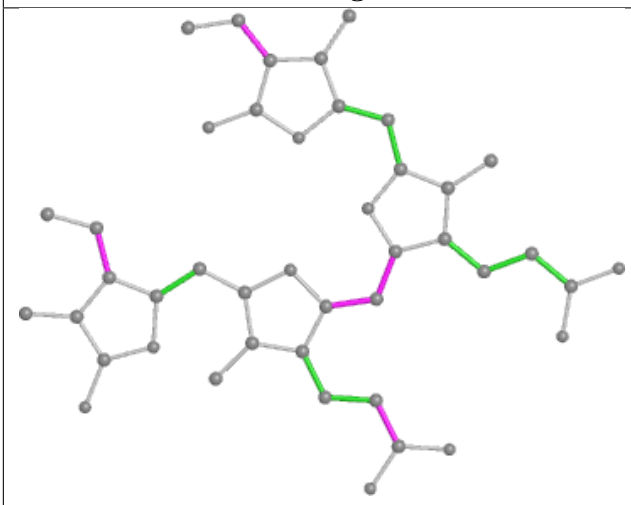

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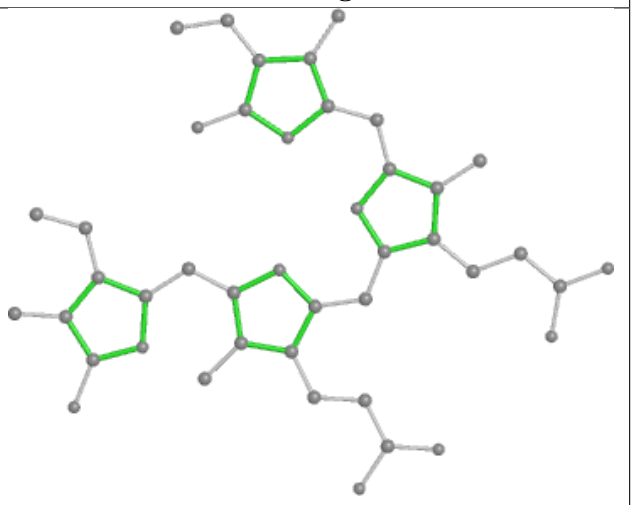
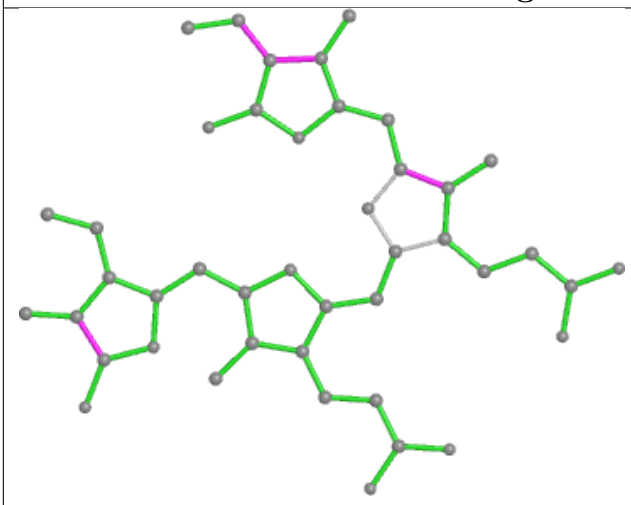


Rings

Ligand PEB aw 202



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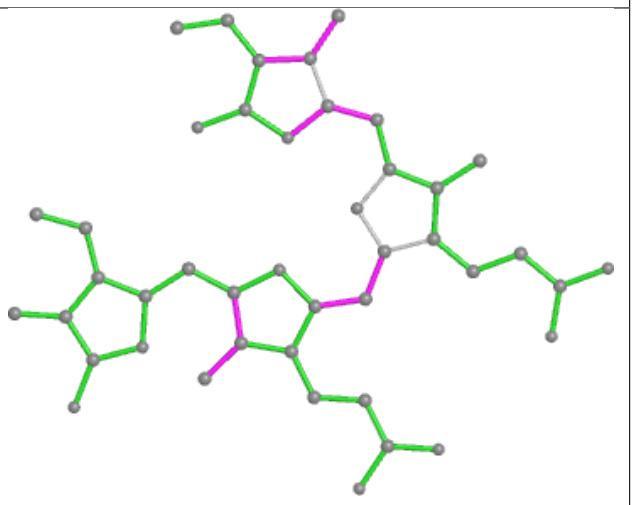

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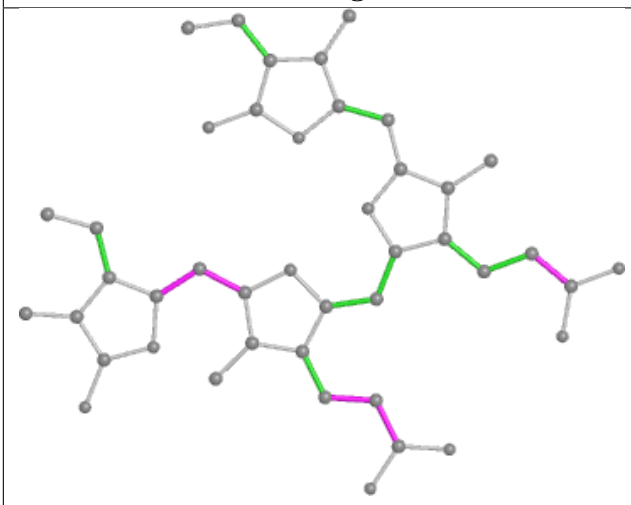
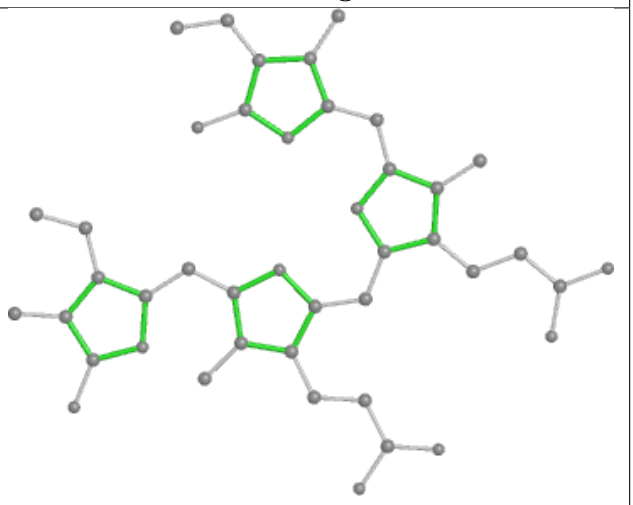
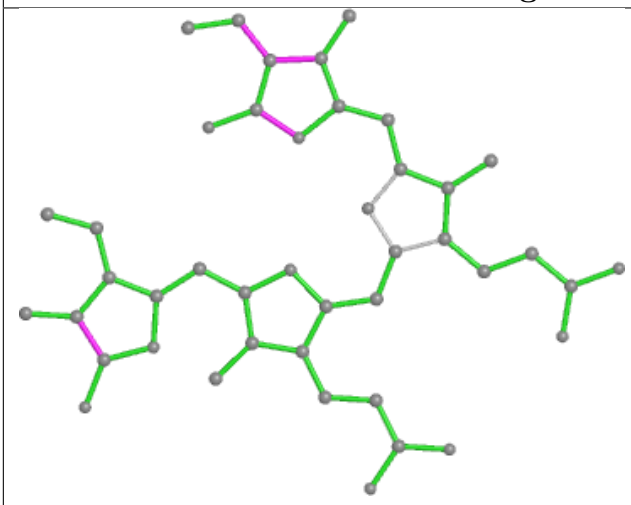


Torsions



Rings

Ligand PEB g5 201



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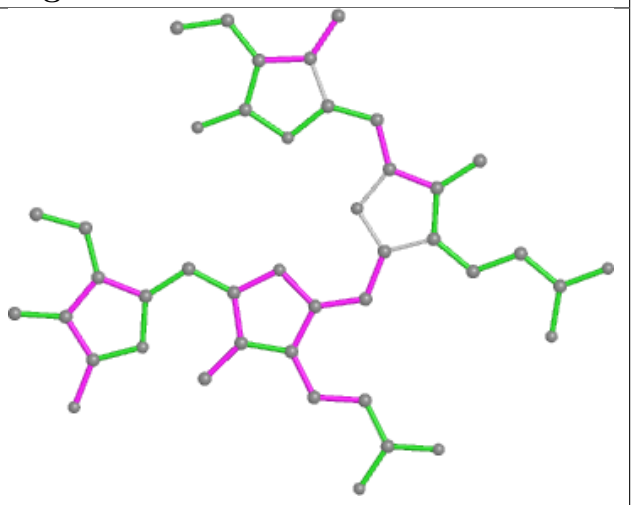

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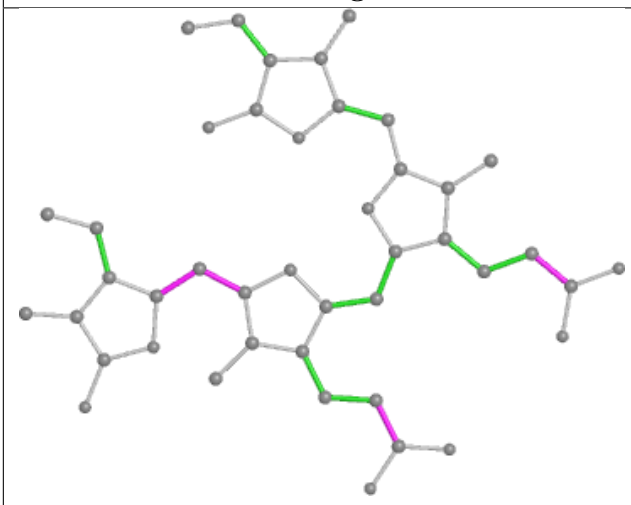

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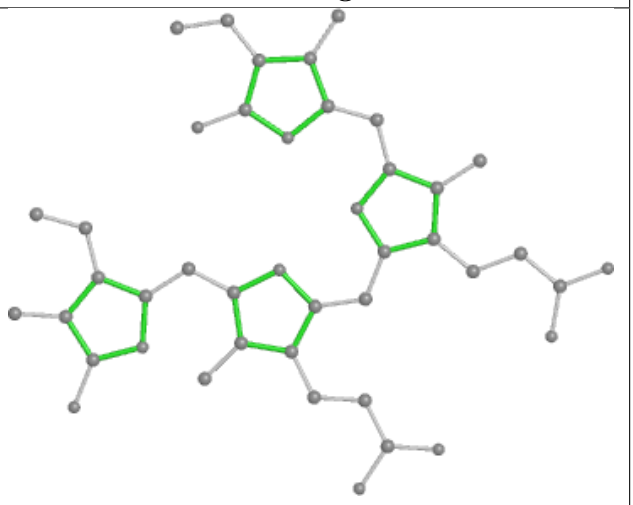
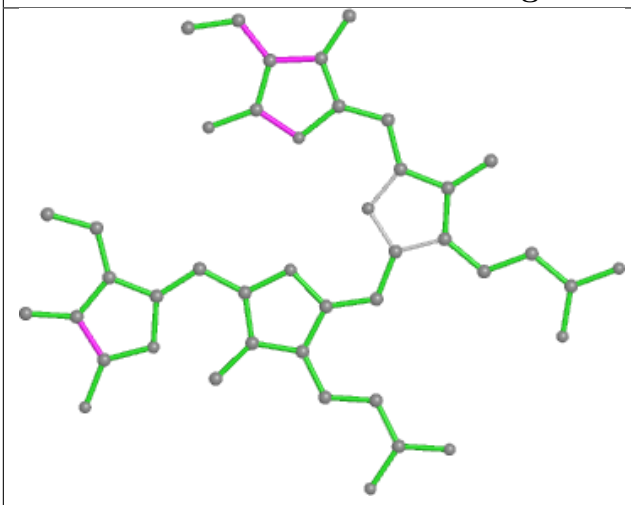


Rings

Ligand PEB bj 202



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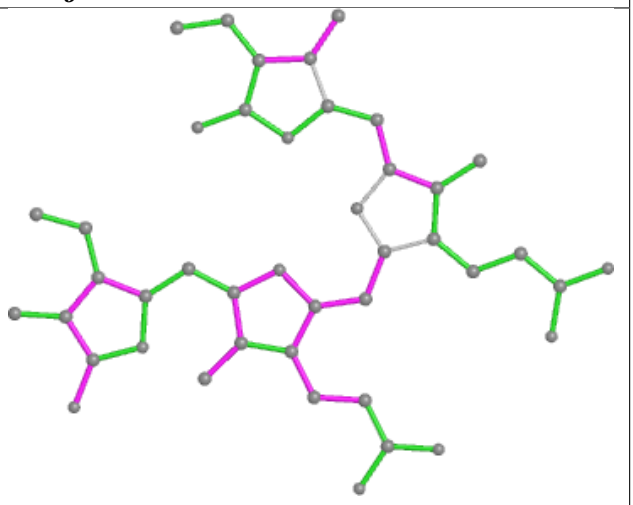

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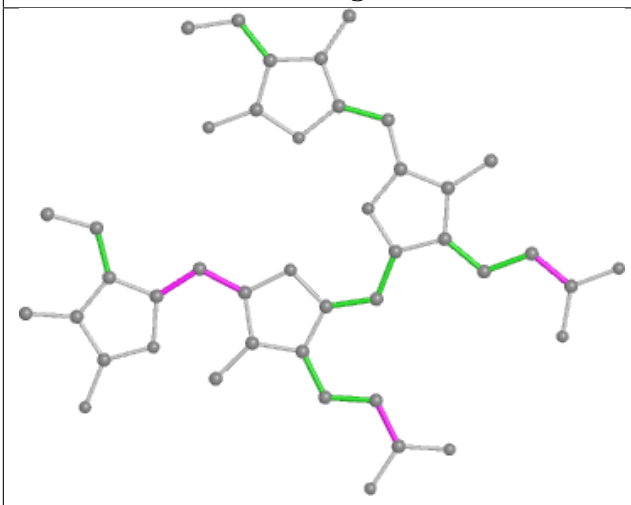

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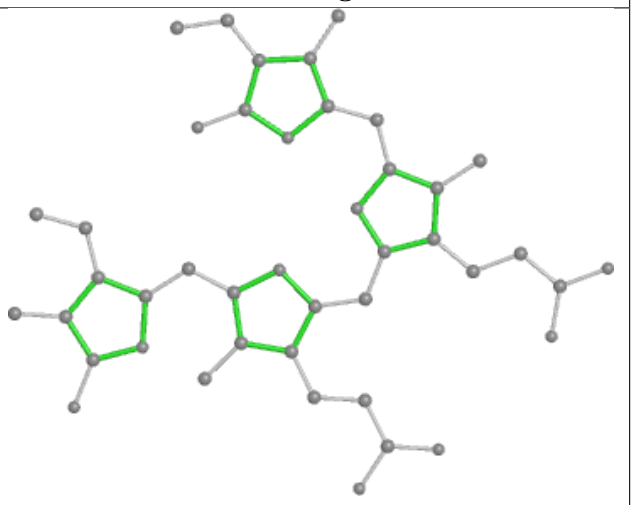
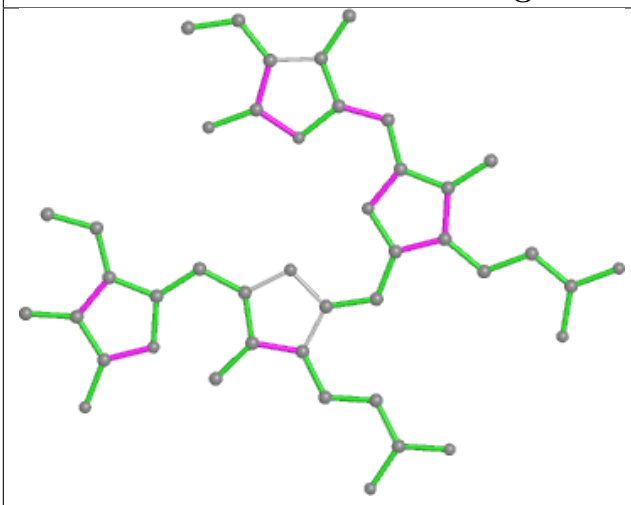


Rings

Ligand PUB cR 203



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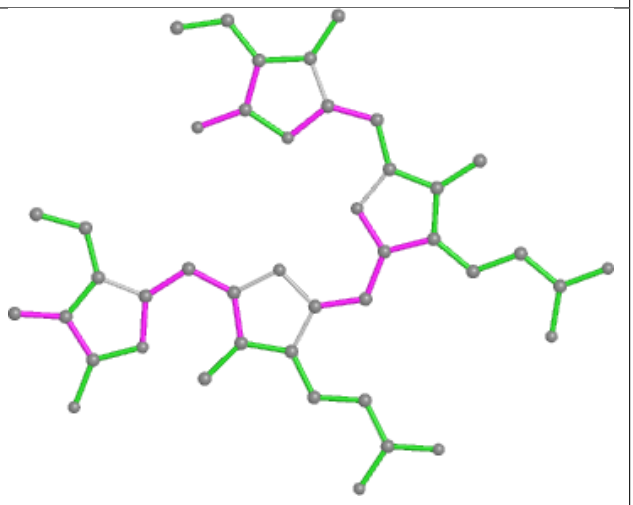

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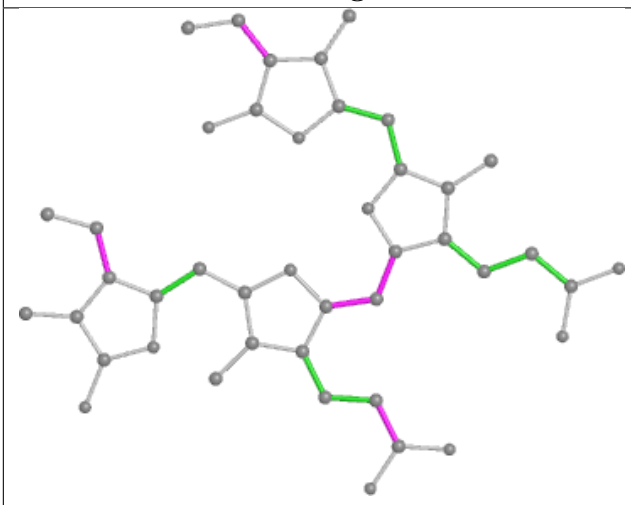

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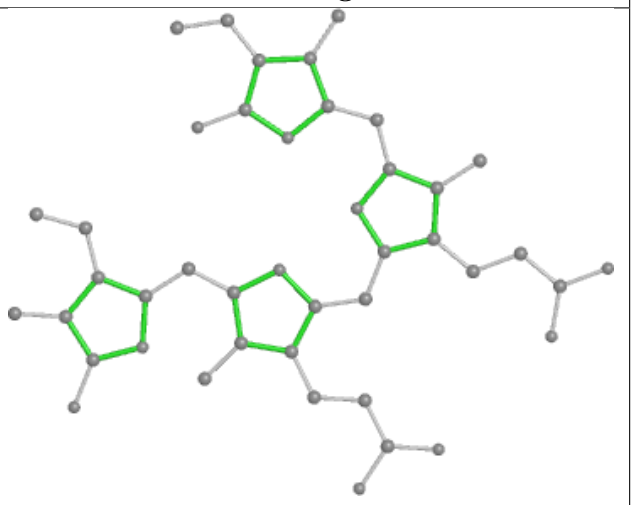
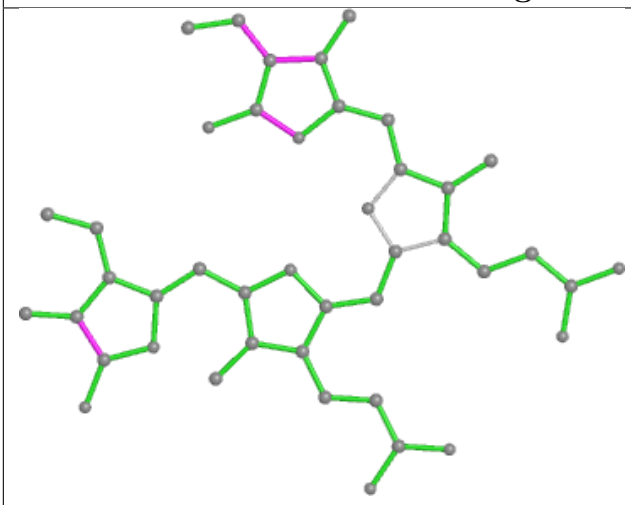


Rings

Ligand PEB bQ 201



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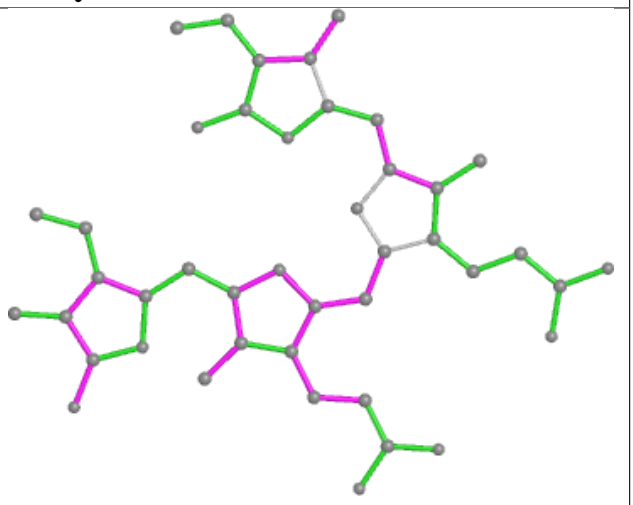

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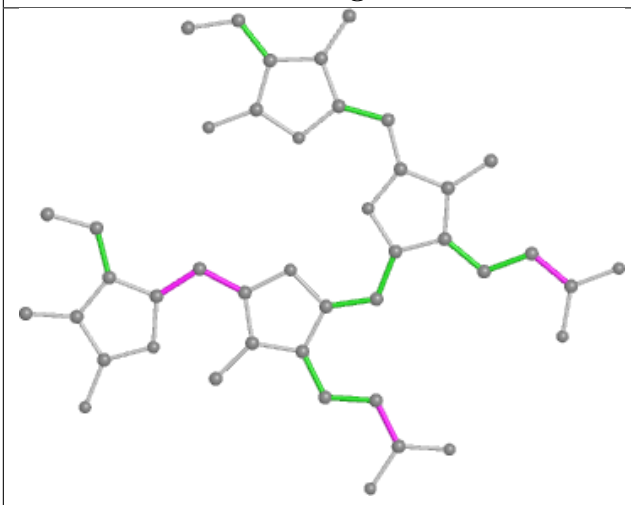

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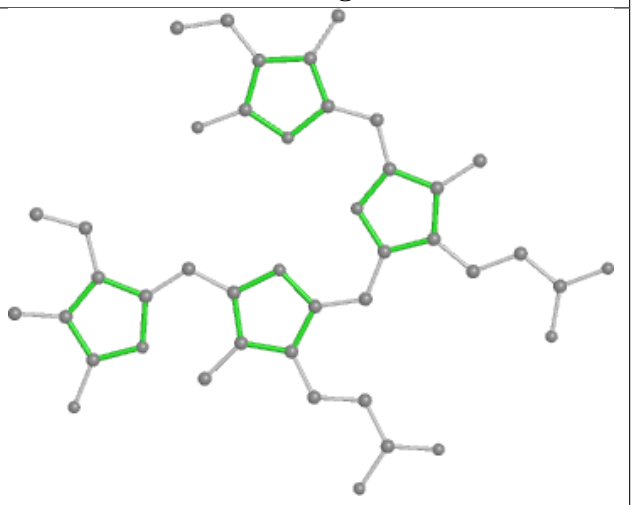
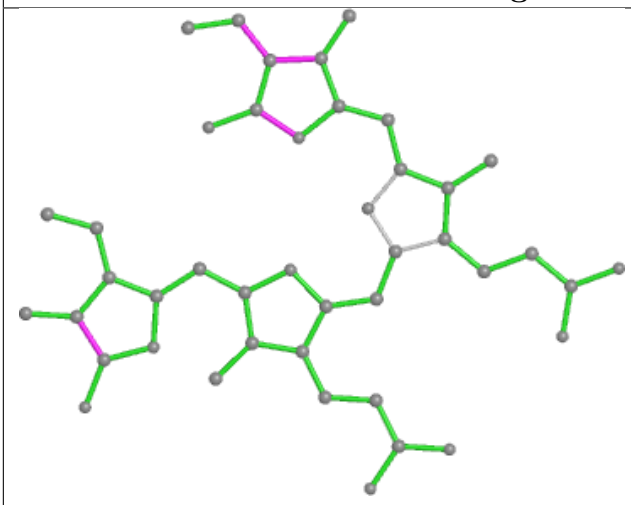


Rings

Ligand PEB y9 1002



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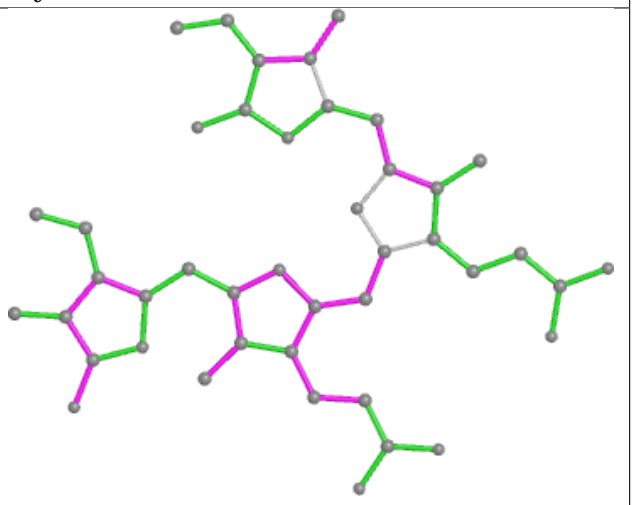

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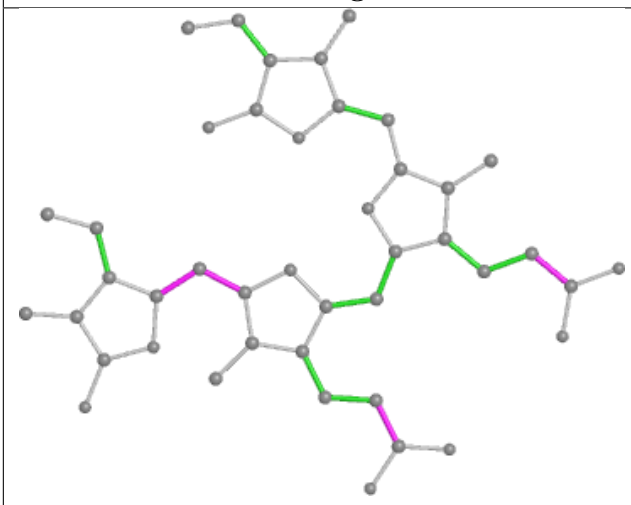

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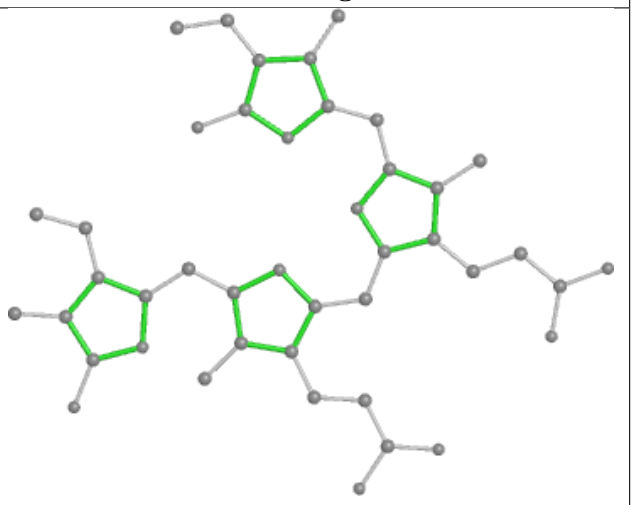
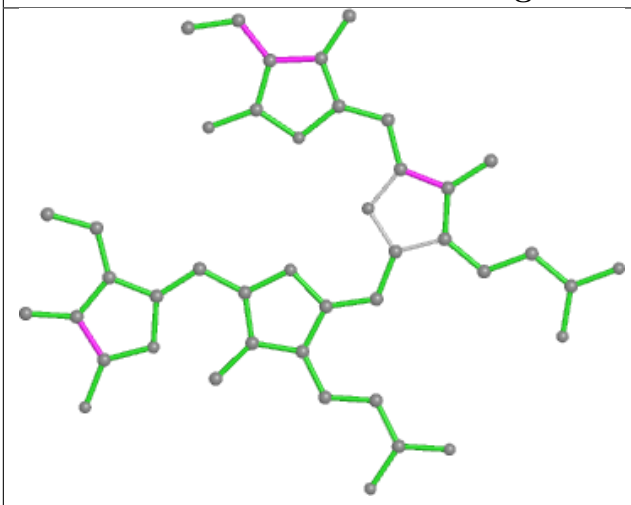


Rings

Ligand PEB em 202



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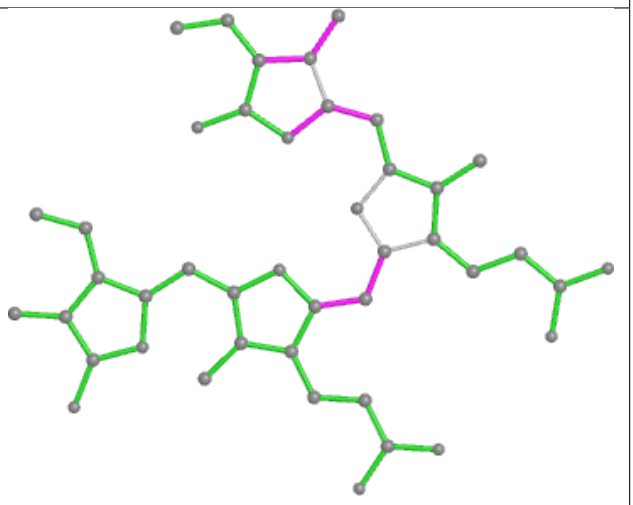

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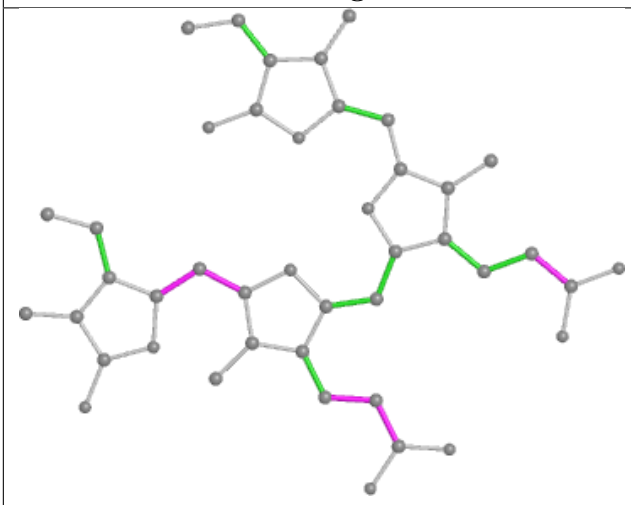

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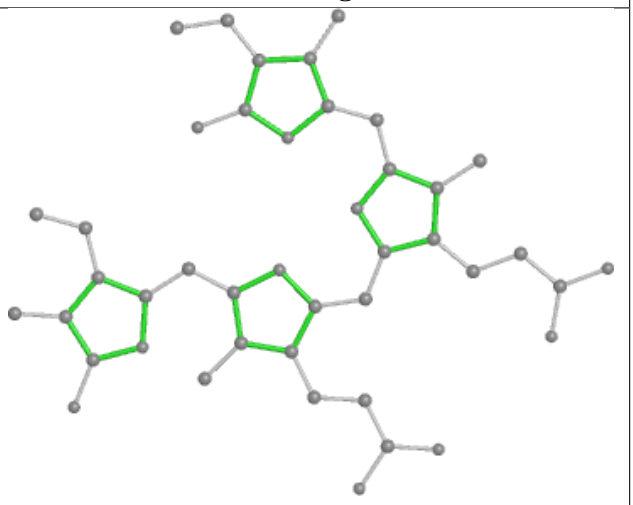
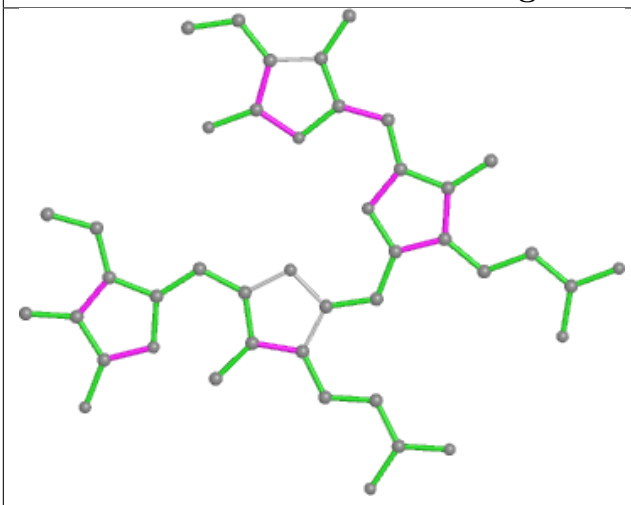


Rings

Ligand PUB c8 305



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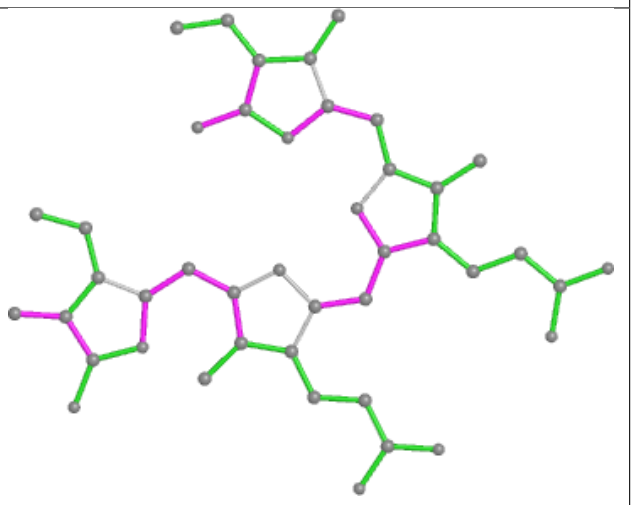

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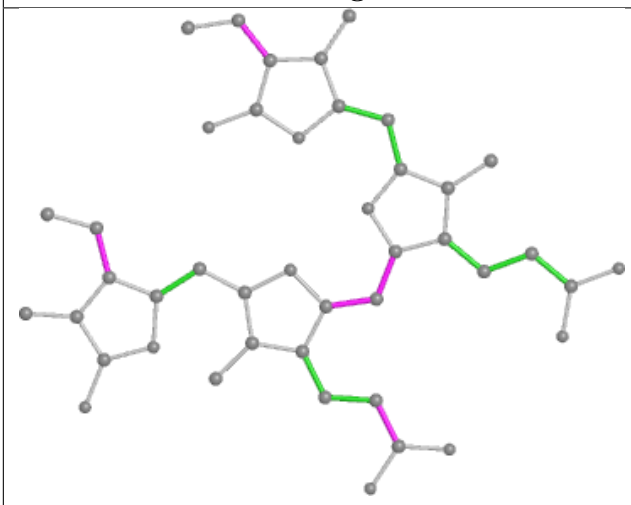

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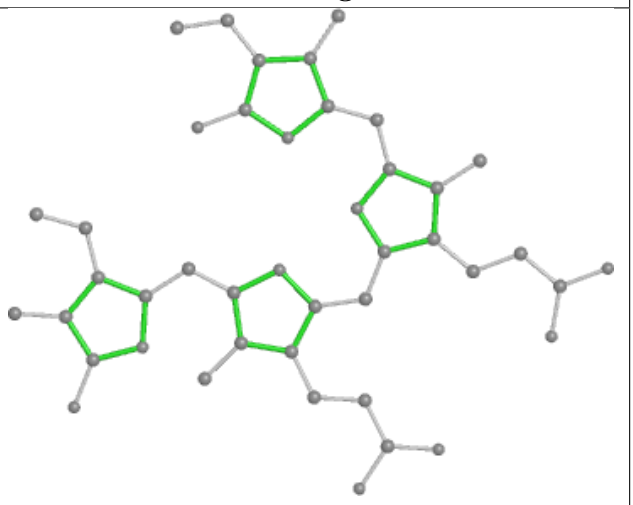
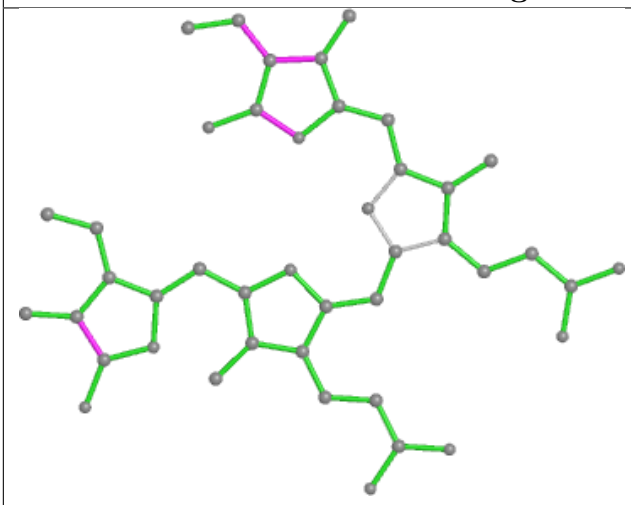


Rings

Ligand PEB W2 202



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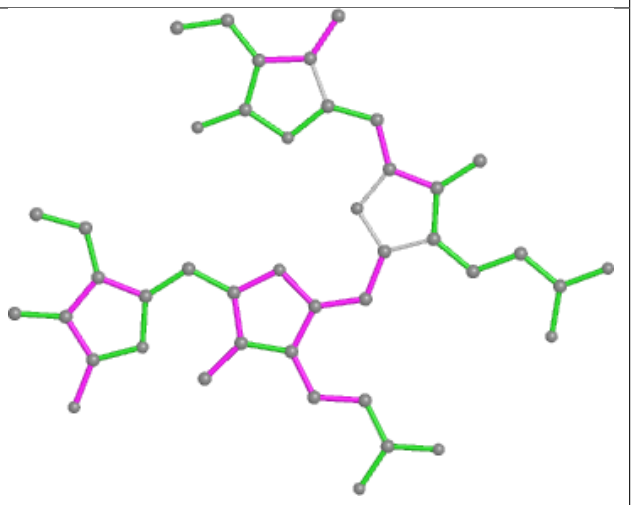

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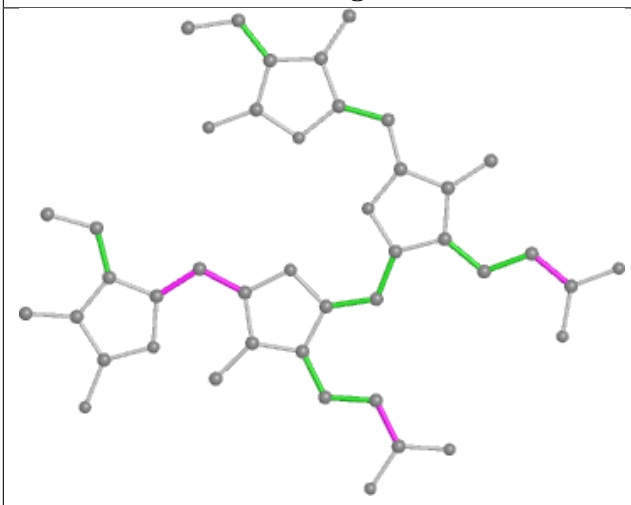

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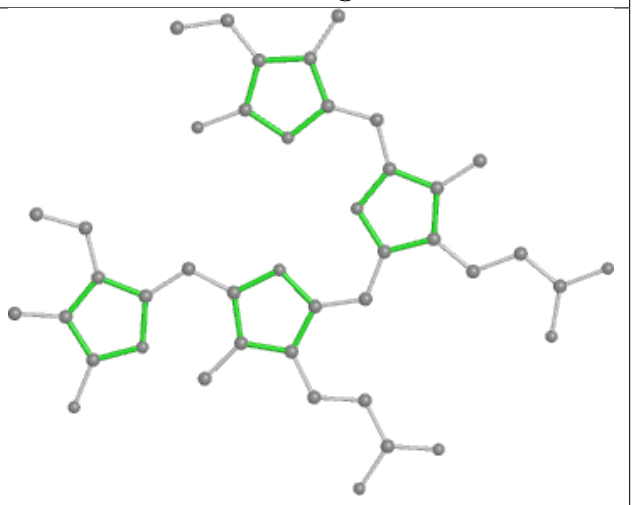

Rings

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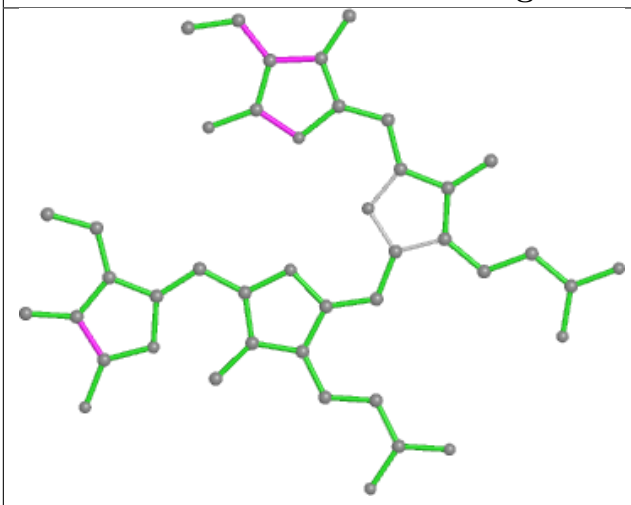

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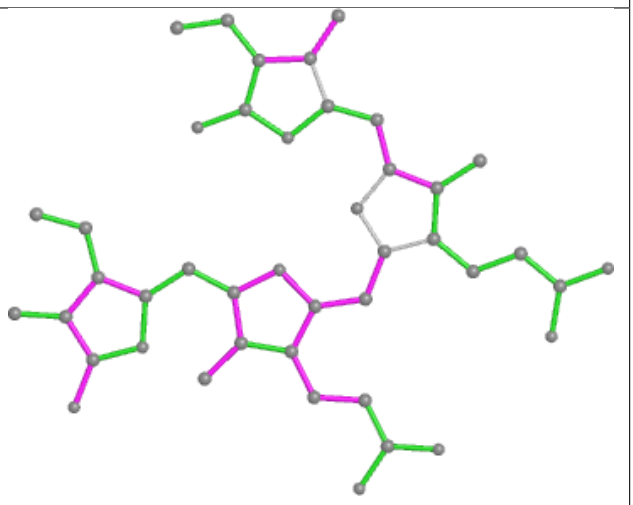

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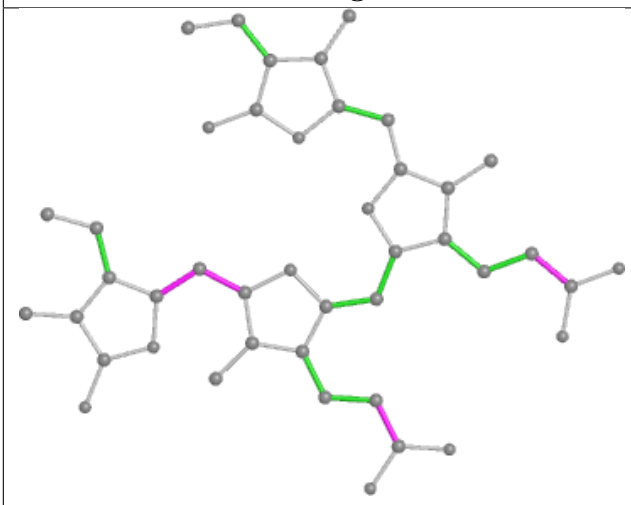

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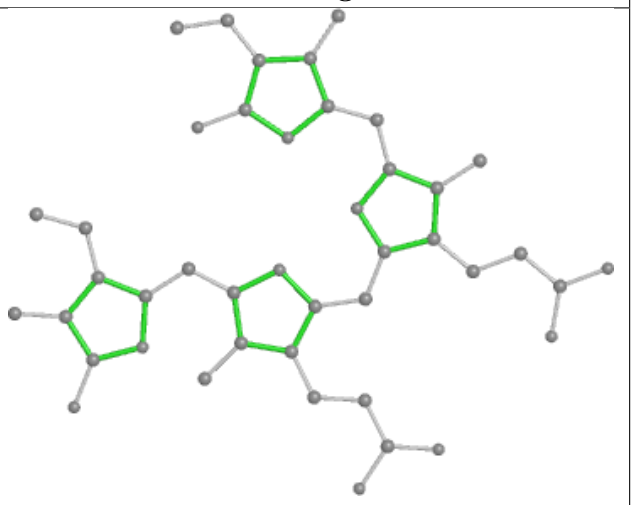
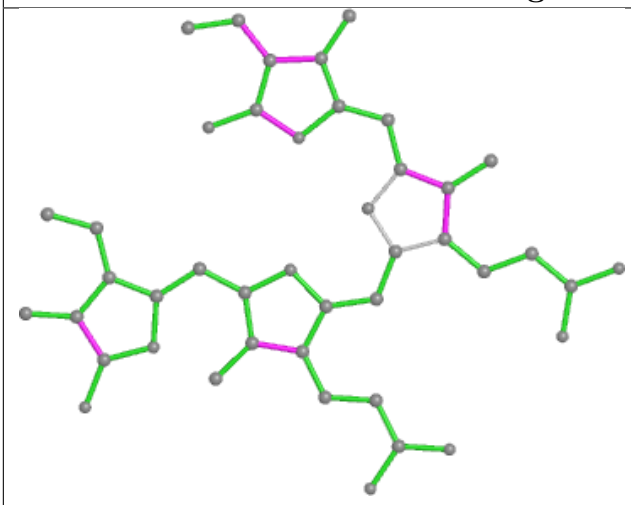


Rings

Ligand PEB ff 202



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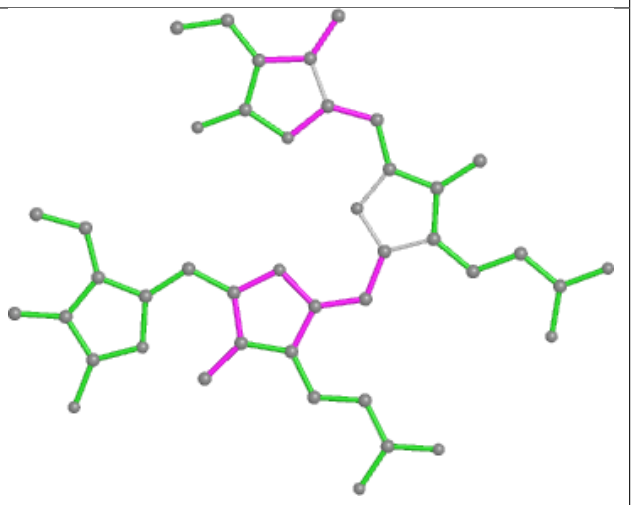

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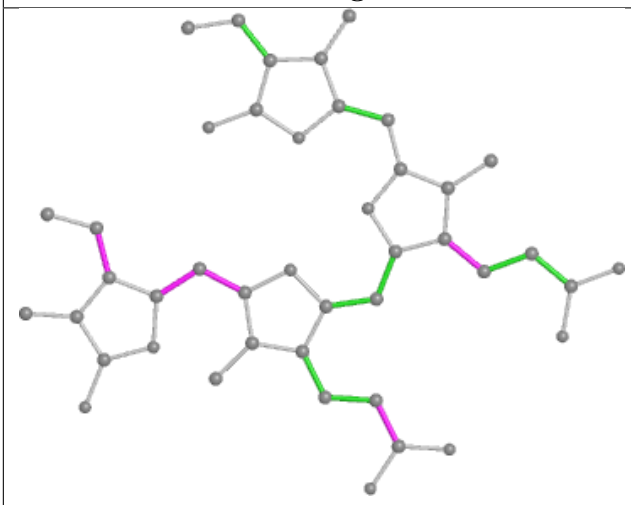

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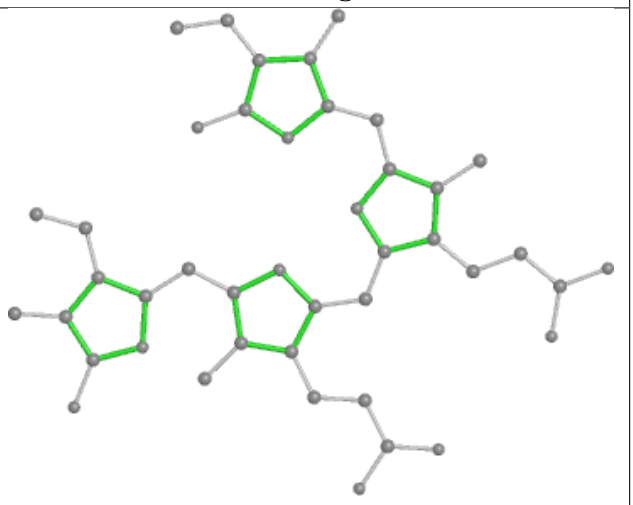
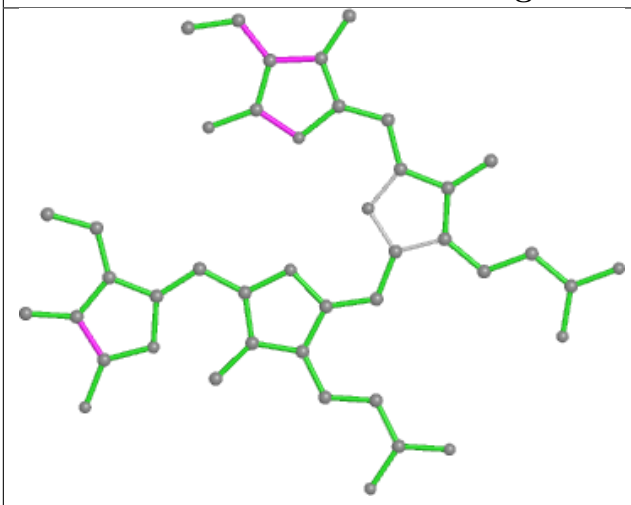


Rings

Ligand PEB U6 201



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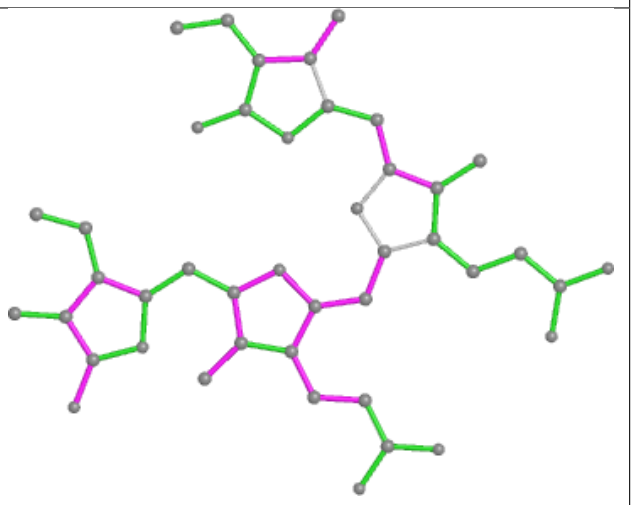

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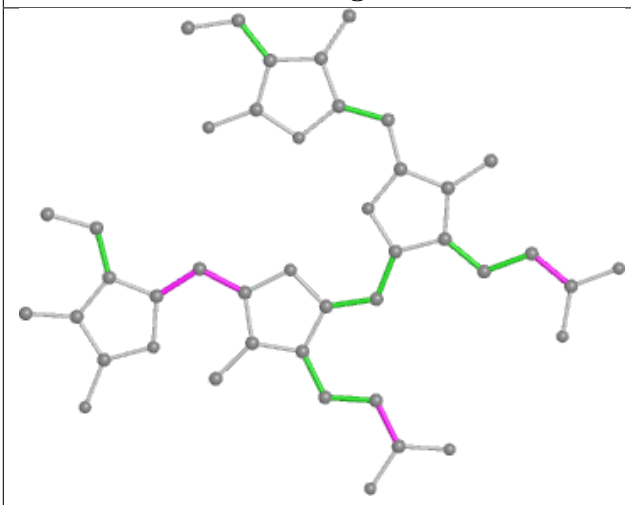

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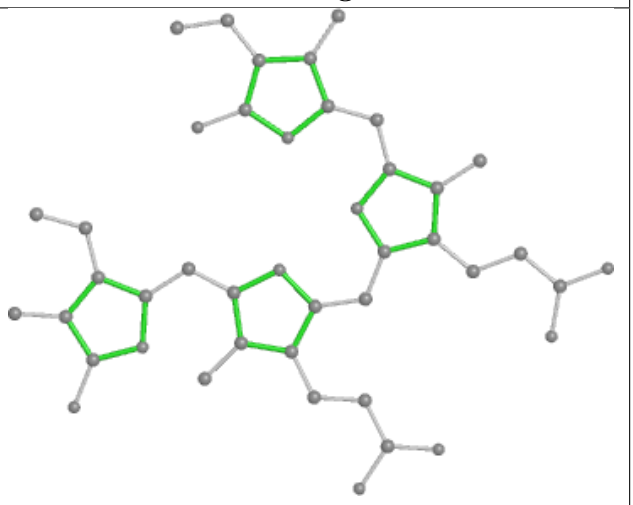
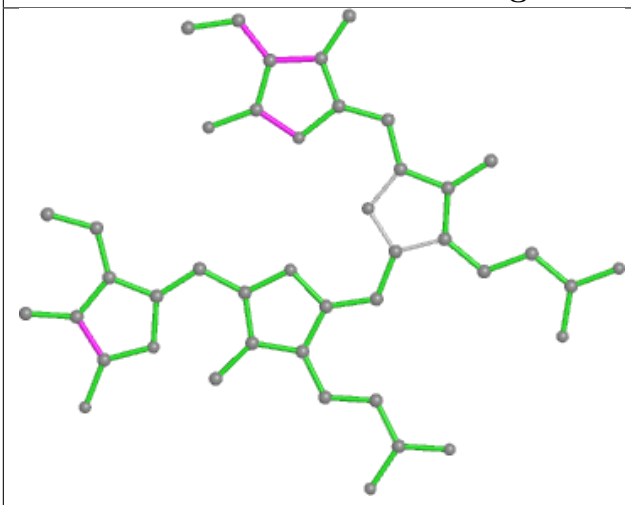


Rings

Ligand PEB b8 1001



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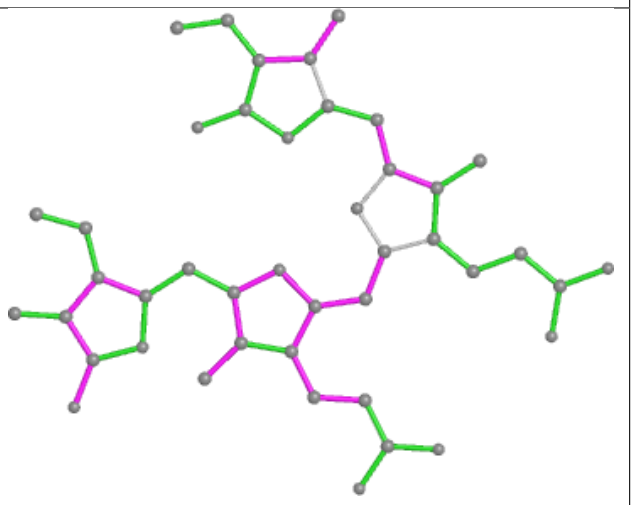

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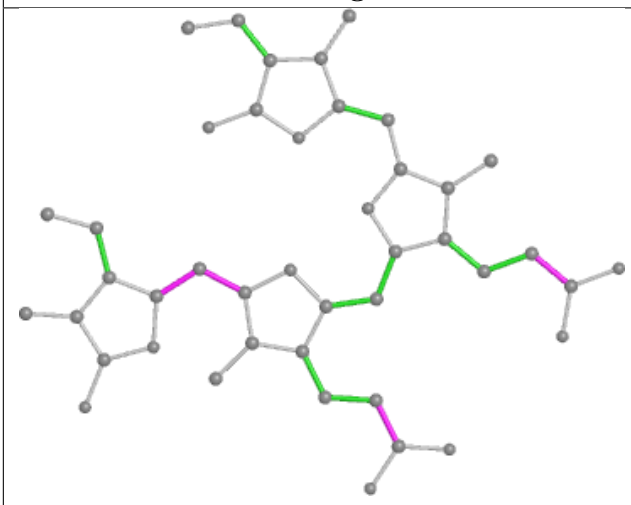

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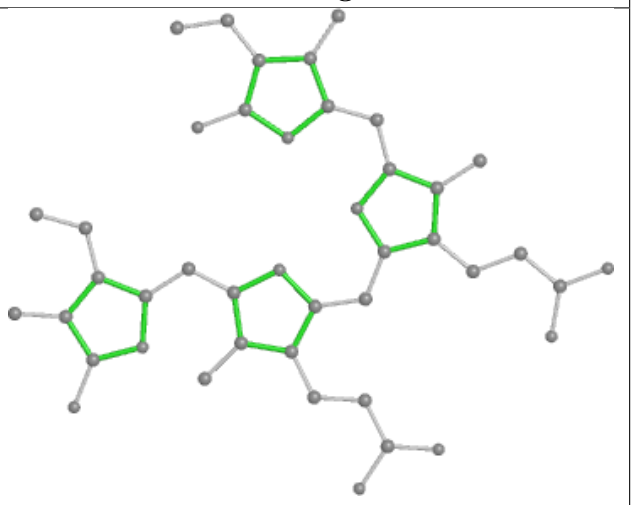
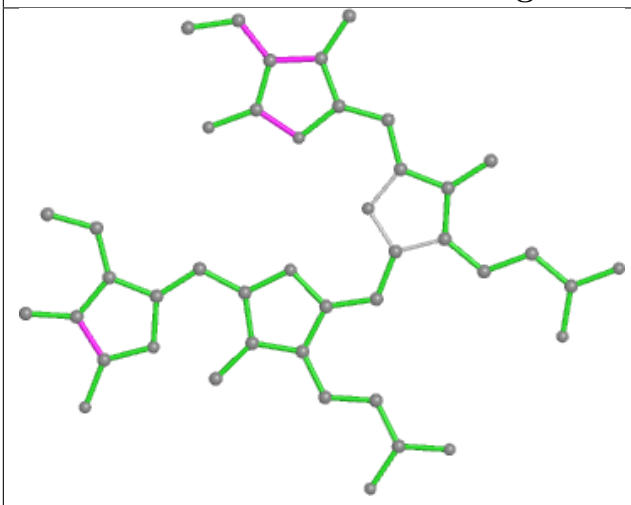


Rings

Ligand PEB P8 202



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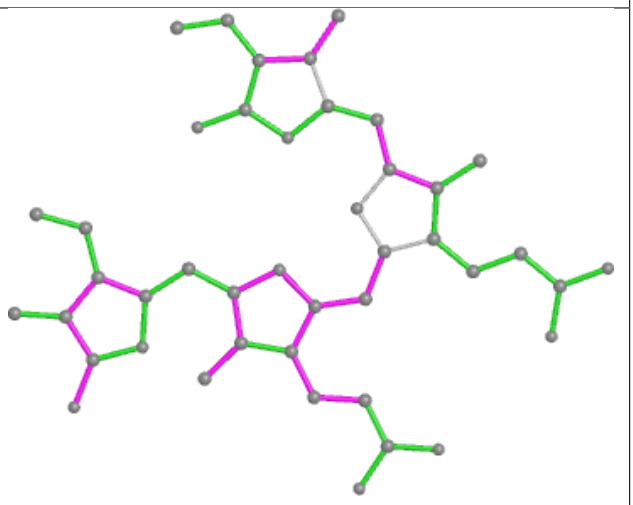

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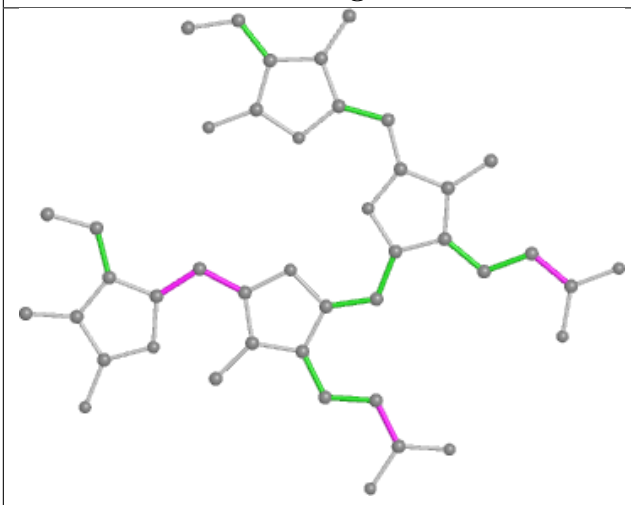
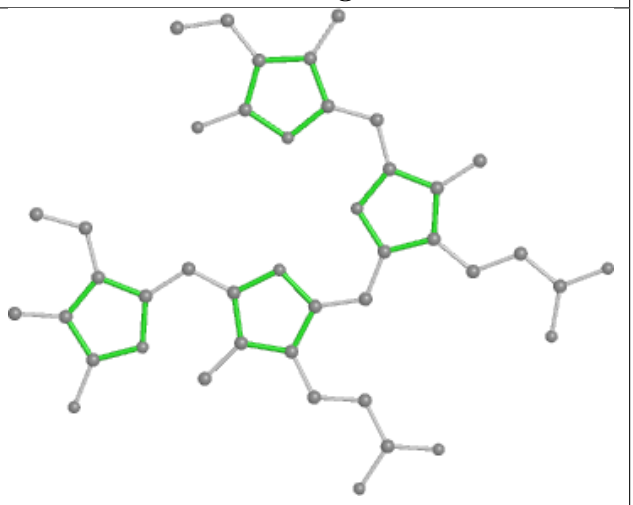
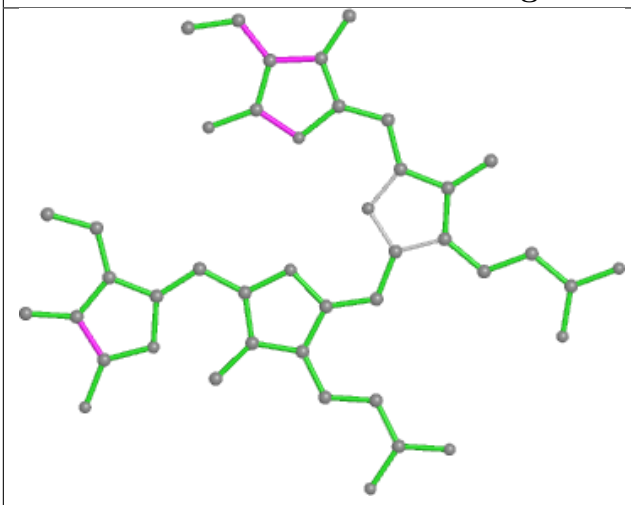


Torsions



Rings

Ligand PEB ds 201



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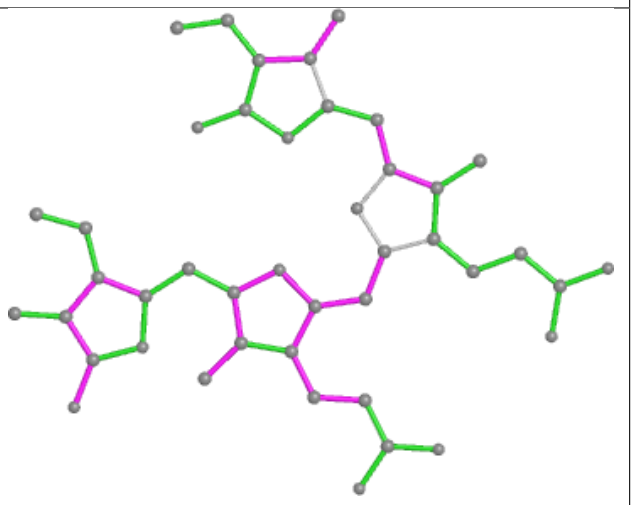

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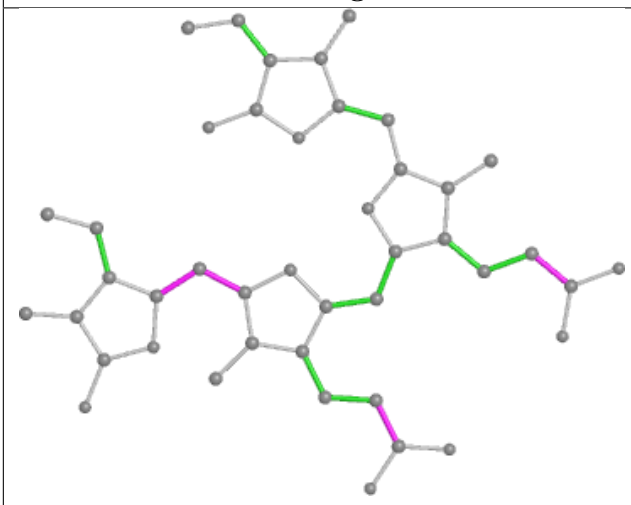

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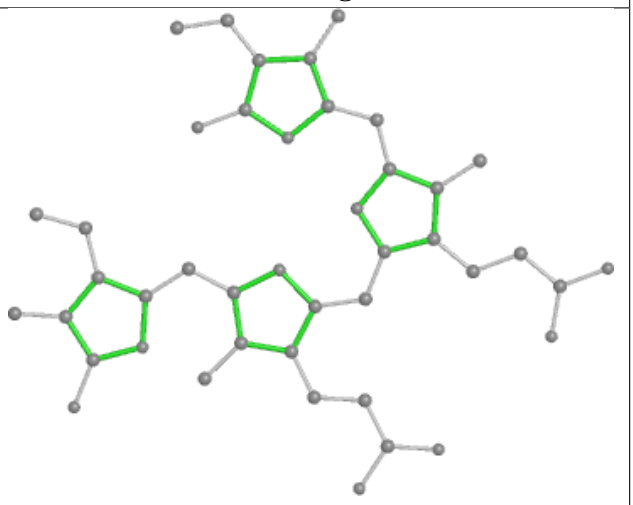
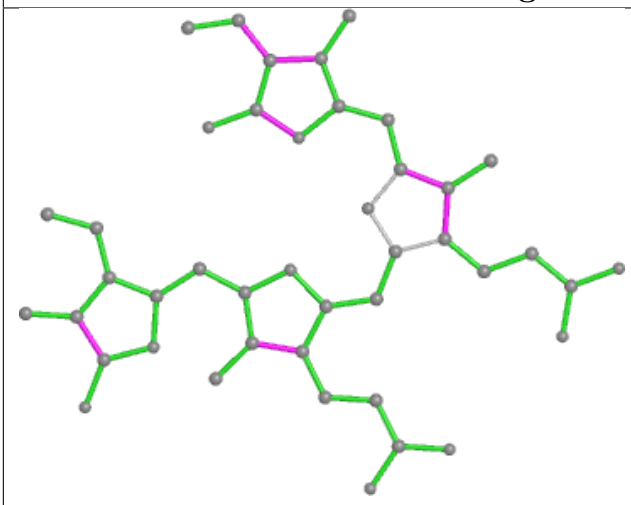


Rings

Ligand PEB n3 202



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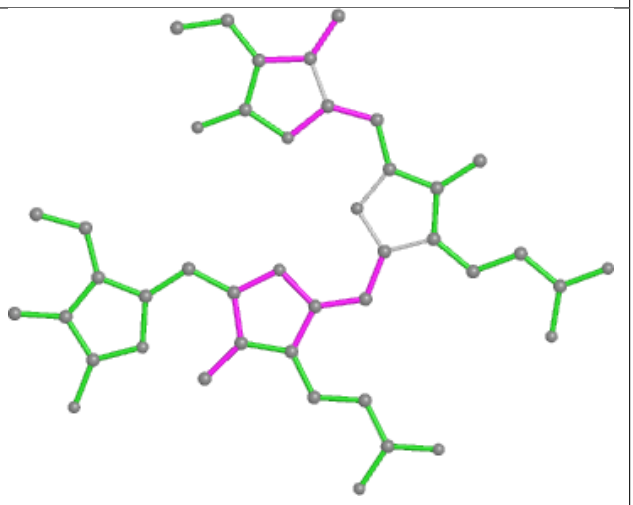

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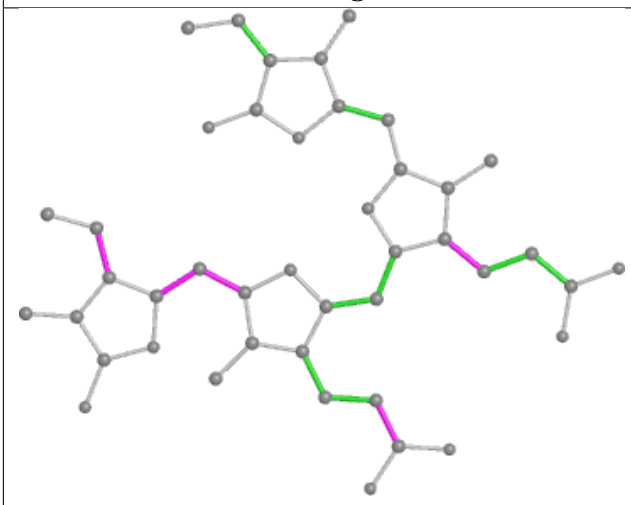

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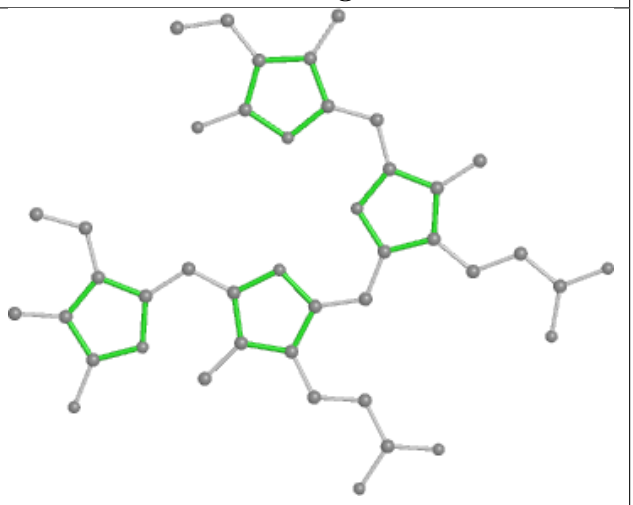
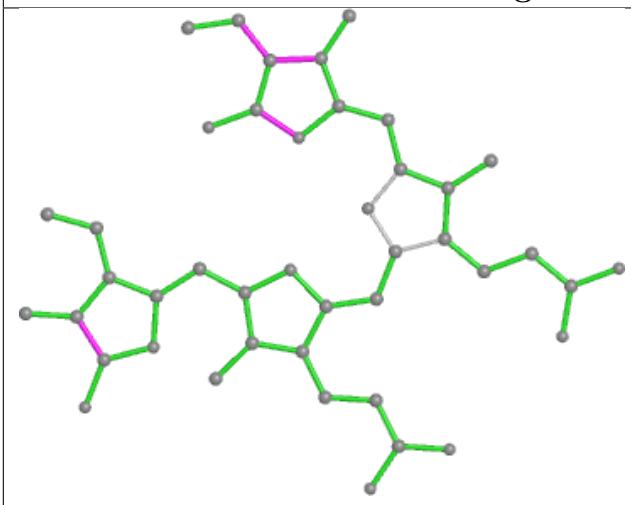


Rings

Ligand PEB dA 202



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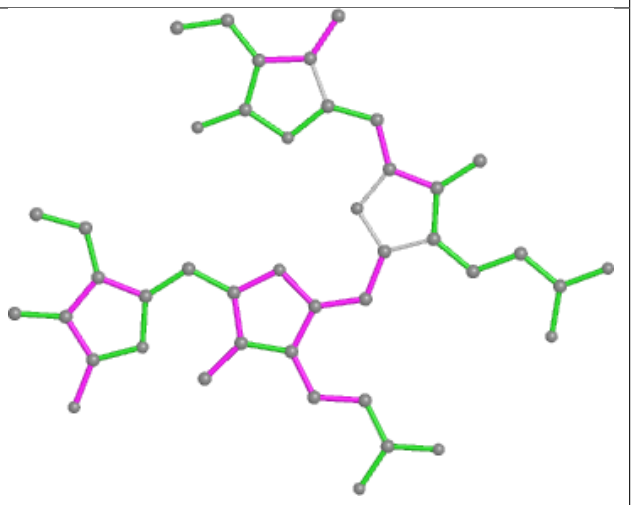

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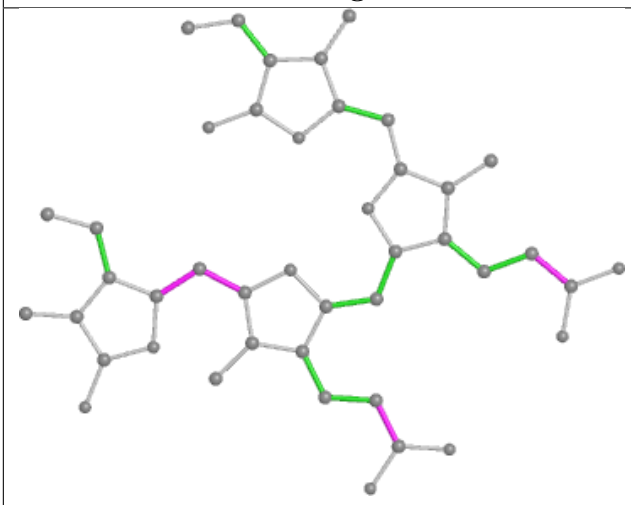

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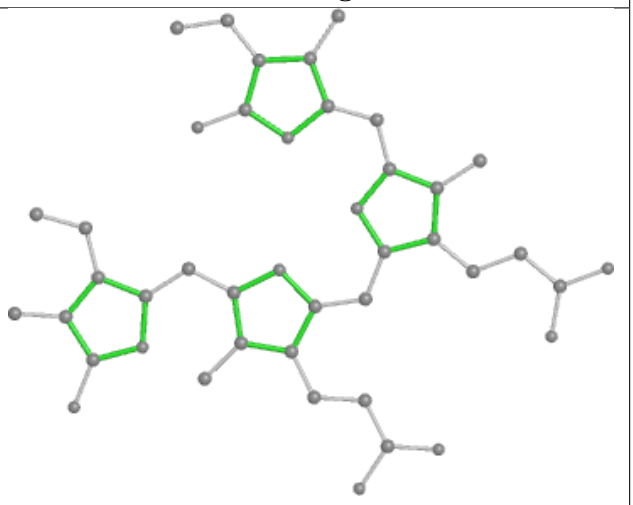
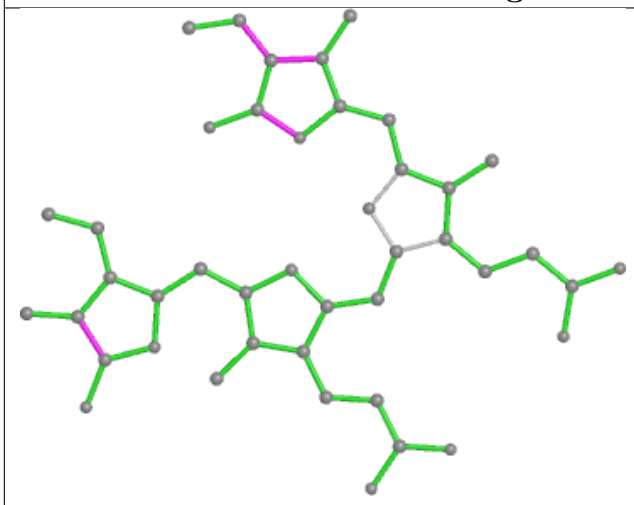


Rings

Ligand PEB am 1001



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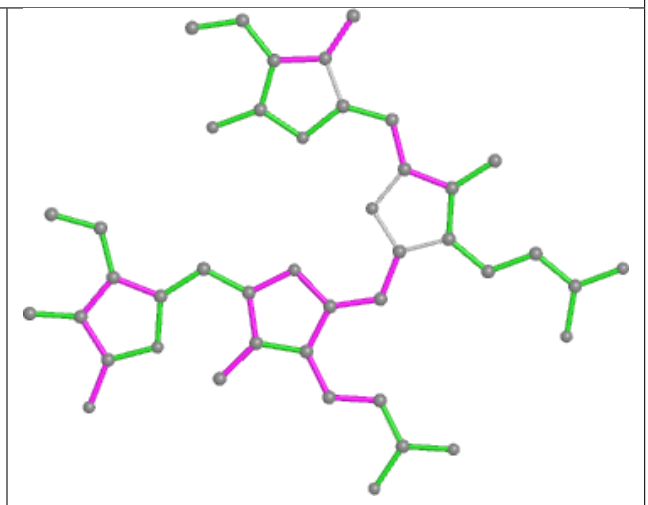

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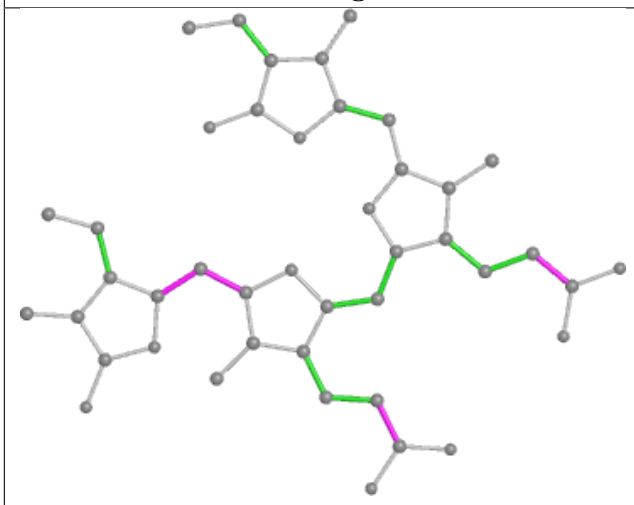

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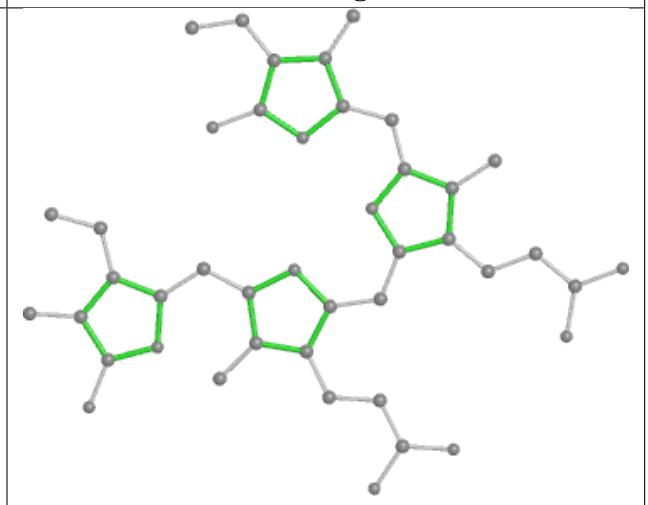
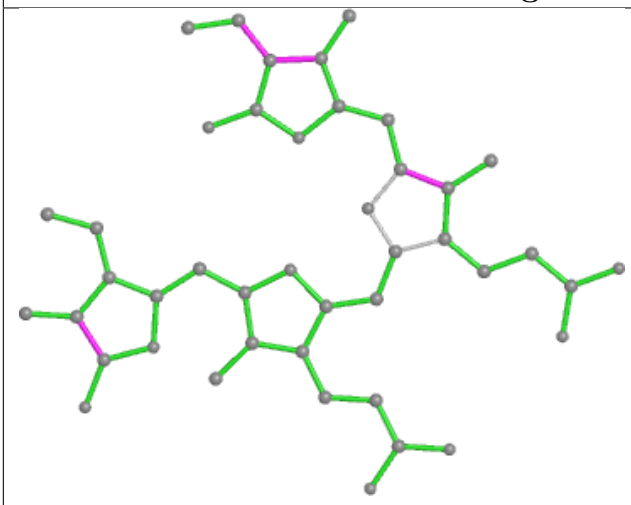


Rings

Ligand PEB r8 202



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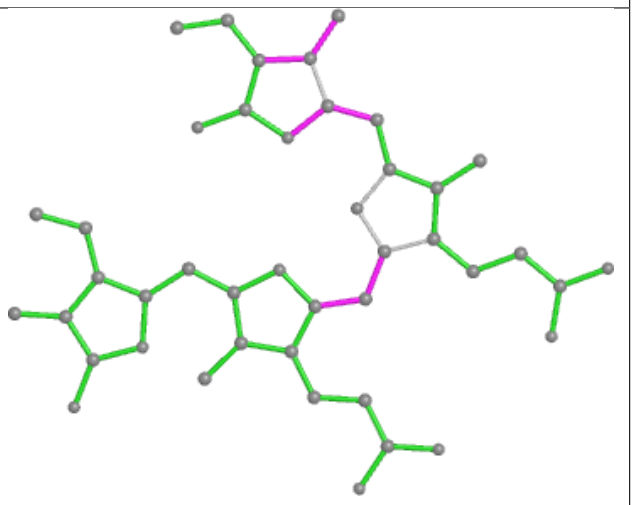

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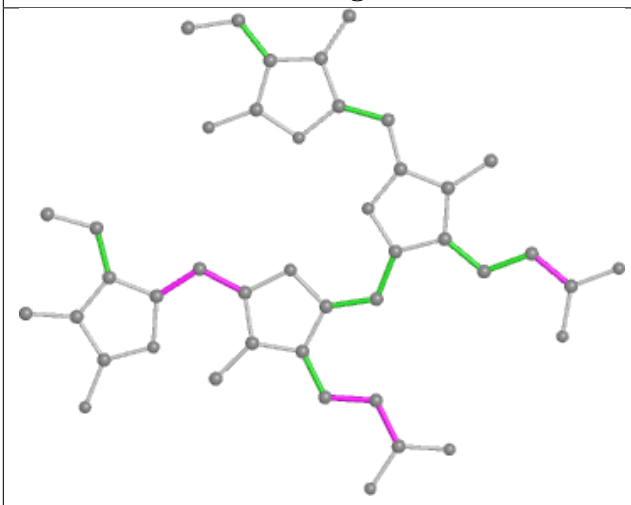

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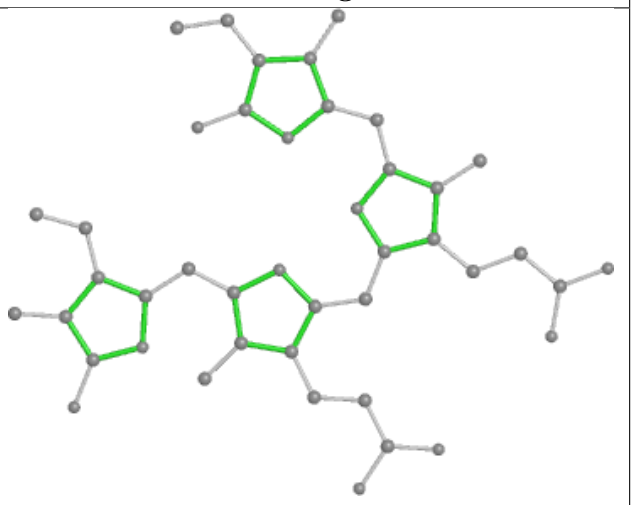
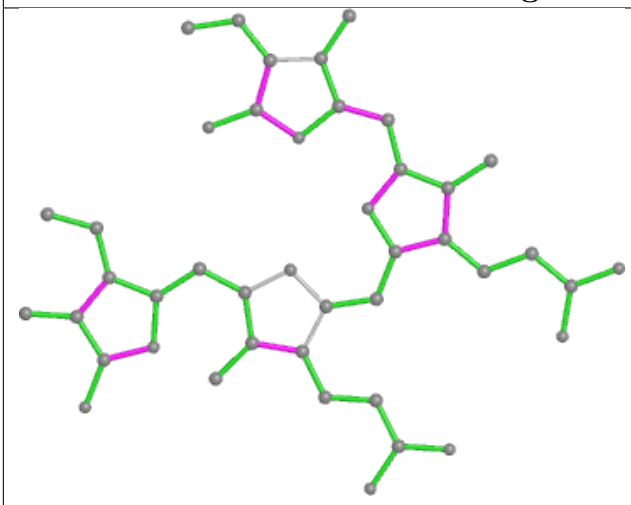


Rings

Ligand PUB j2 203



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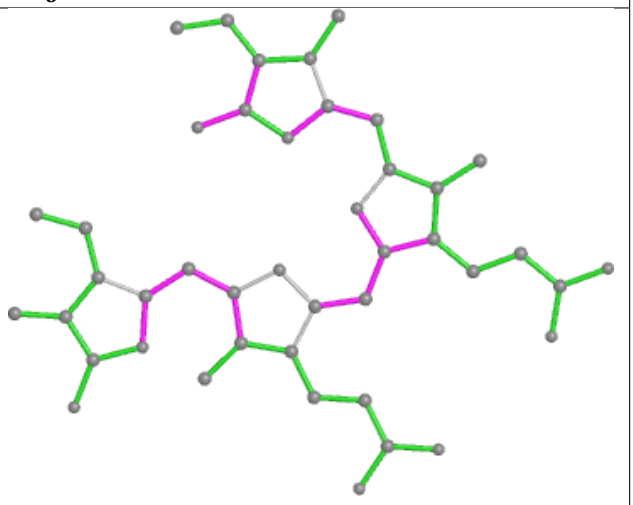

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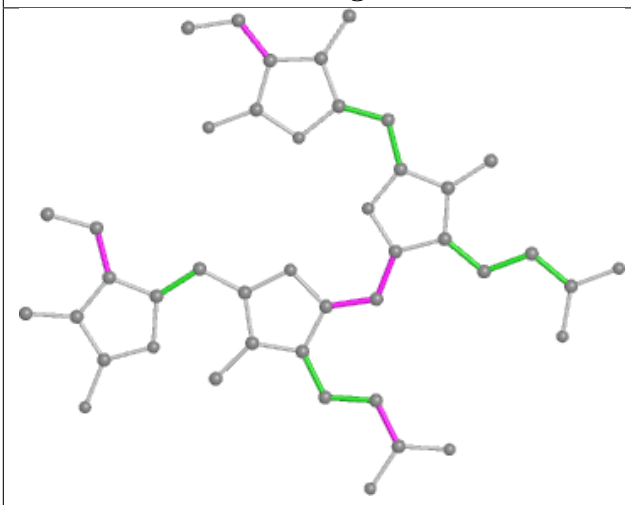

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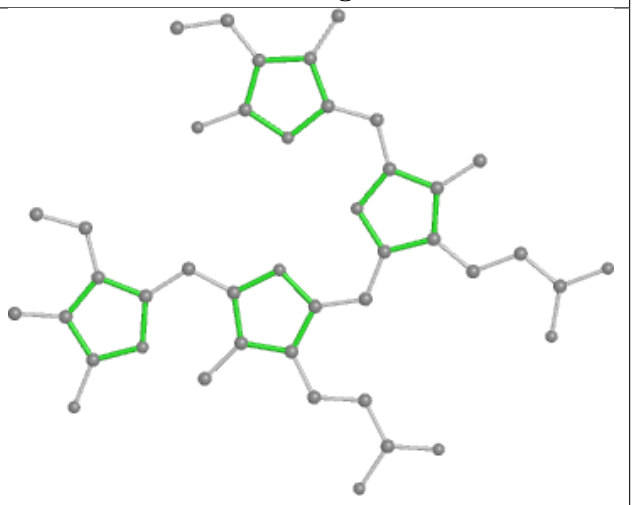

Rings

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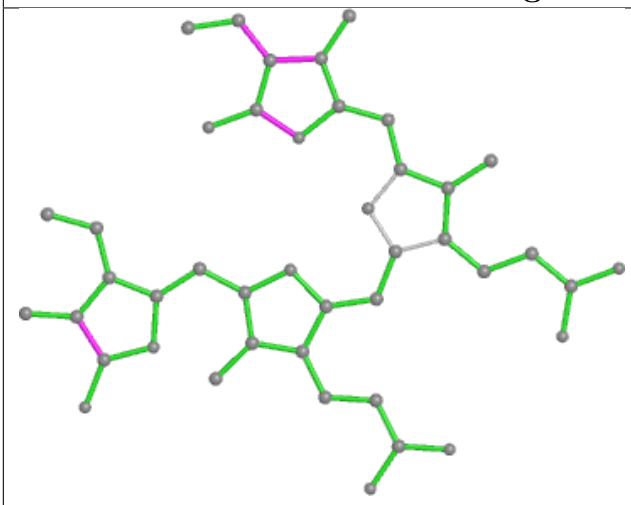

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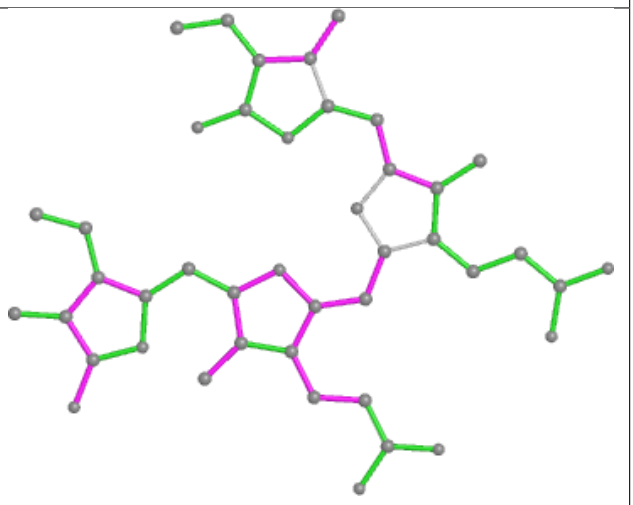

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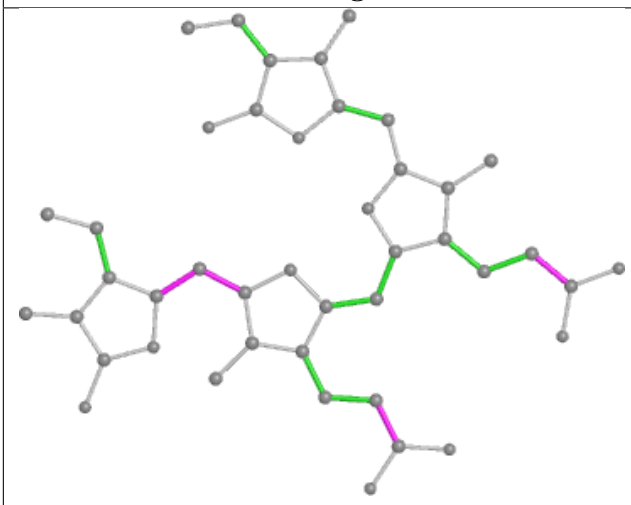

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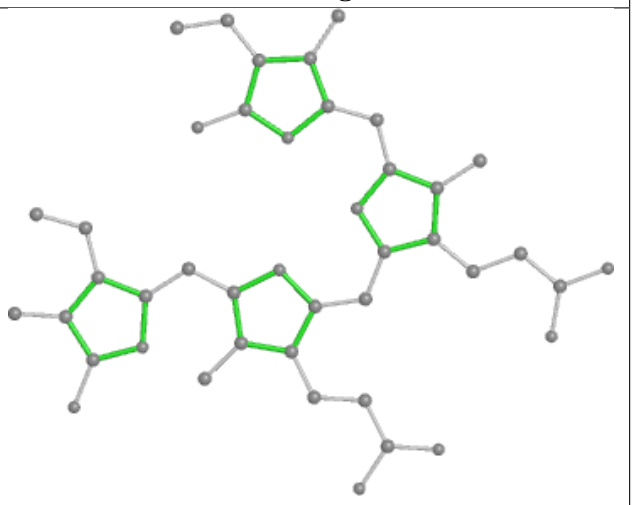
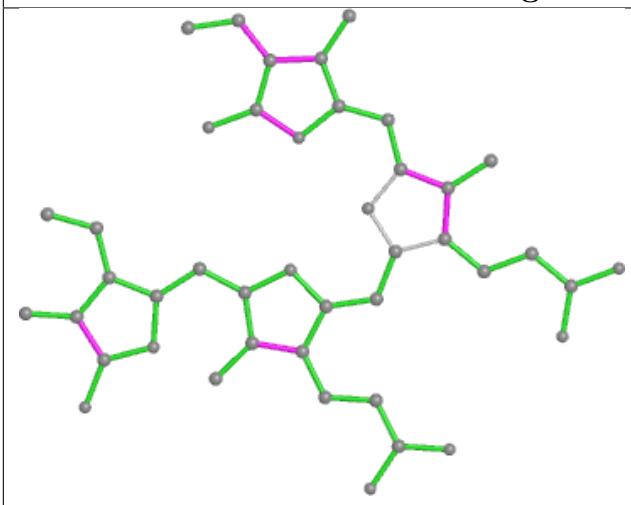


Rings

Ligand PEB gt 202



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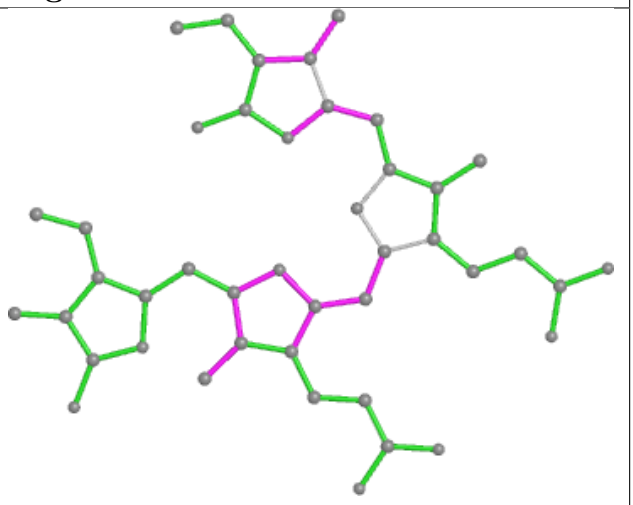

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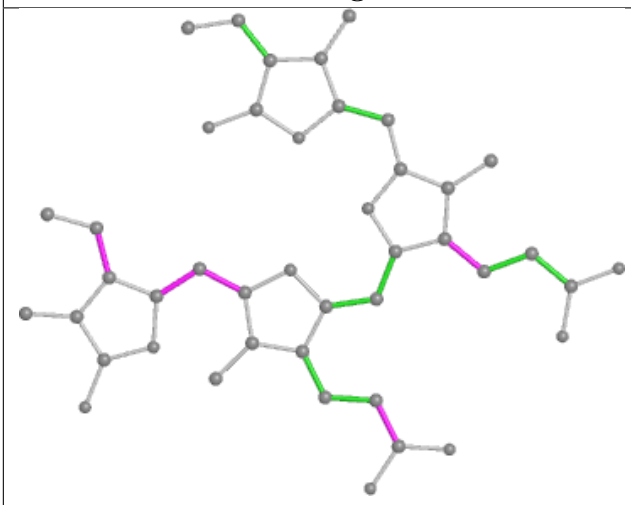

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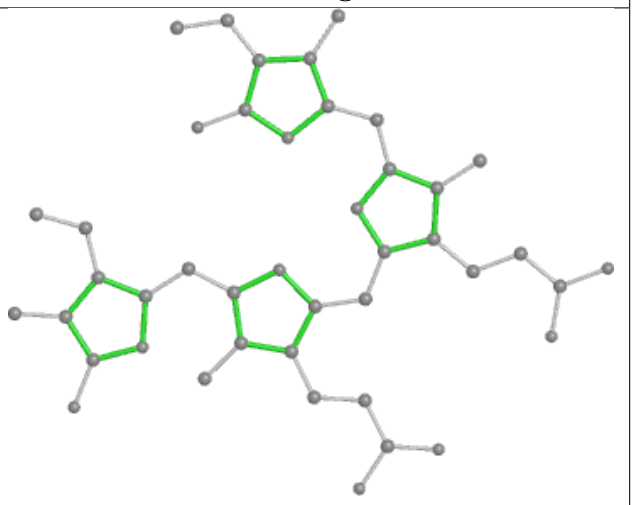
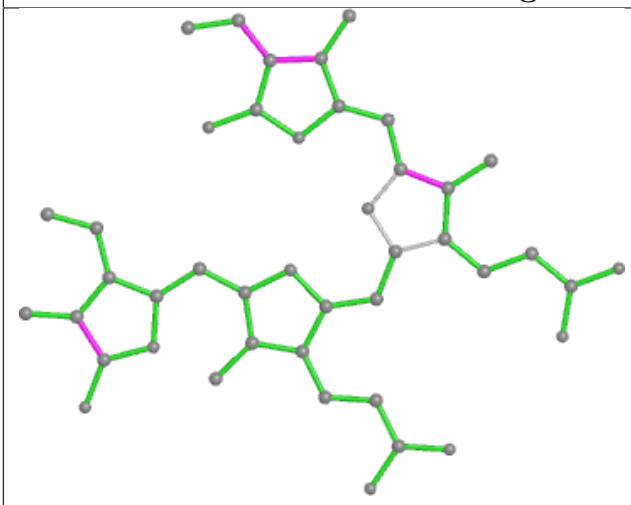


Rings

Ligand PEB o8 201



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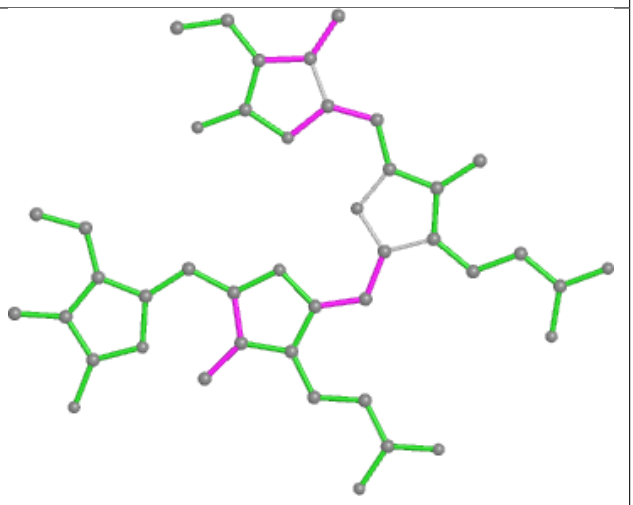

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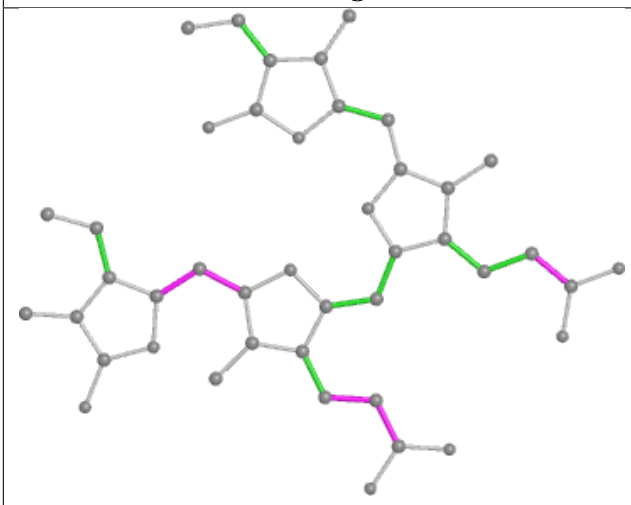

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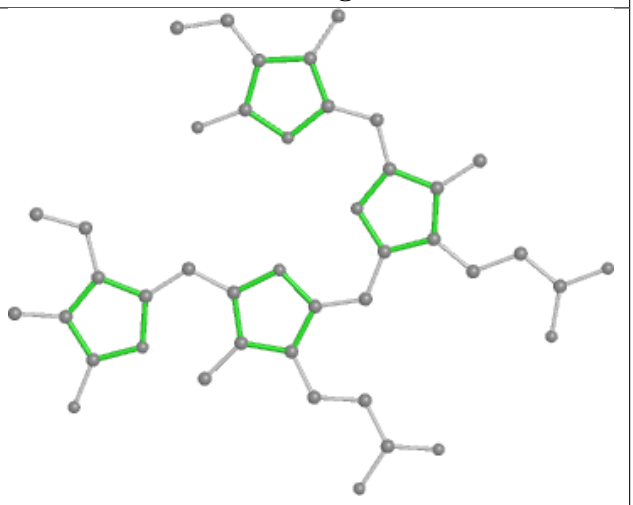
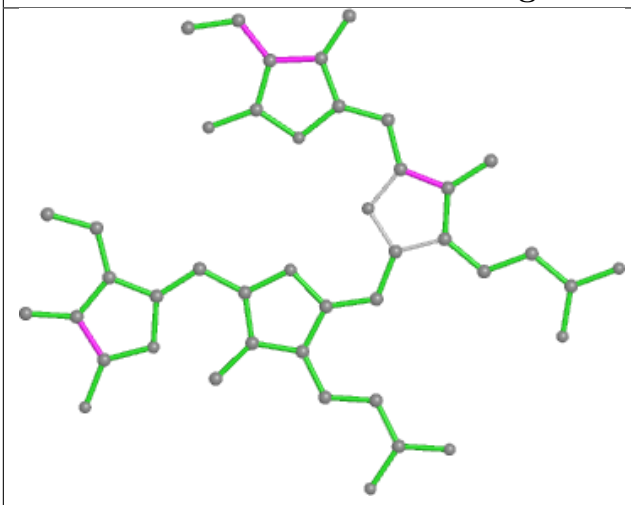


Rings

Ligand PEB S7 202



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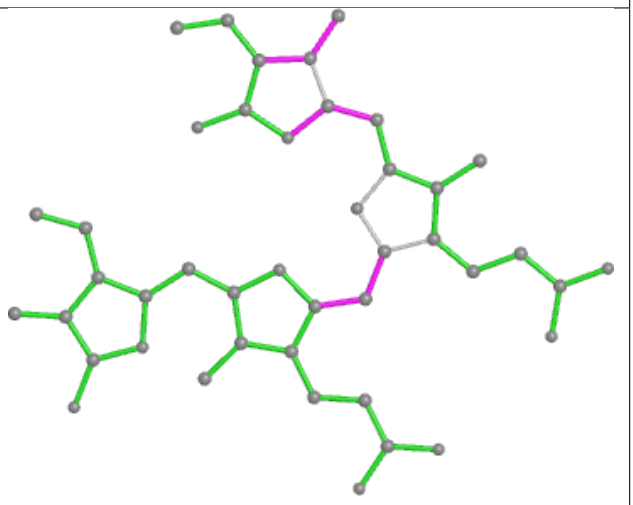

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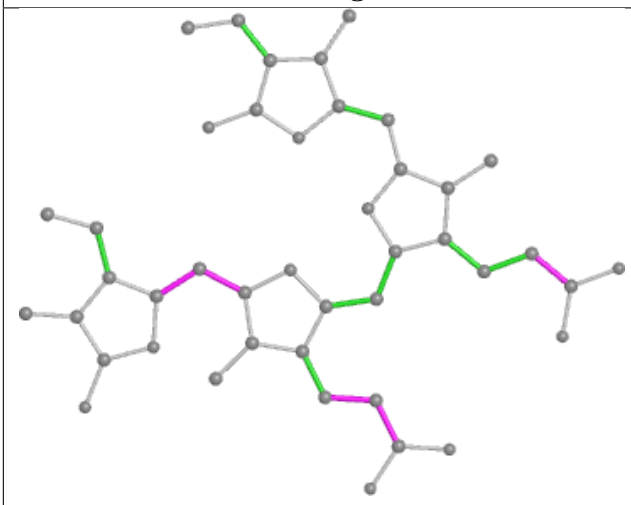

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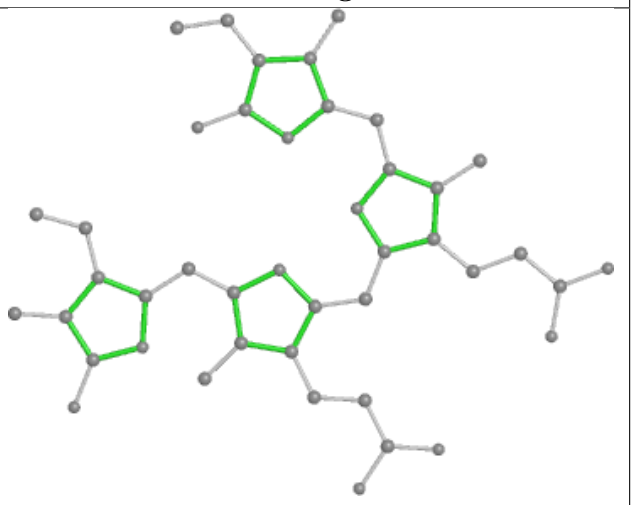
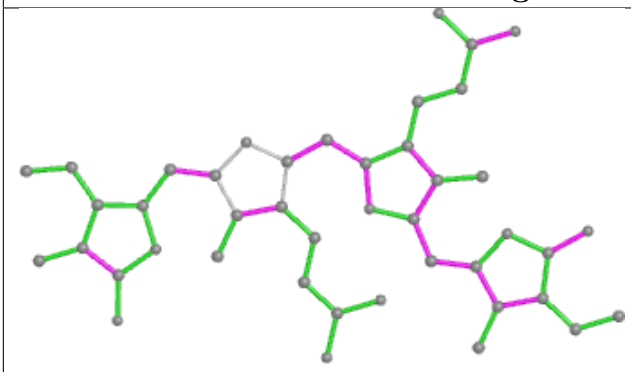


Rings

Ligand CYC i1 1001



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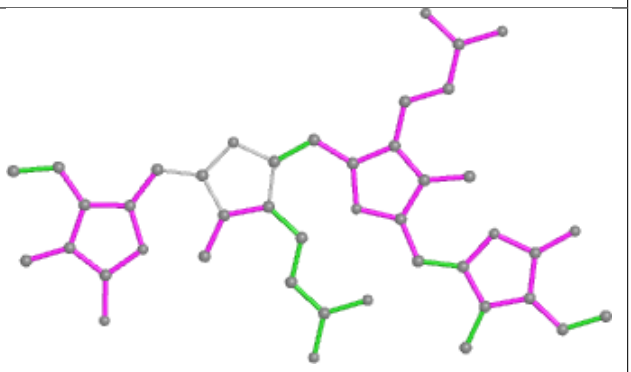

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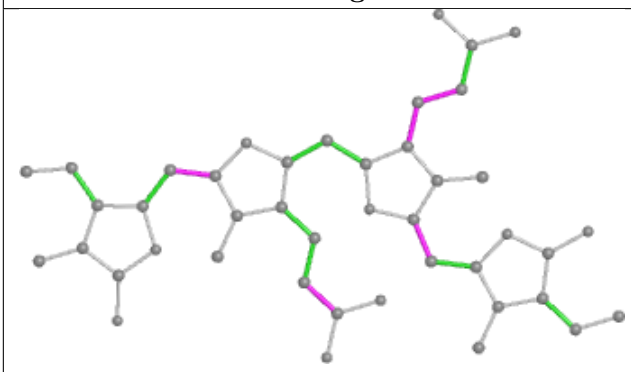

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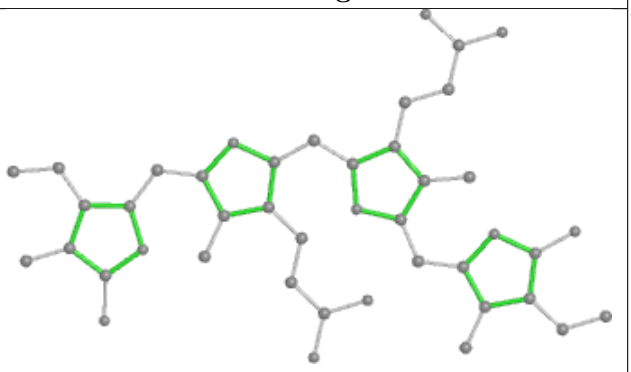
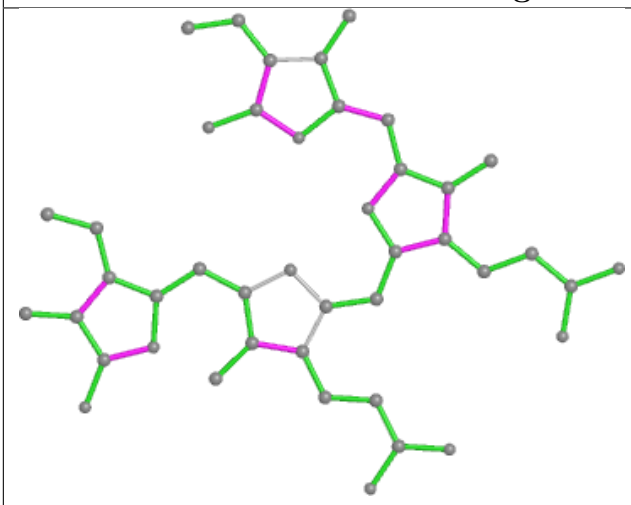


Rings

Ligand PUB dP 203



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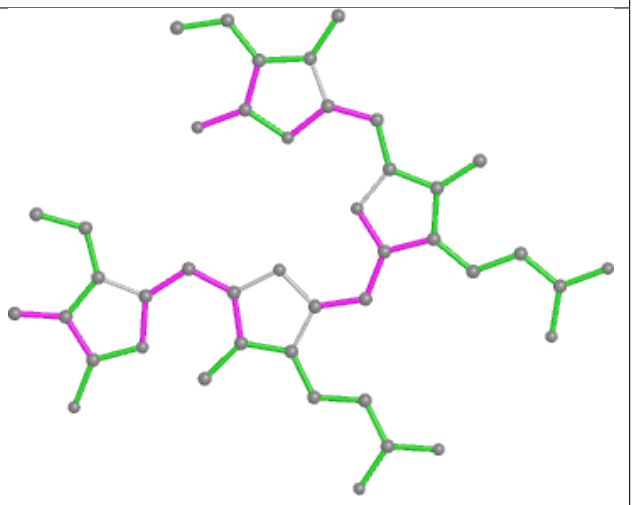

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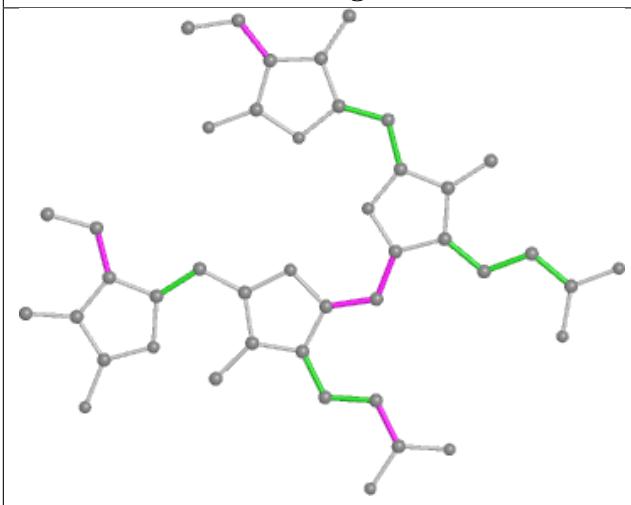

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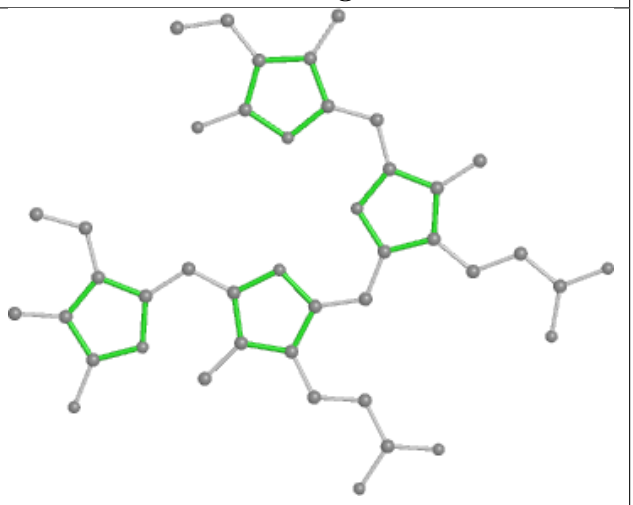
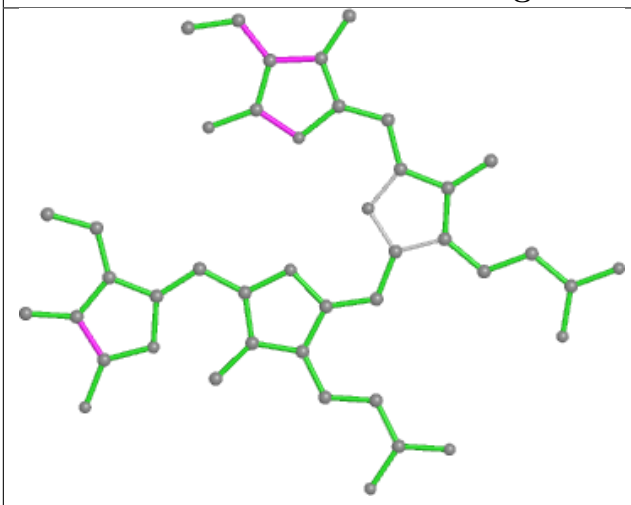


Rings

Ligand PEB hN 201



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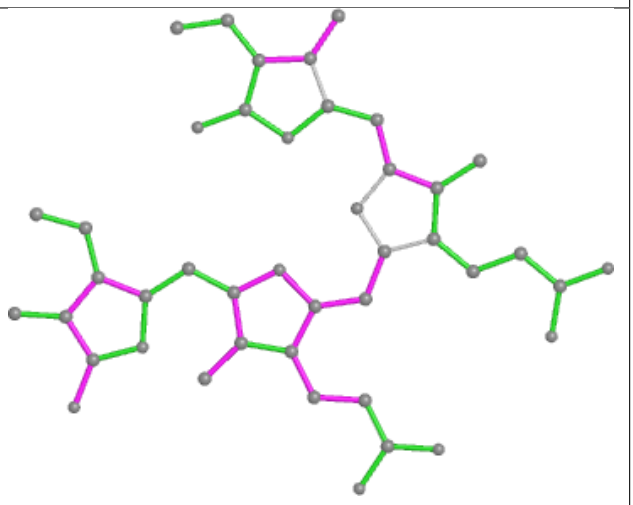
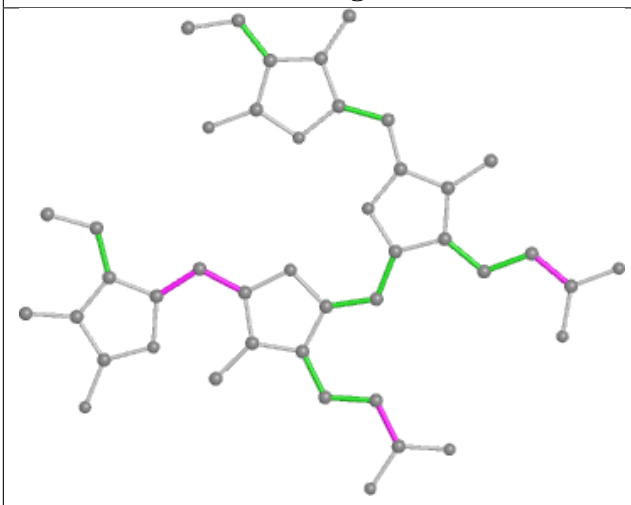


Bond angles



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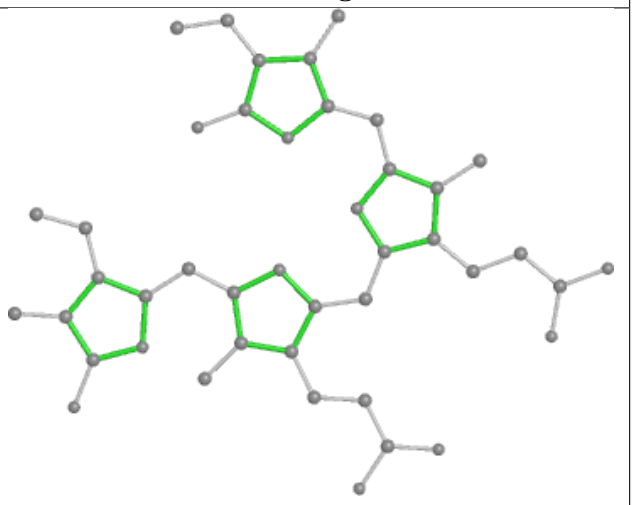
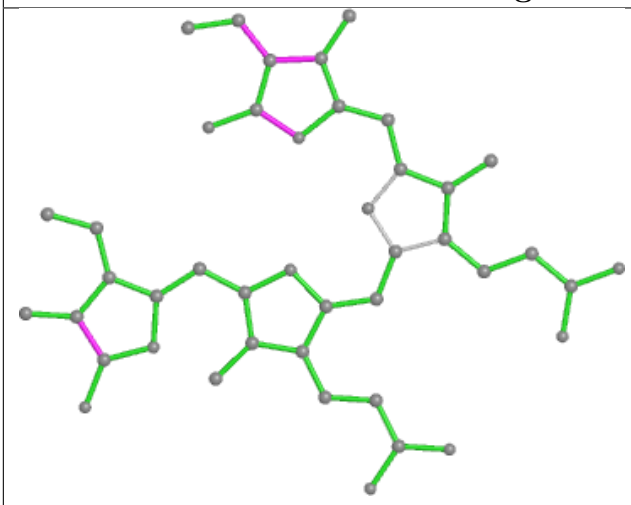
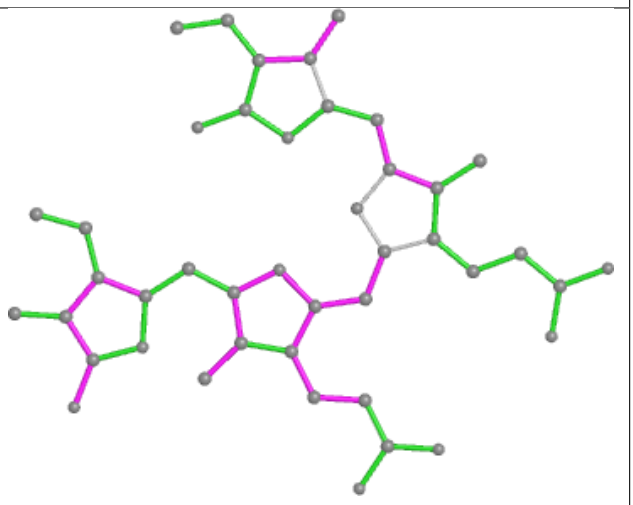


Rings

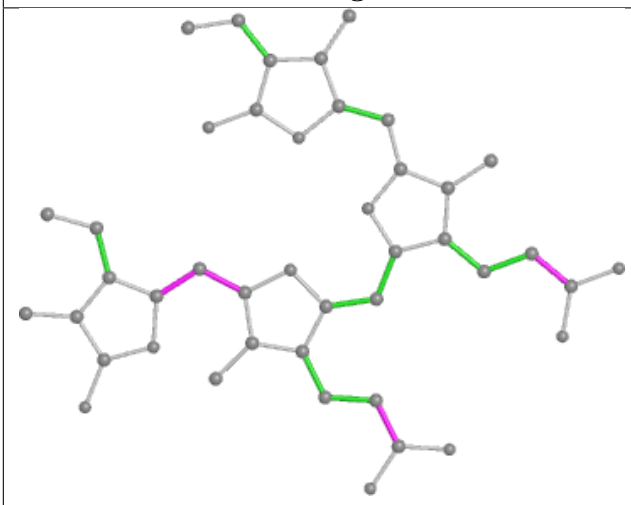
Ligand PEB dw 403



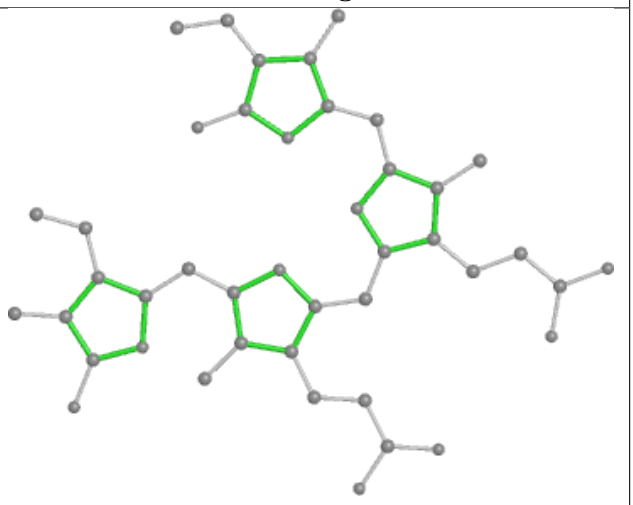
Bond lengths



Bond angles

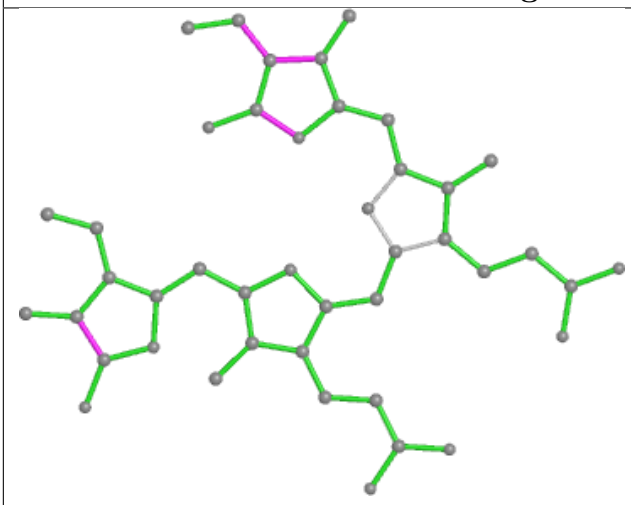


Torsions



Rings

Ligand PEB c9 302



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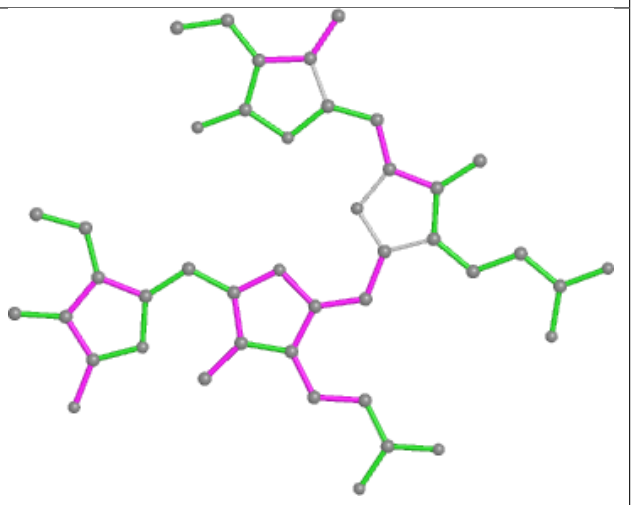

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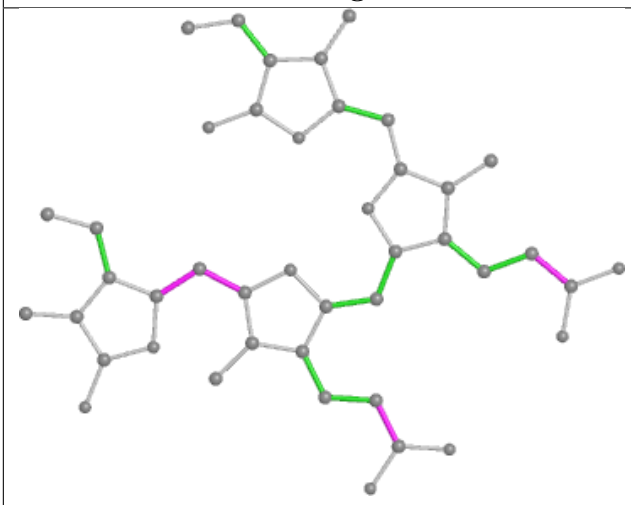

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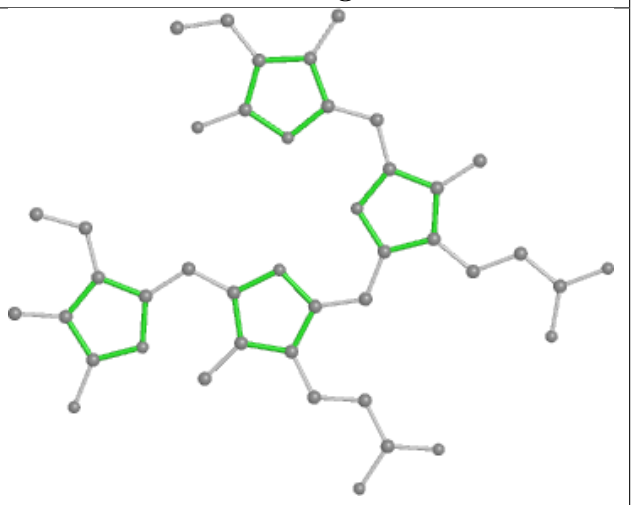
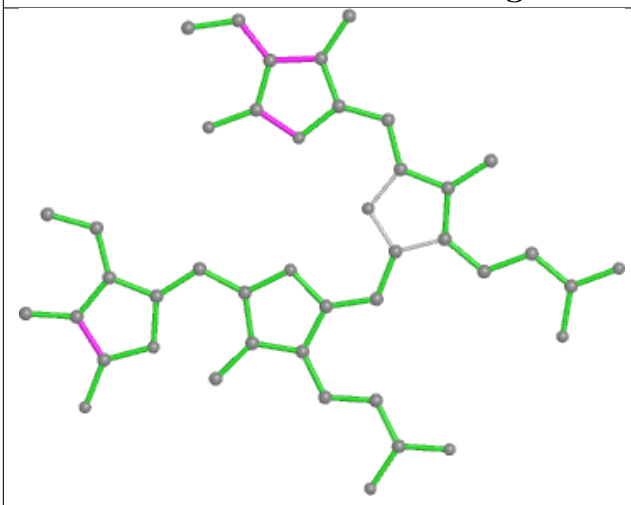


Rings

Ligand PEB cm 1001



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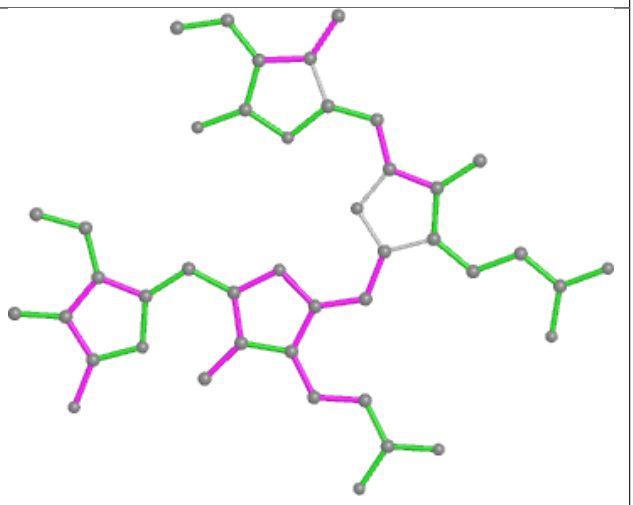

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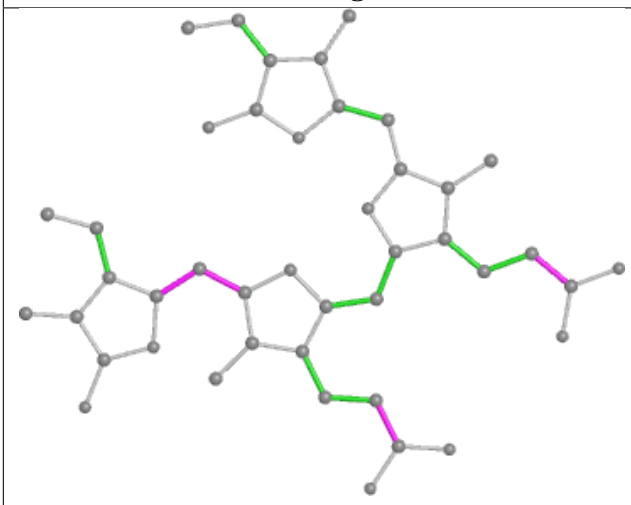

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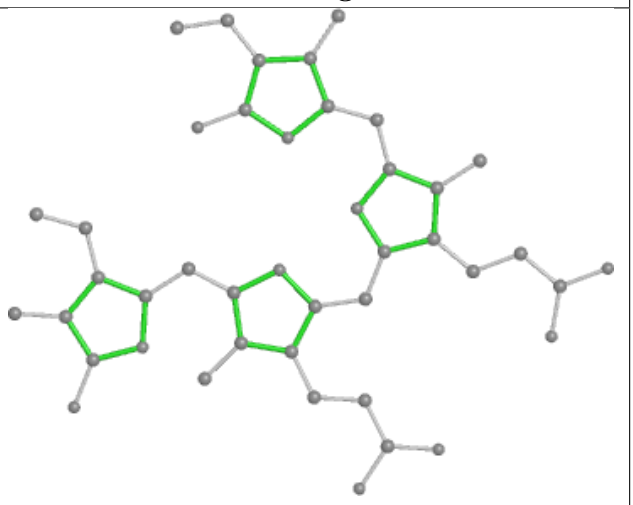
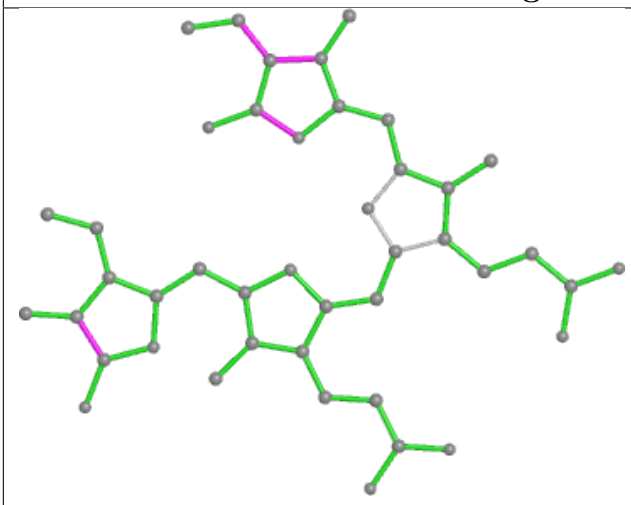


Rings

Ligand PEB bi 201



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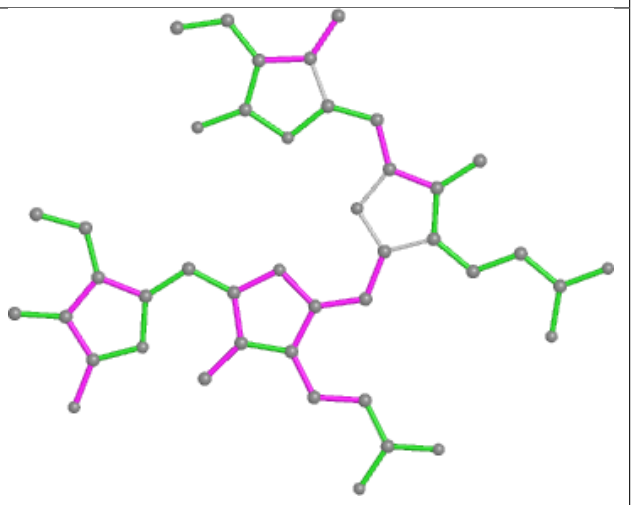

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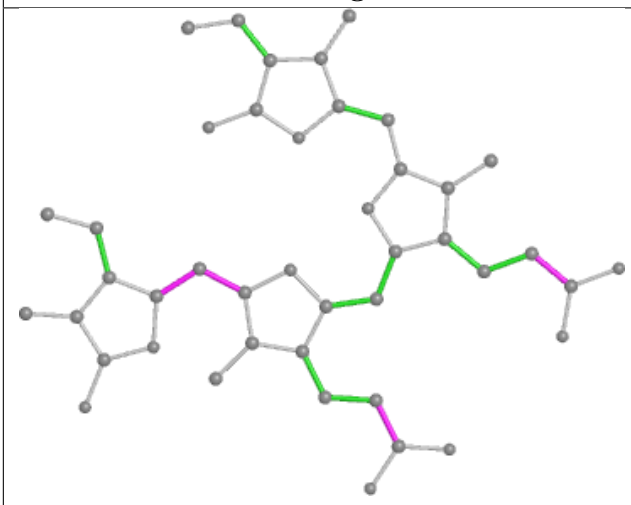

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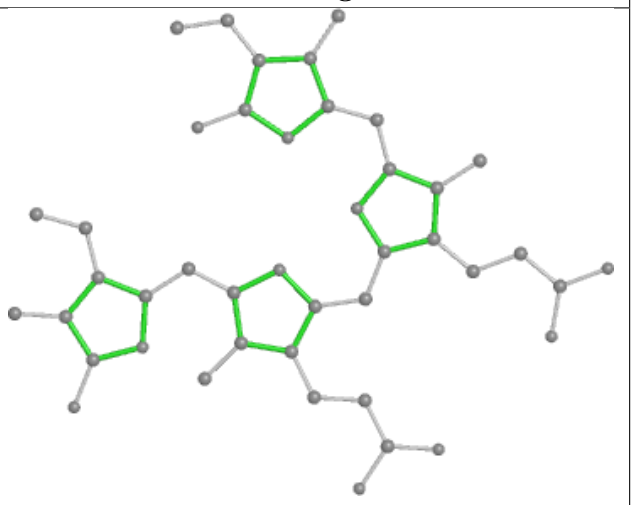
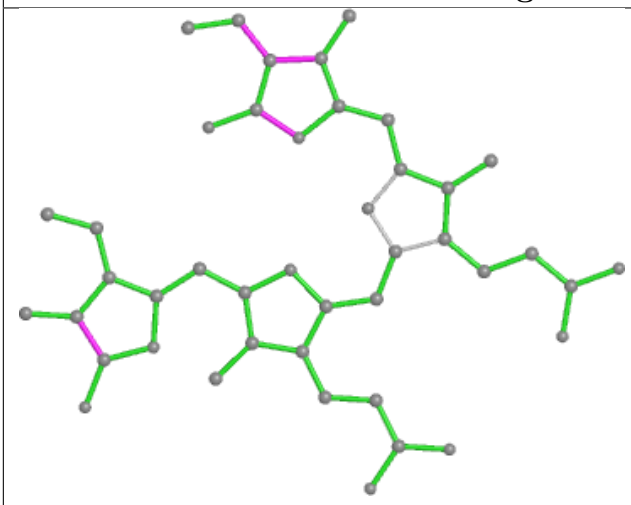


Rings

Ligand PEB cQ 201



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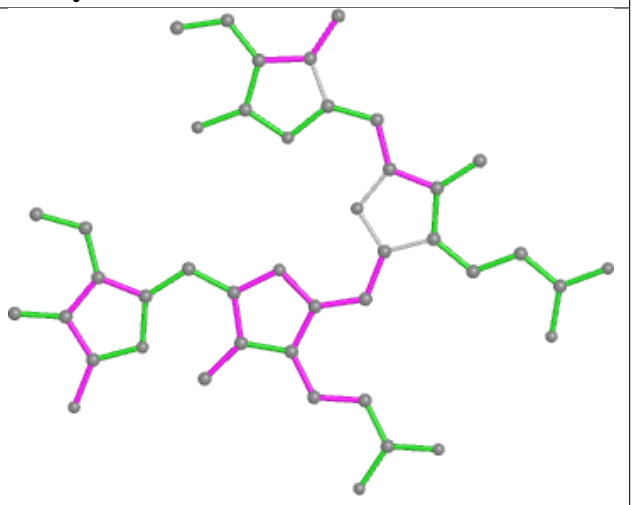

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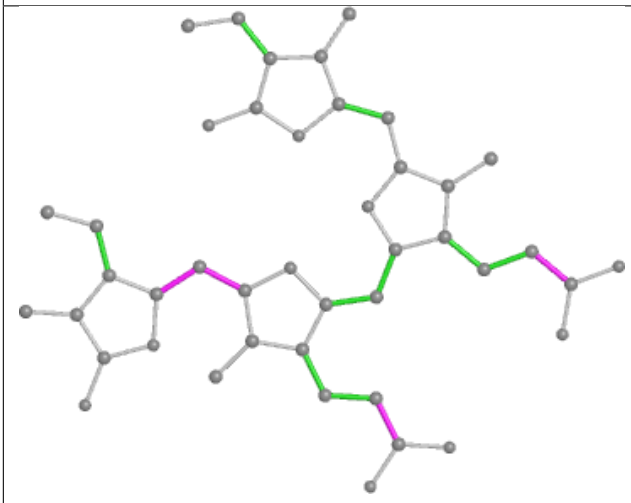

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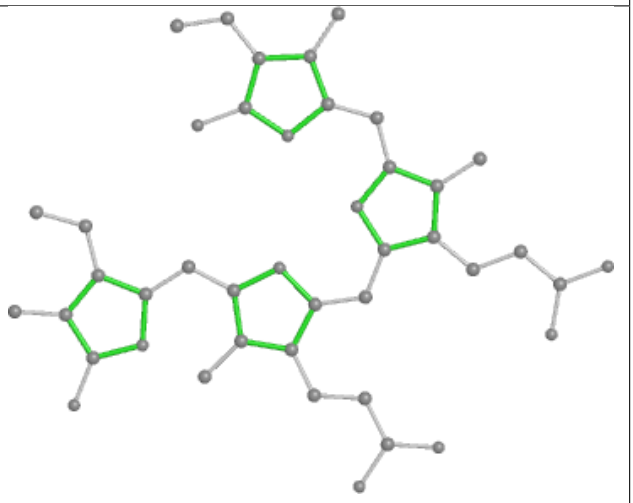

Rings

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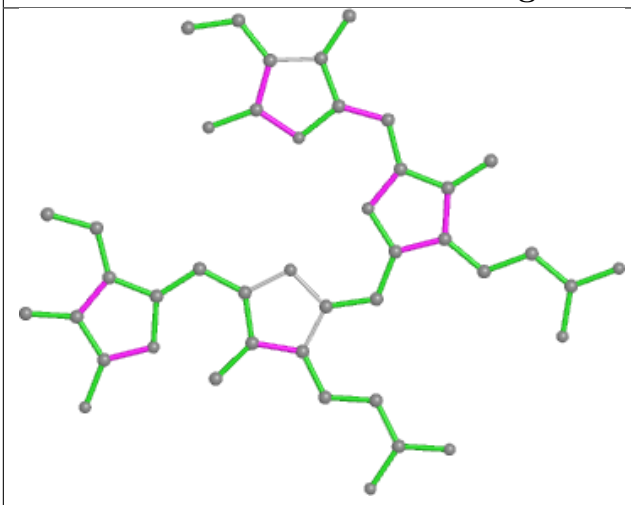

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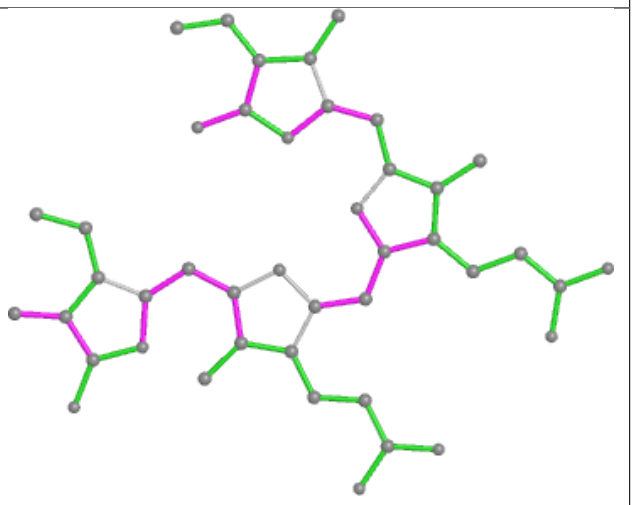

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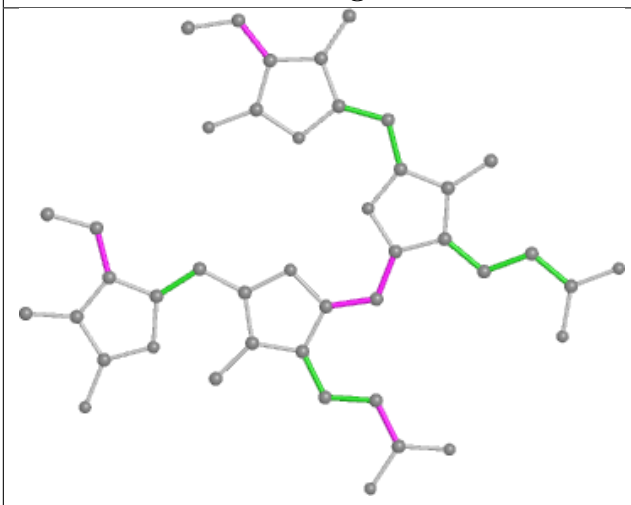

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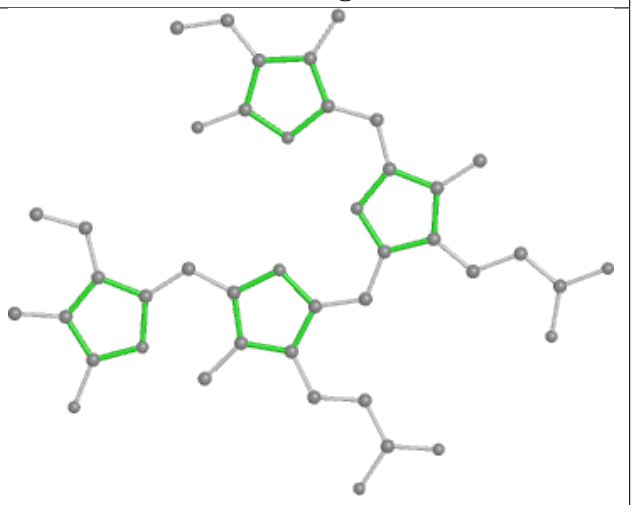

Rings

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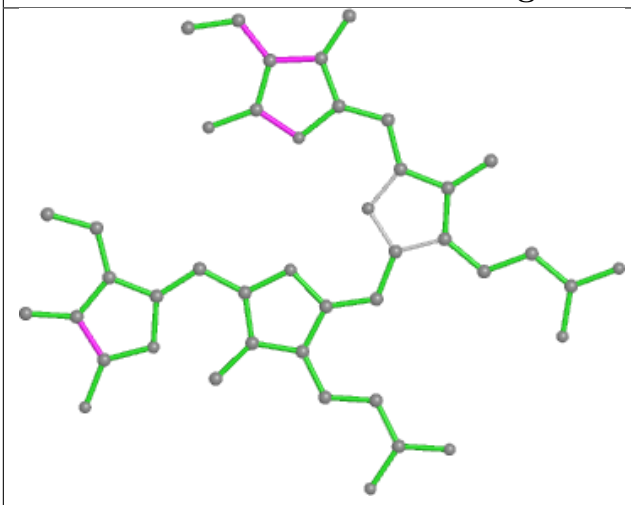

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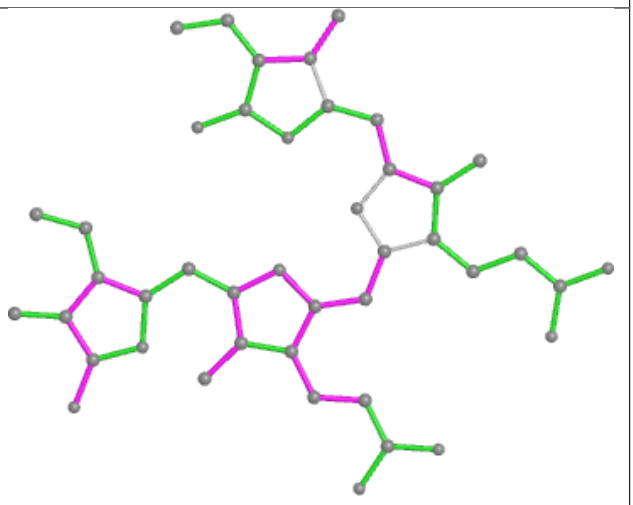

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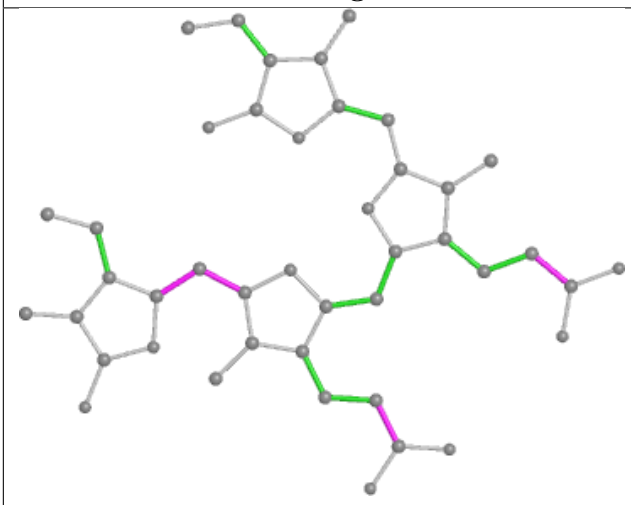

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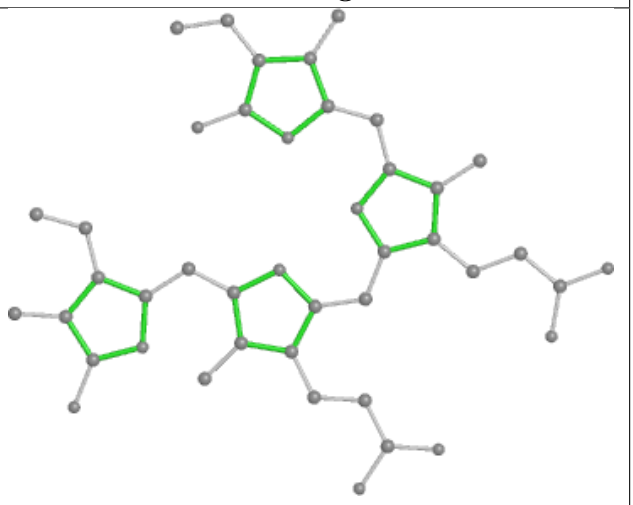

Rings

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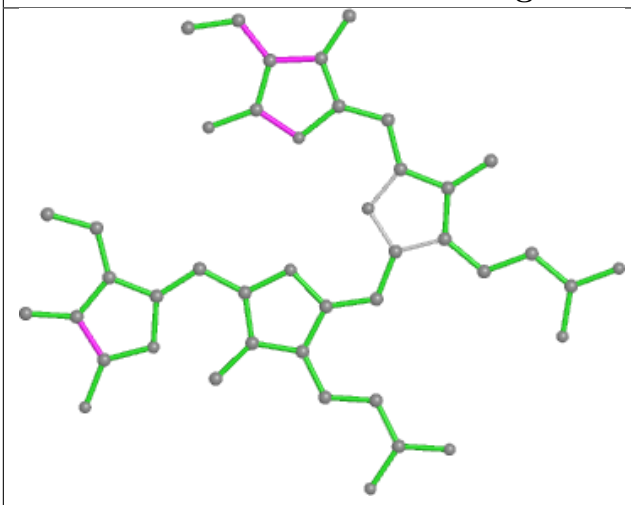

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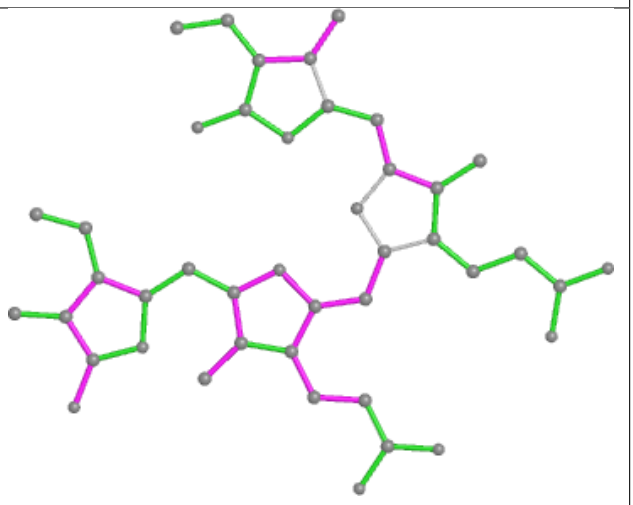

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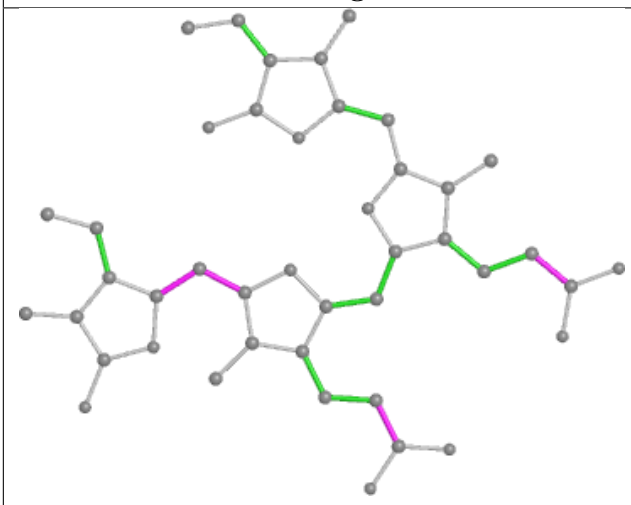

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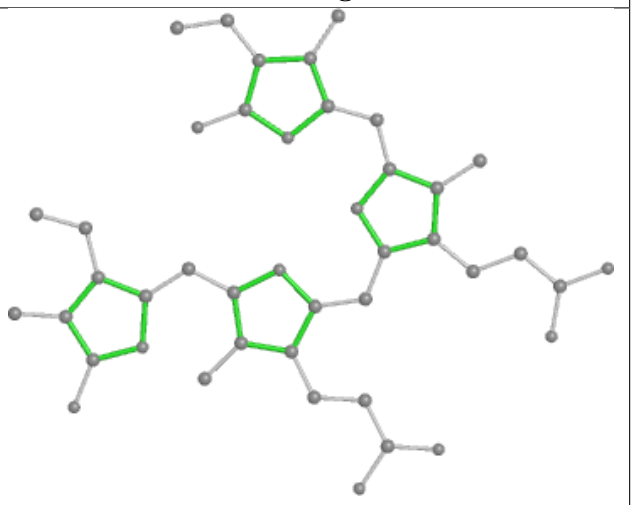
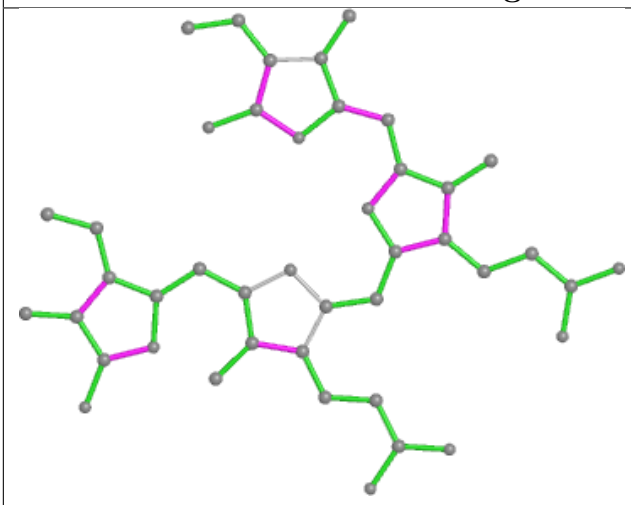


Rings

Ligand PUB kQ 1003



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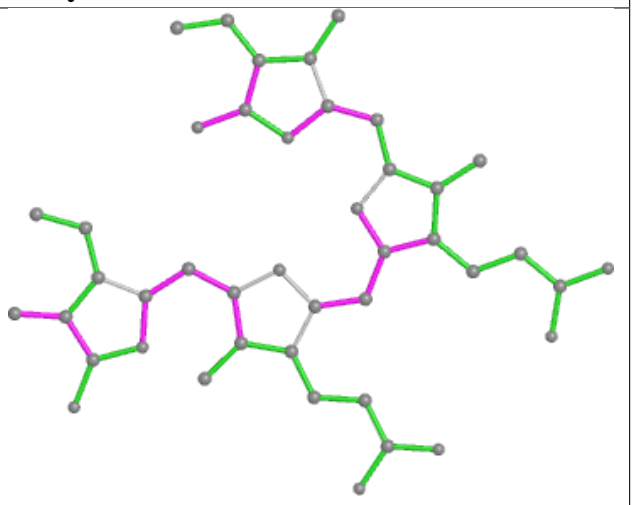

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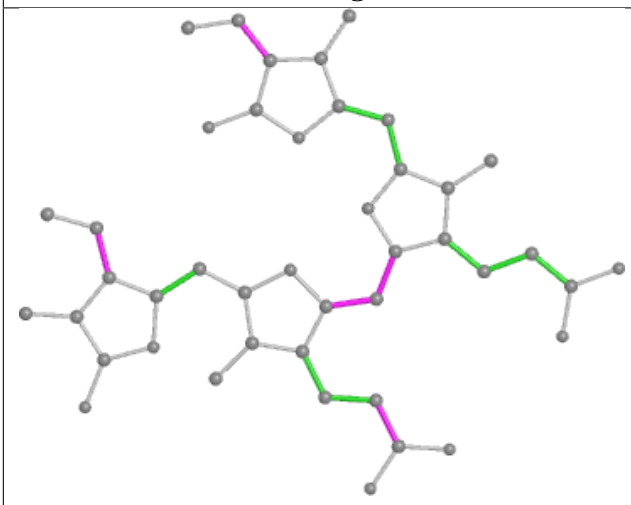

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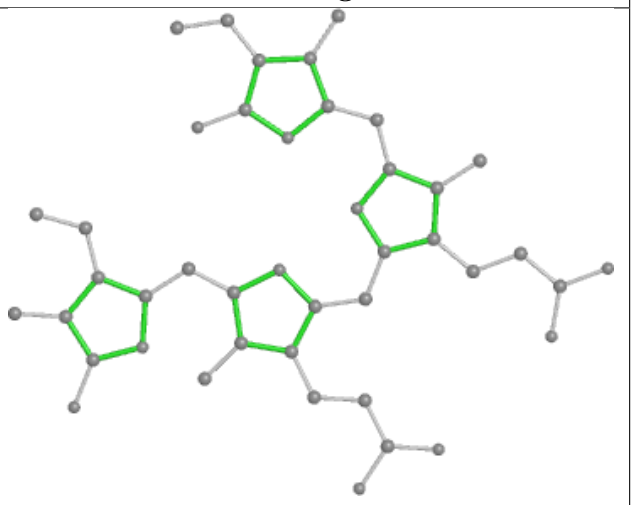

Rings

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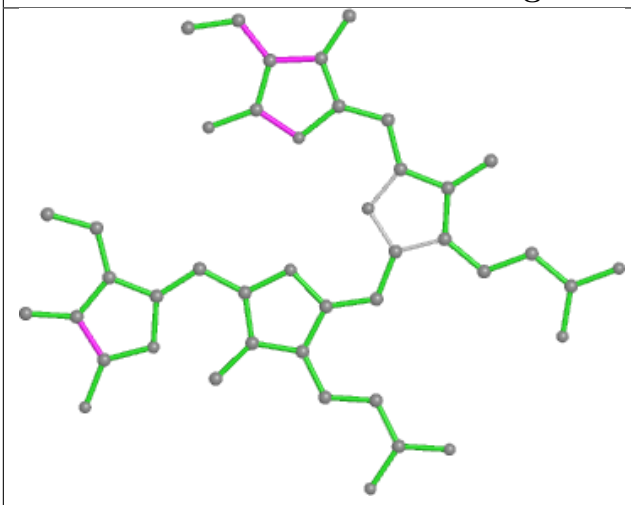

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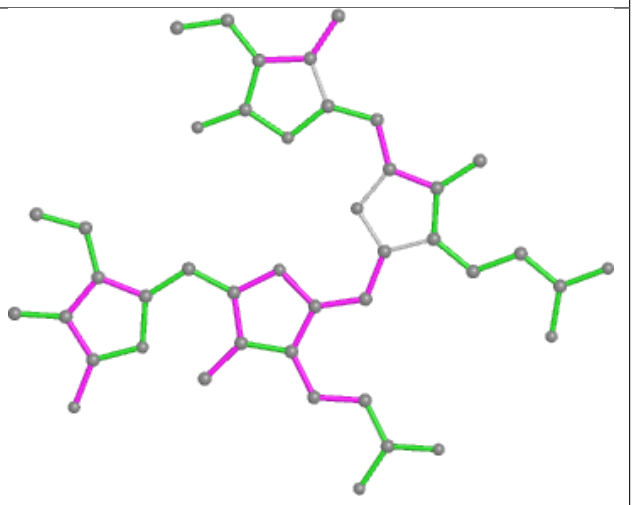

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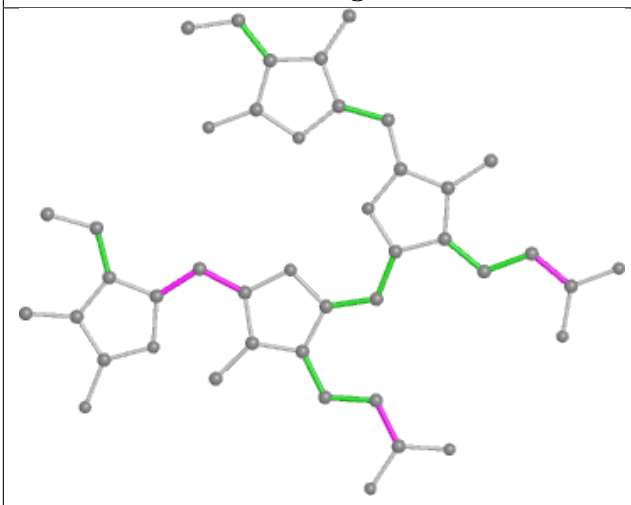

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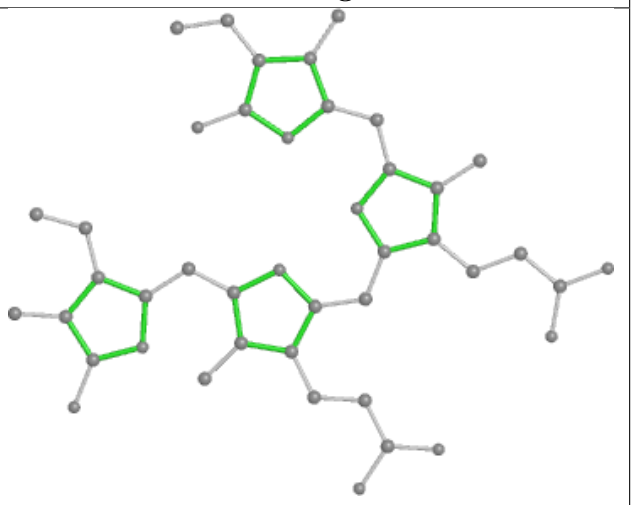
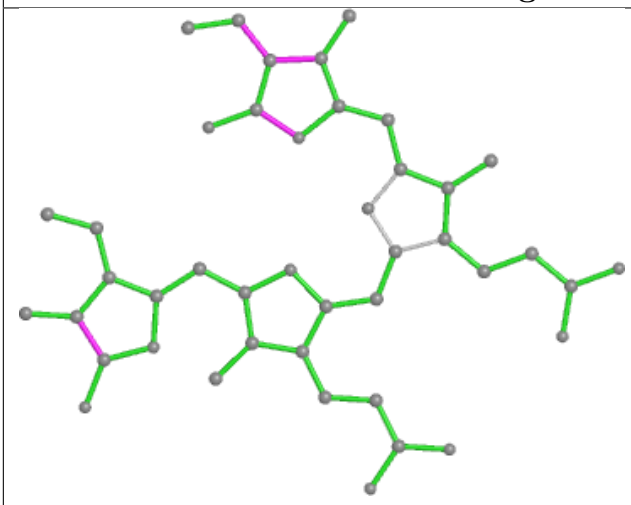


Rings

Ligand PEB cZ 201



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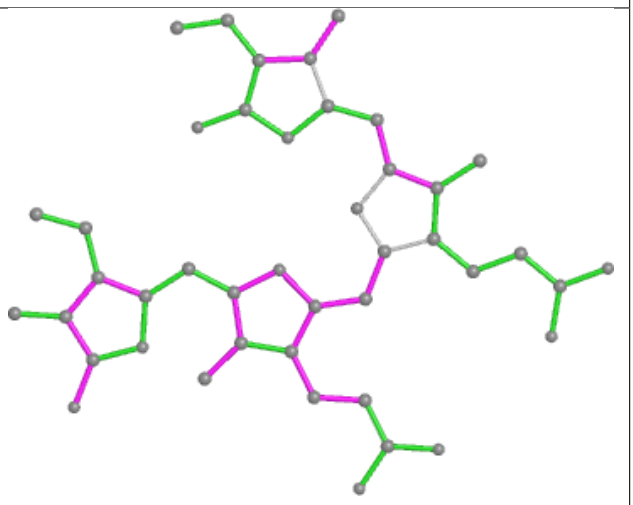

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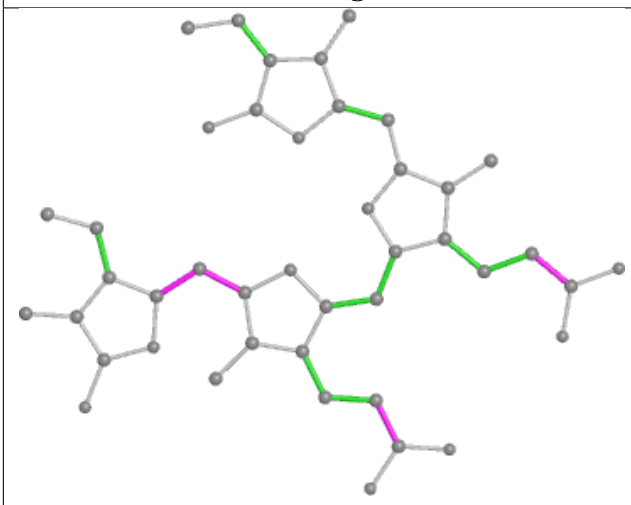

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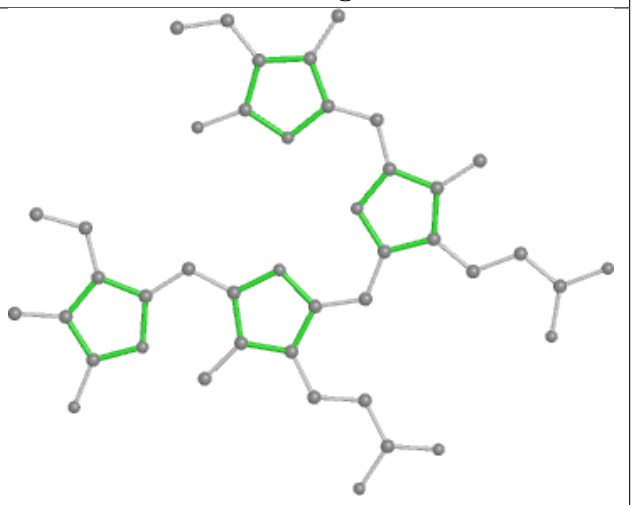
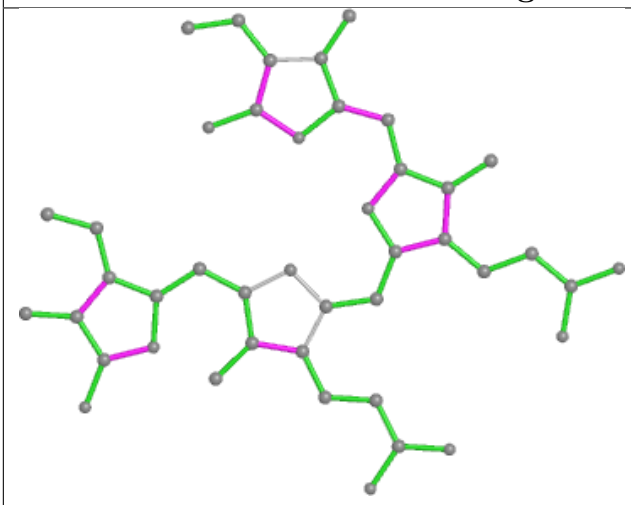


Rings

Ligand PUB J4 203



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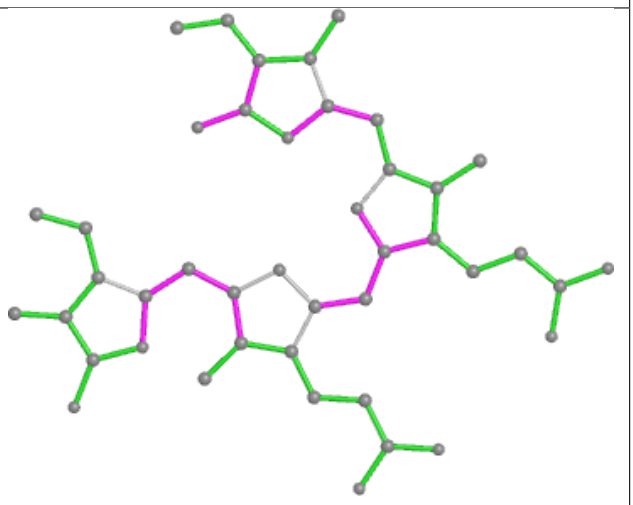

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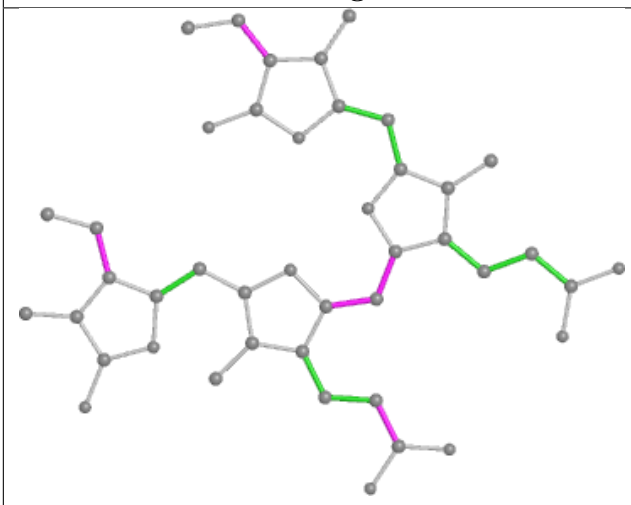

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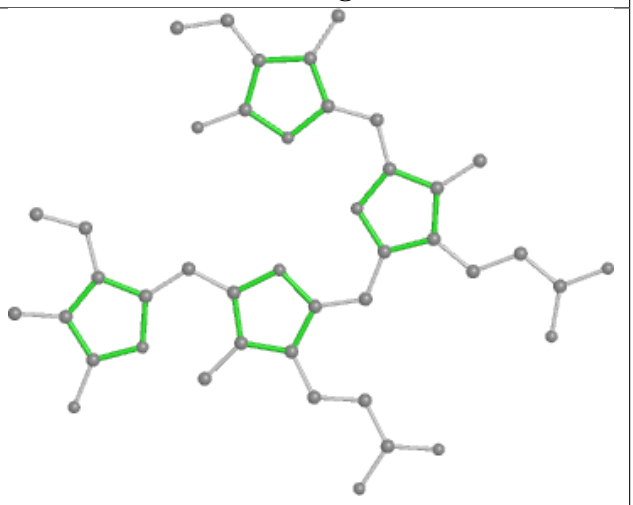

Rings

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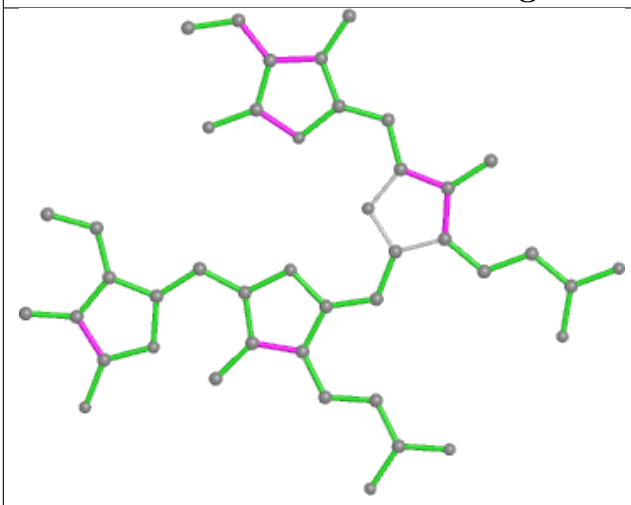

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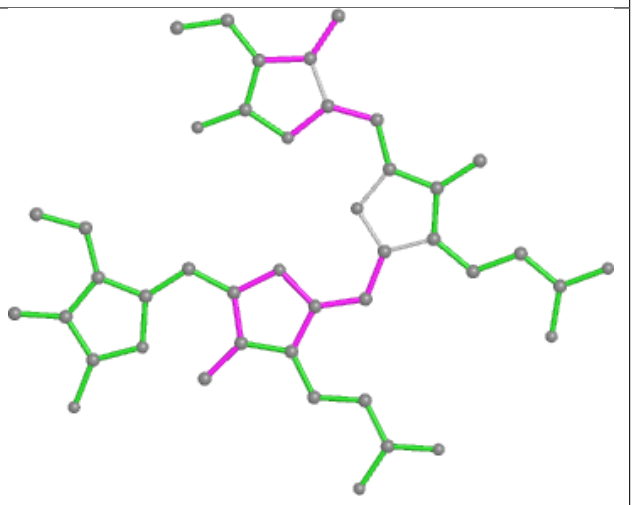

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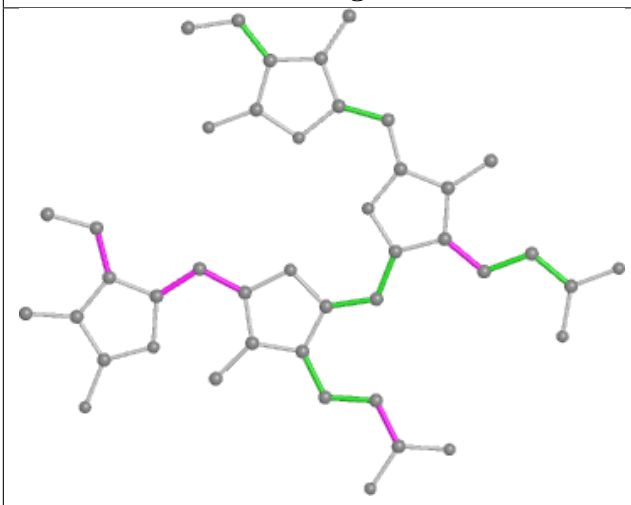

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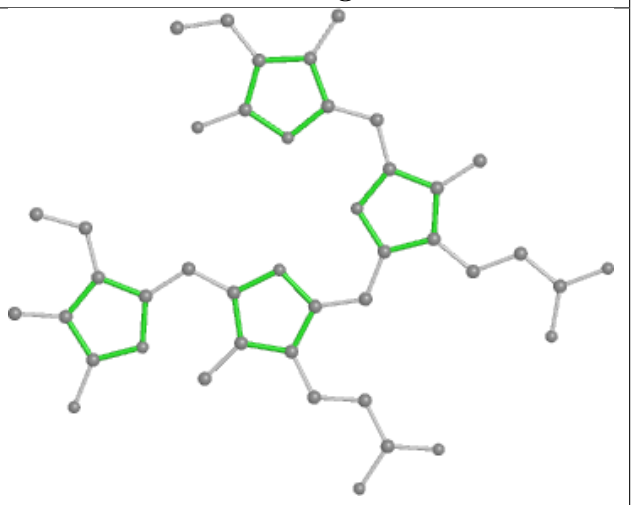
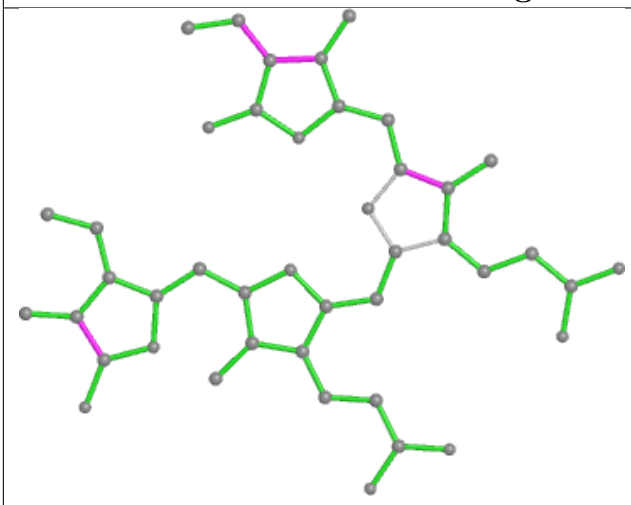


Rings

Ligand PEB K3 202



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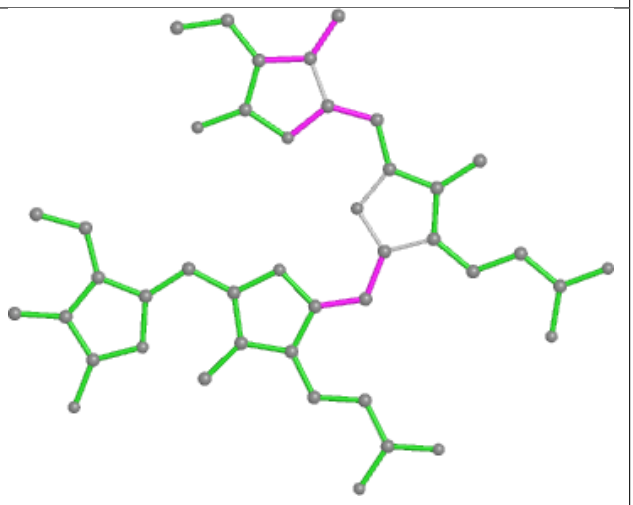
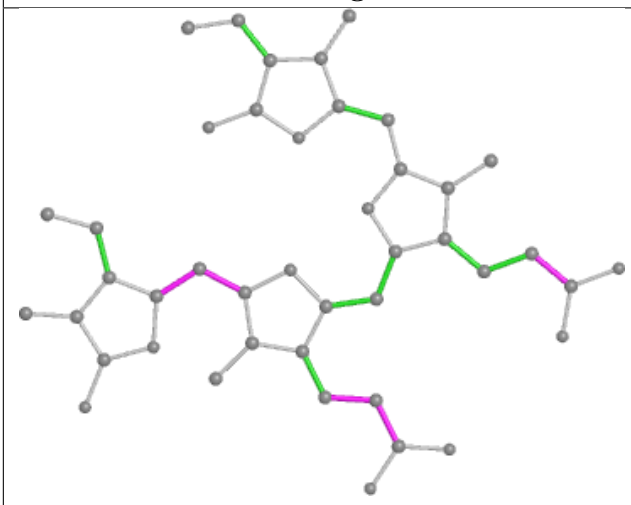
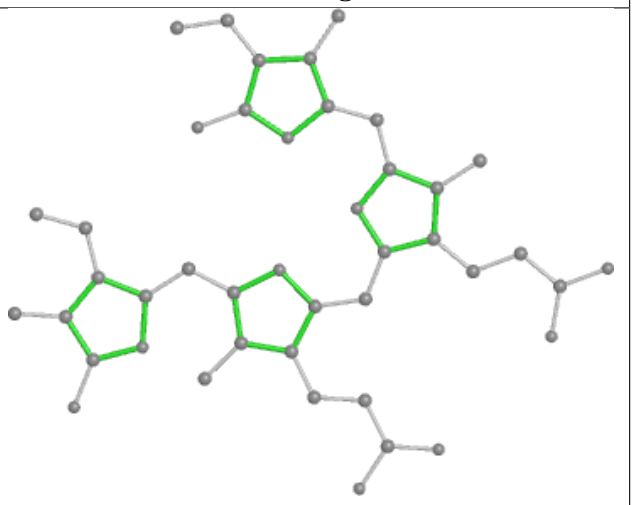


Bond angles

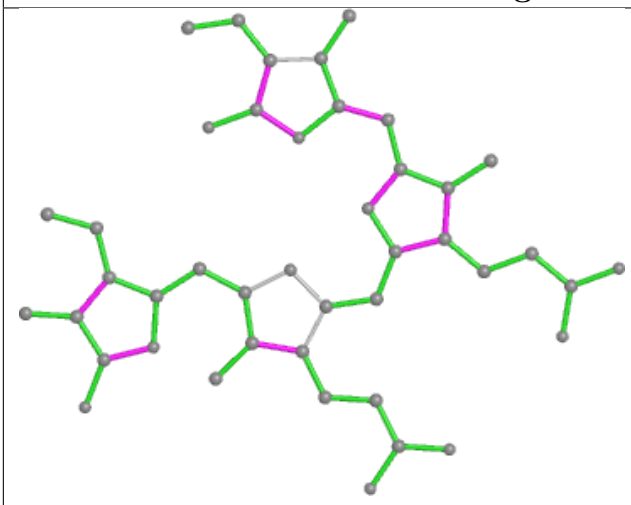


Torsions



Rings

Ligand PUB eY 404



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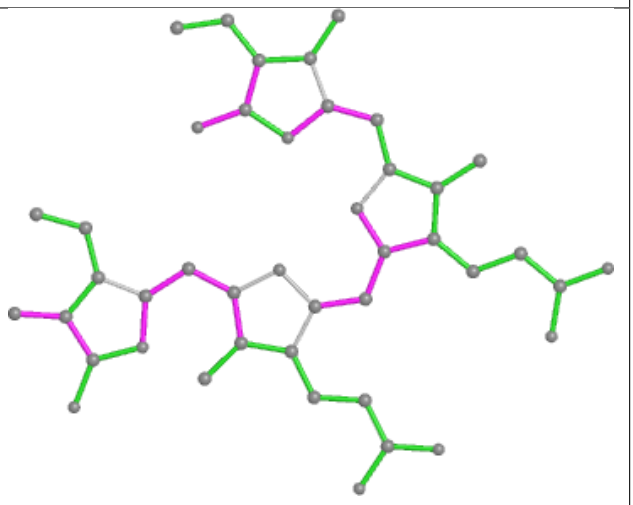
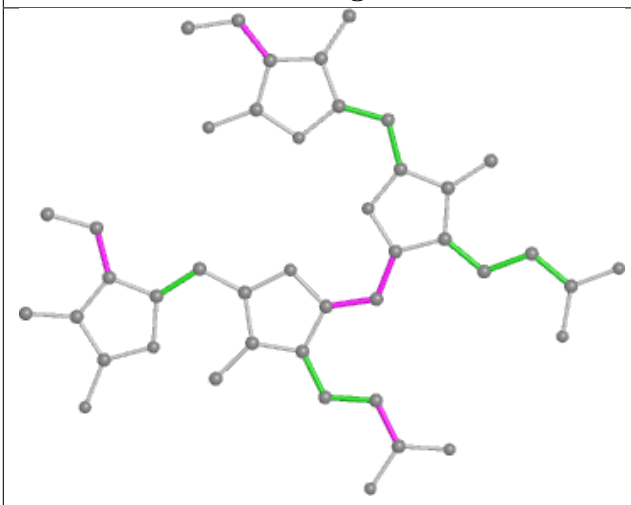
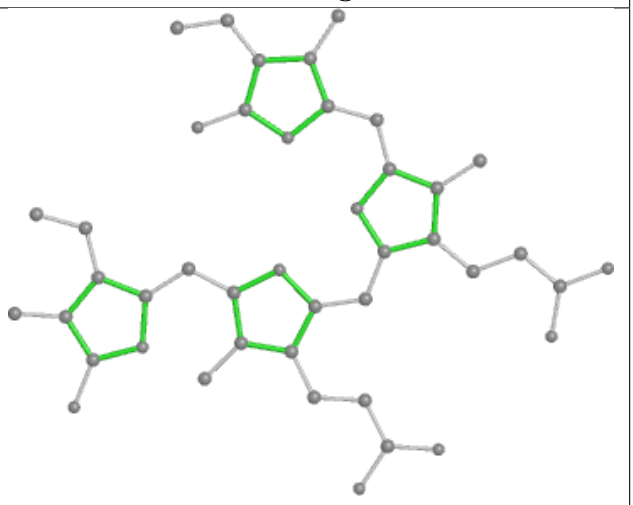


Bond angles

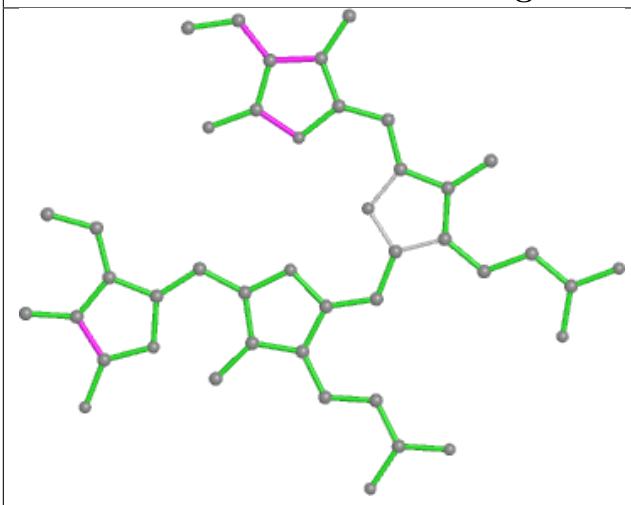


Torsions



Rings

Ligand PEB V6 201



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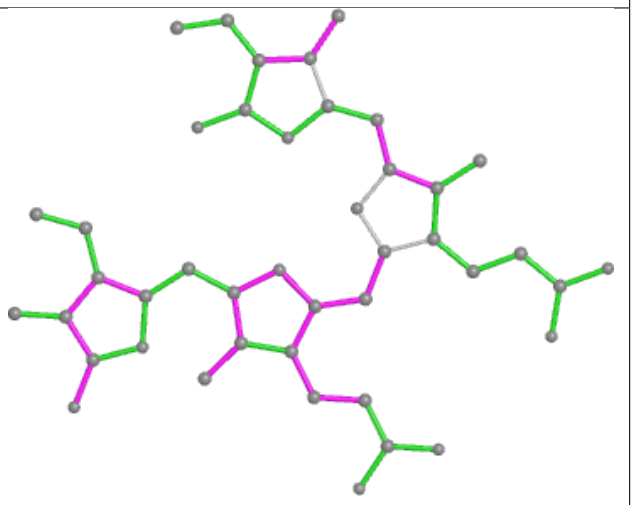
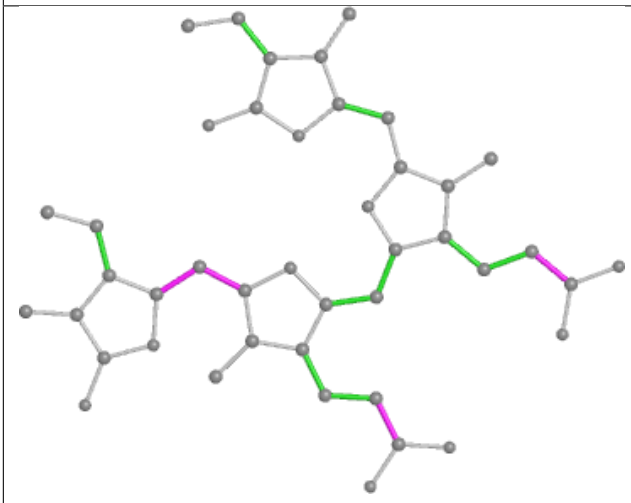


Bond angles



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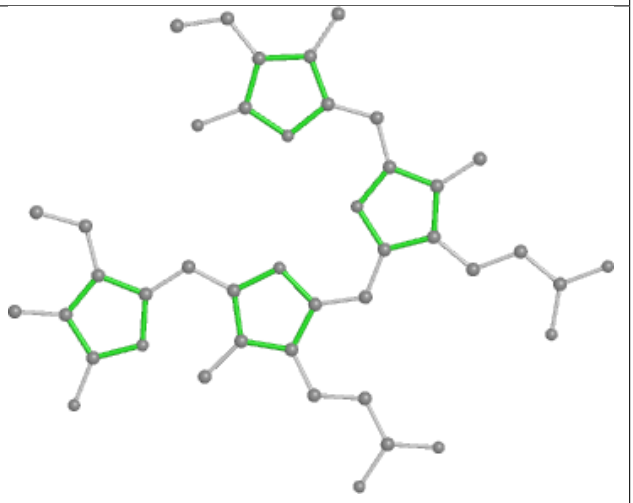
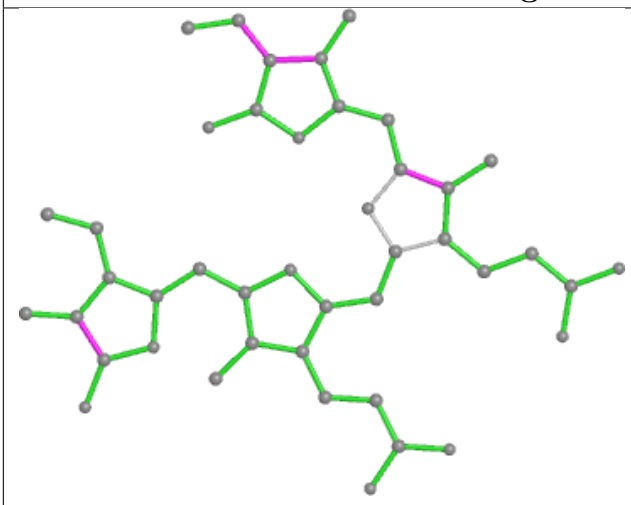


Rings

Ligand PEB c4 201



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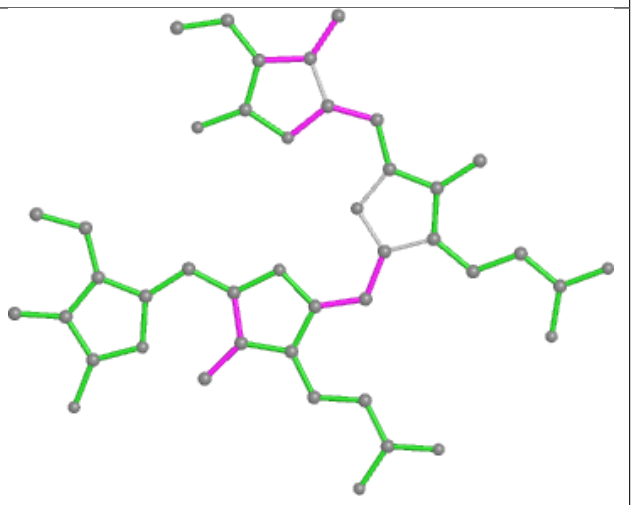
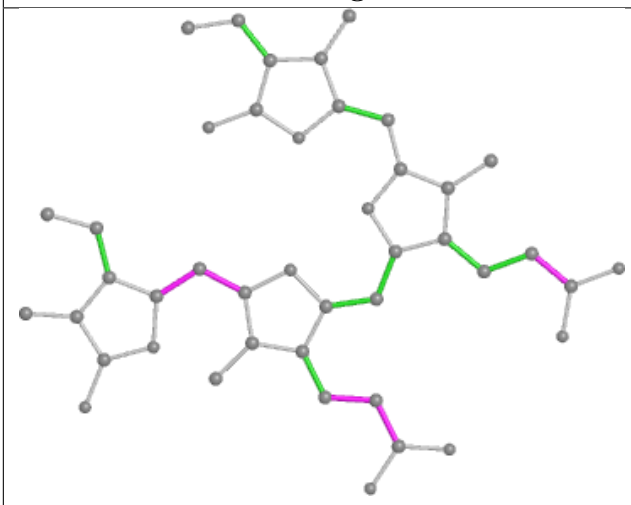


Bond angles



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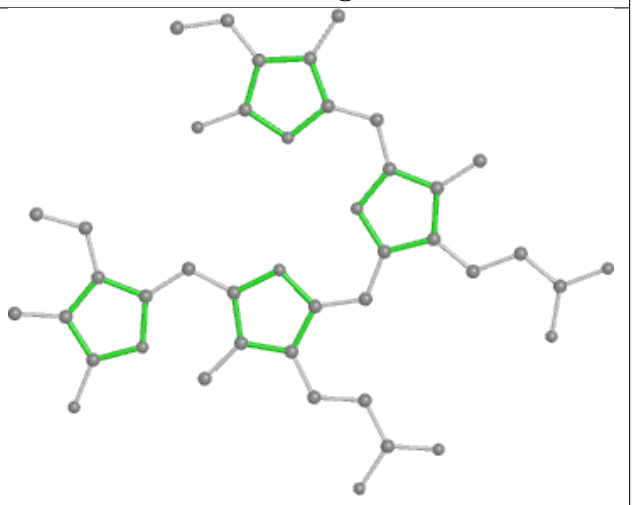
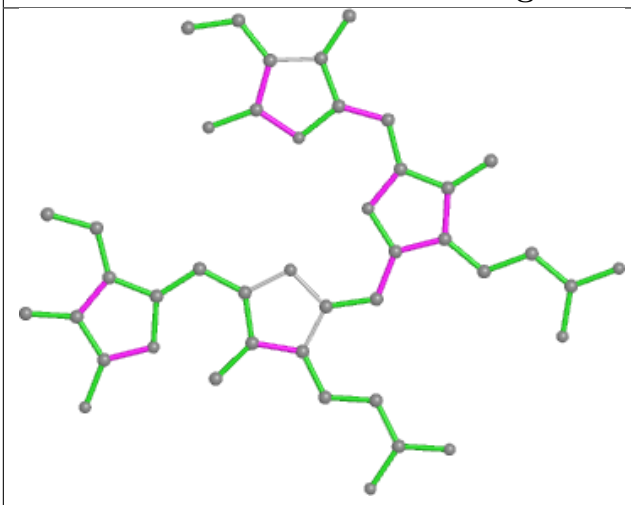


Rings

Ligand PUB eZ 403



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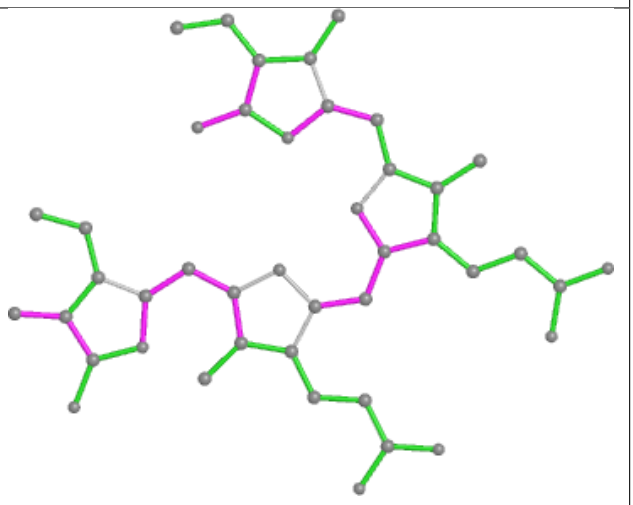
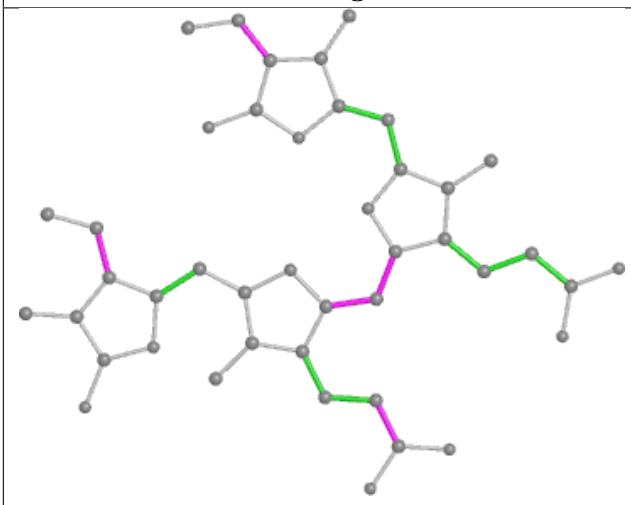


Bond angles



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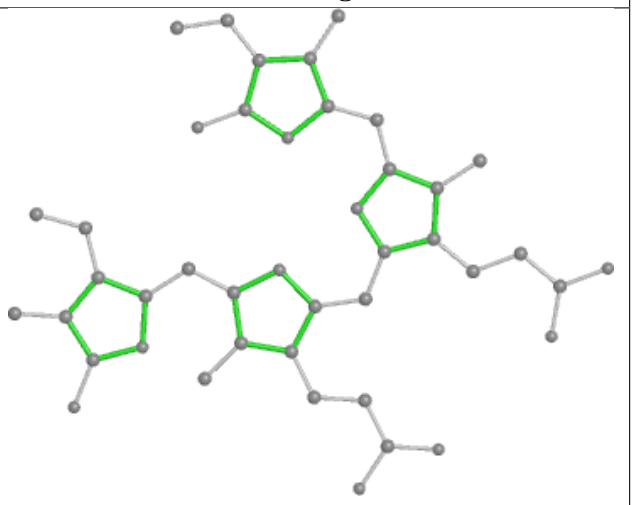
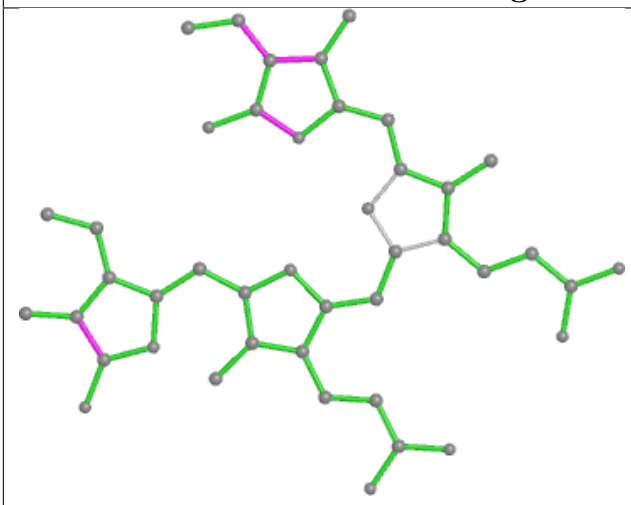


Rings

Ligand PEB W8 202



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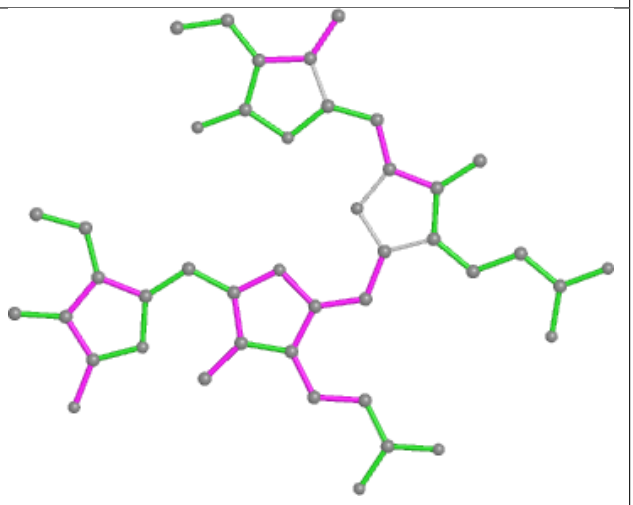

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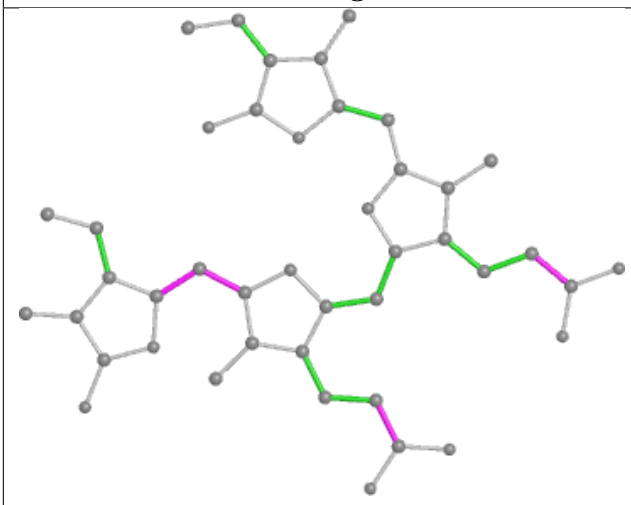

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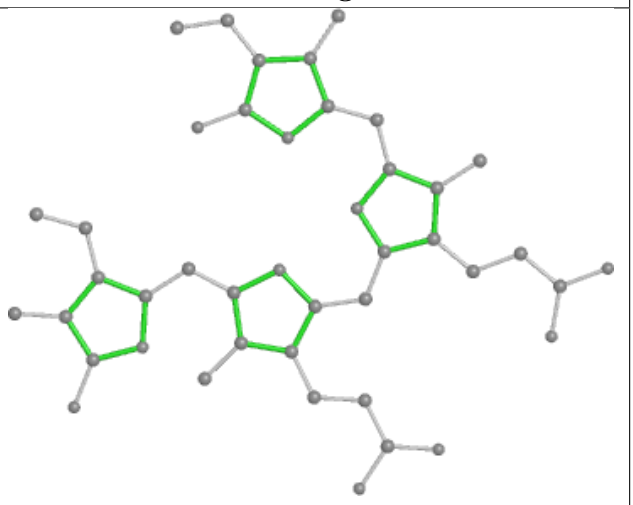
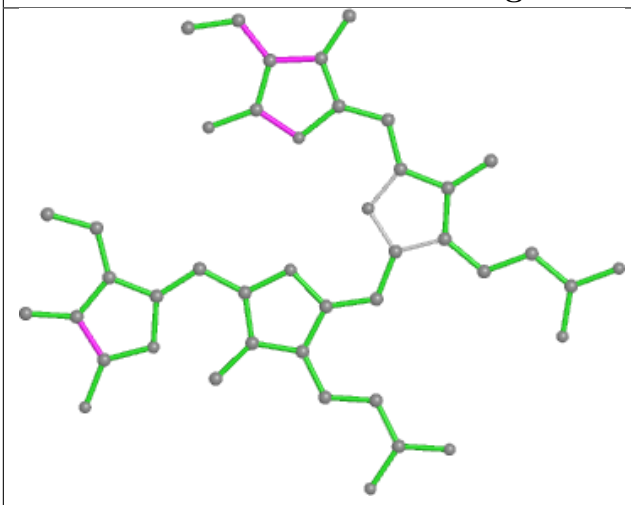


Rings

Ligand PEB bY 1001



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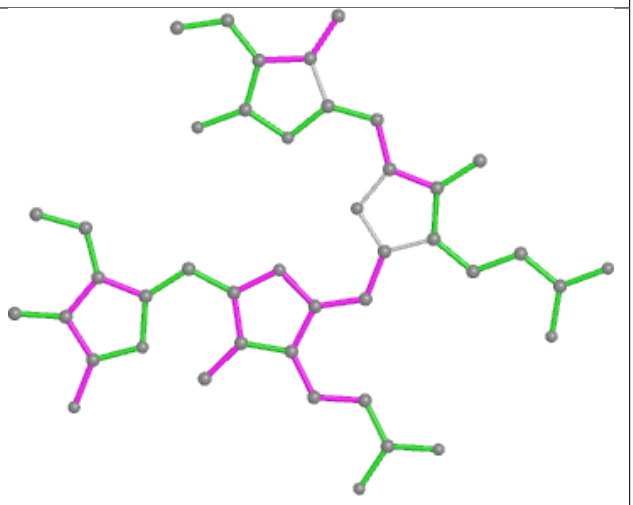
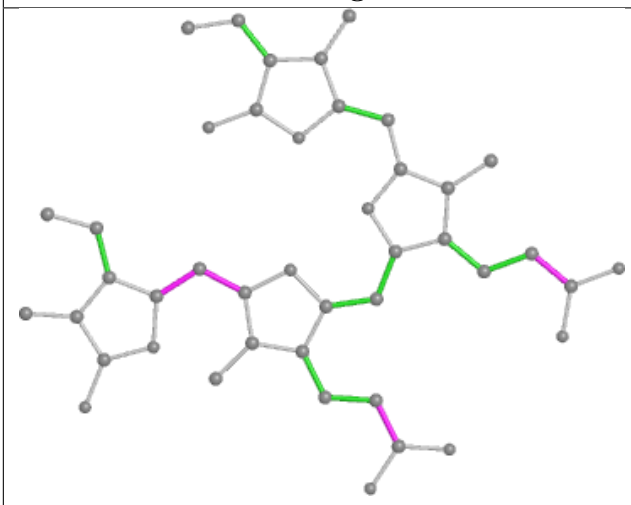


Bond angles



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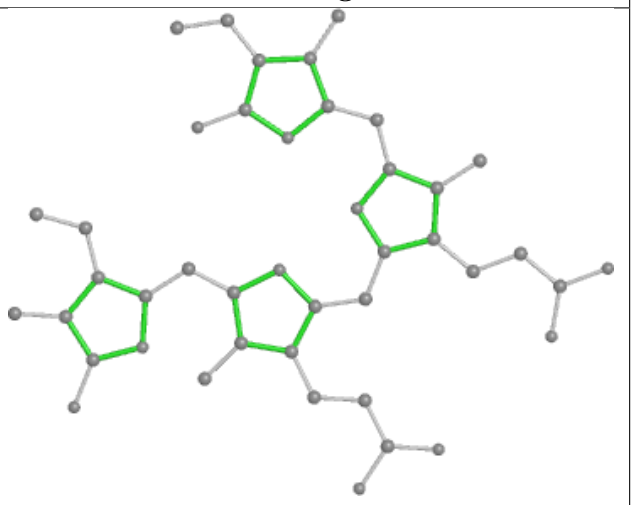

Rings

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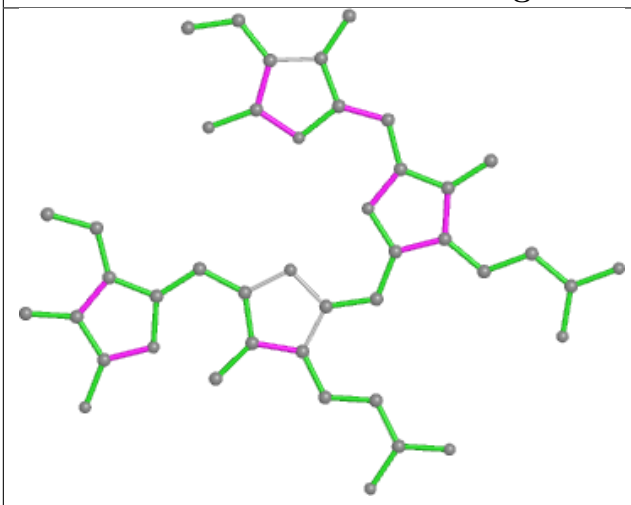

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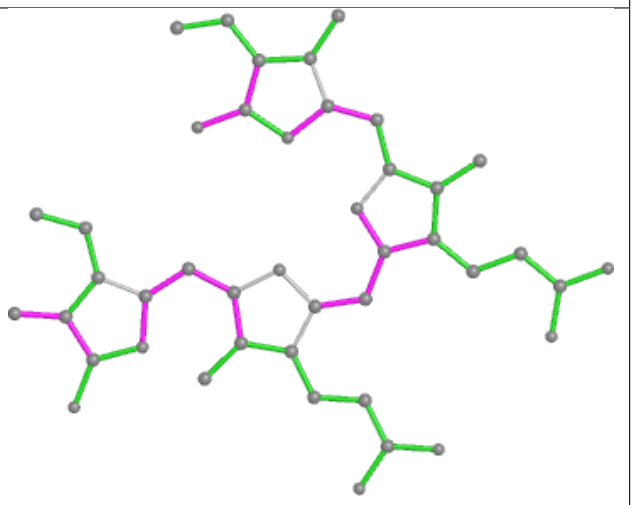

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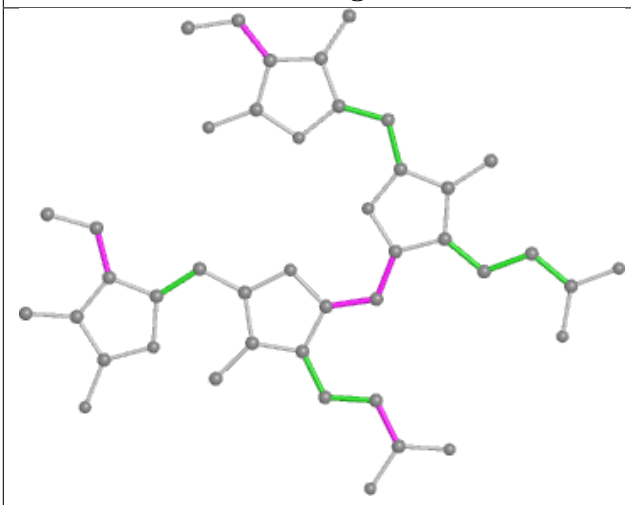

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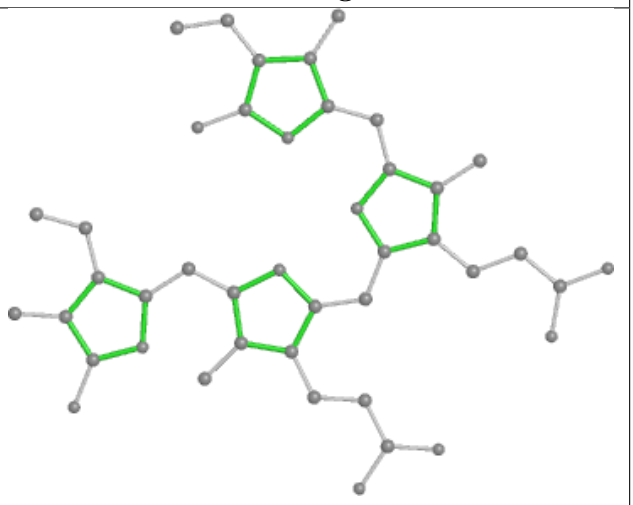
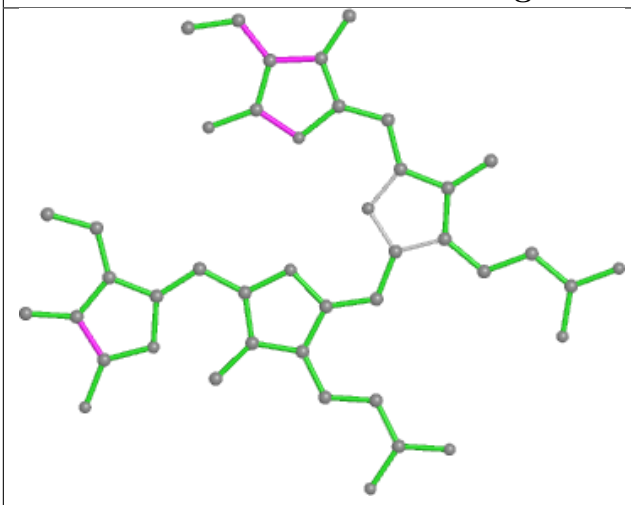


Rings

Ligand PEB hX 201



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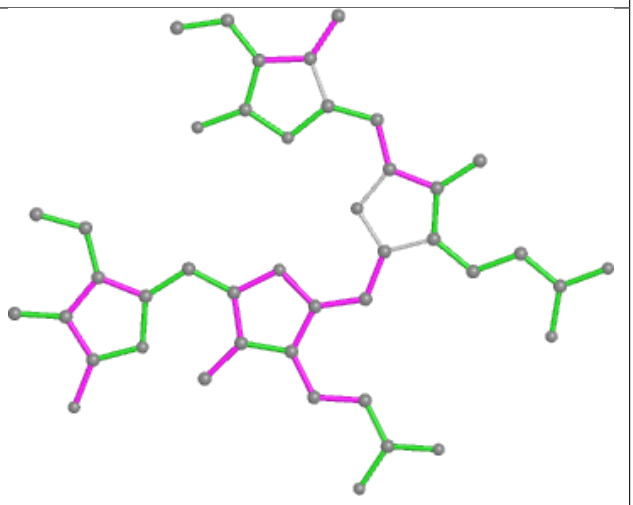
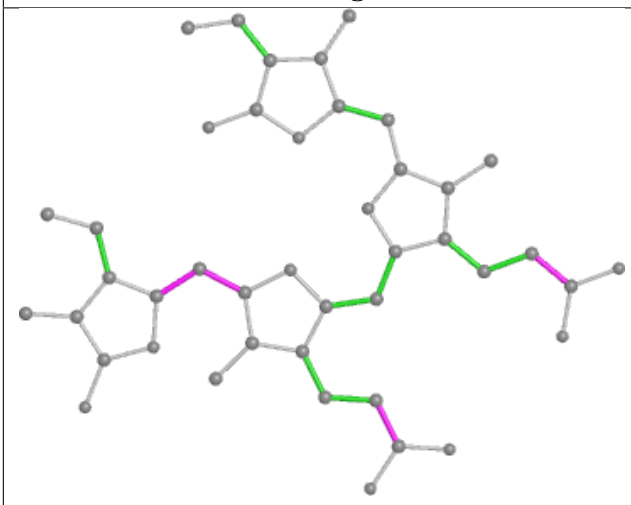
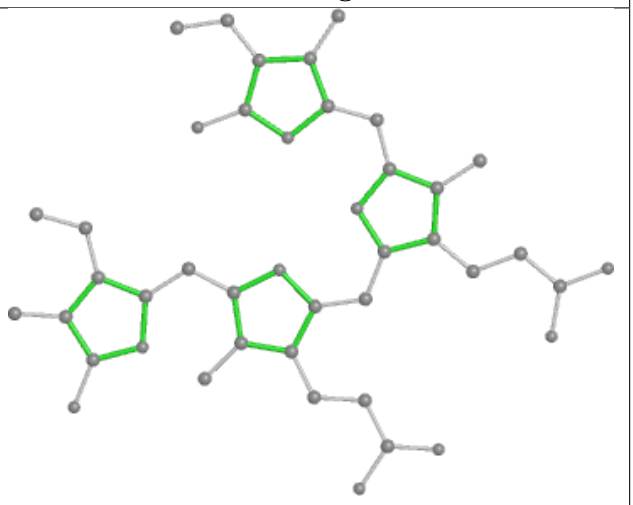


Bond angles

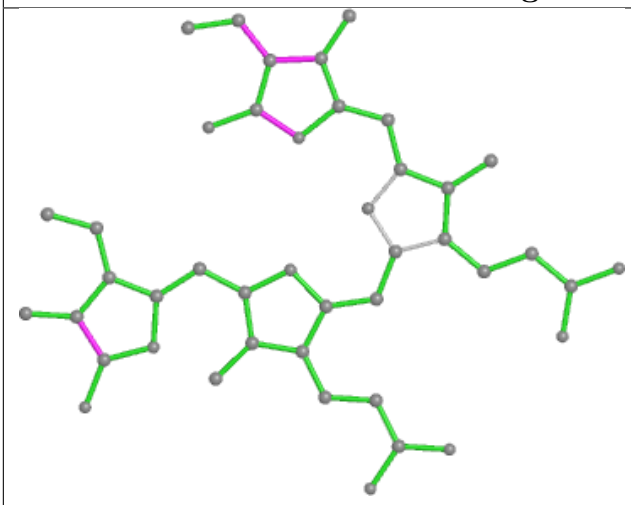


Torsions



Rings

Ligand PEB r5 201



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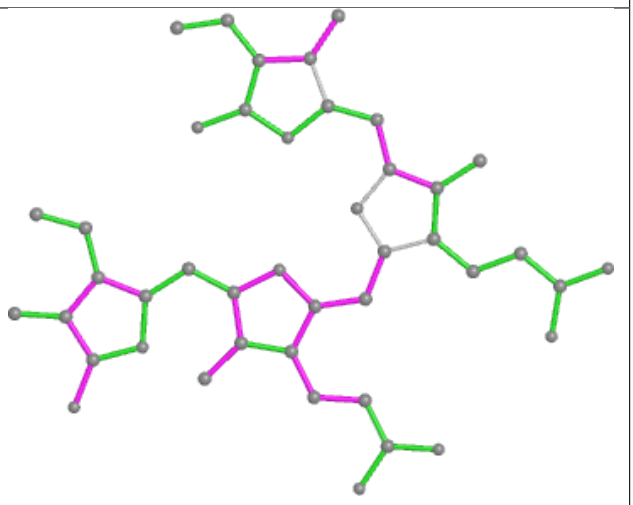
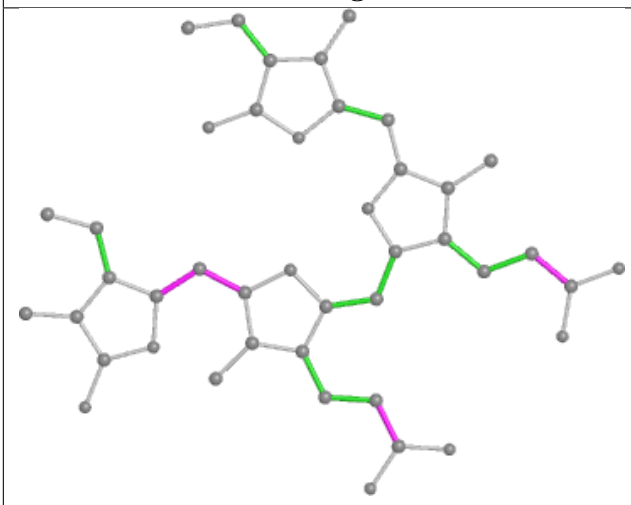


Bond angles



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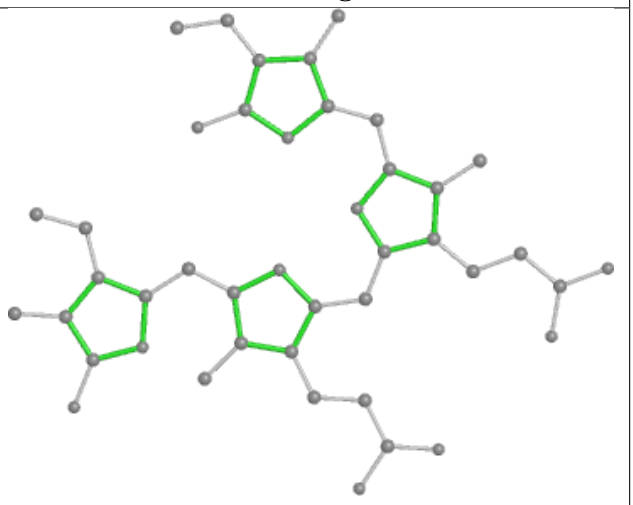
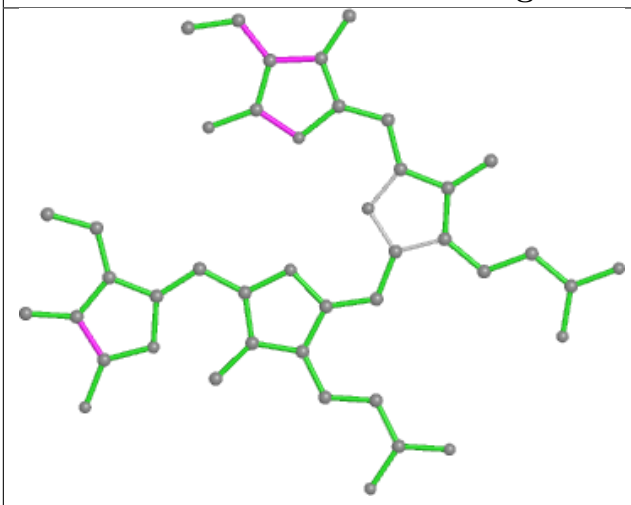


Rings

Ligand PEB bF 201



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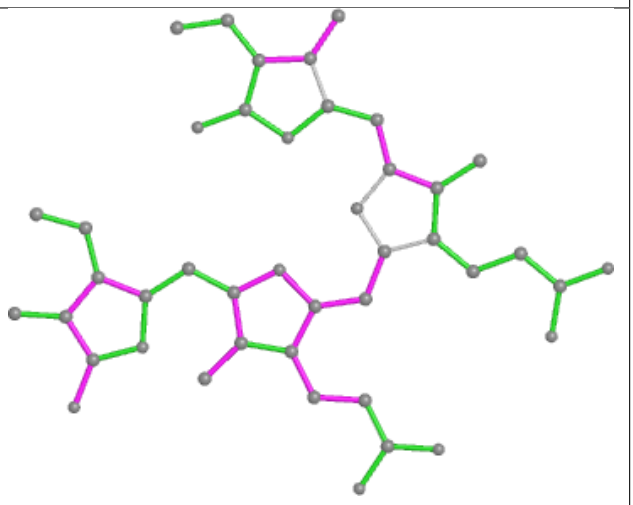
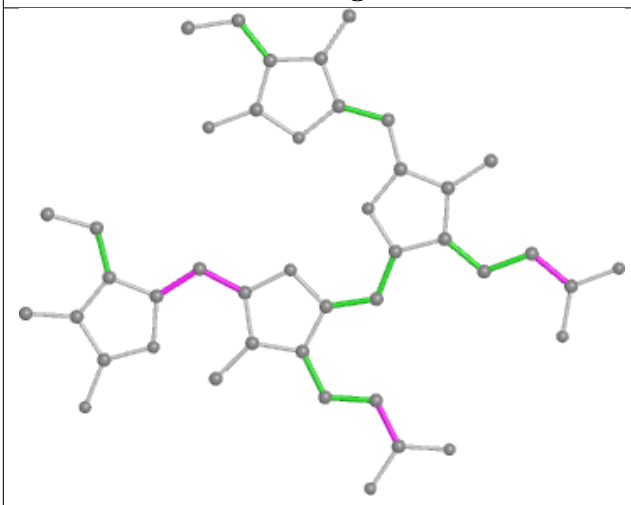


Bond angles



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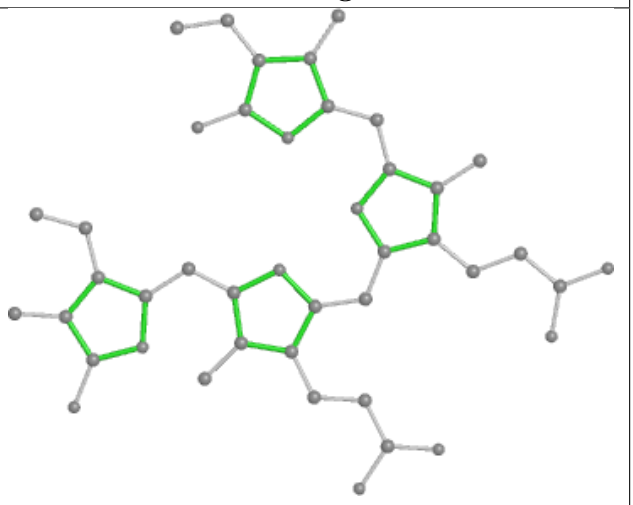
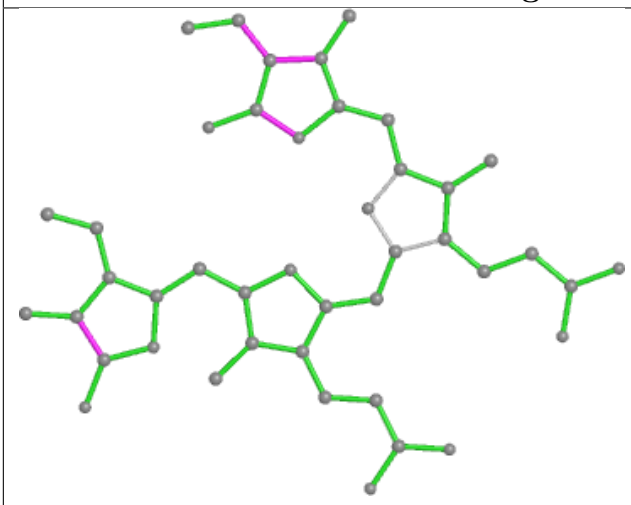


Rings

Ligand PEB I3 201



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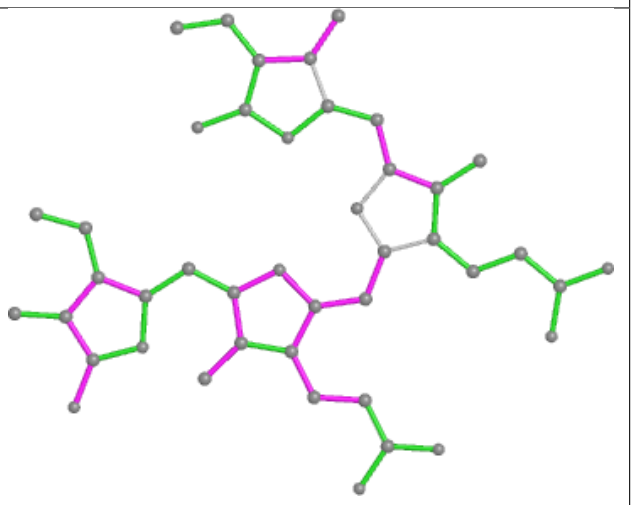

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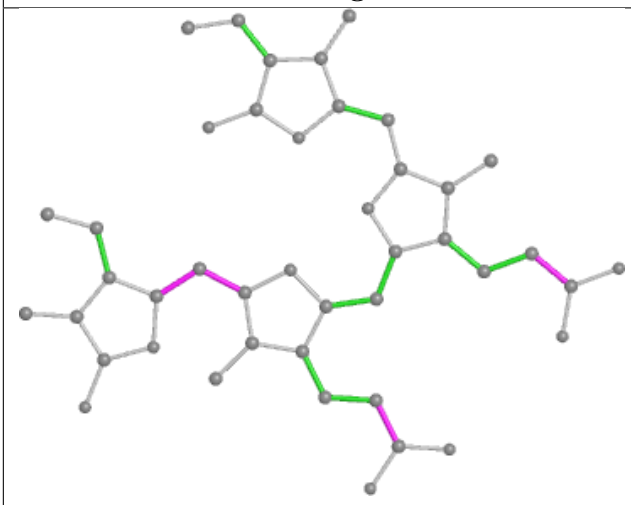
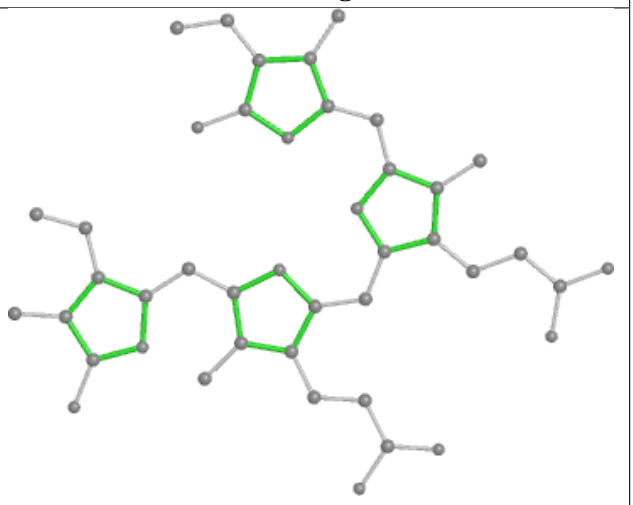
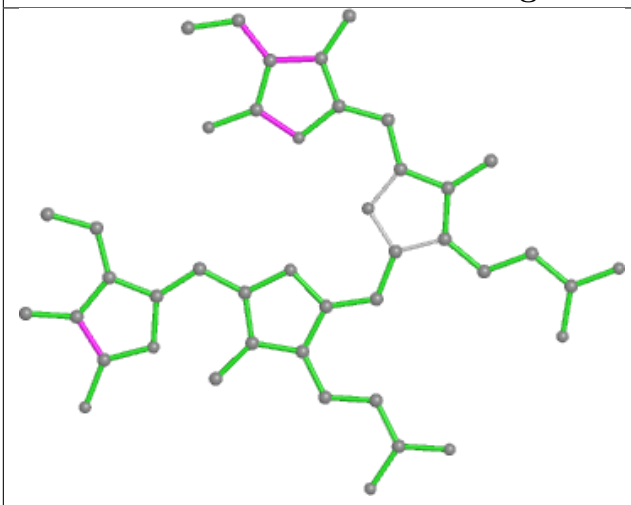


Torsions



Rings

Ligand PEB dz 402



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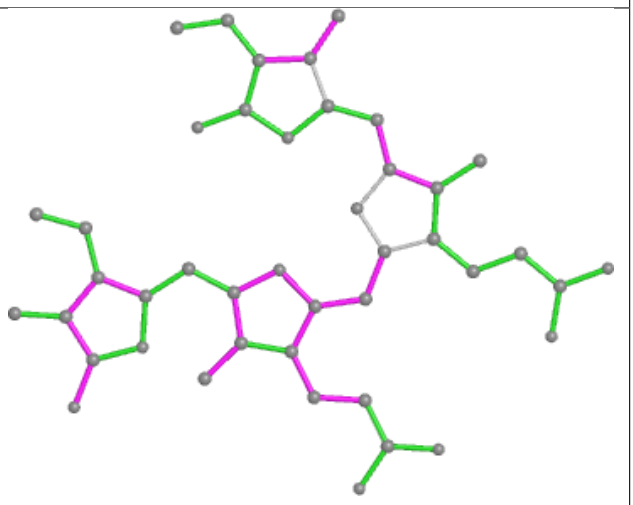
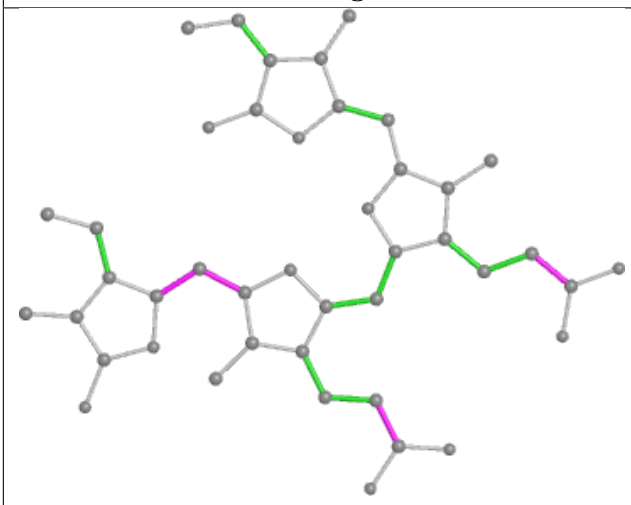


Bond angles



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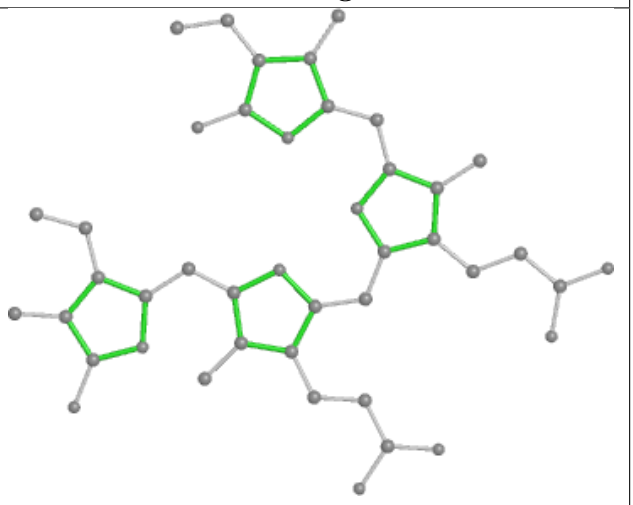
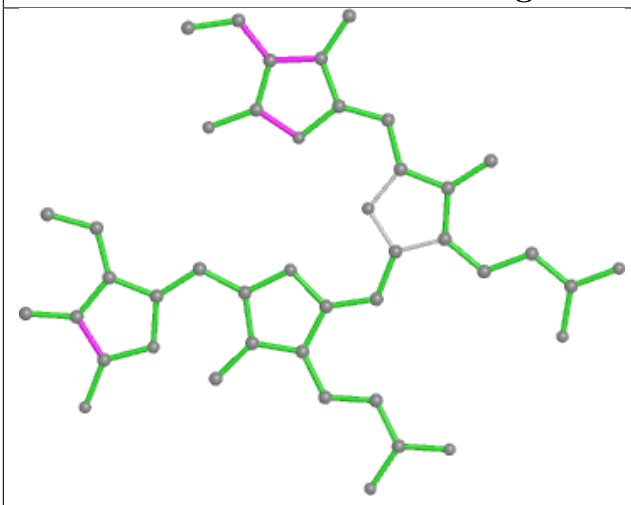


Rings

Ligand PEB R4 201



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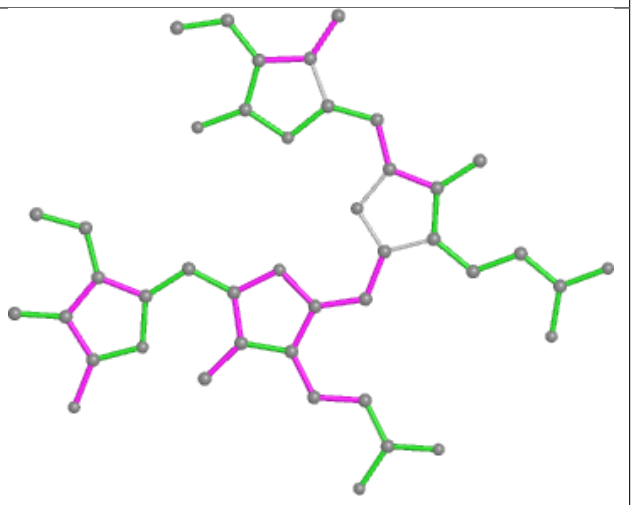
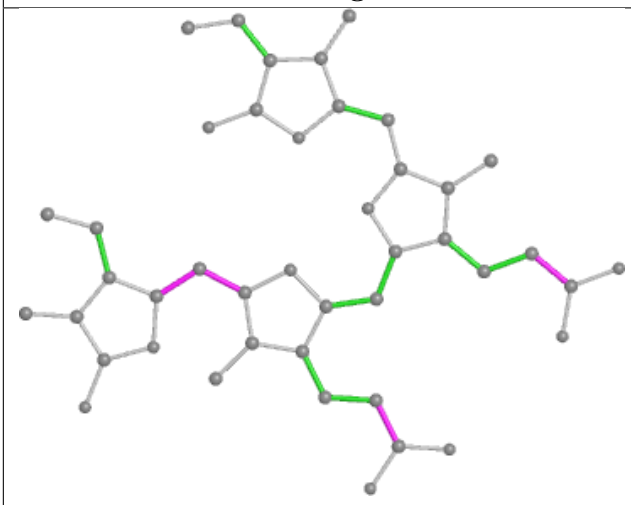
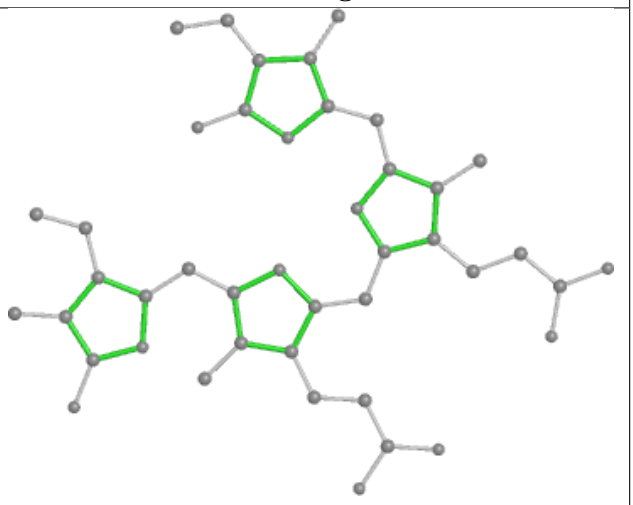


Bond angles

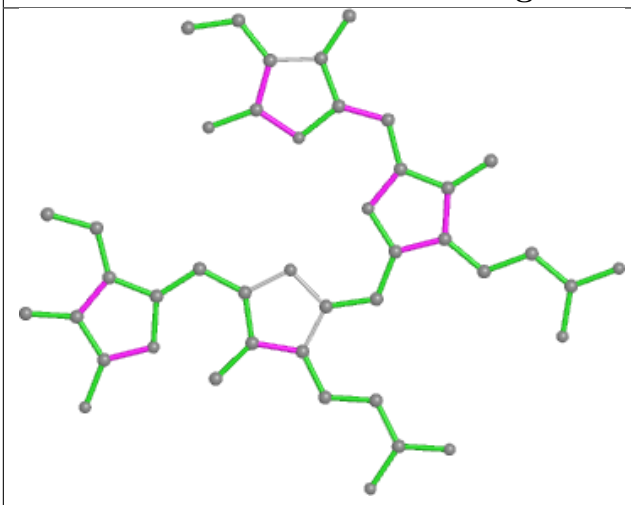


Torsions



Rings

Ligand PUB bp 202



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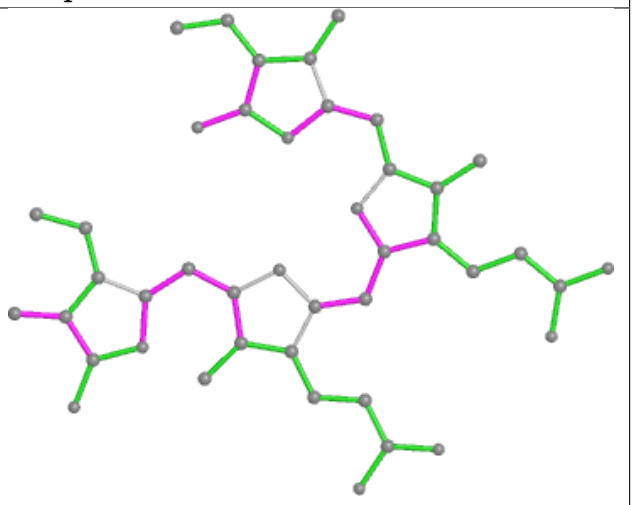
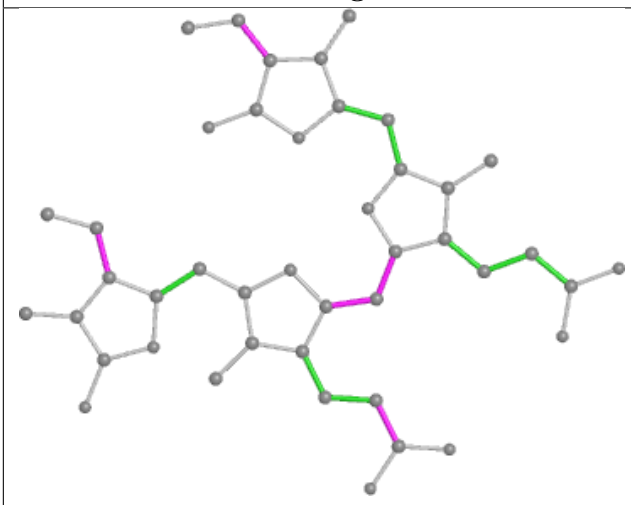


Bond angles



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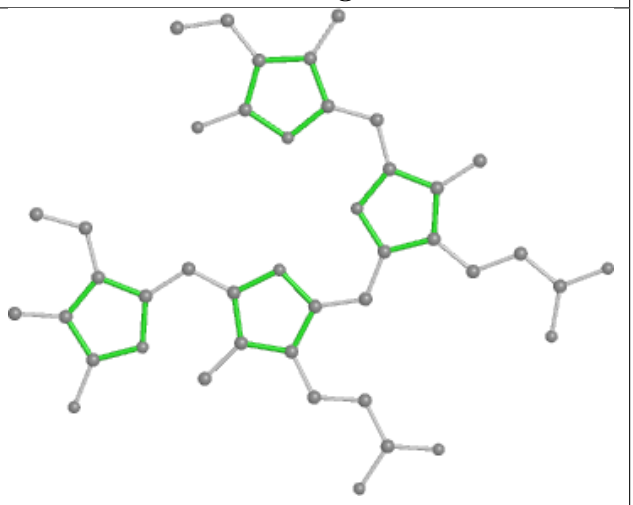
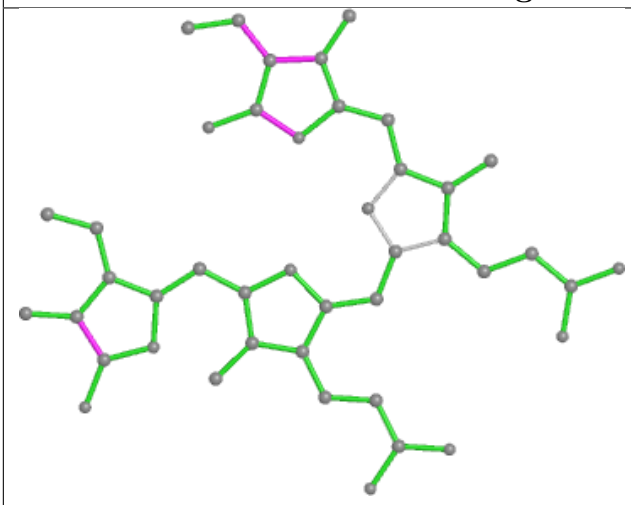


Rings

Ligand PEB Q8 201



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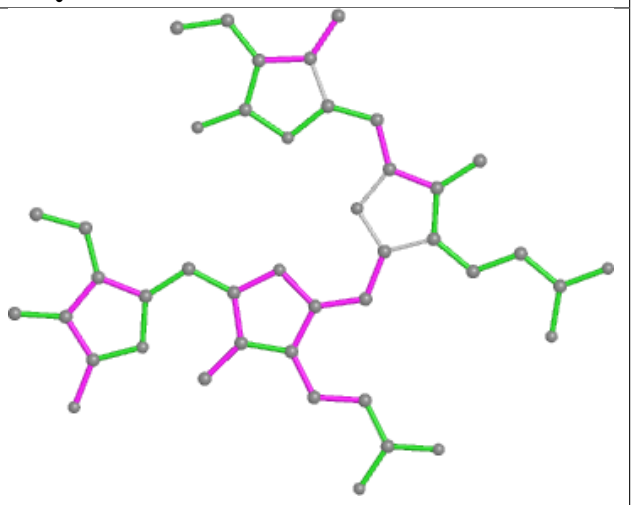

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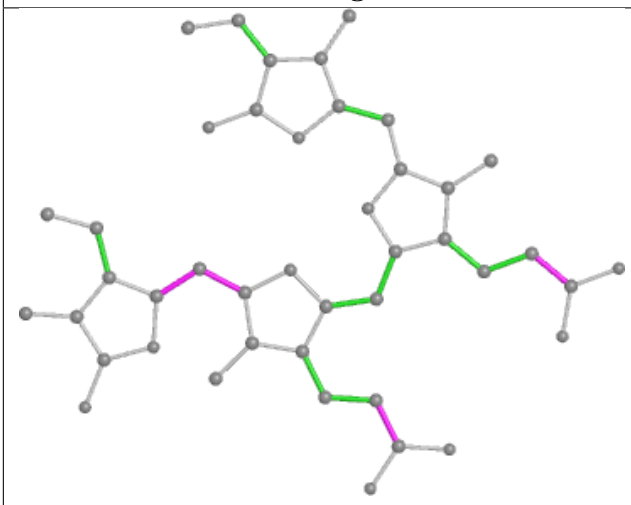

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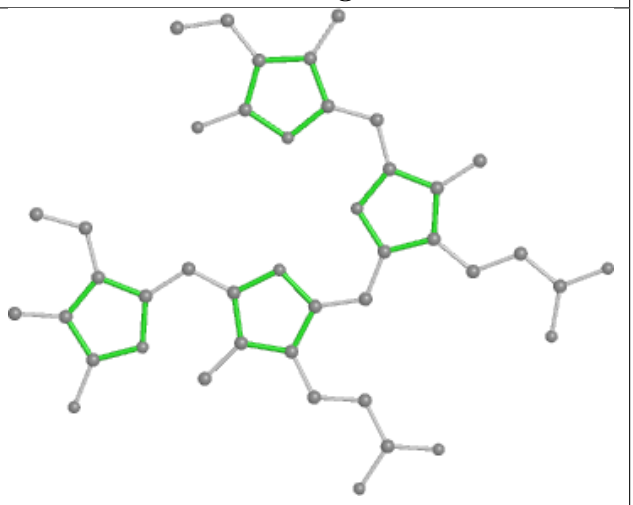
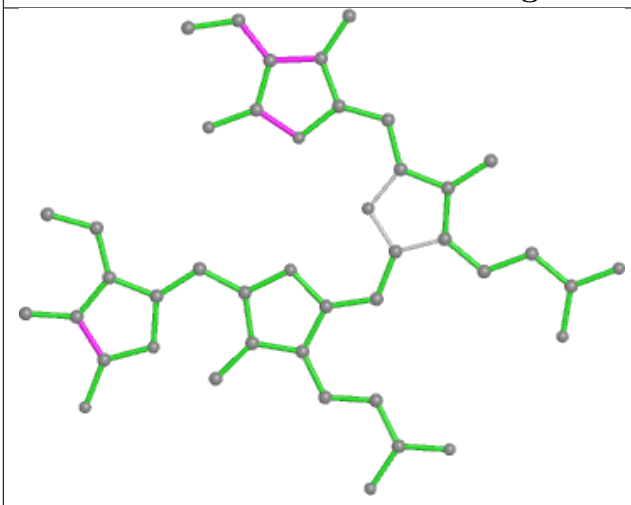


Rings

Ligand PEB bI 201



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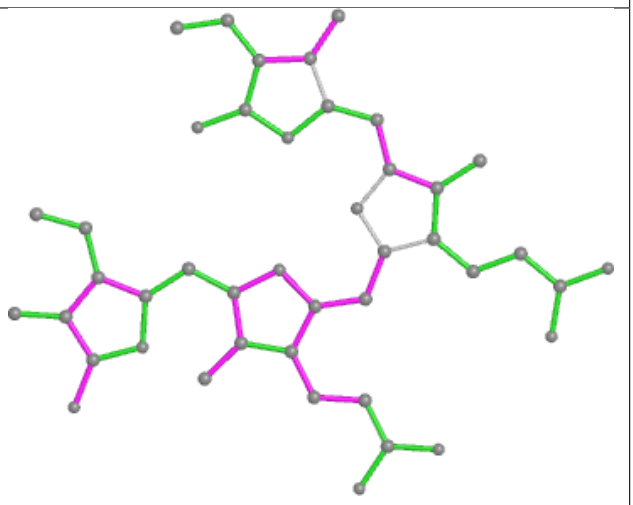

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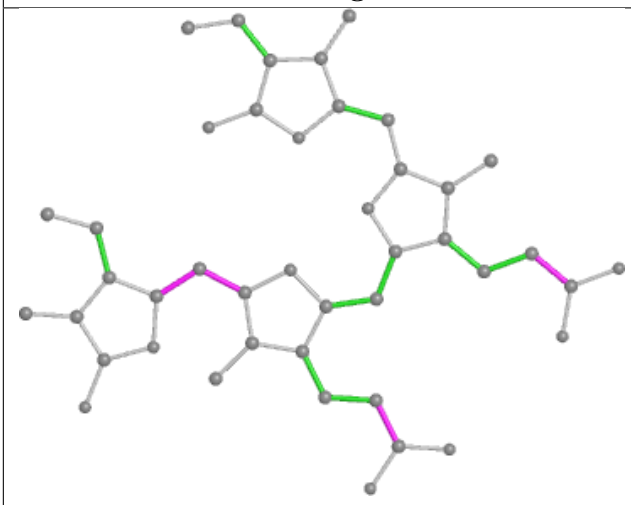

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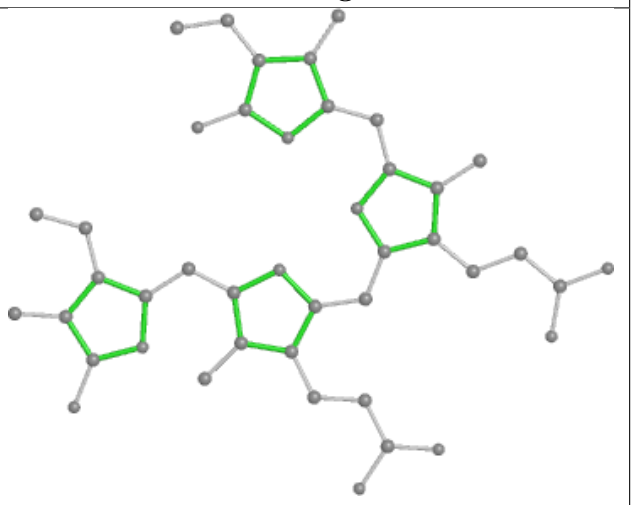
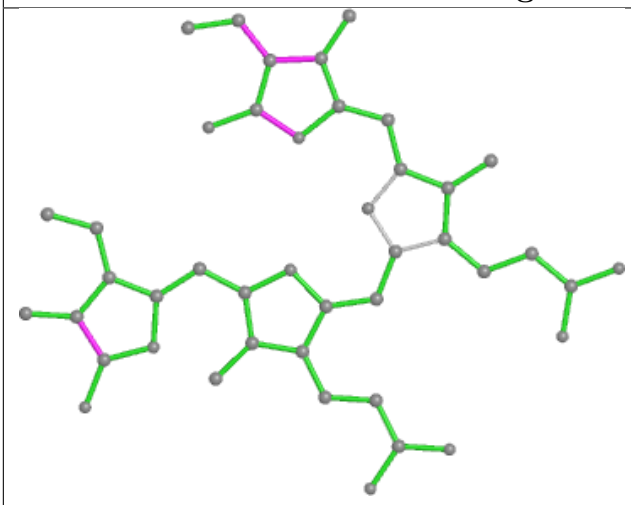


Rings

Ligand PEB eC 201



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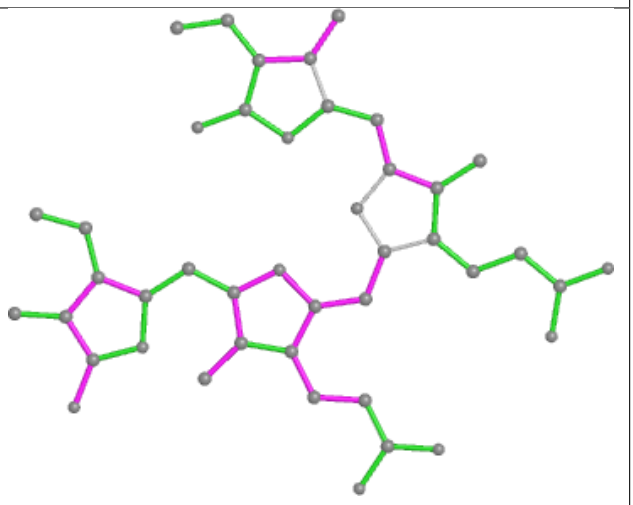

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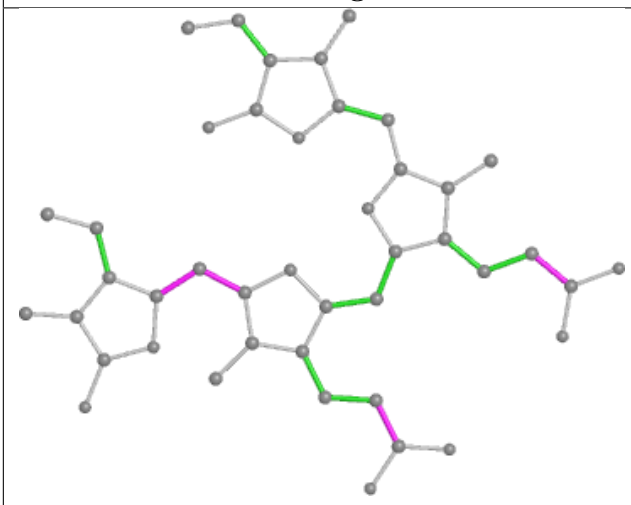

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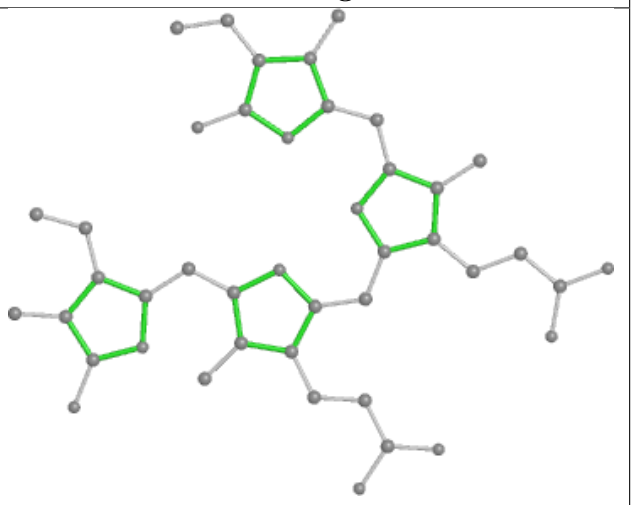
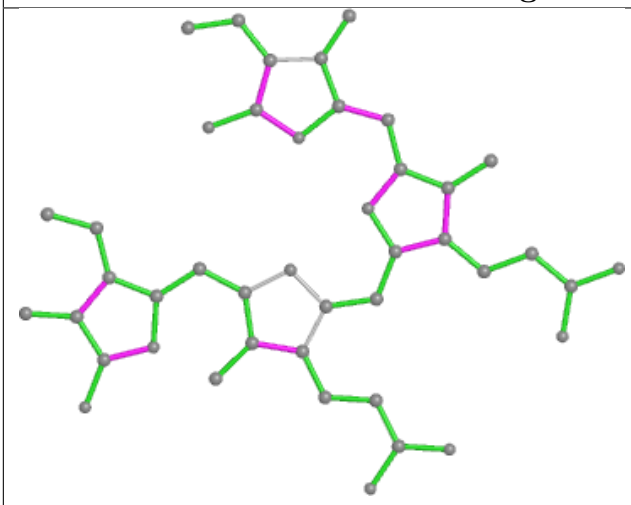


Rings

Ligand PUB t5 203



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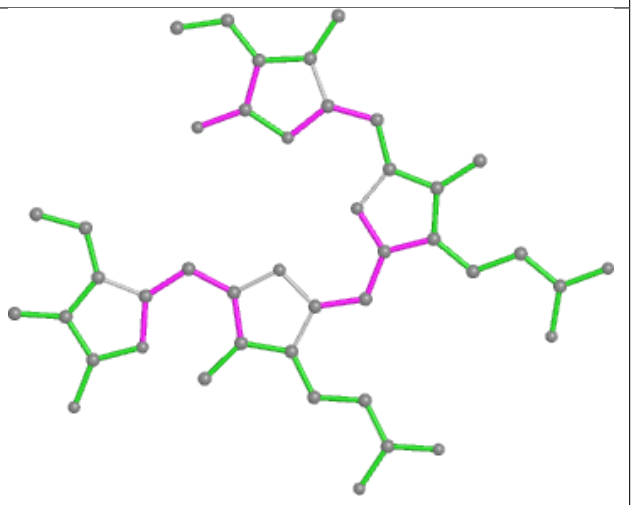

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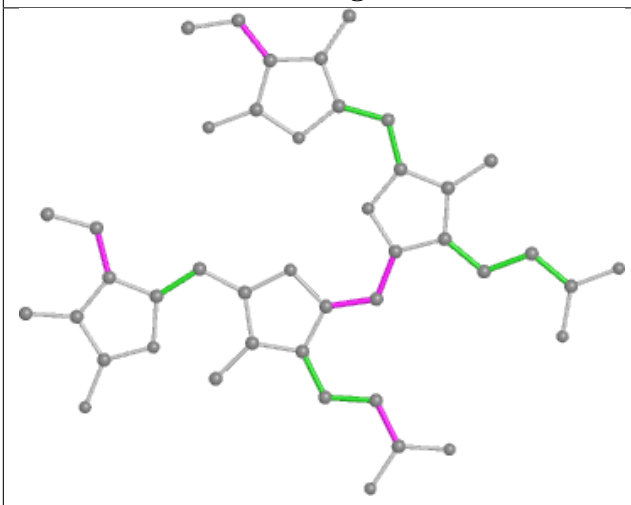

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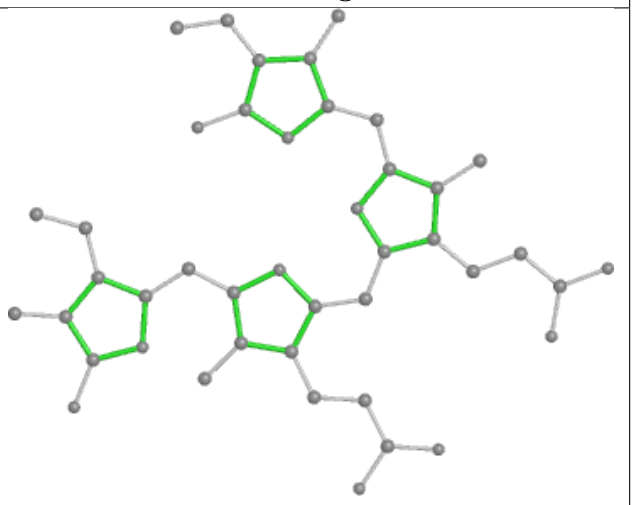

Rings

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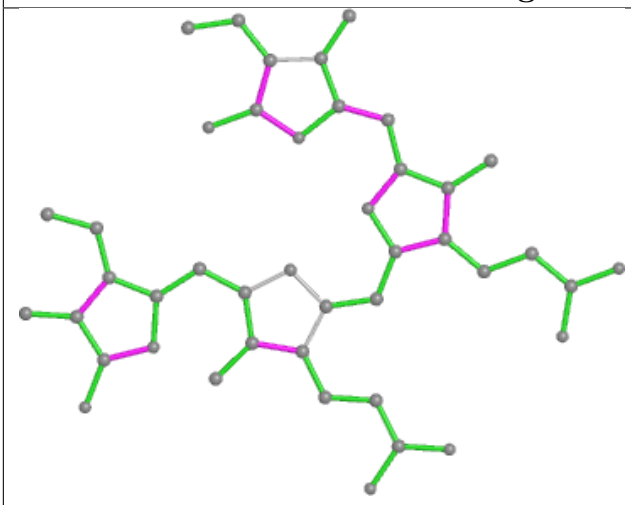

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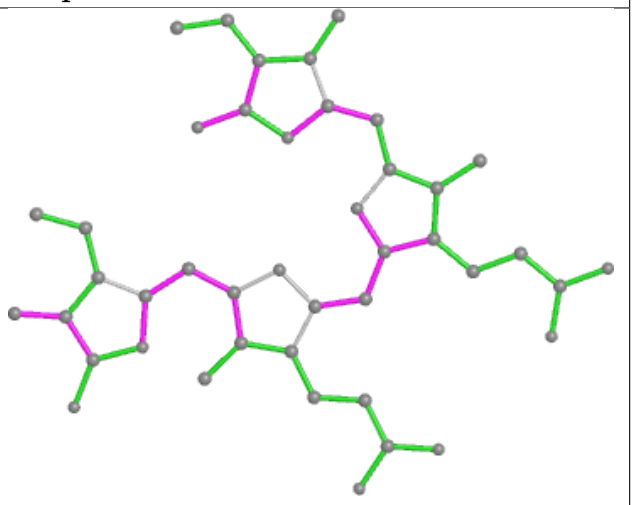

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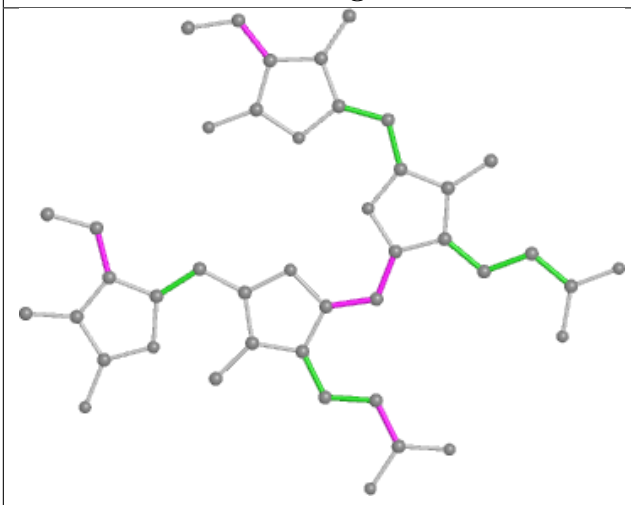

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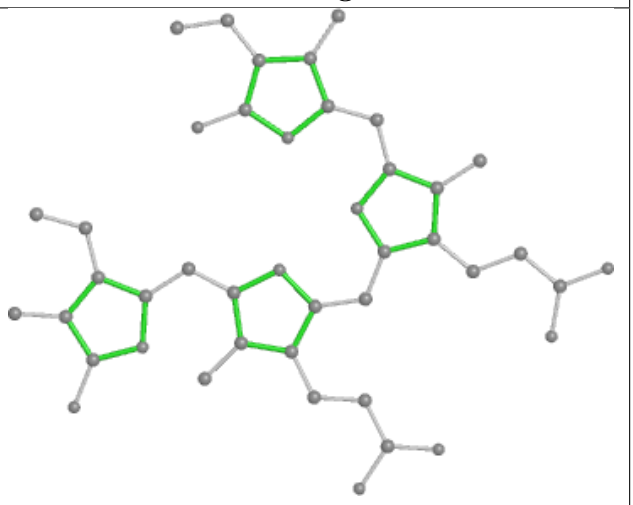
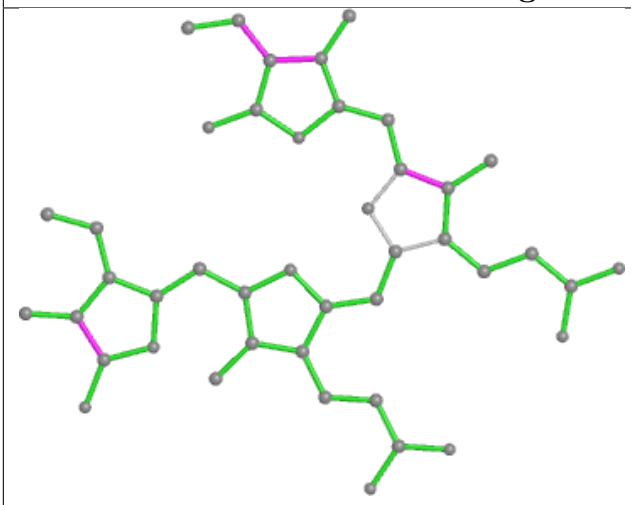


Rings

Ligand PEB d3 301



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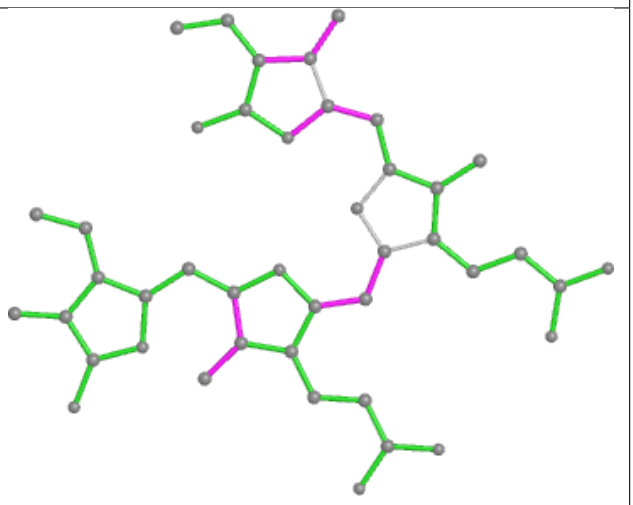

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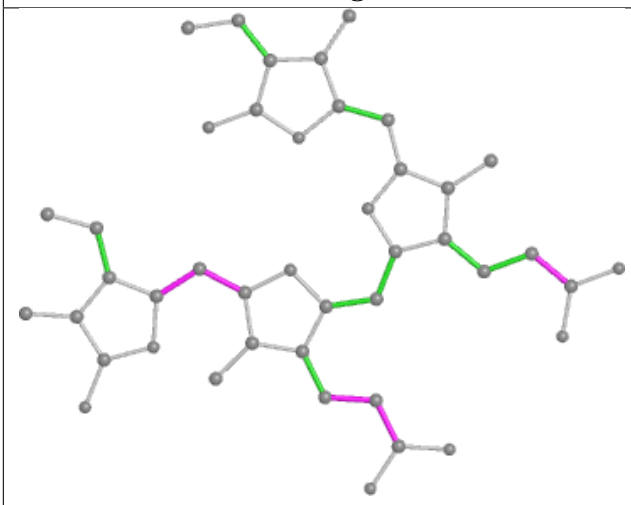

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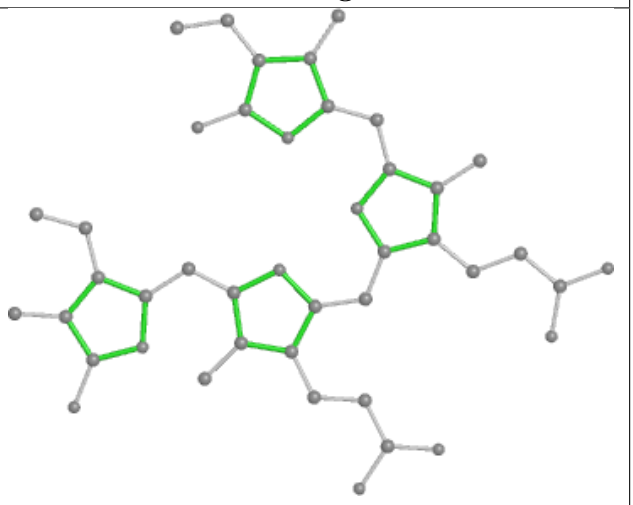
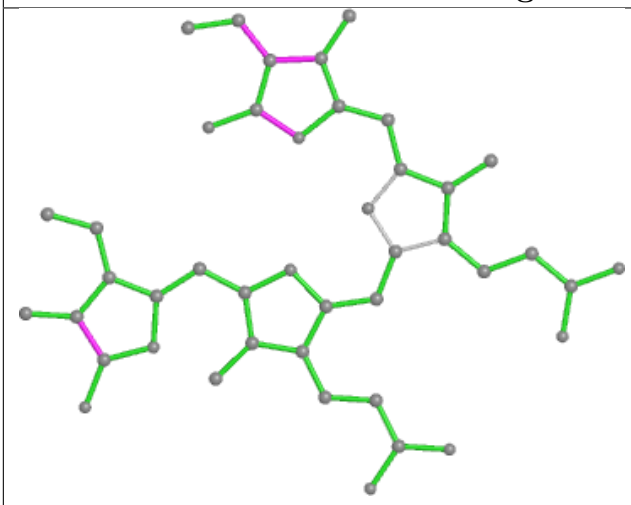


Rings

Ligand PEB eB 202



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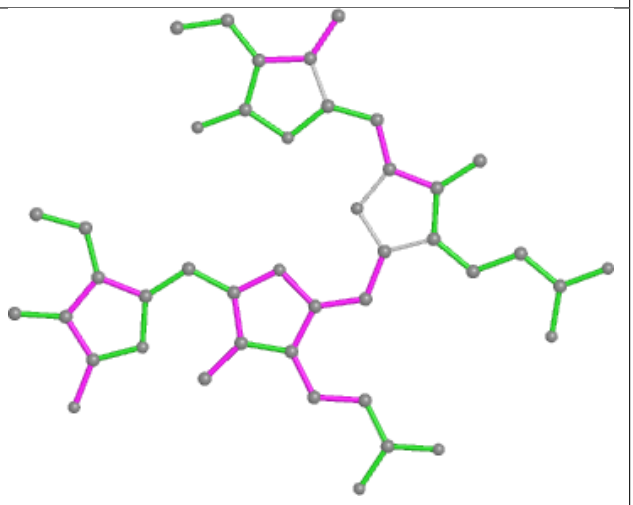

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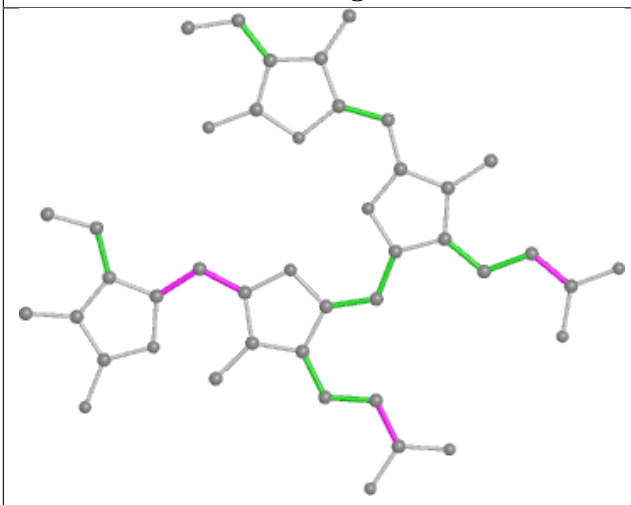

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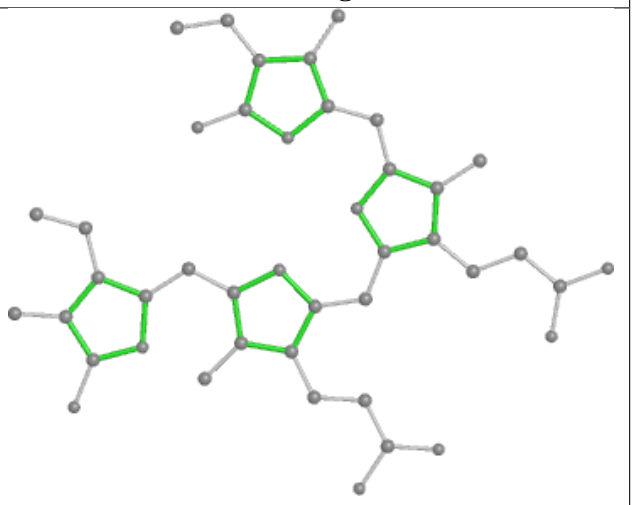
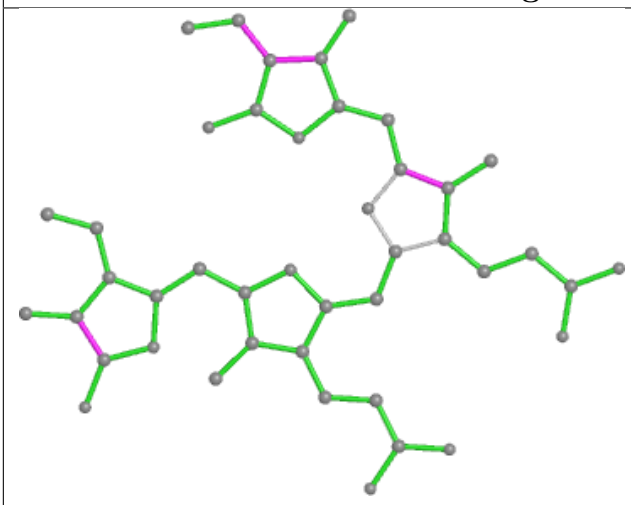


Rings

Ligand PEB I9 202



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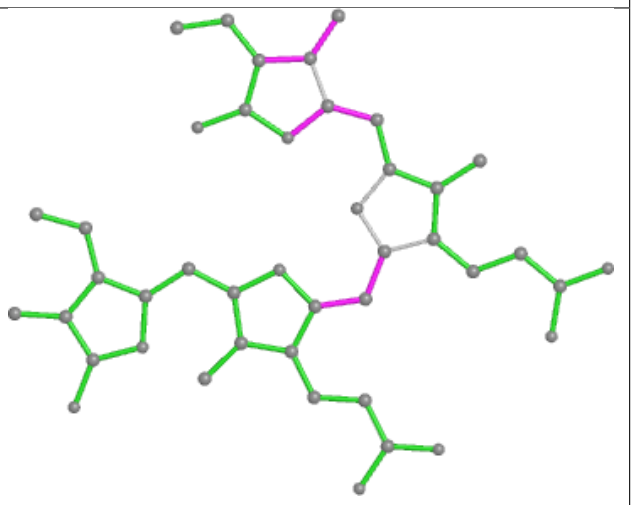

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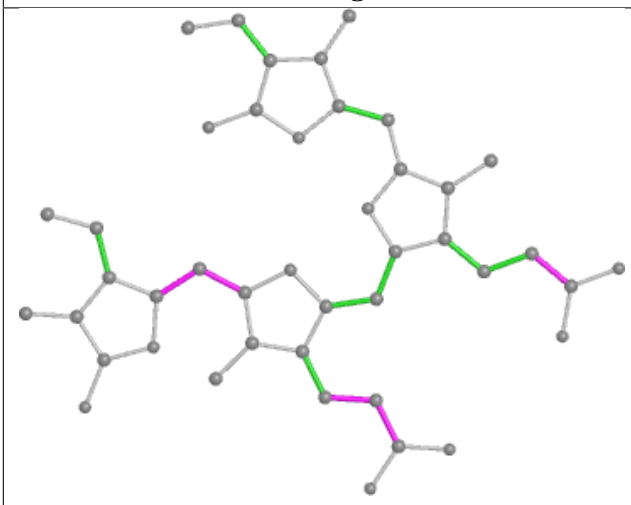

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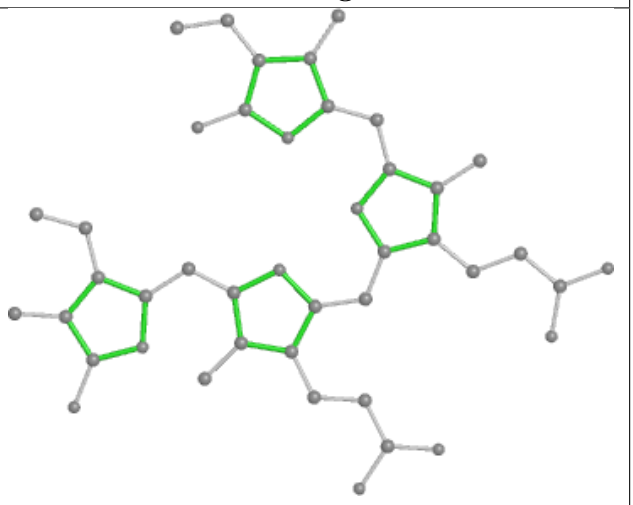
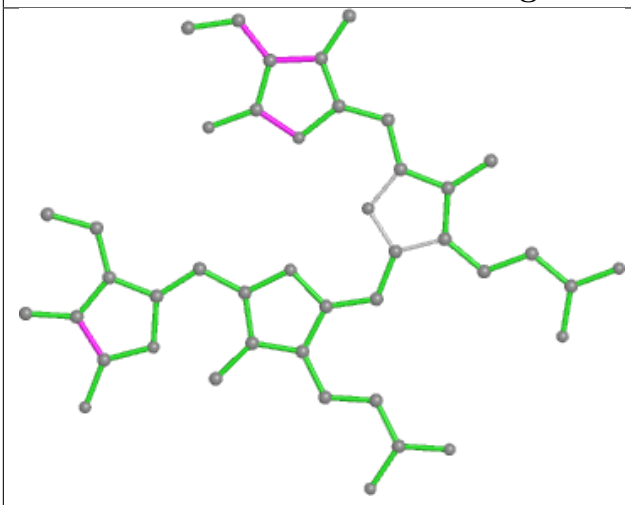


Rings

Ligand PEB cS 201



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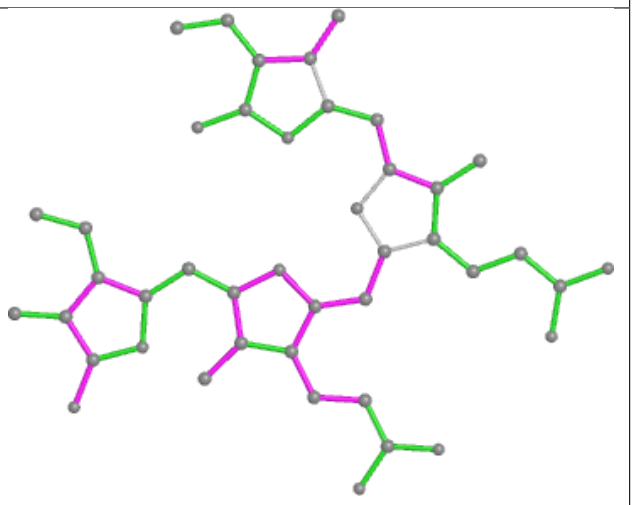

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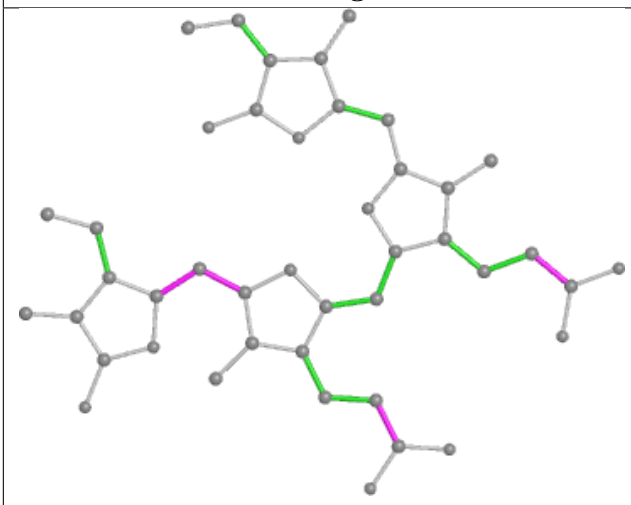

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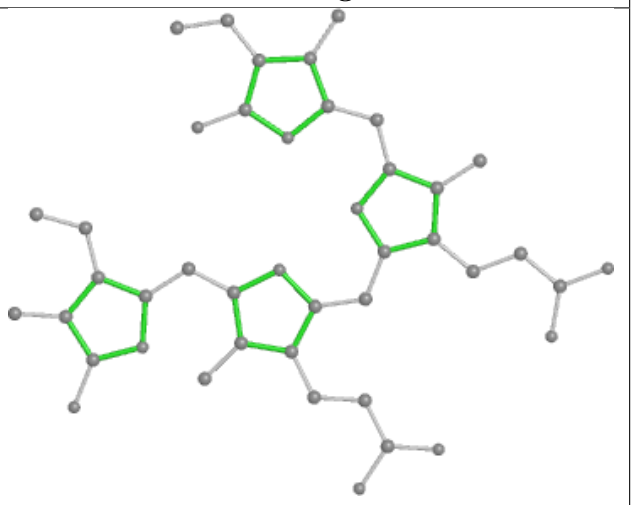
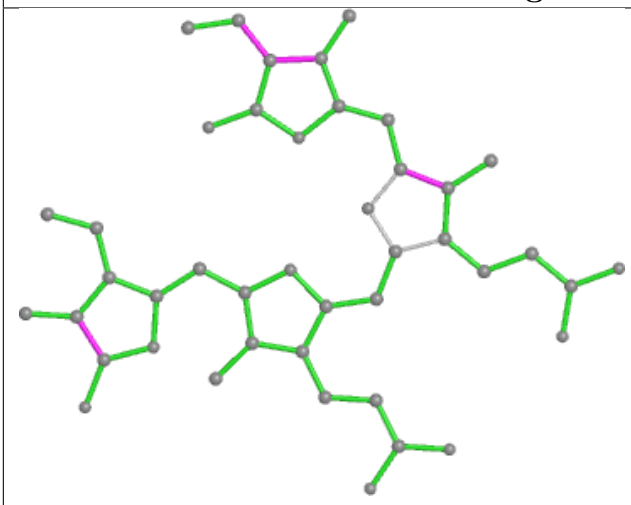


Rings

Ligand PEB ls 202



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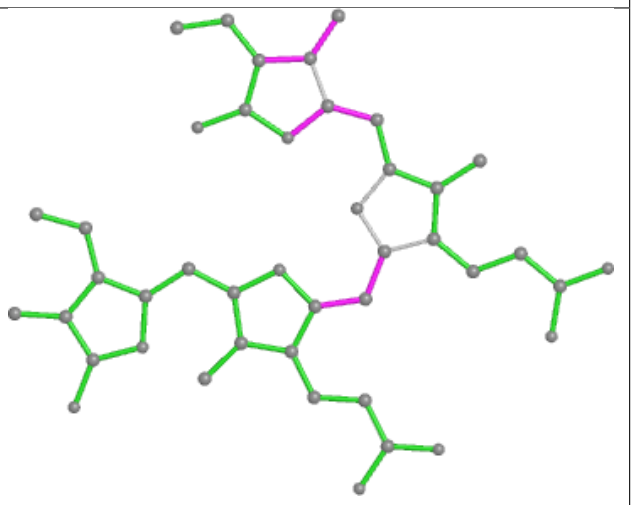

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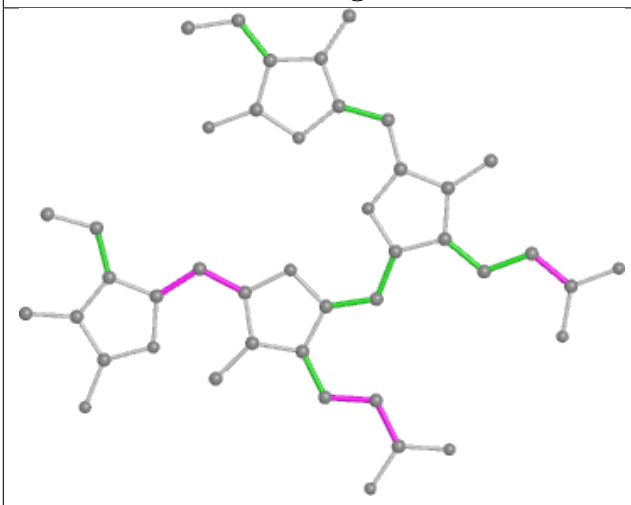

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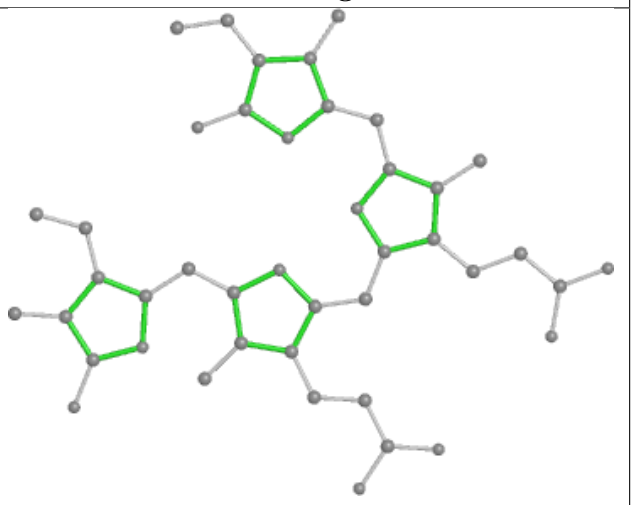
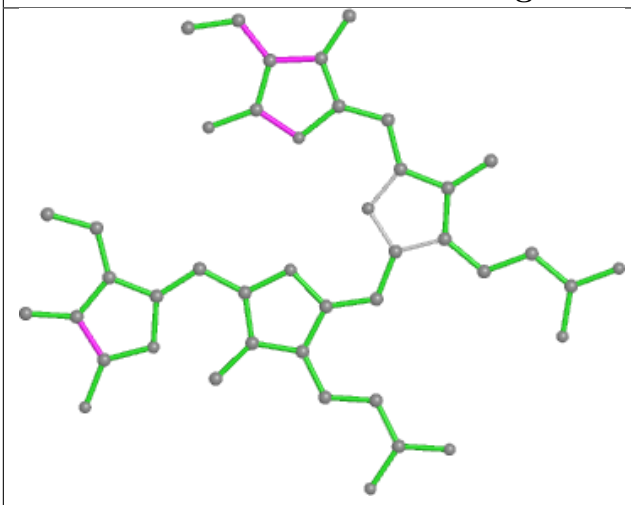


Rings

Ligand PEB V9 201



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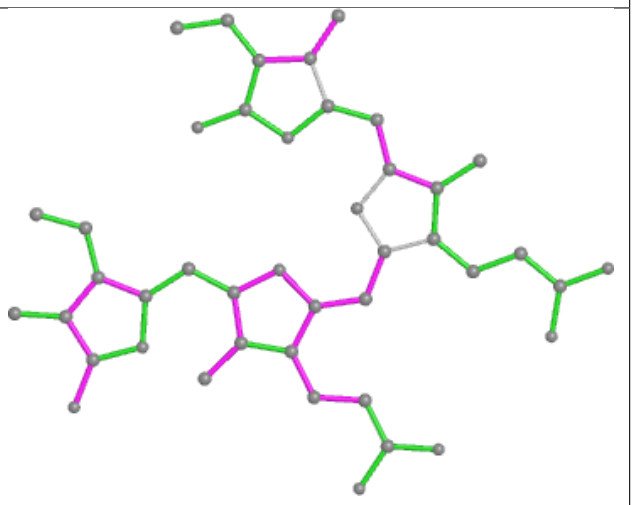
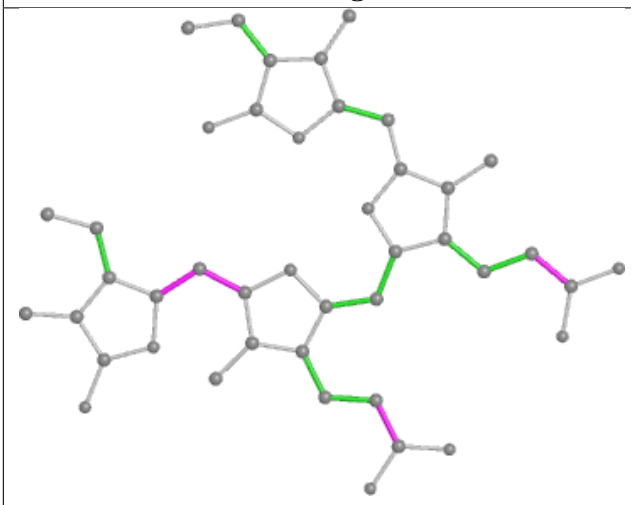


Bond angles



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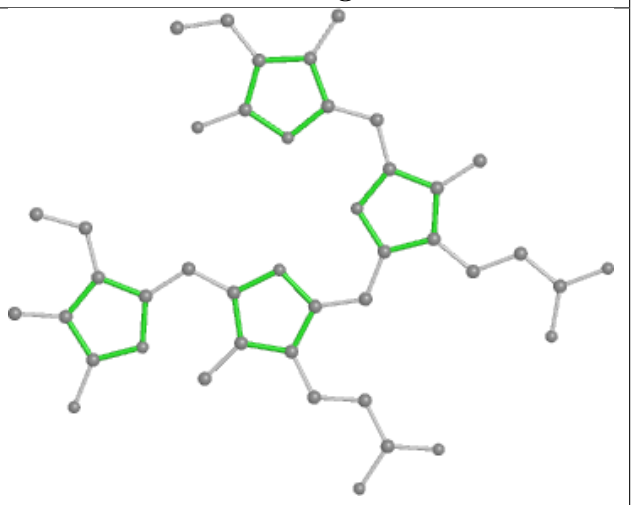
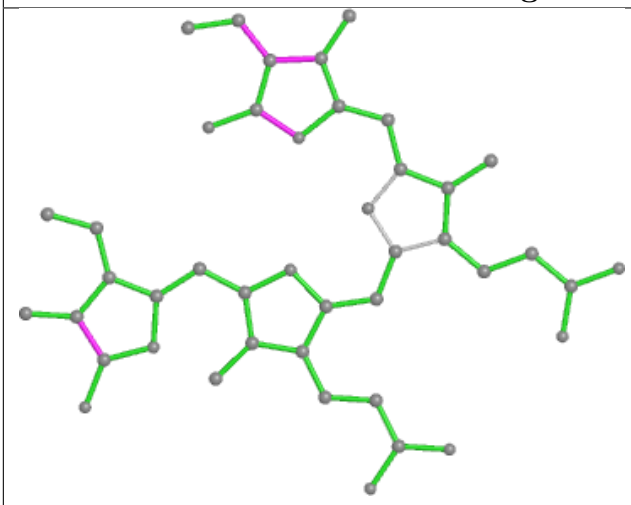


Rings

Ligand PEB z2 201



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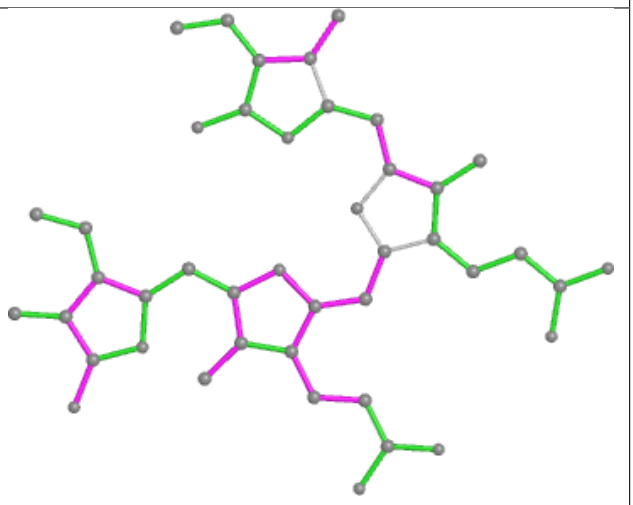
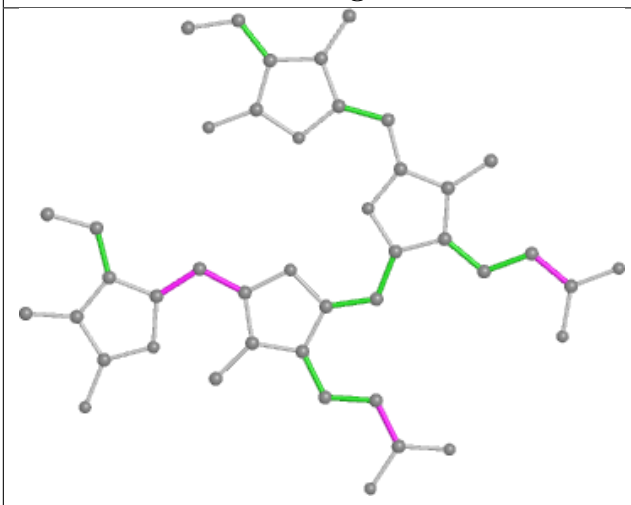


Bond angles



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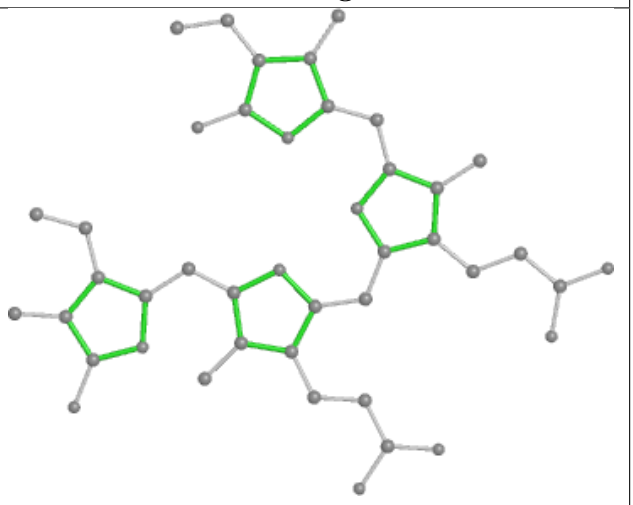
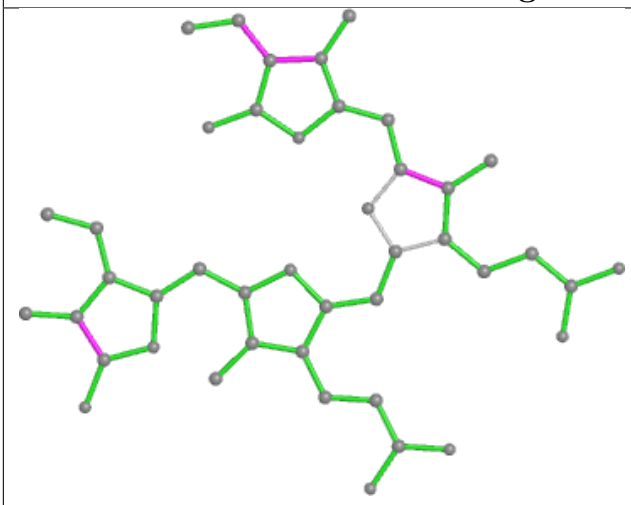
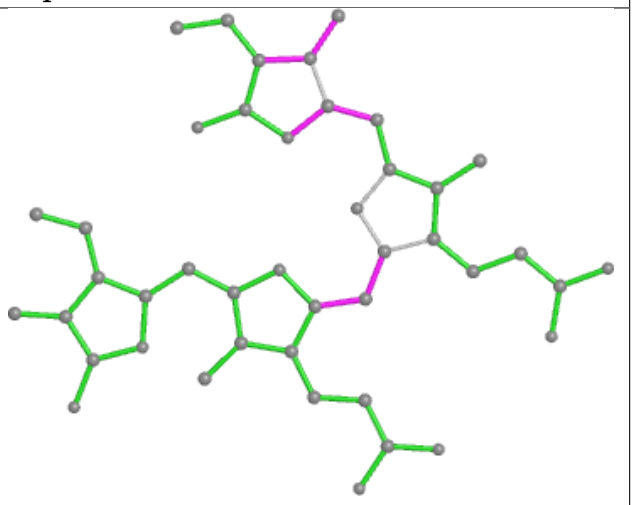


Rings

Ligand PEB p6 202



Bond lengths



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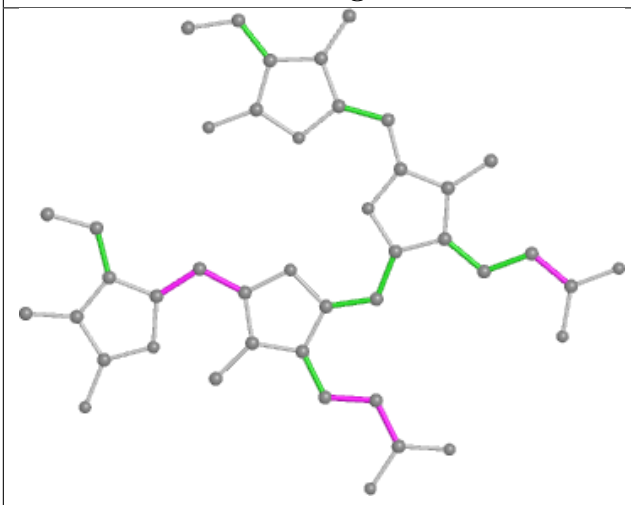
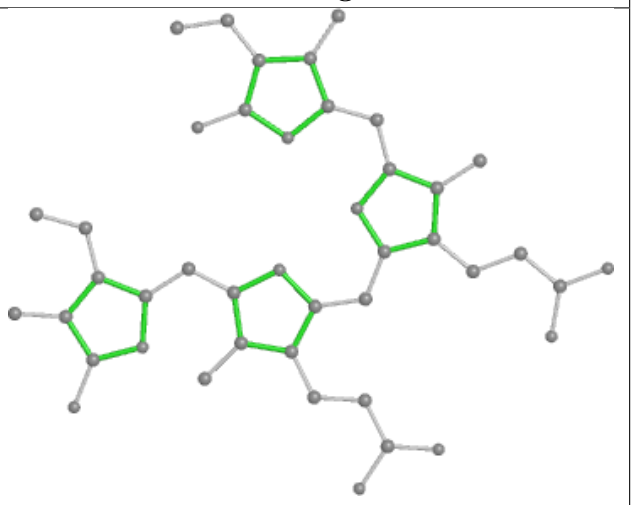
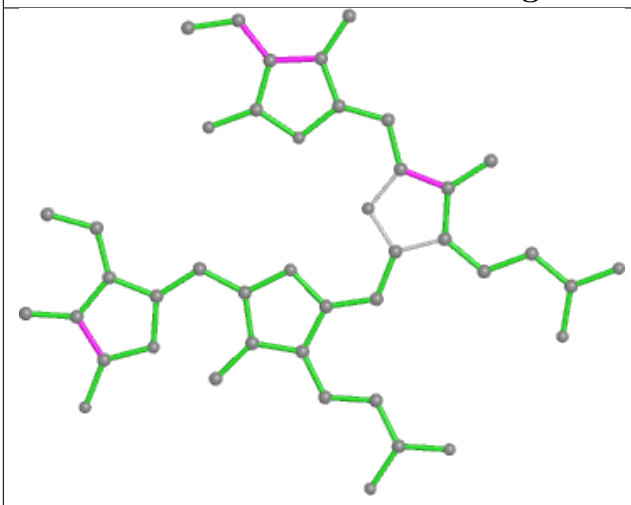


Torsions



Rings

Ligand PEB s8 202



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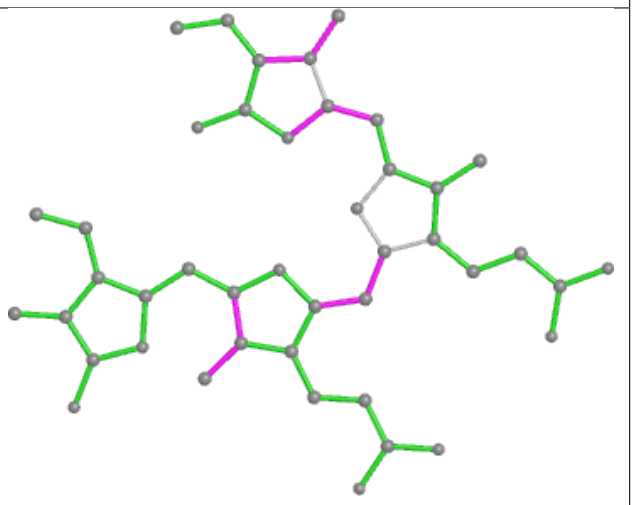

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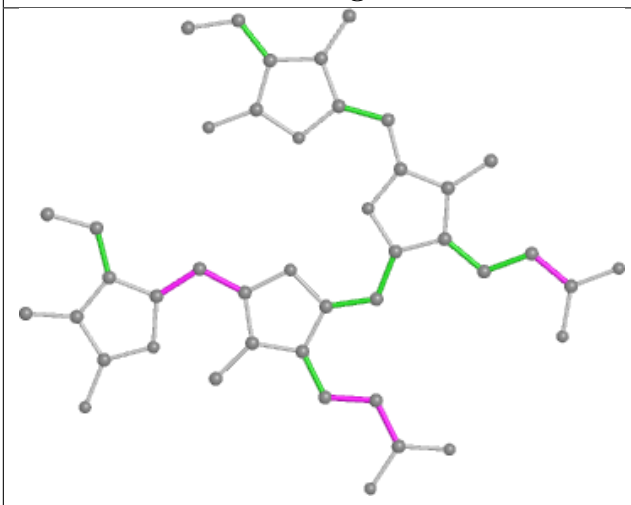

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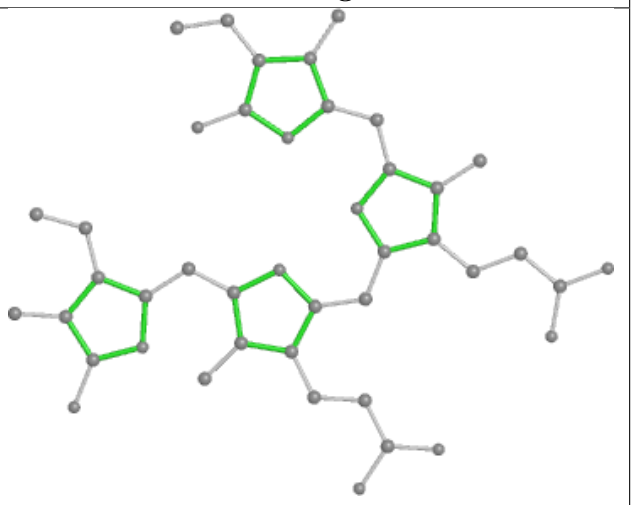
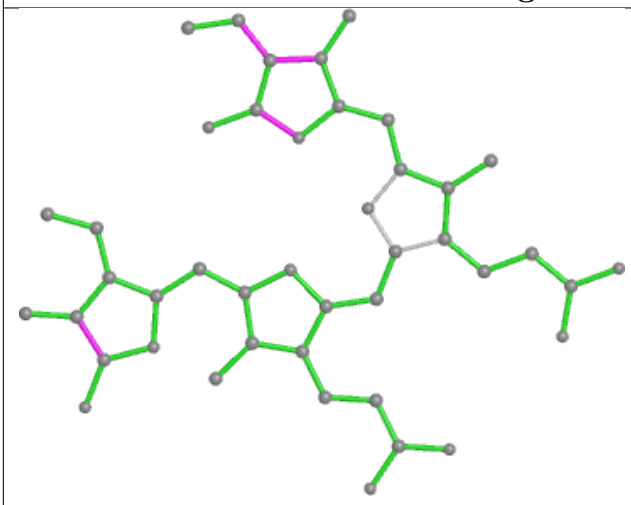


Rings

Ligand PEB Z6 202



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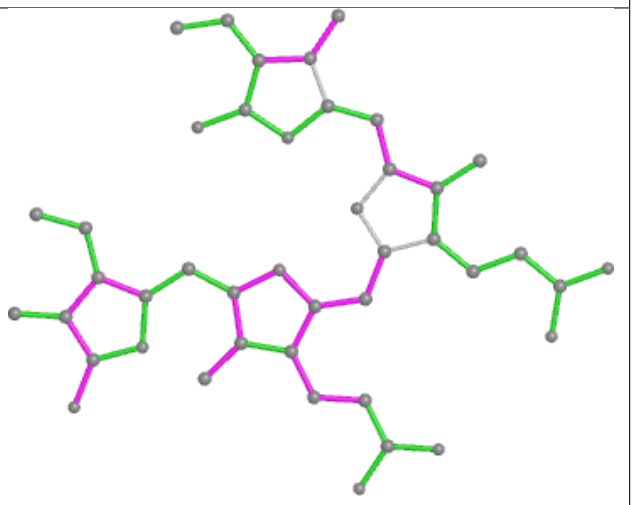

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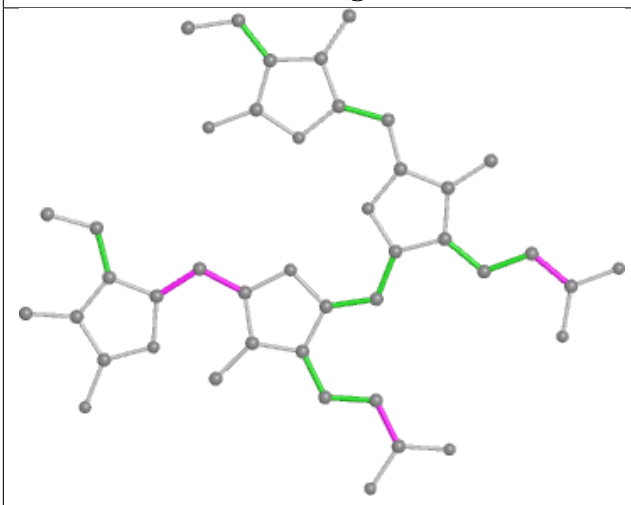

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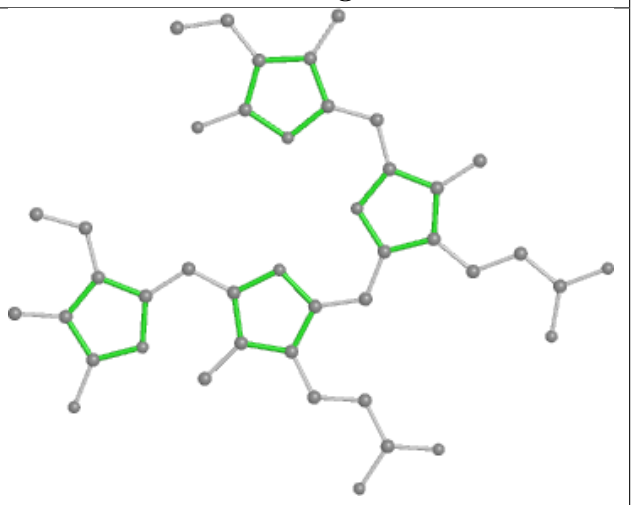
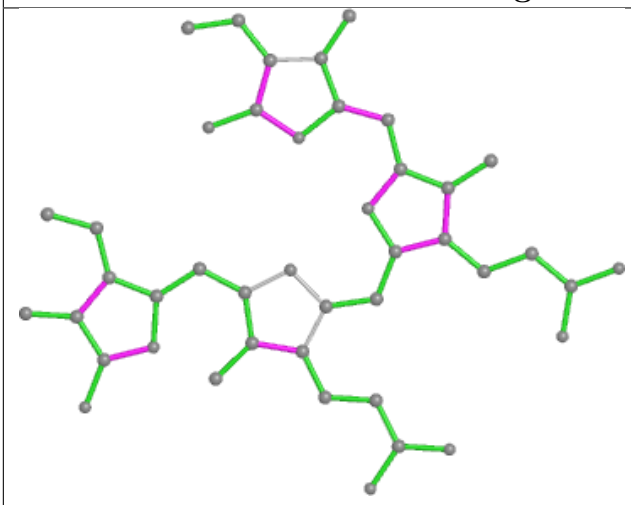


Rings

Ligand PUB B4 203



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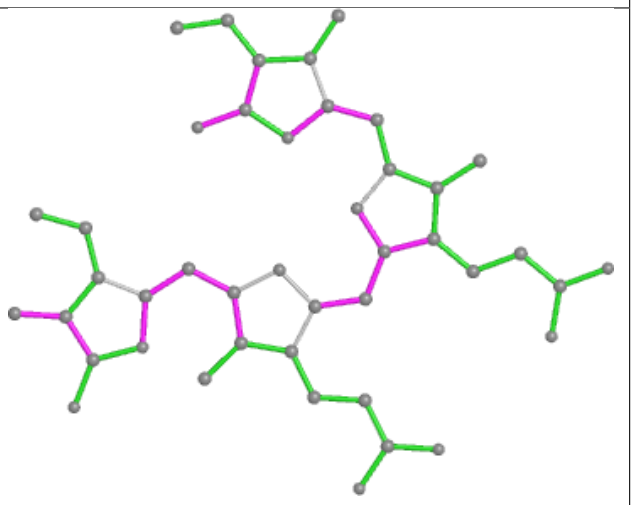

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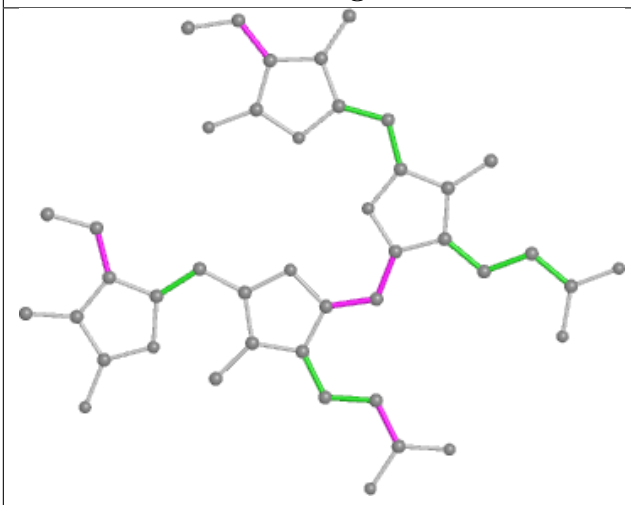

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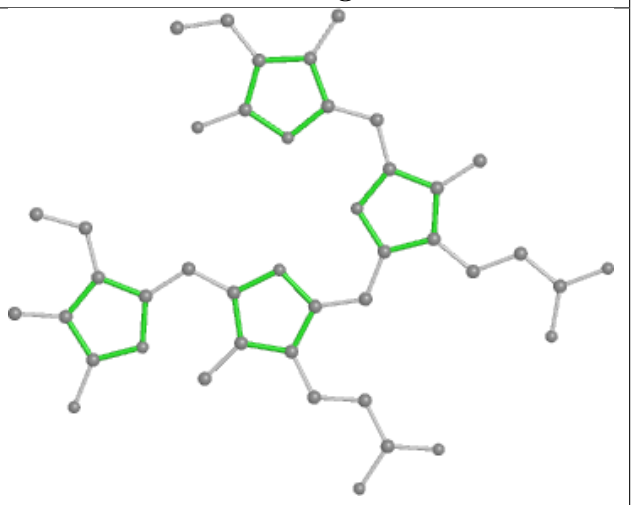
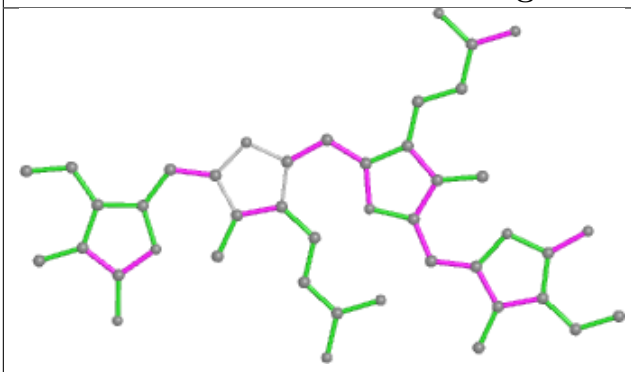


Rings

Ligand CYC k1 201



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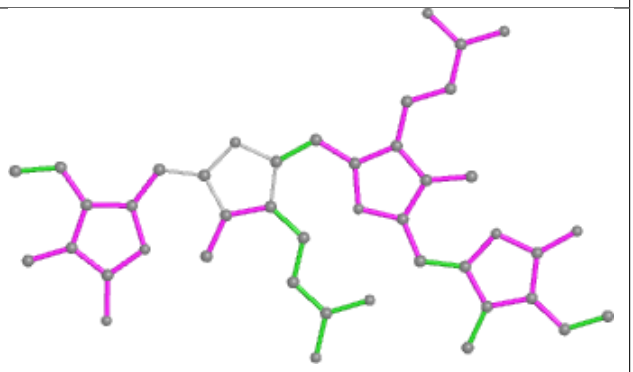

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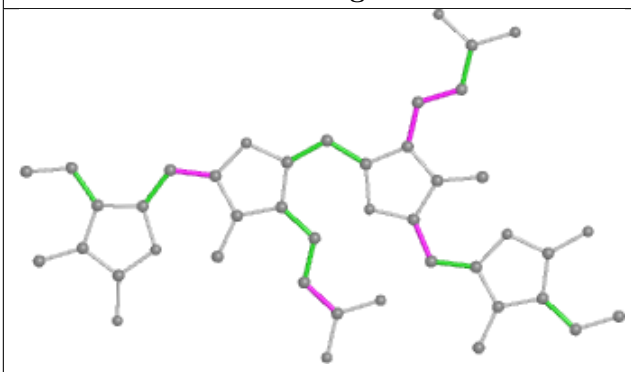

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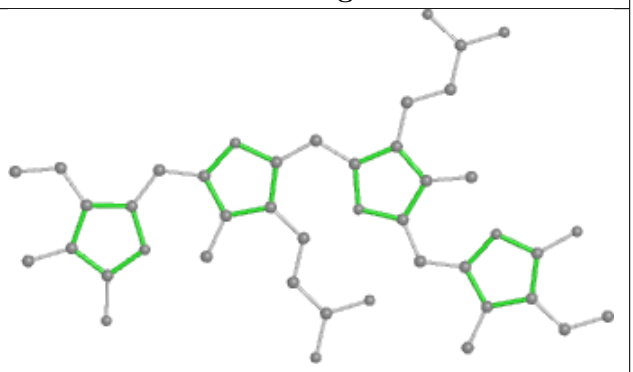

Rings

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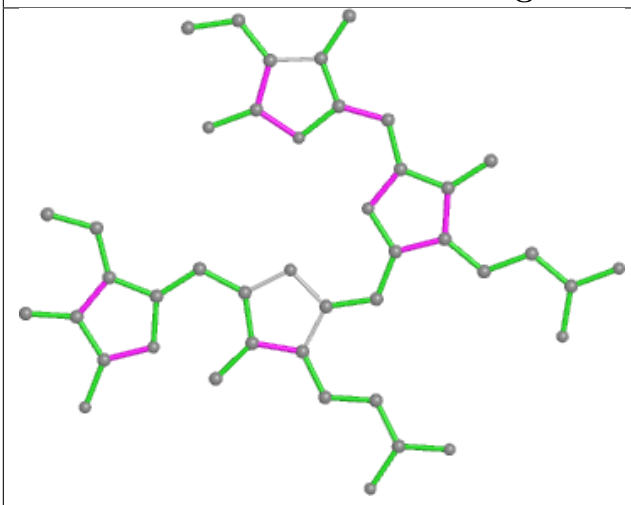

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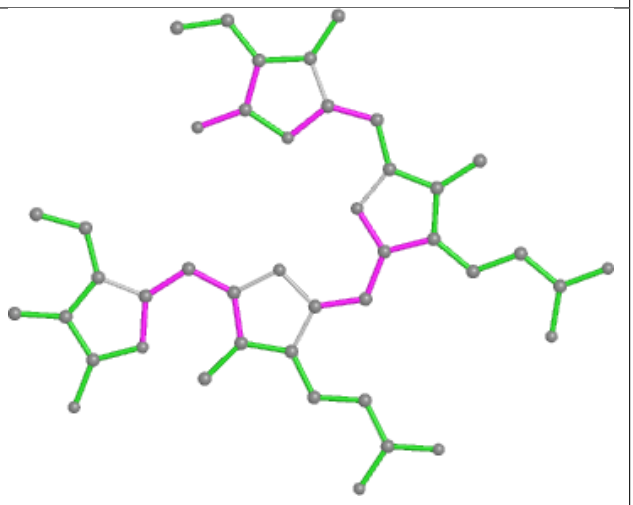

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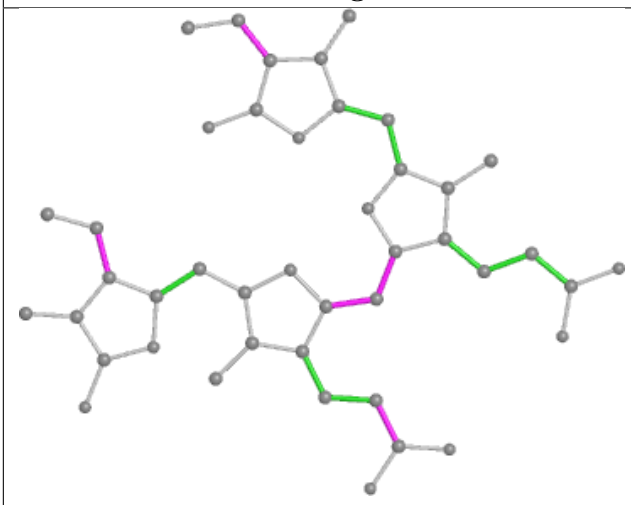

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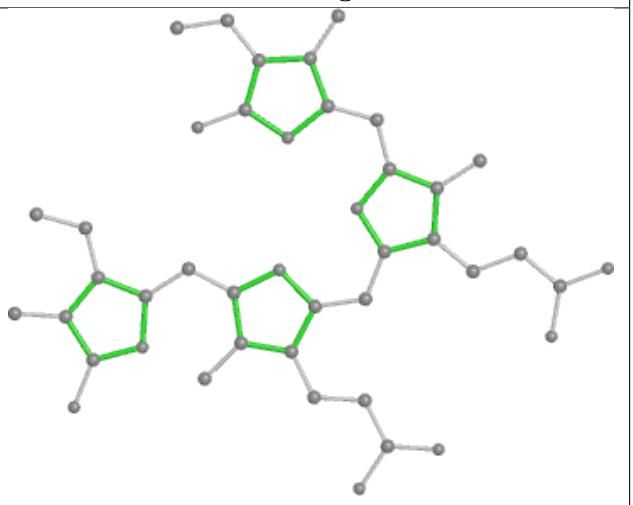

Rings

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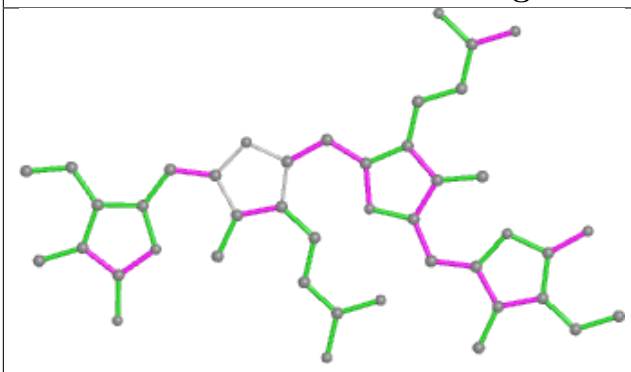

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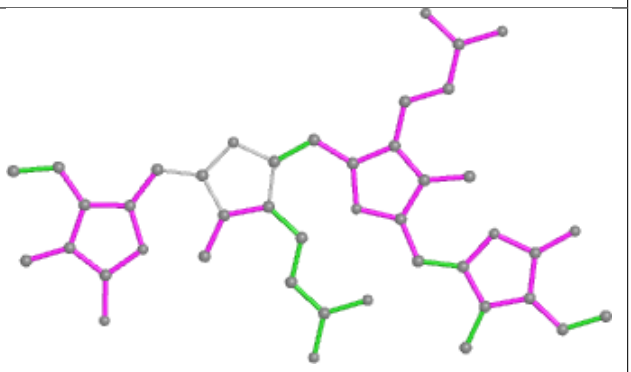

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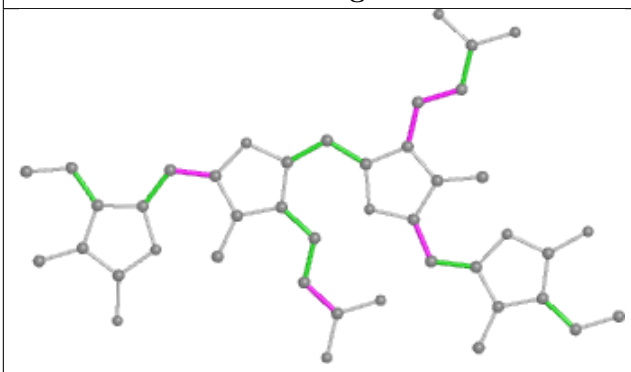

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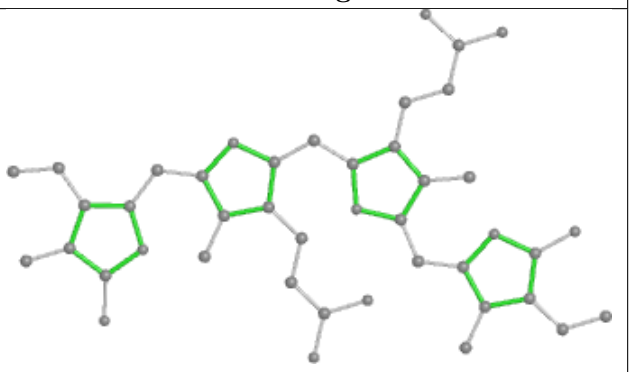

Rings

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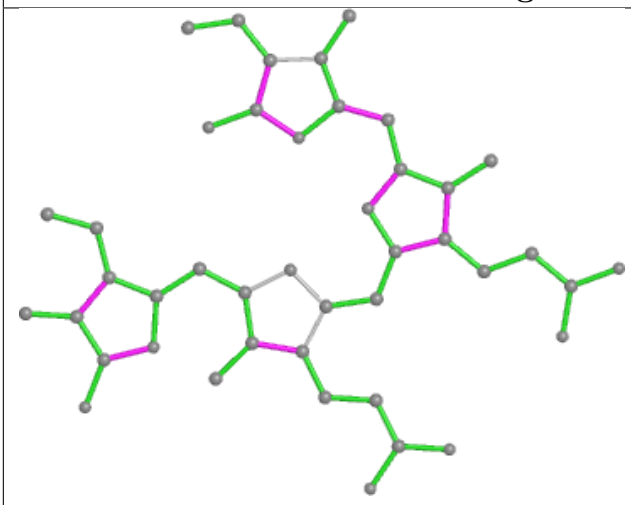

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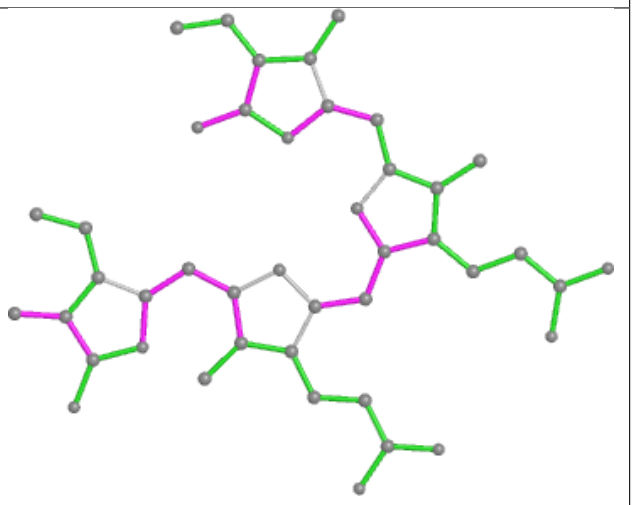

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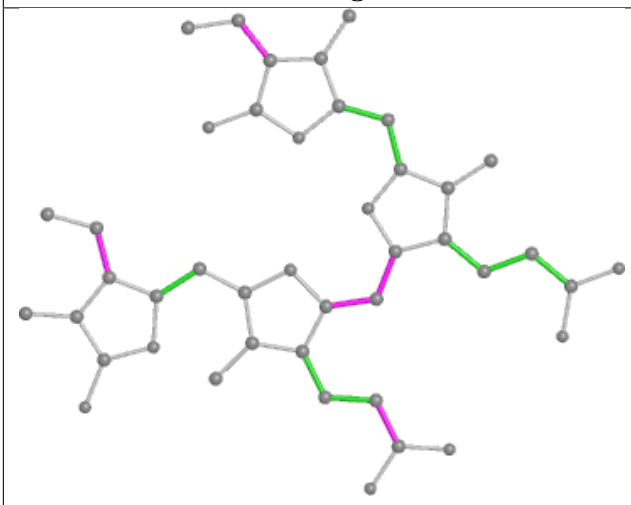

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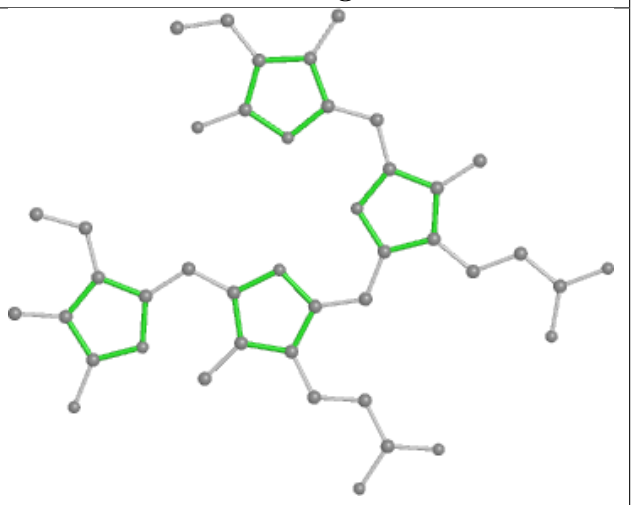

Rings

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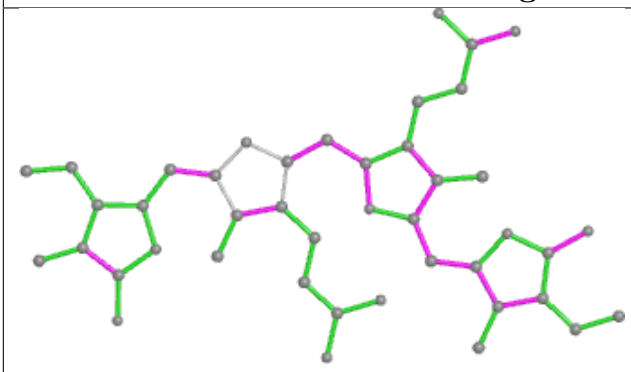

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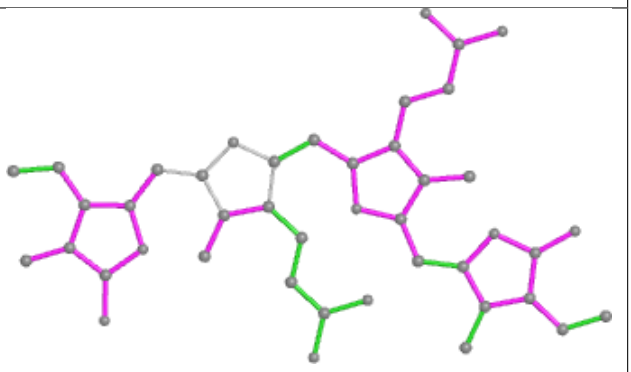

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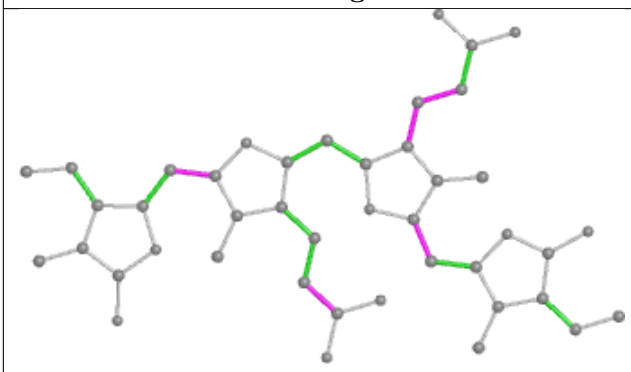

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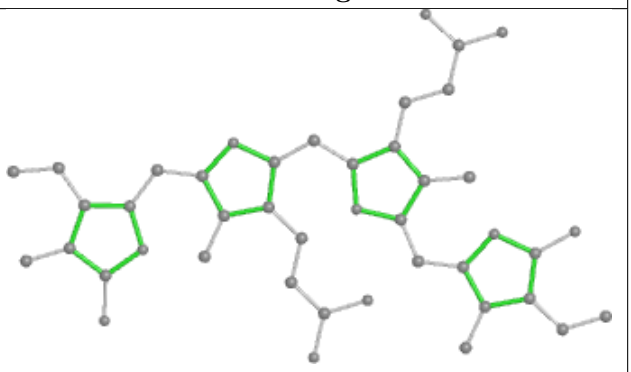
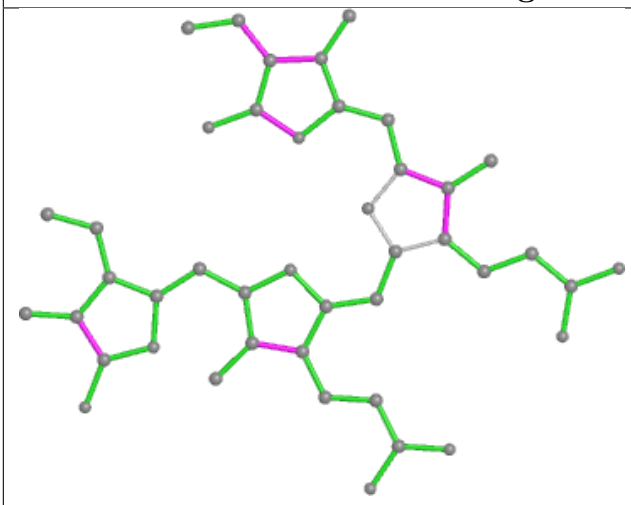


Rings

Ligand PEB Z2 202



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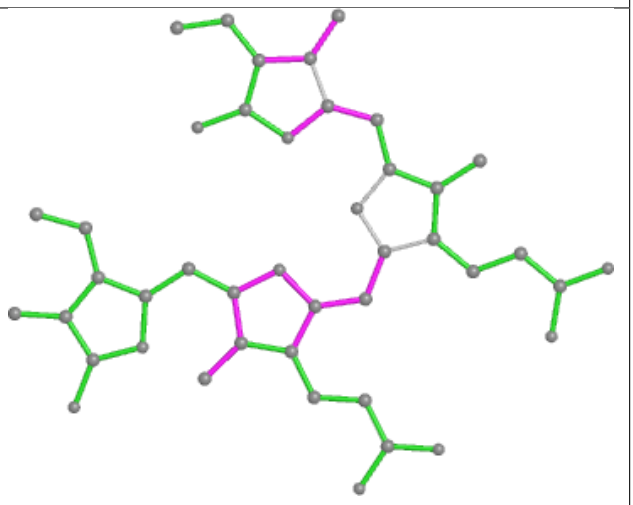

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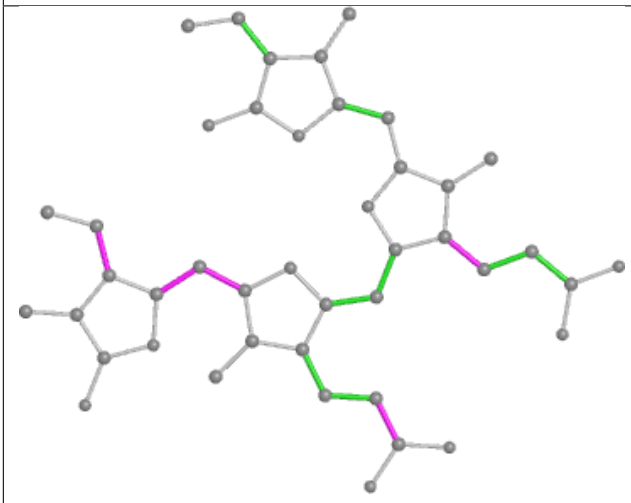

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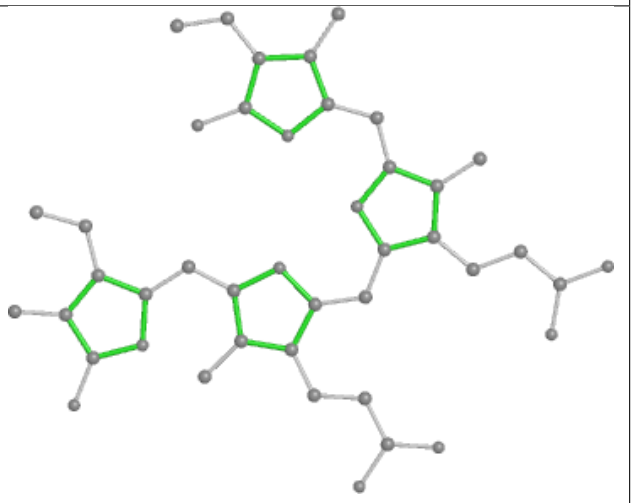

Rings

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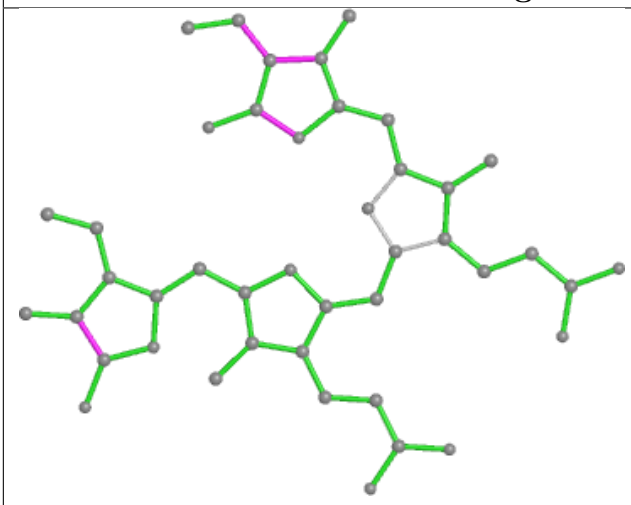

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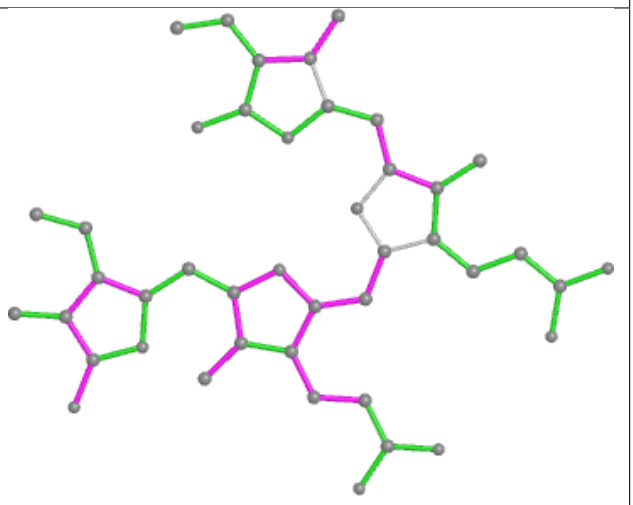

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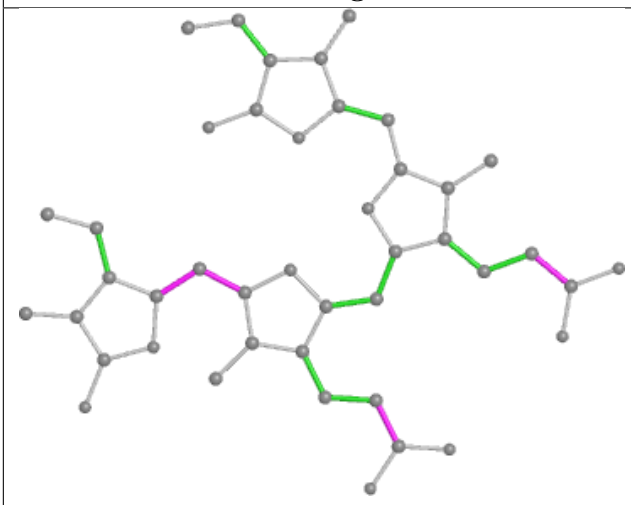

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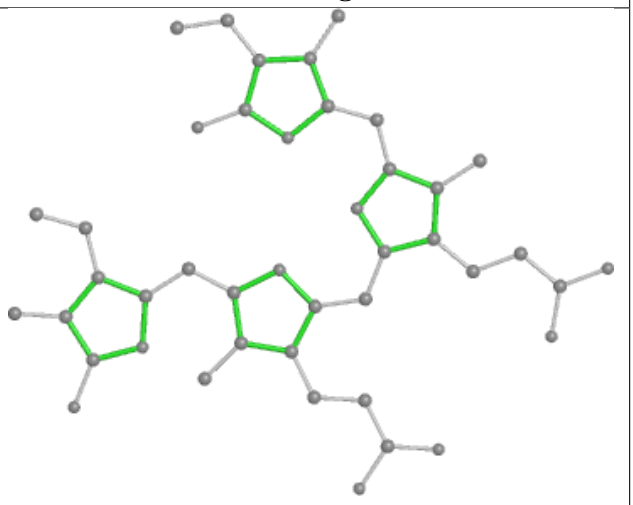
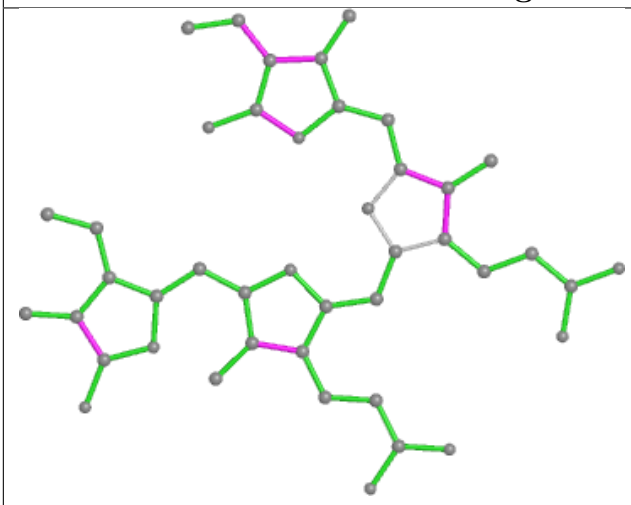


Rings

Ligand PEB D7 202



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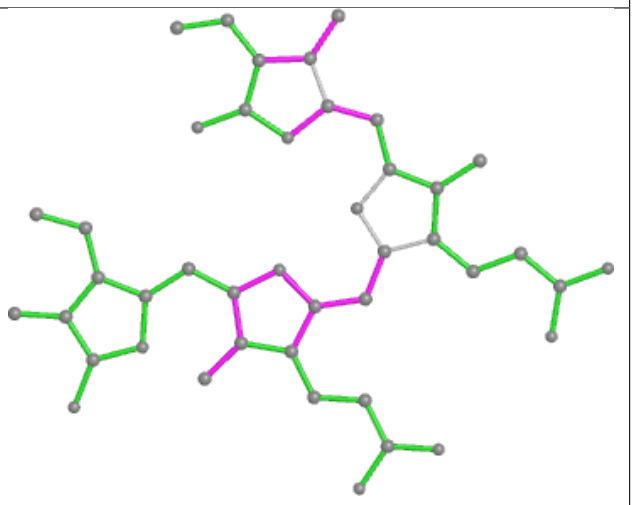

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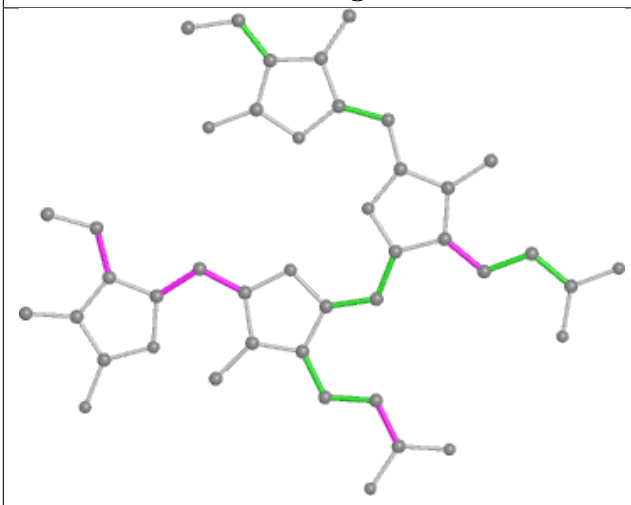

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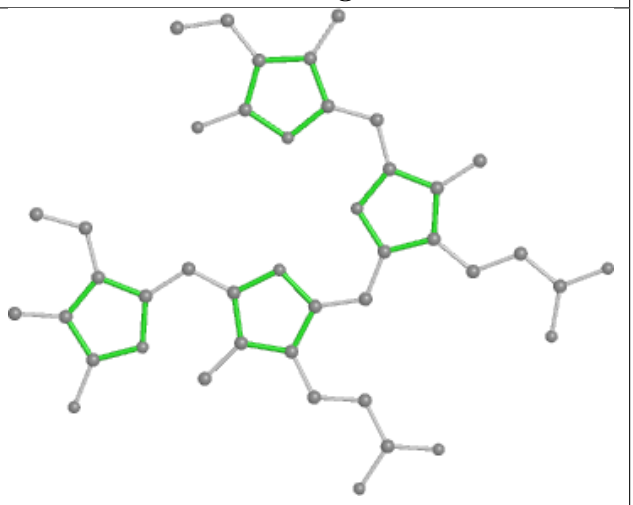
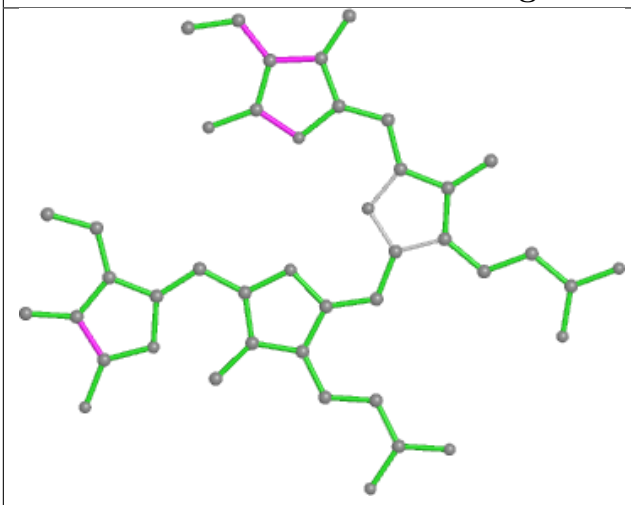


Rings

Ligand PEB ap 201



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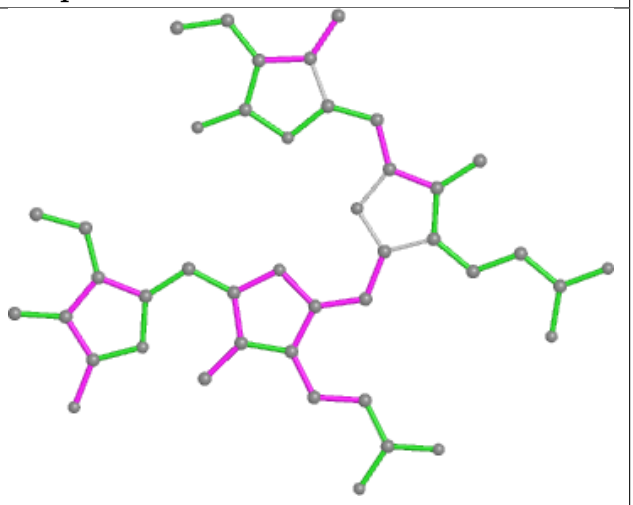
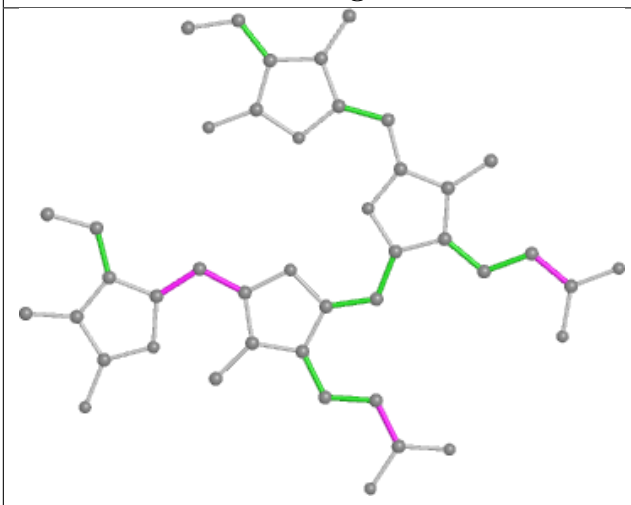


Bond angles



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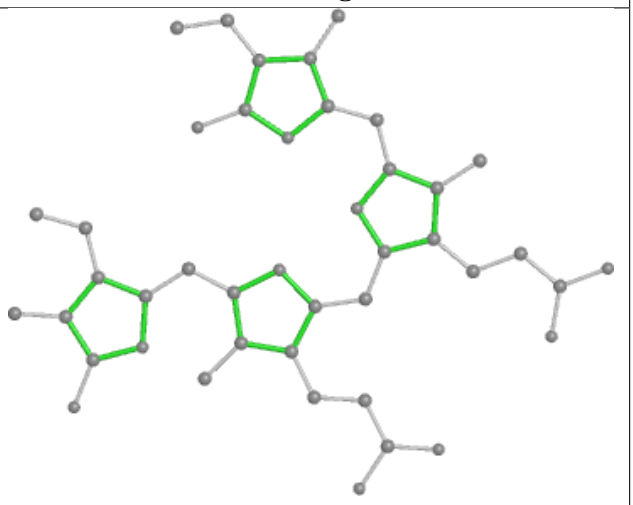
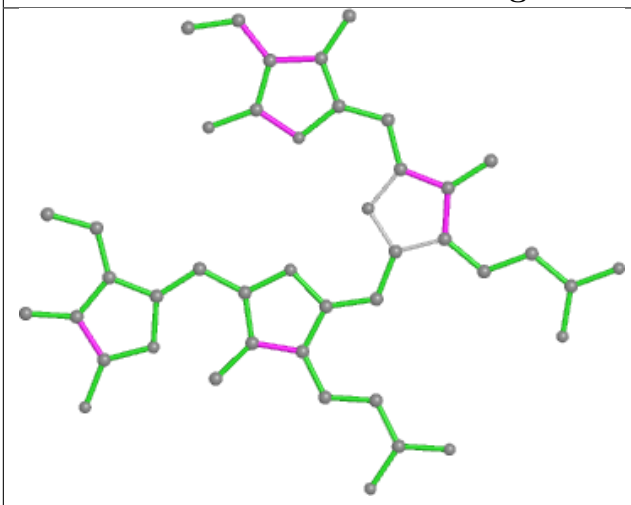


Rings

Ligand PEB jK 1002



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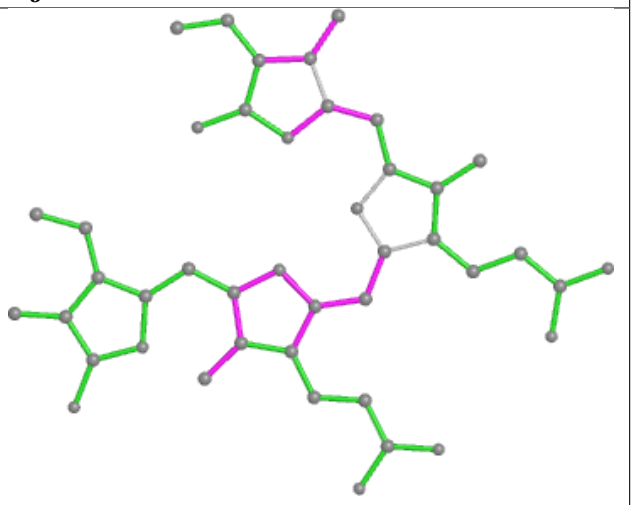
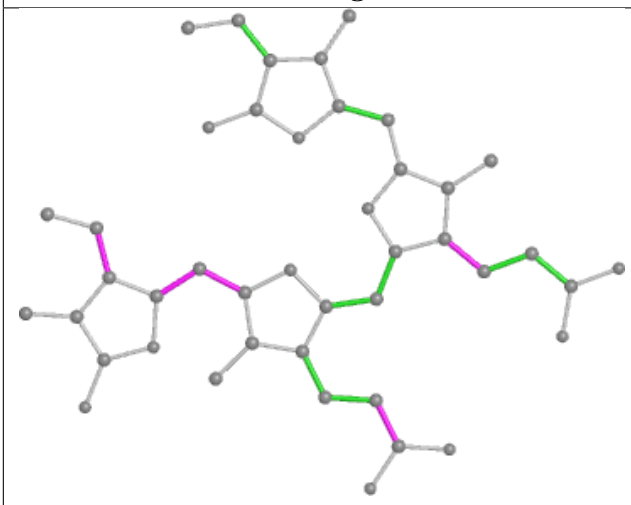
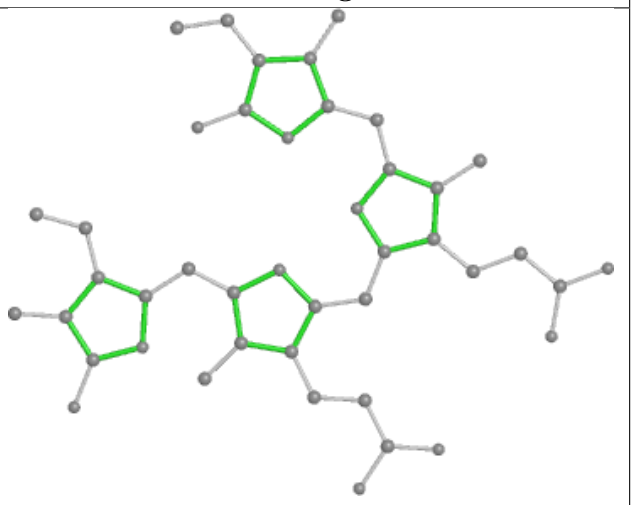


Bond angles

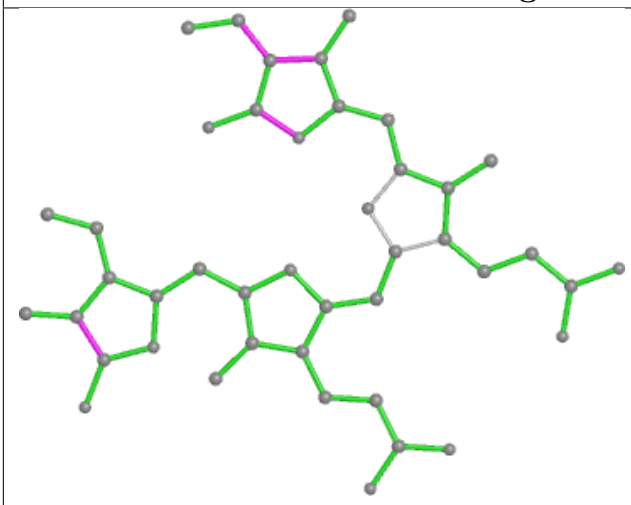


Torsions



Rings

Ligand PEB bc 201



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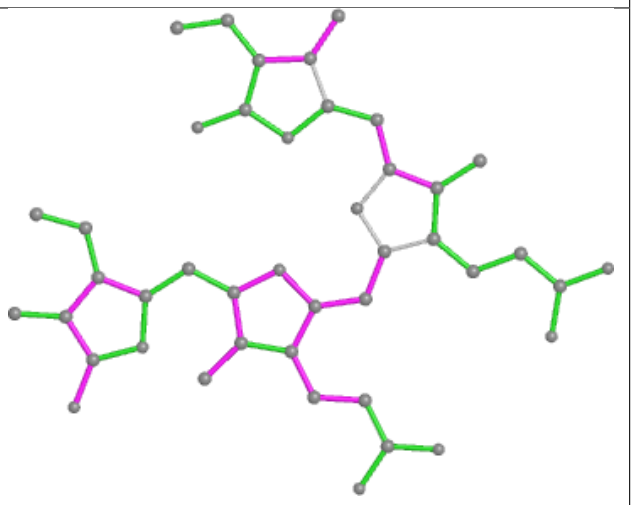

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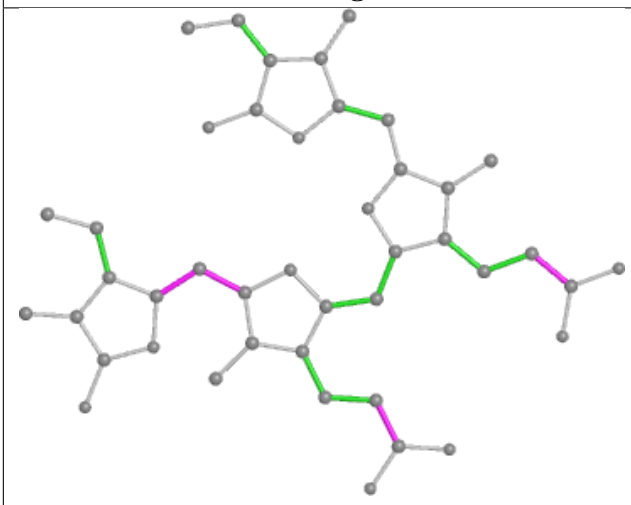

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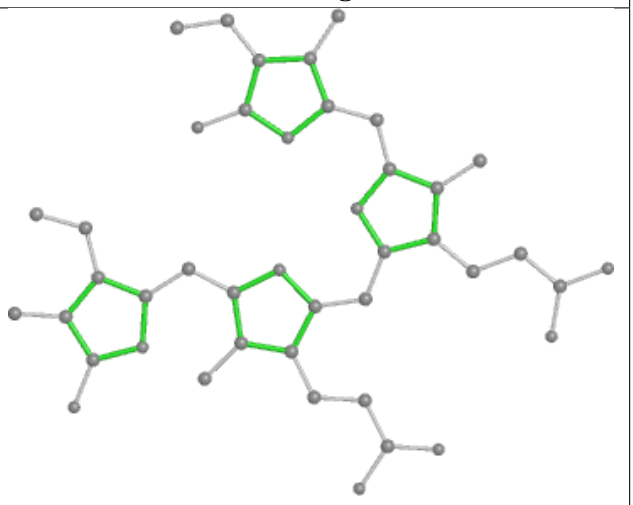
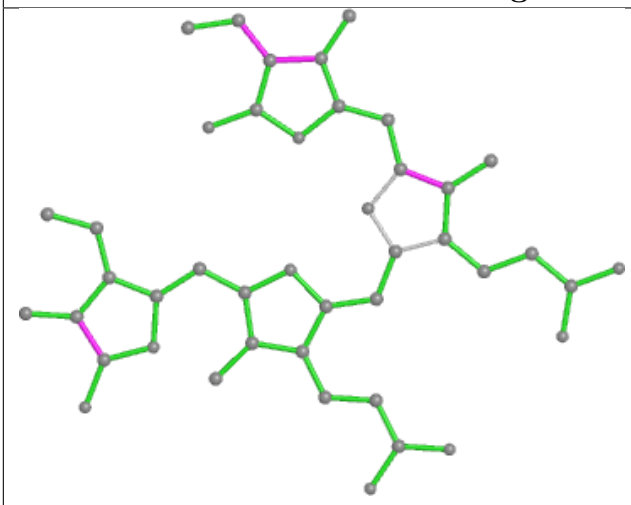


Rings

Ligand PEB W7 202



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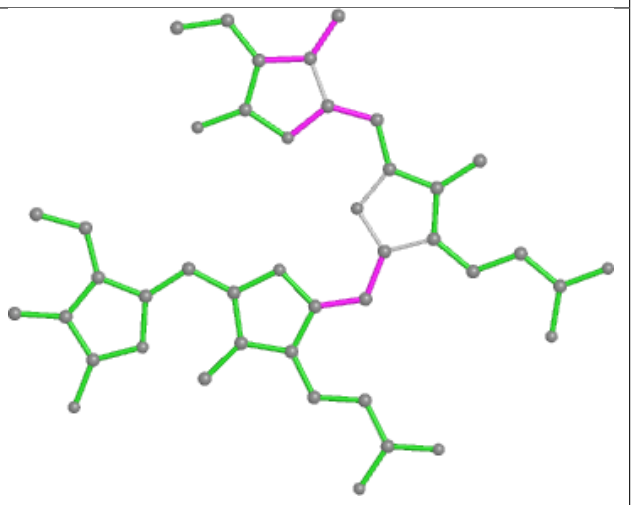

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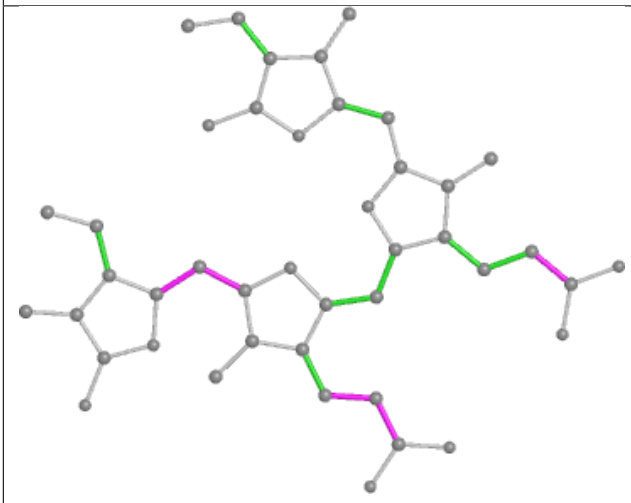

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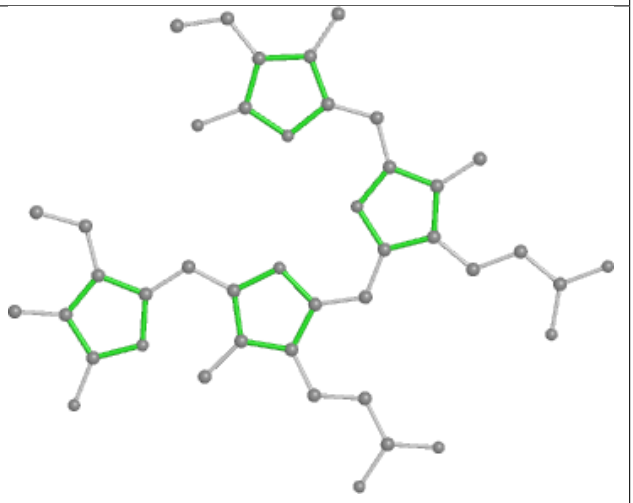
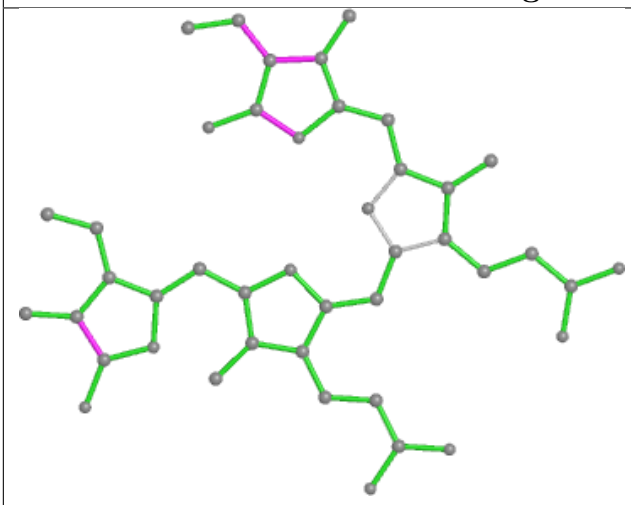


Rings

Ligand PEB fd 301



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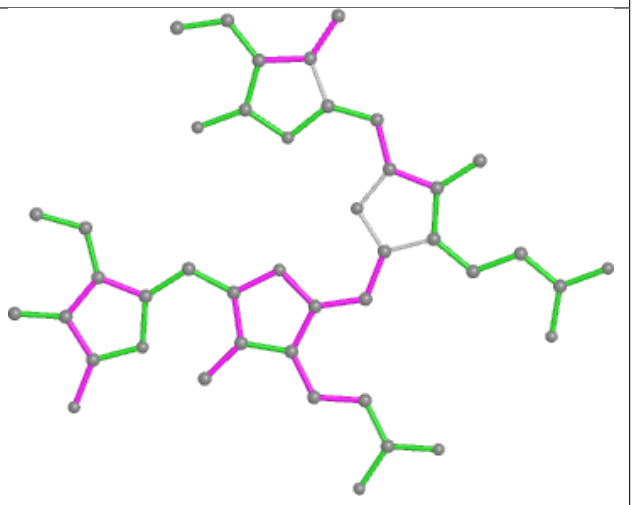

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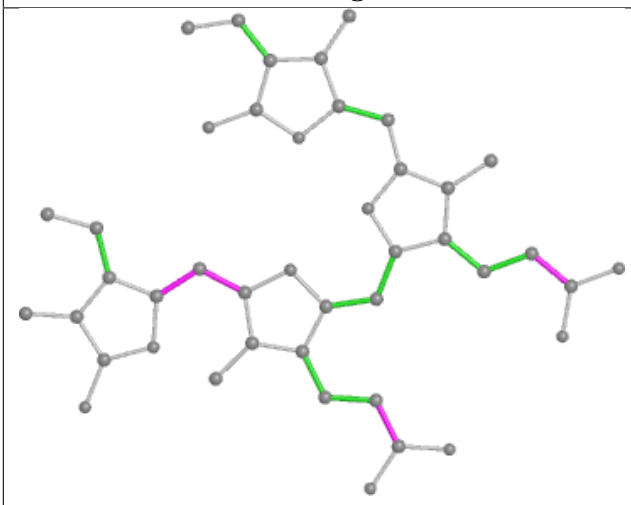

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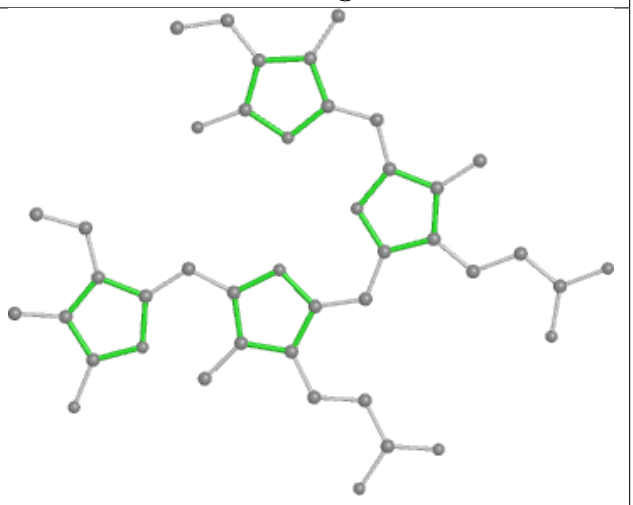
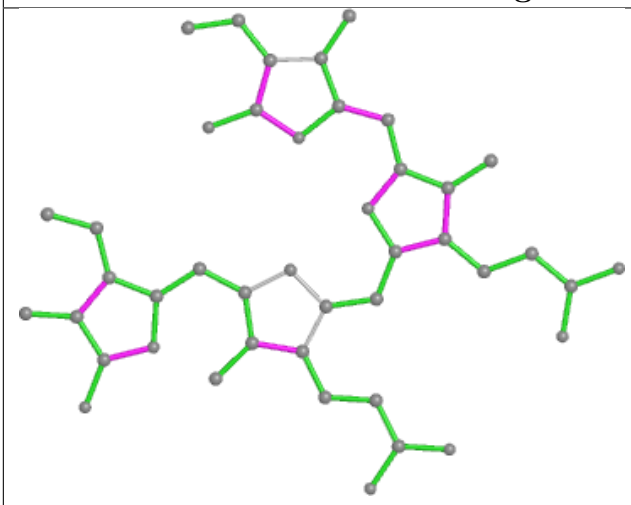


Rings

Ligand PUB P3 203



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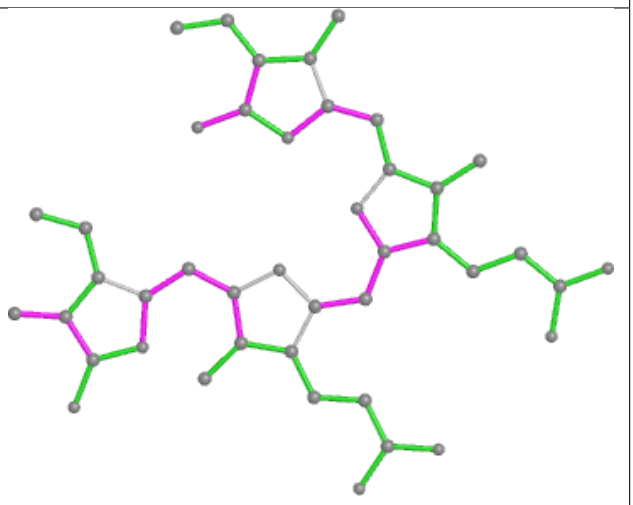

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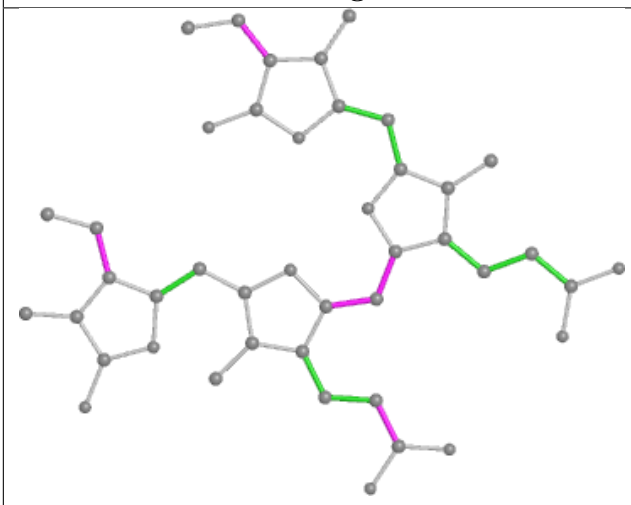

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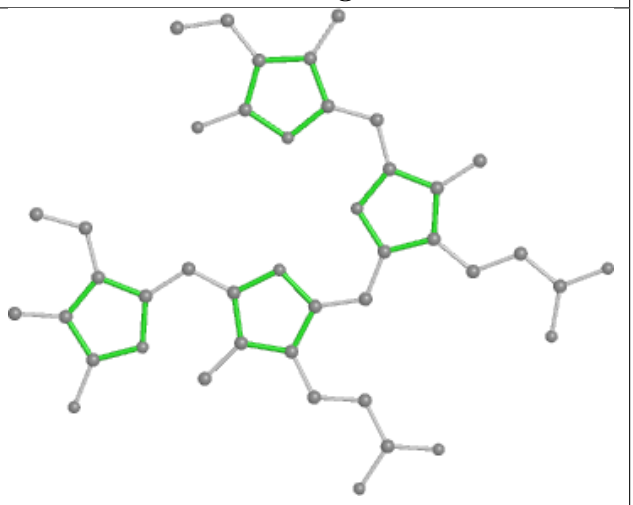
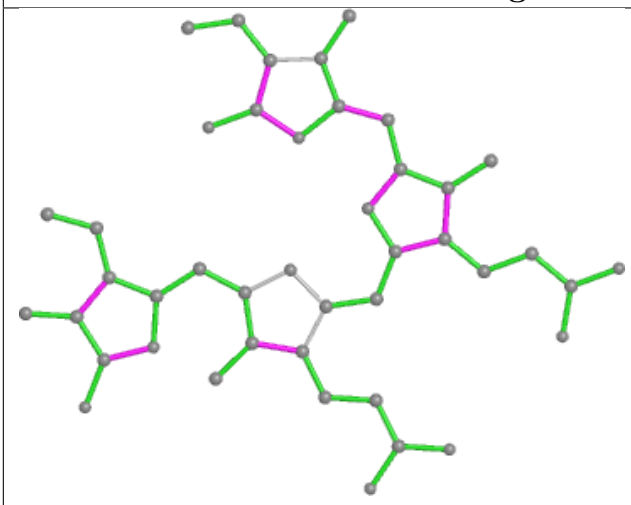


Rings

Ligand PUB 34 1006



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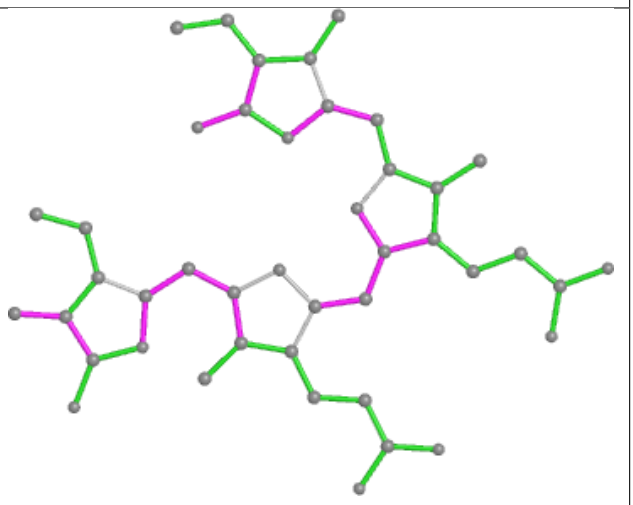

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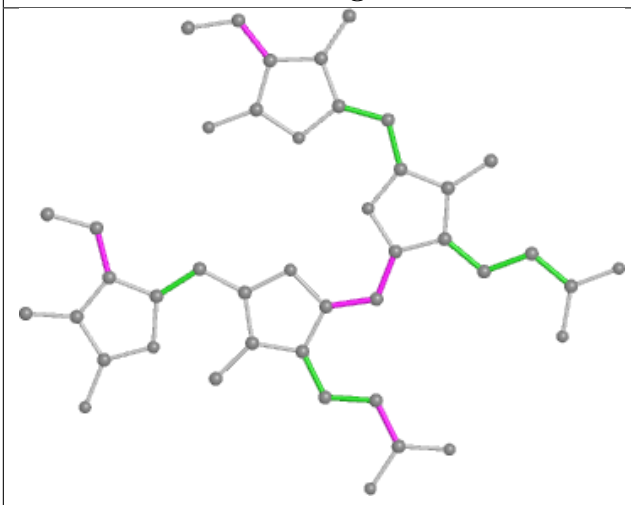

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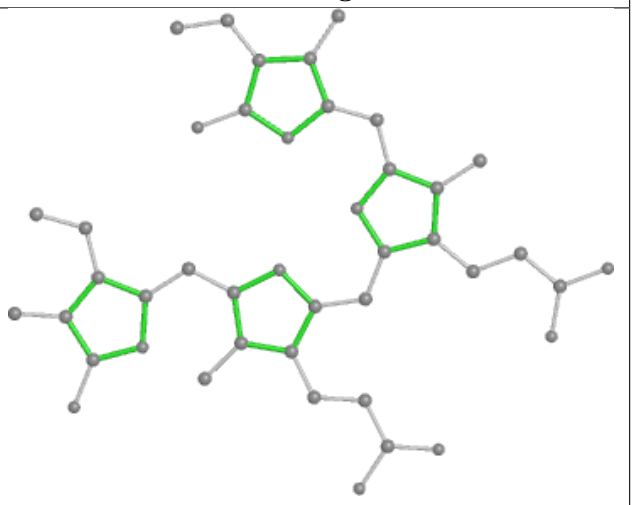

Rings

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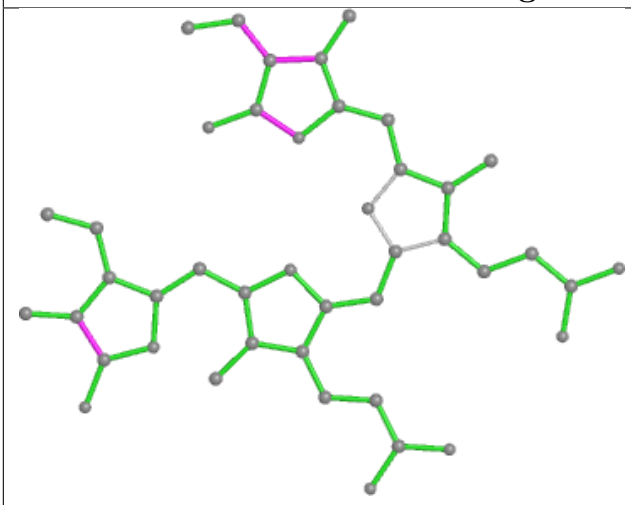

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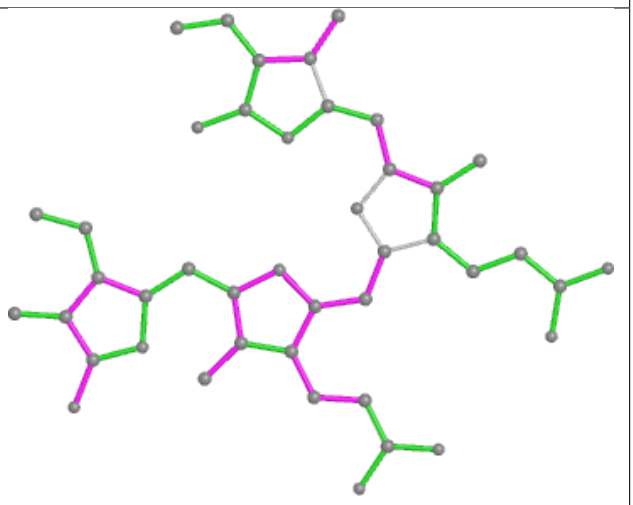

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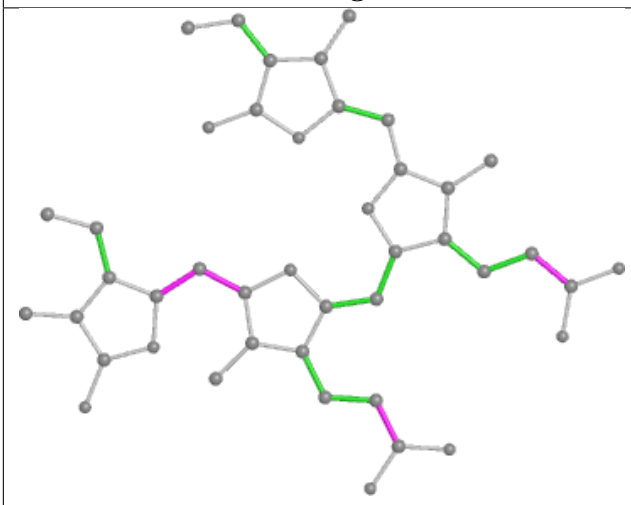

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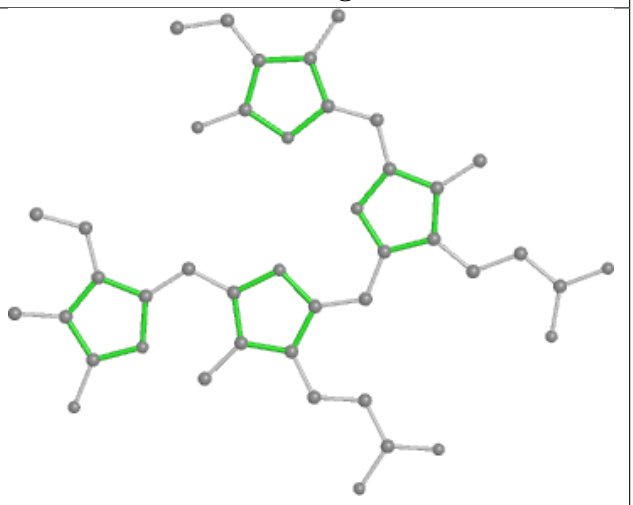

Rings

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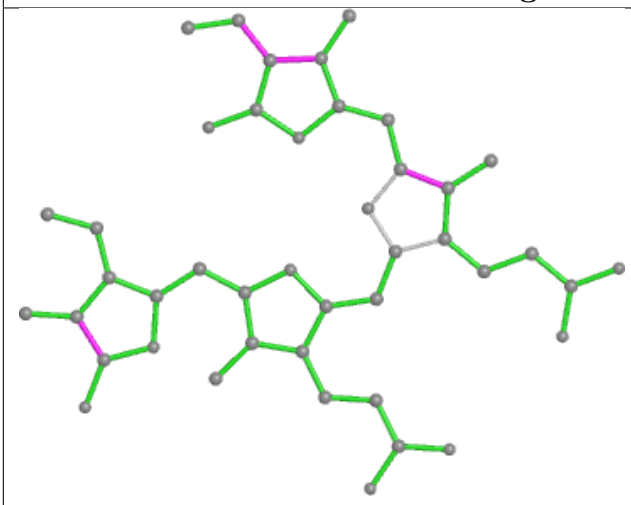

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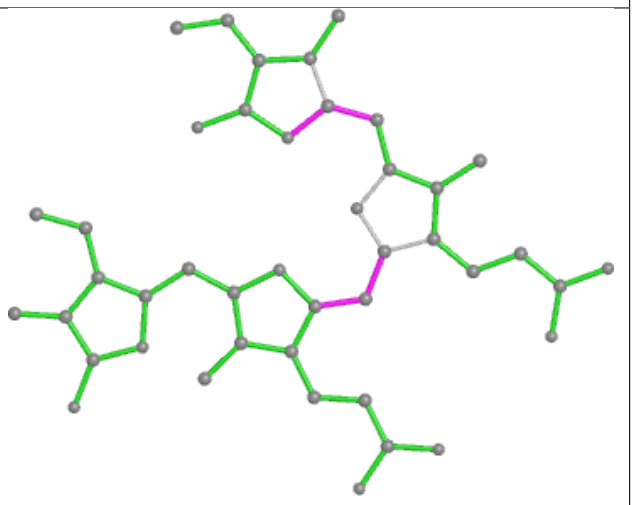

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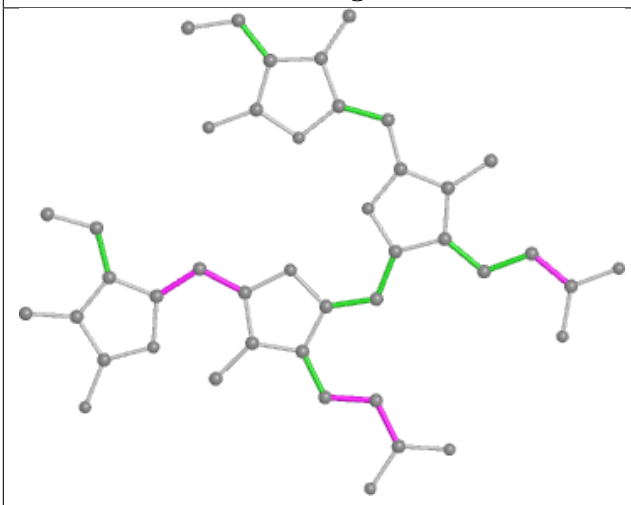

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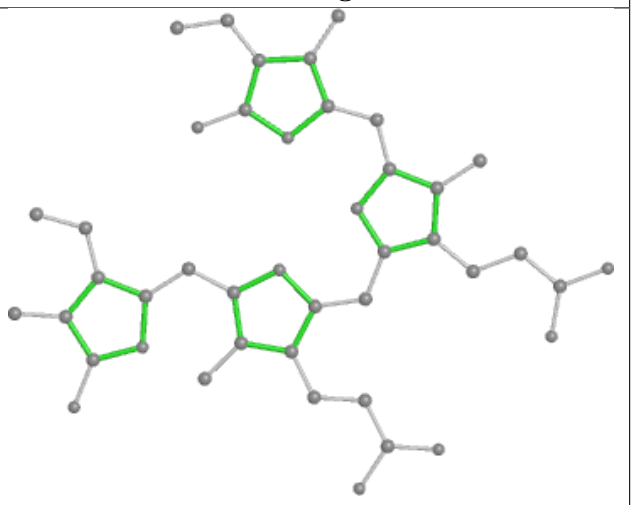
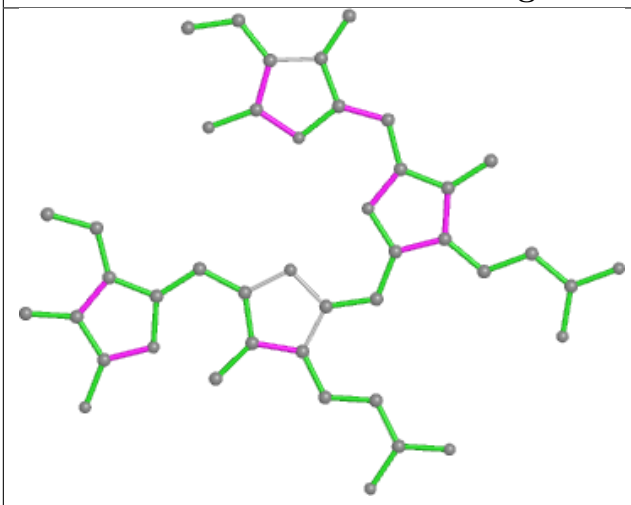


Rings

Ligand PUB av 203



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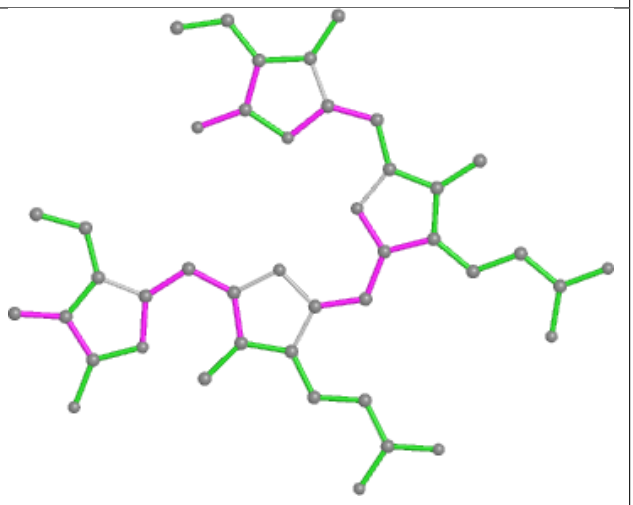

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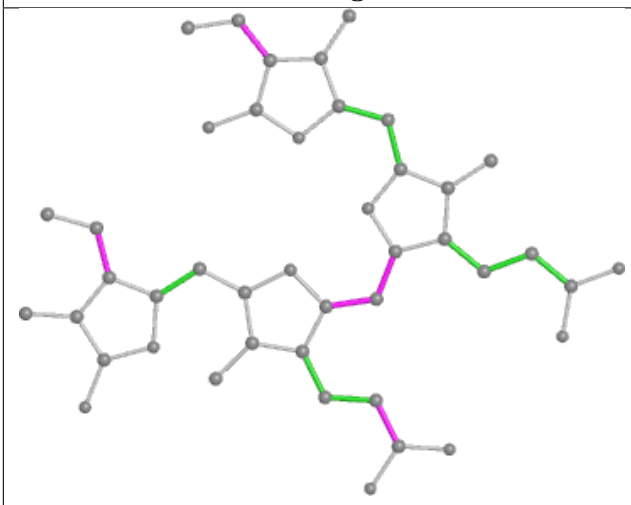

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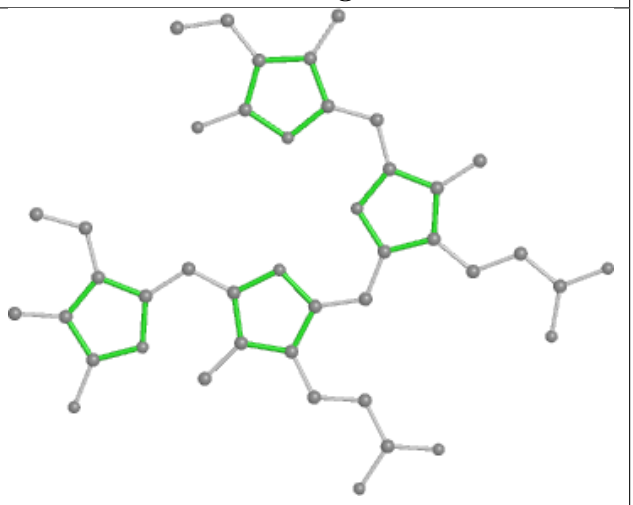
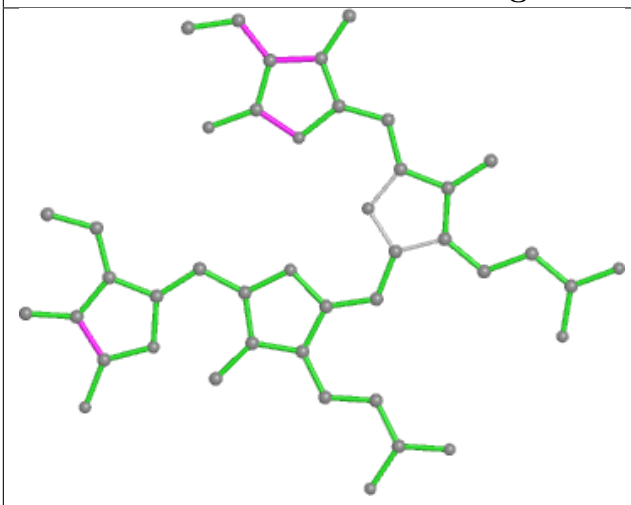


Rings

Ligand PEB b4 1001



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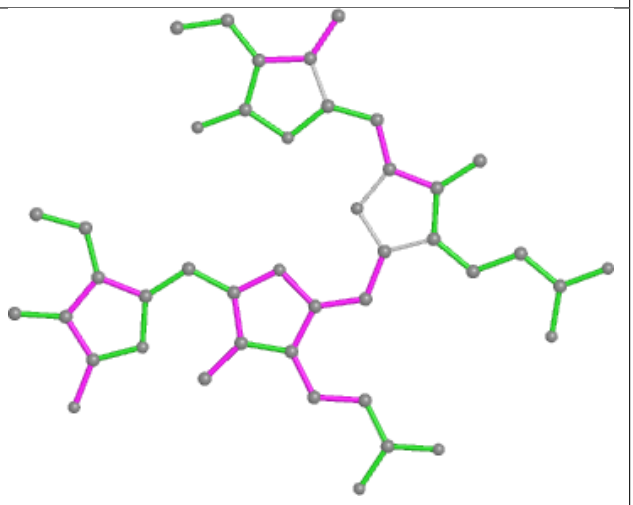

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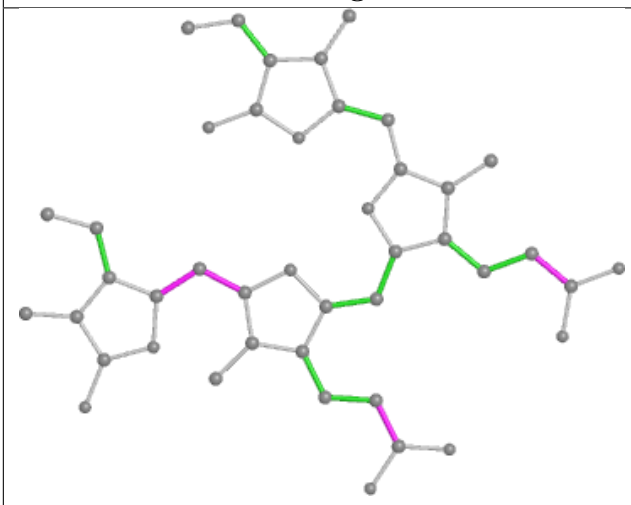

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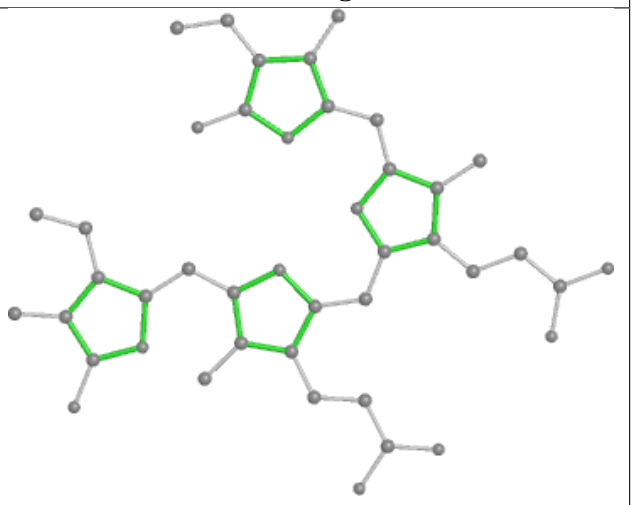
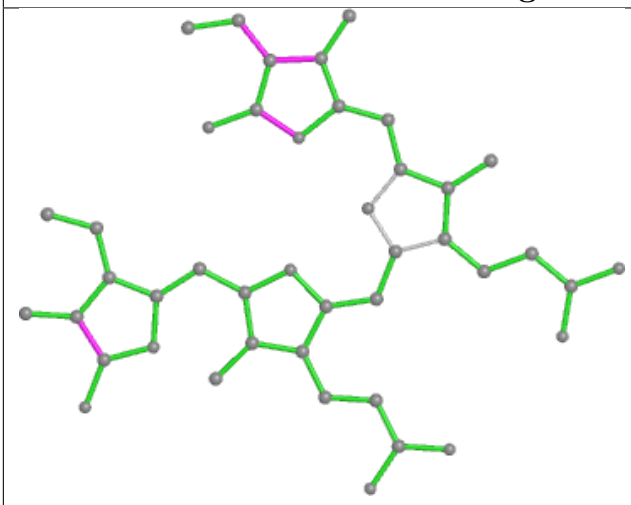


Rings

Ligand PEB d4 201



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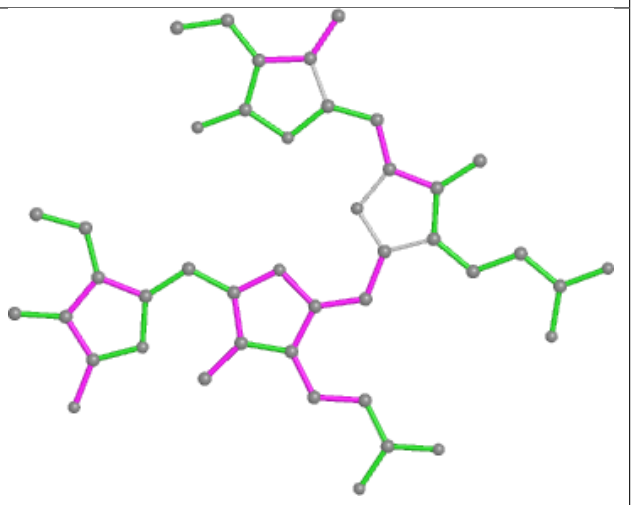

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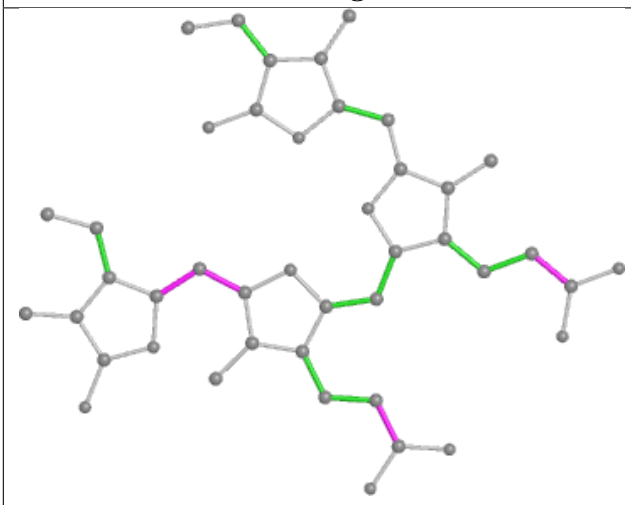

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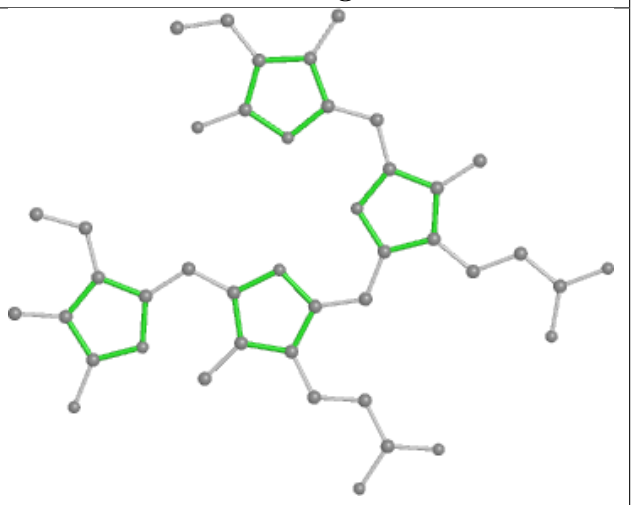

Rings

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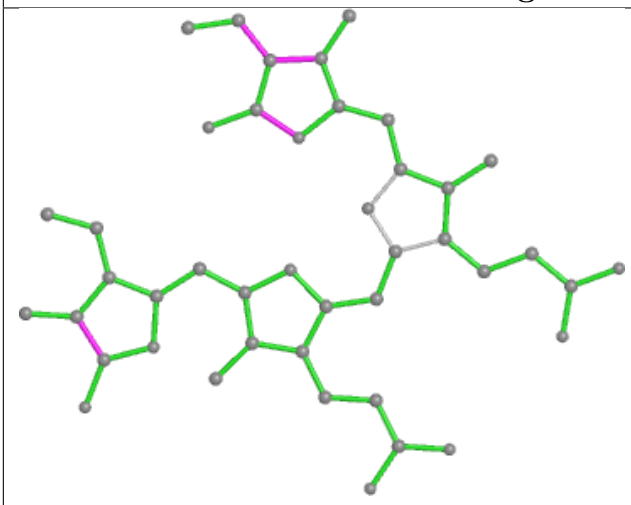

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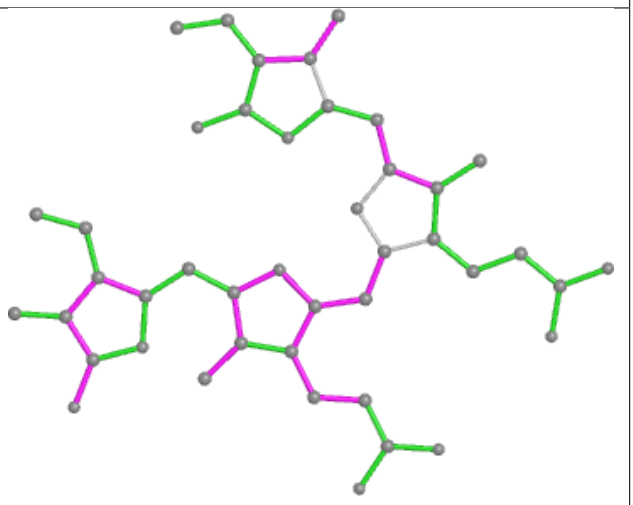

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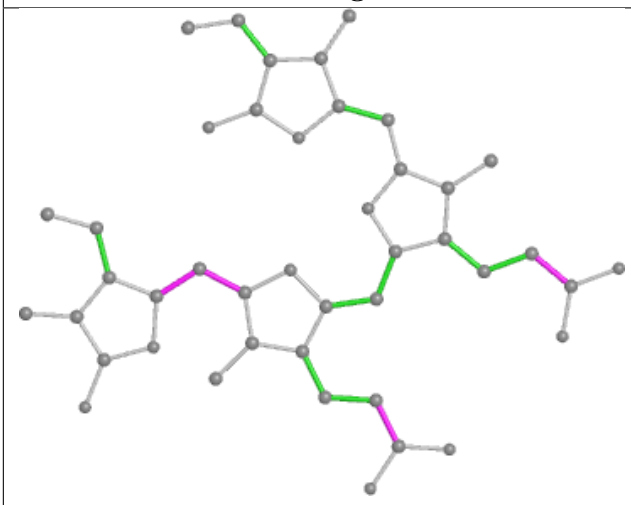

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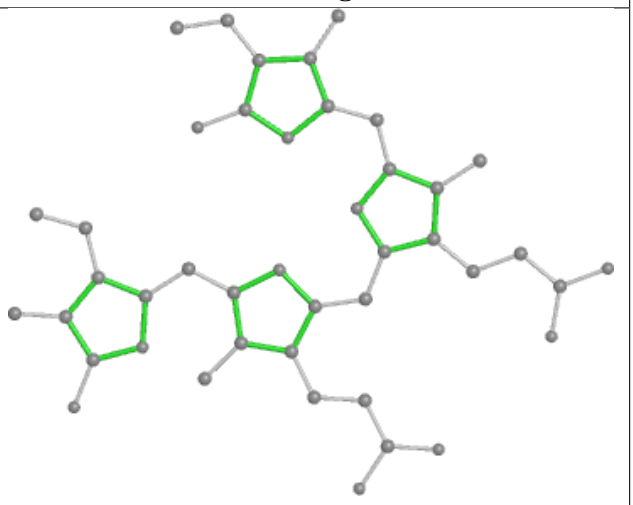

Rings

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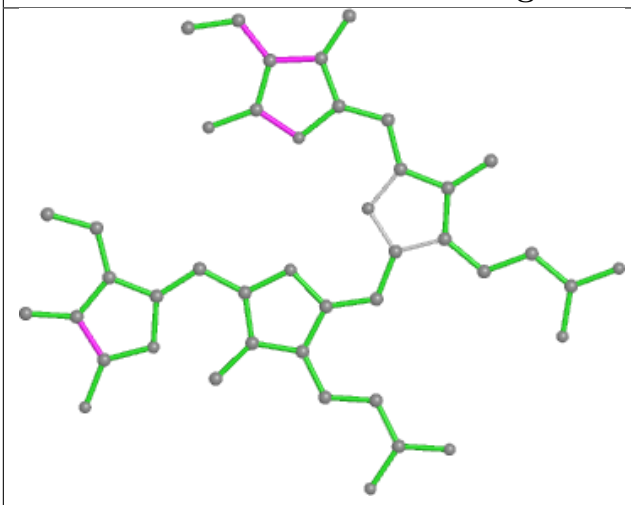

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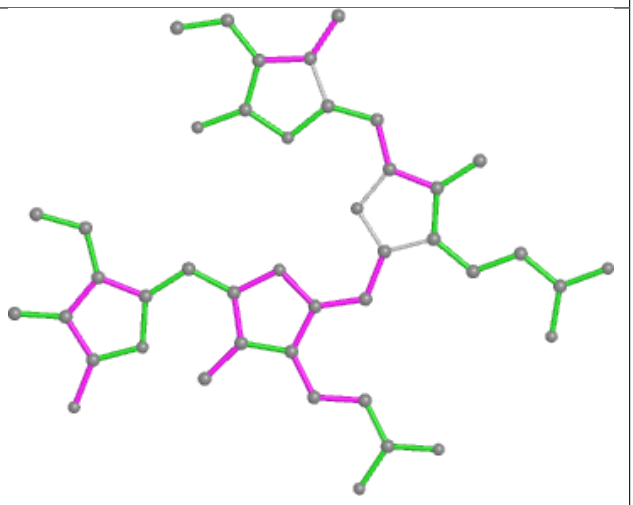

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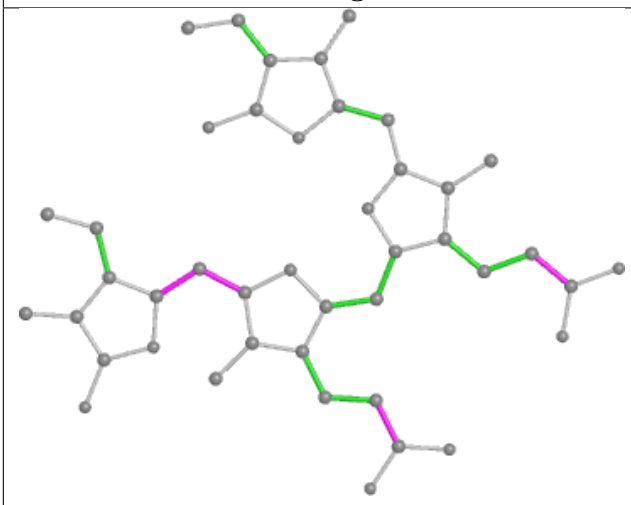

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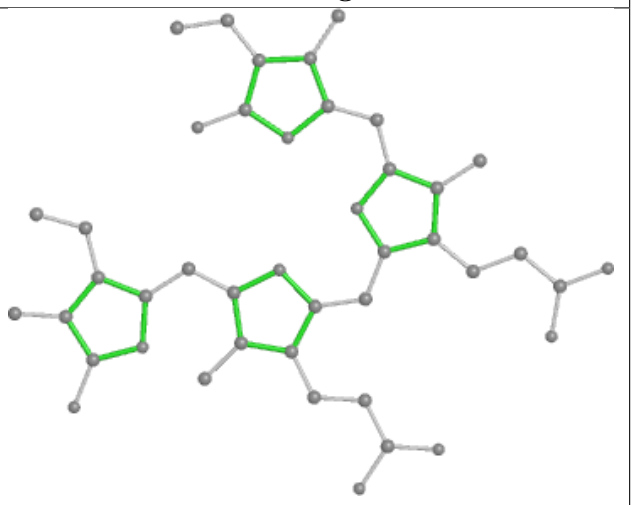
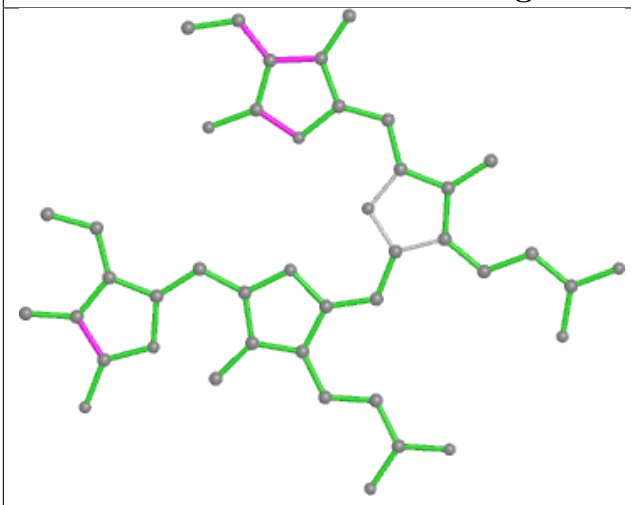


Rings

Ligand PEB aN 201



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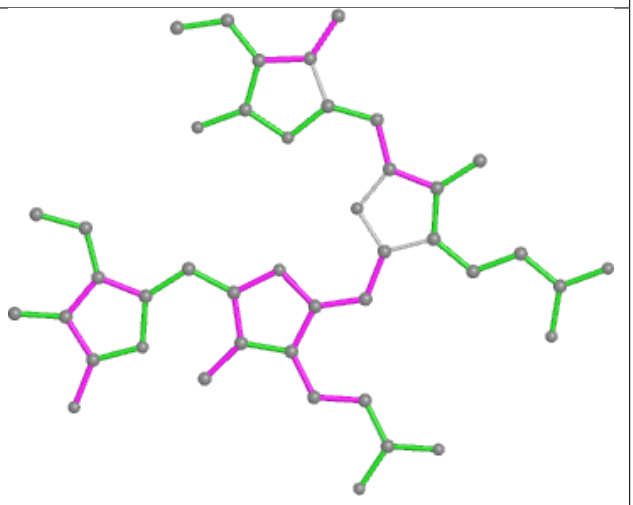
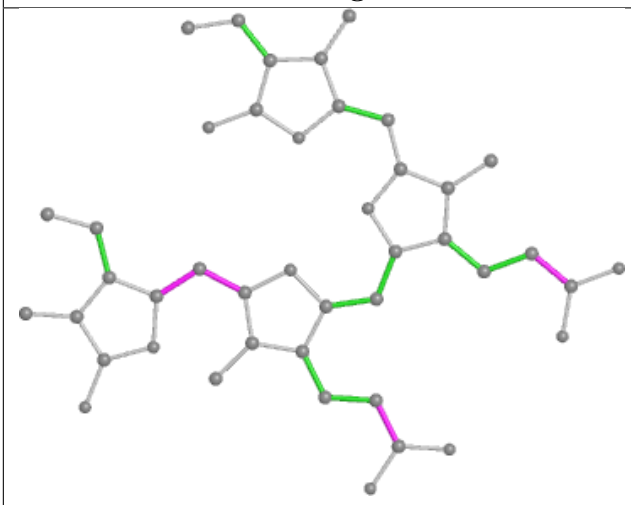
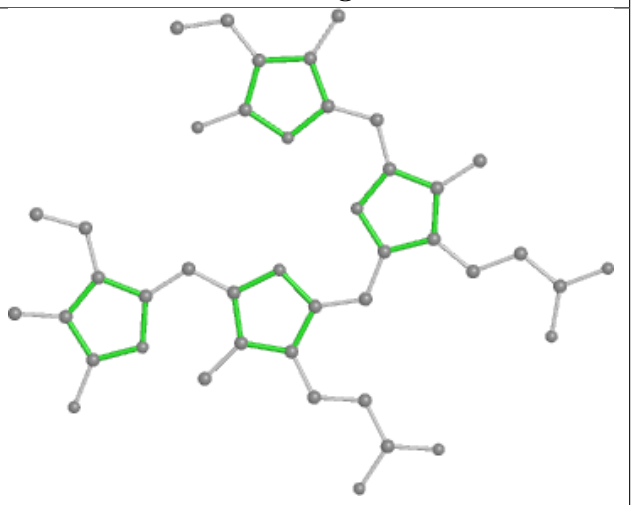


Bond angles

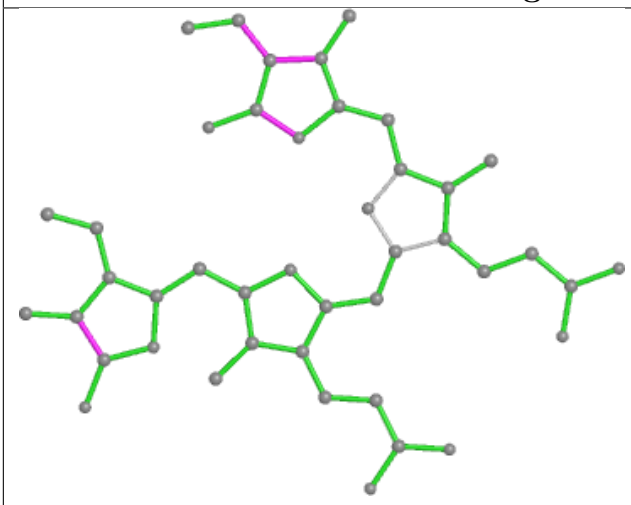


Torsions



Rings

Ligand PEB gf 201



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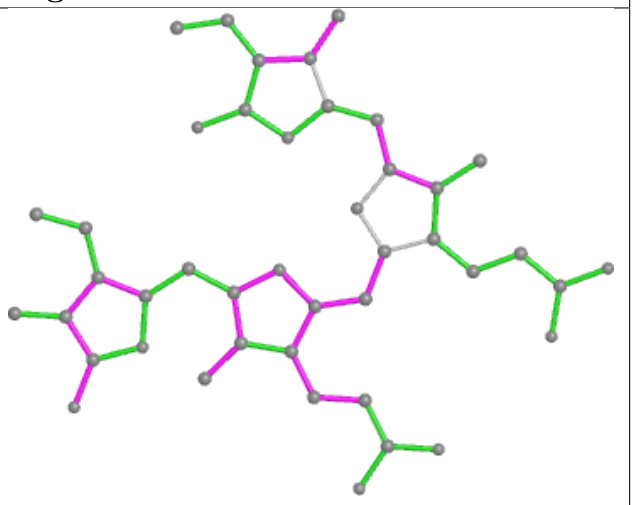

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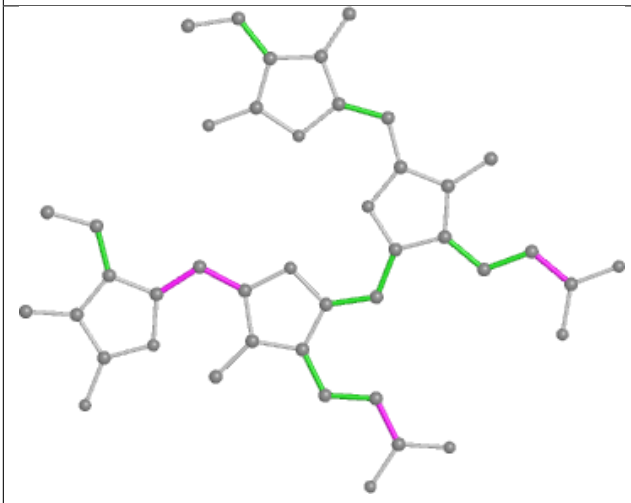

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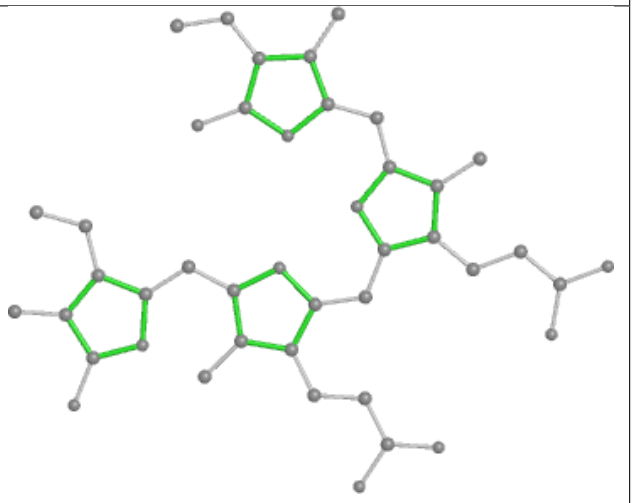
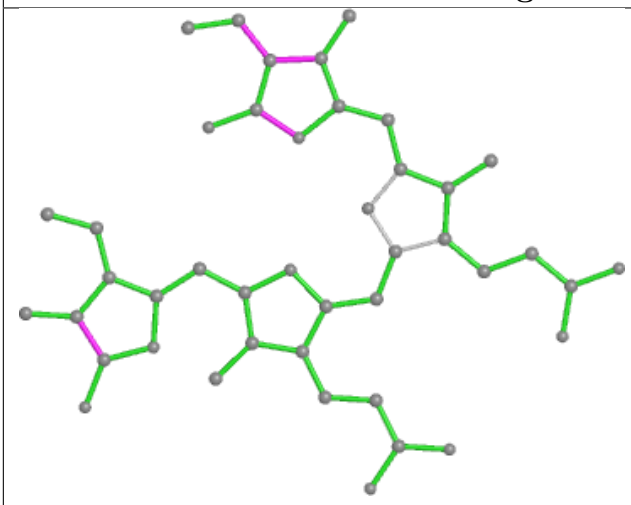


Rings

Ligand PEB cY 201



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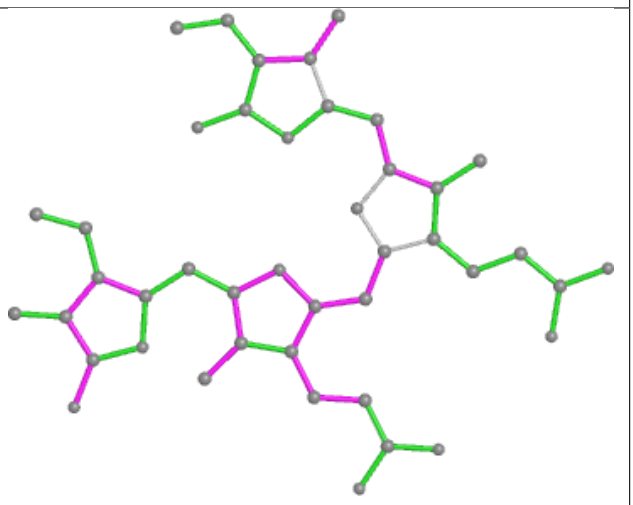

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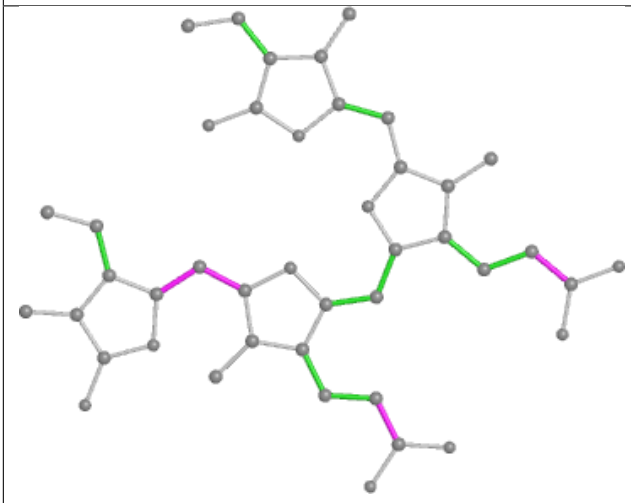

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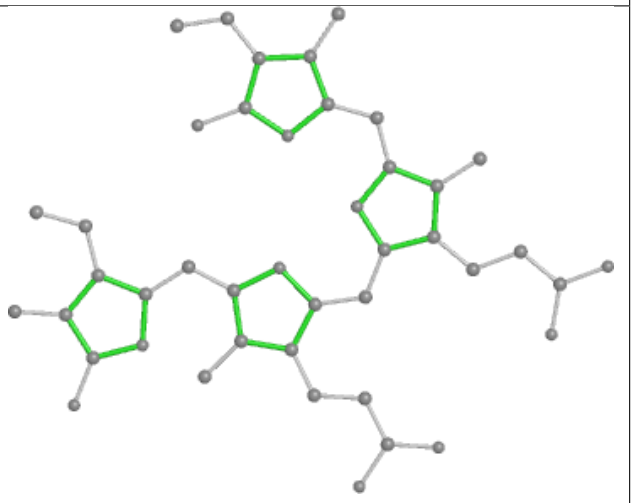
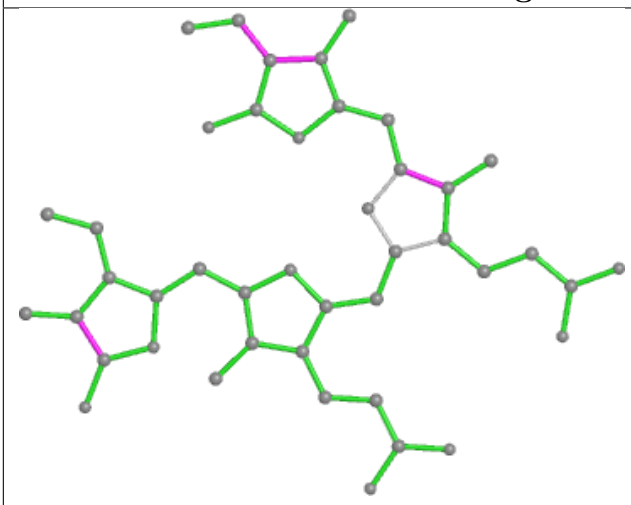


Rings

Ligand PEB U2 202



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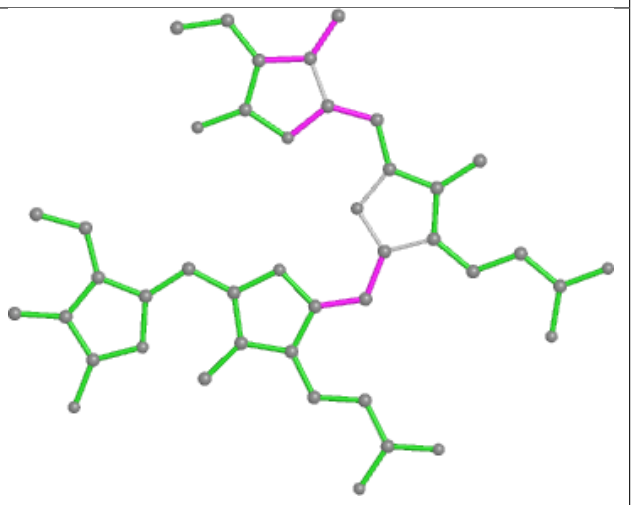

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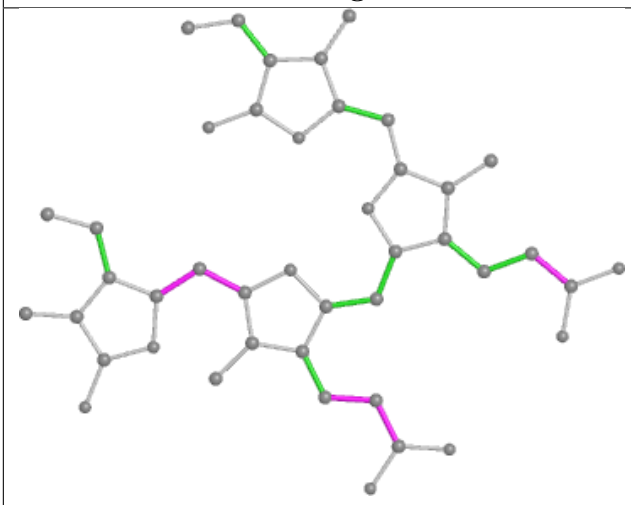

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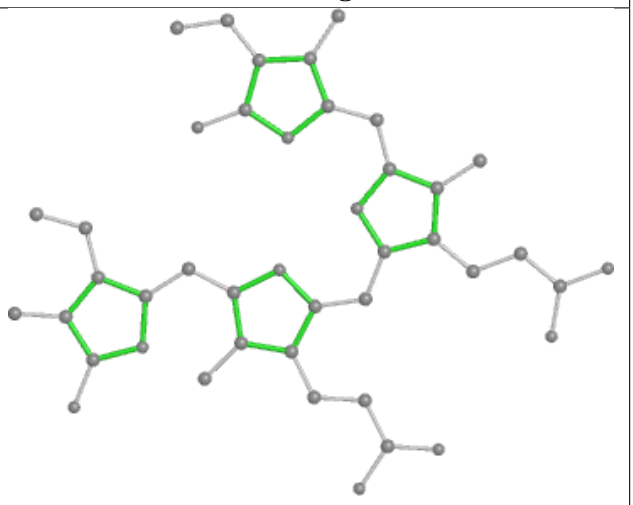
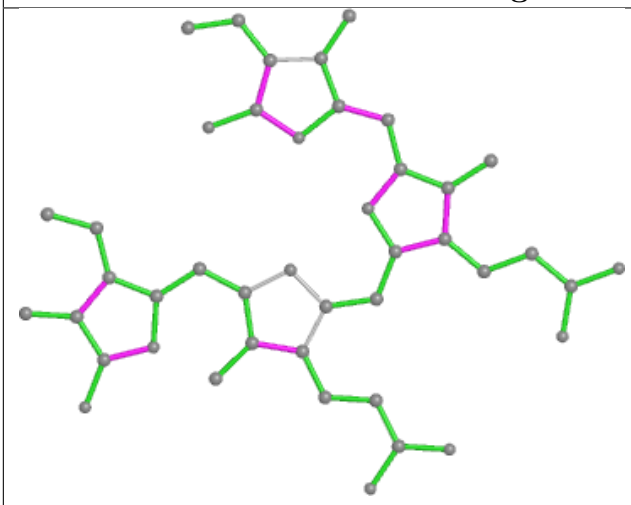


Rings

Ligand PUB ez 1006



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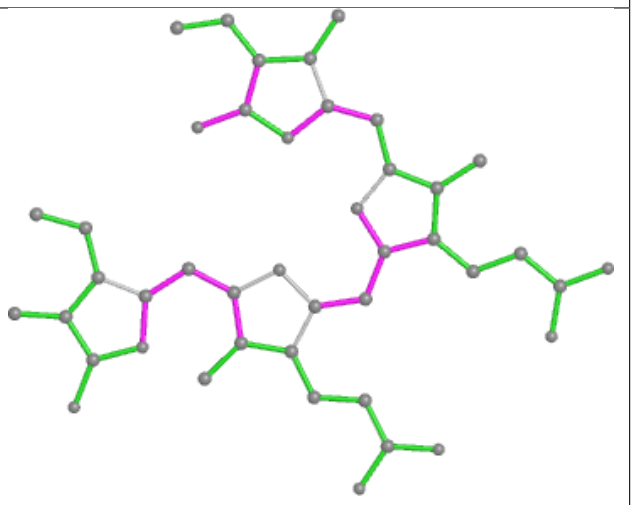

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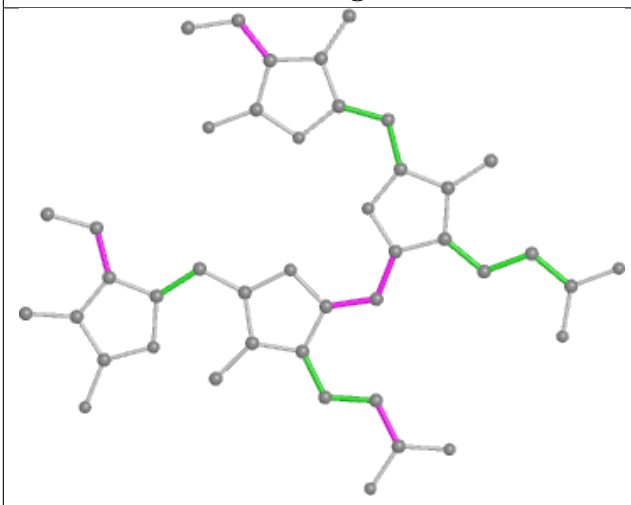

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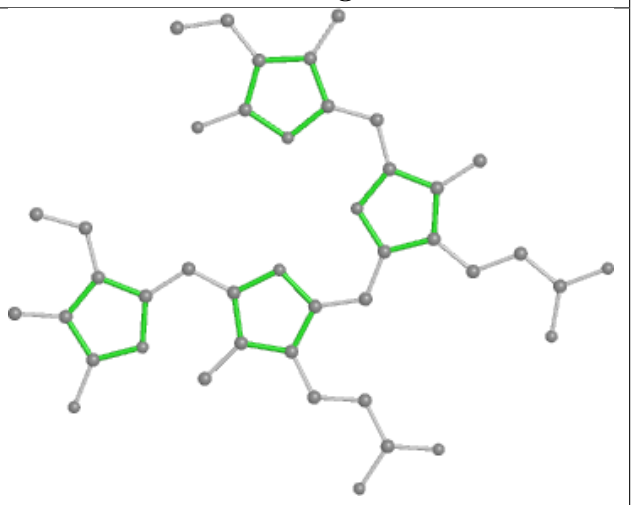
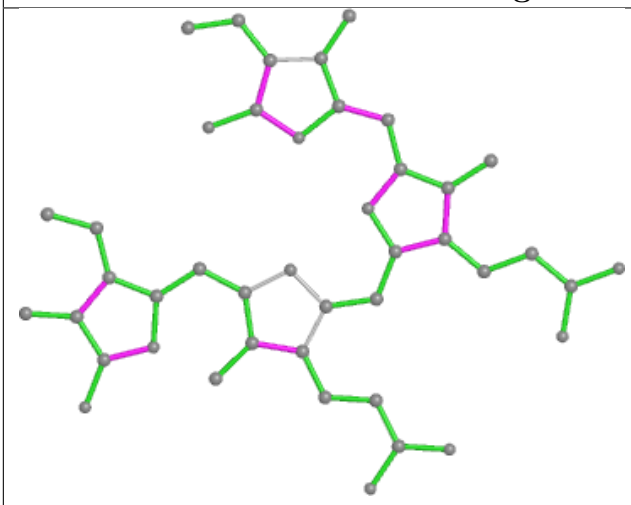


Rings

Ligand PUB R2 203



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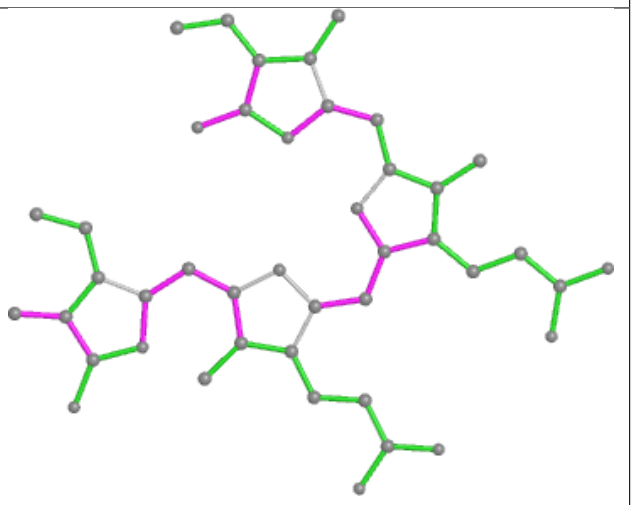

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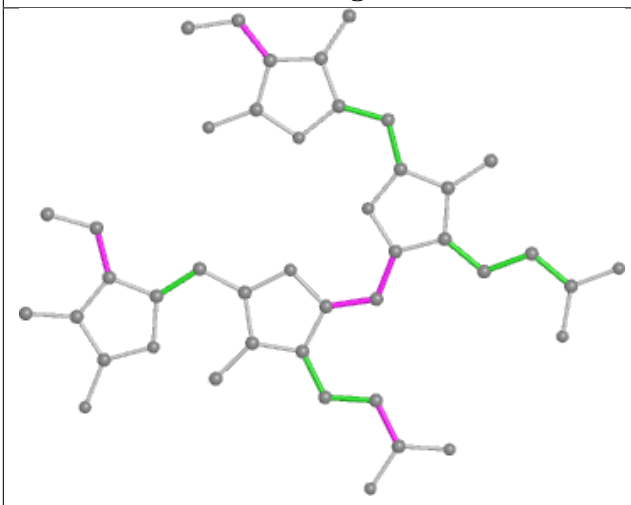

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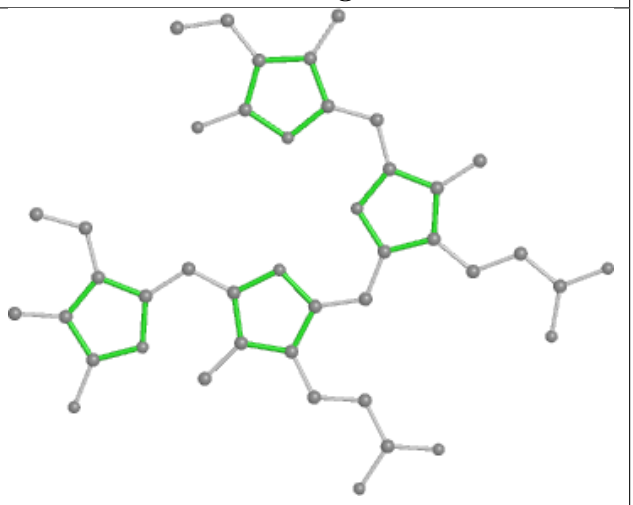
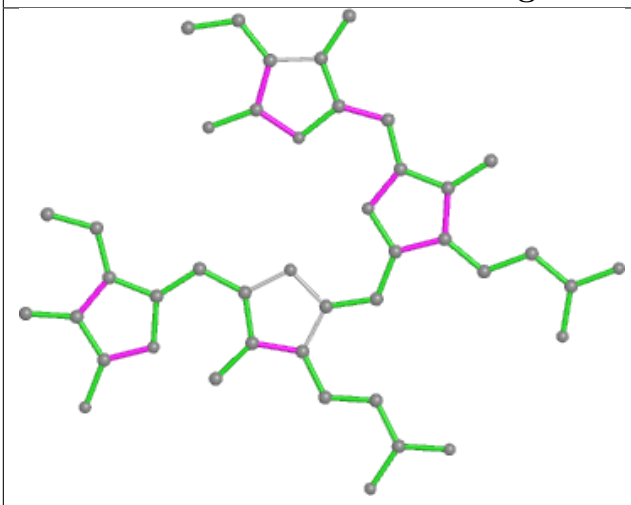


Rings

Ligand PUB a7 203



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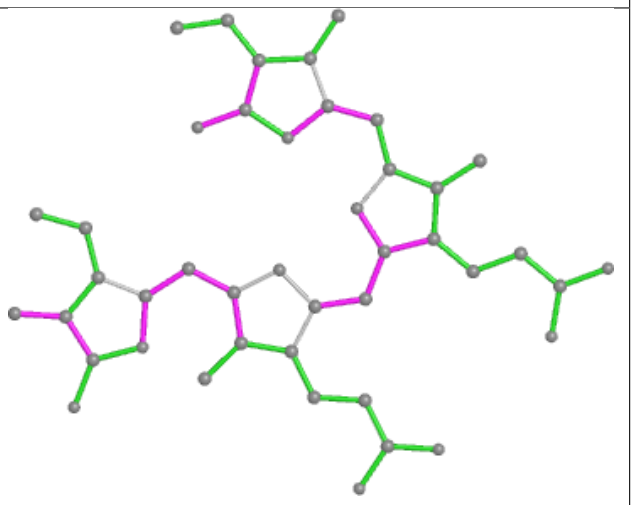

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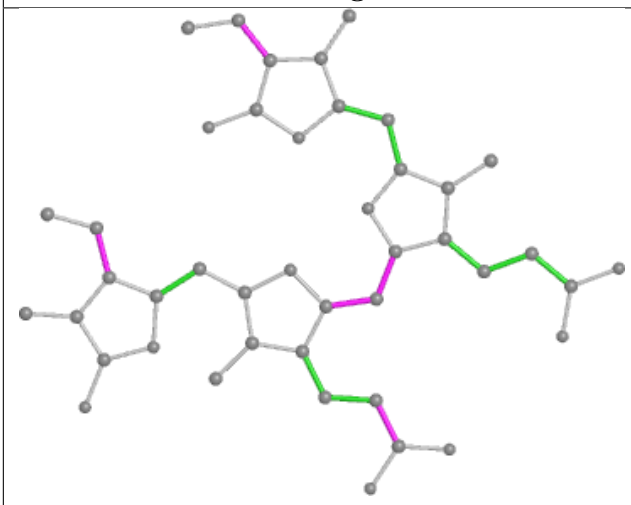

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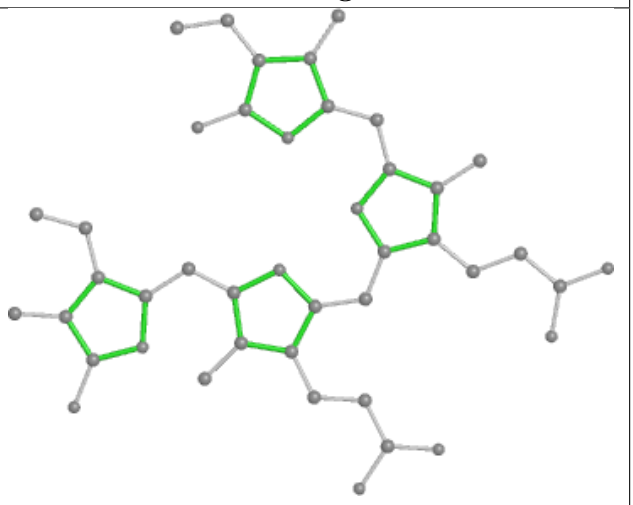
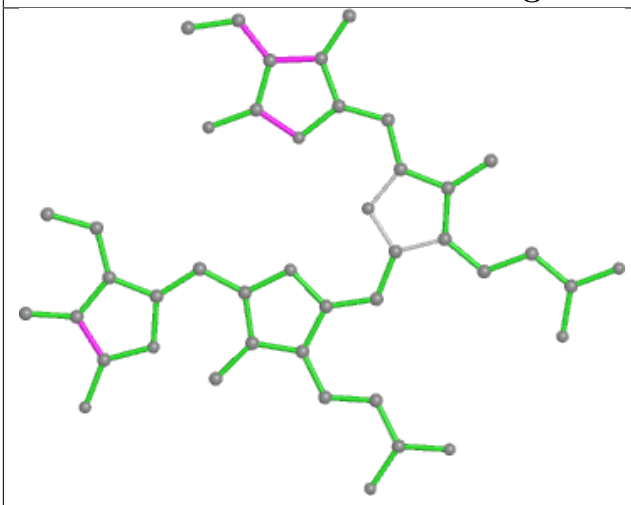


Rings

Ligand PEB j9 202



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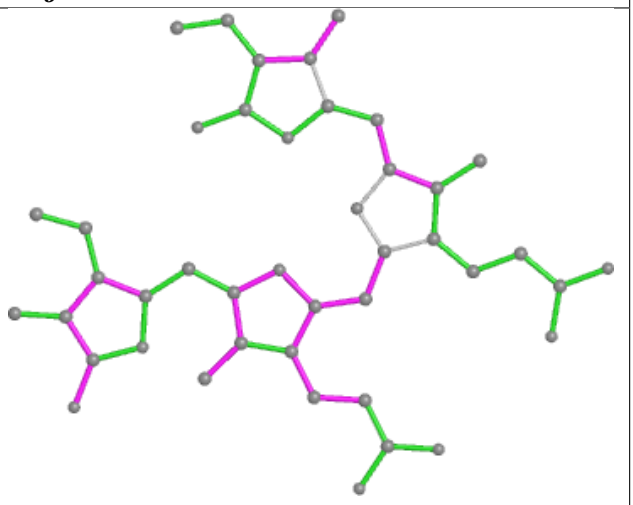

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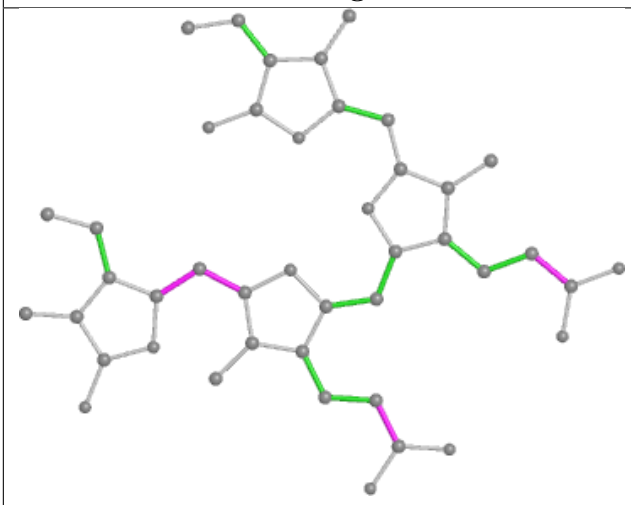

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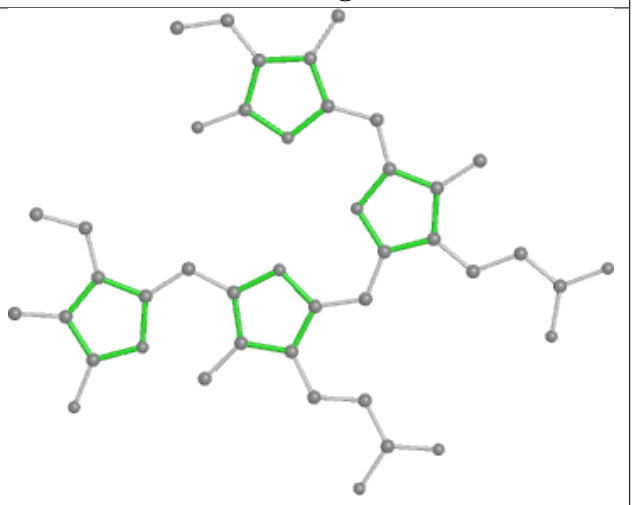
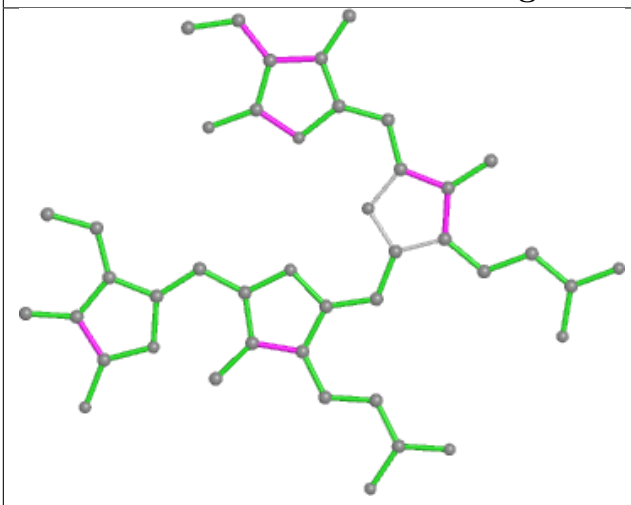


Rings

Ligand PEB gd 201



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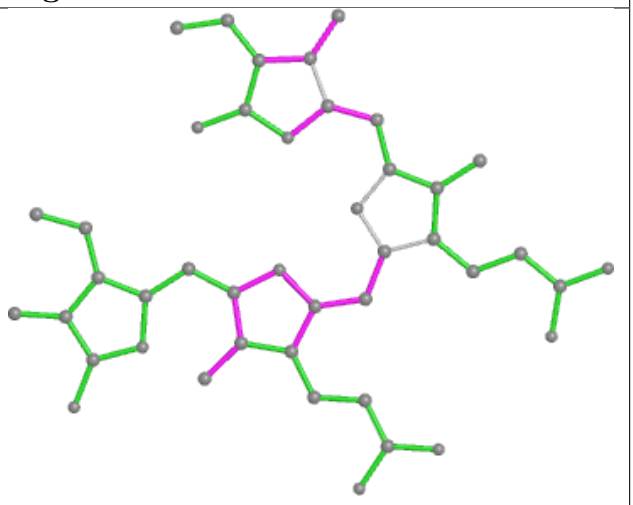

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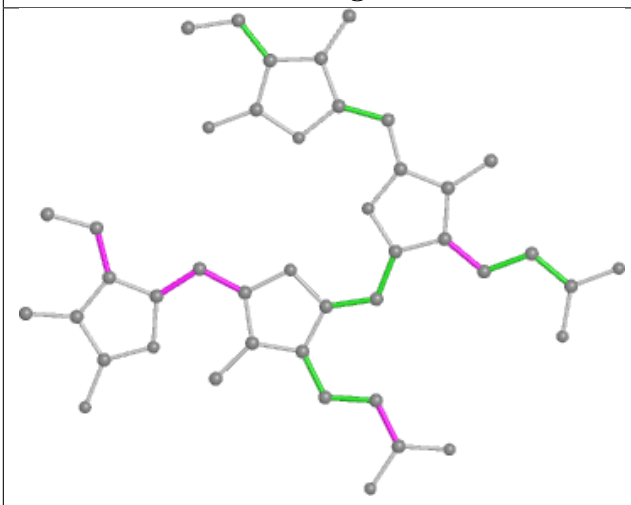

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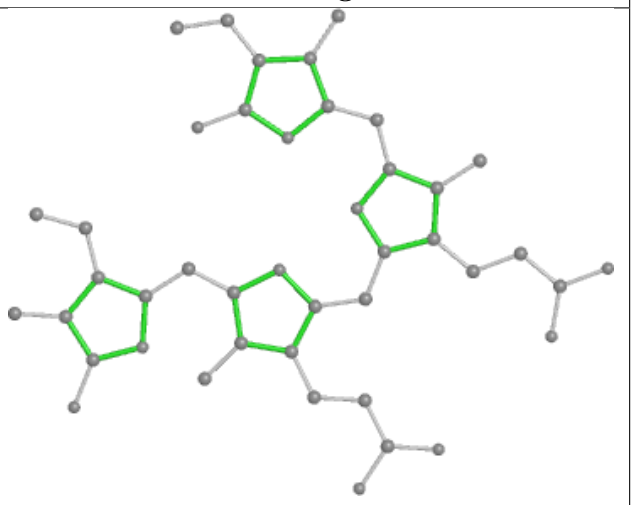

Rings

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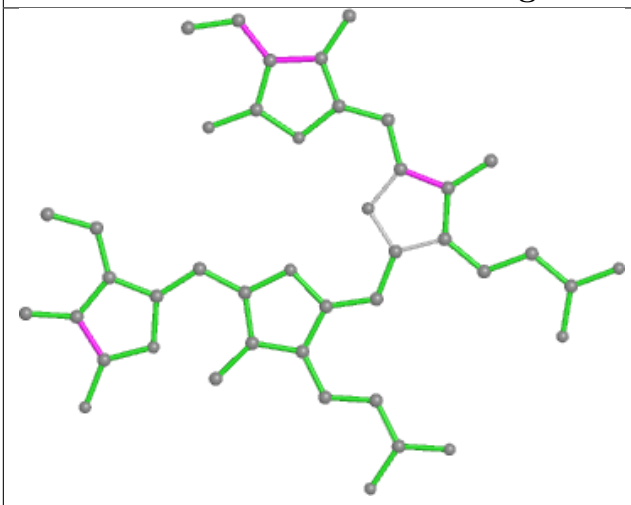

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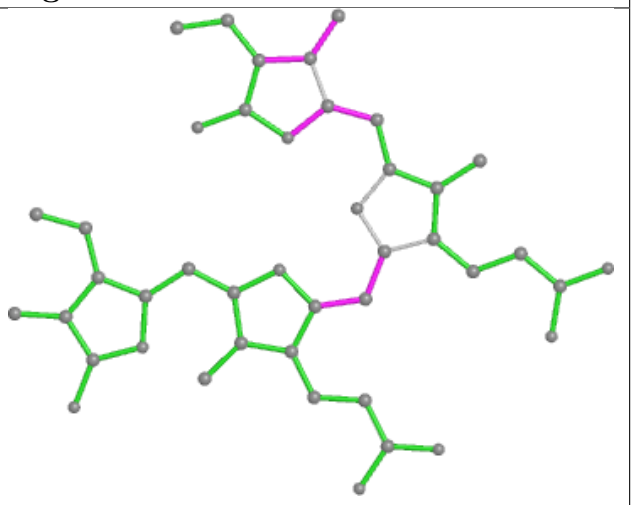

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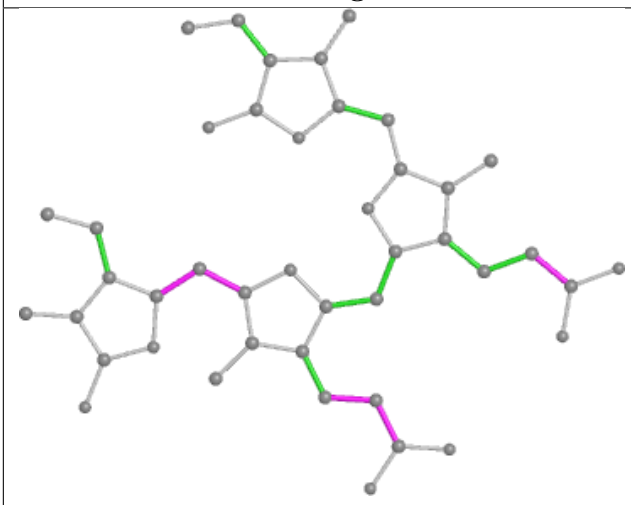

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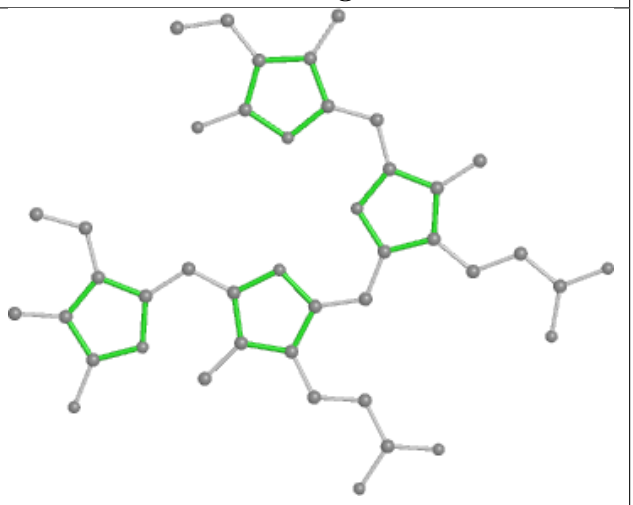
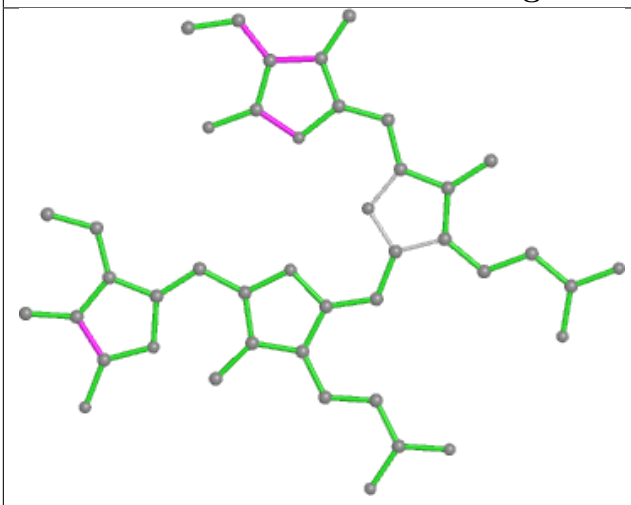


Rings

Ligand PEB eI 201



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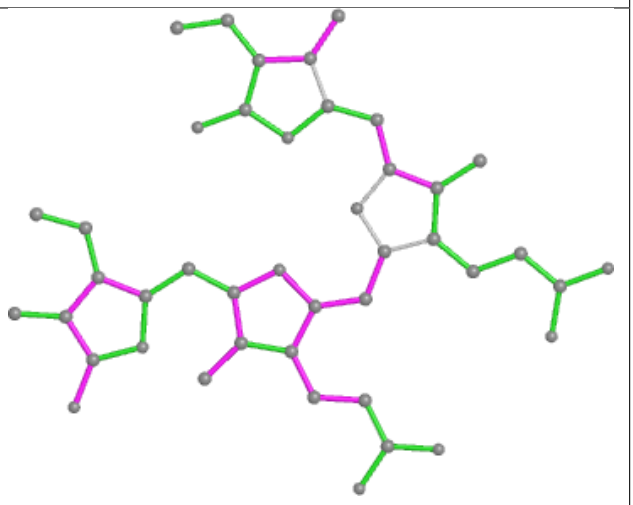

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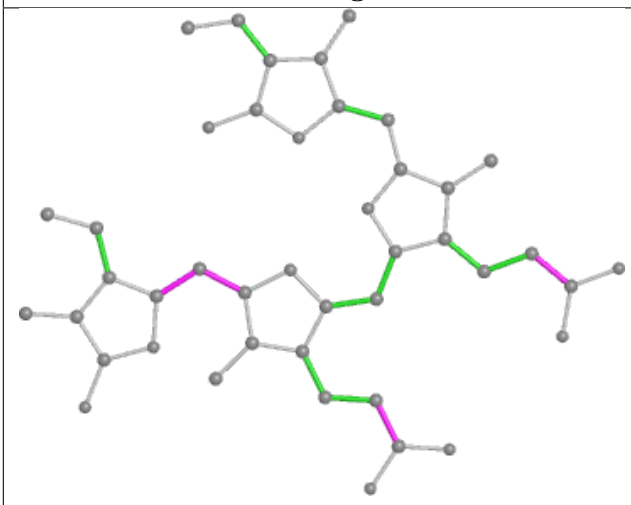

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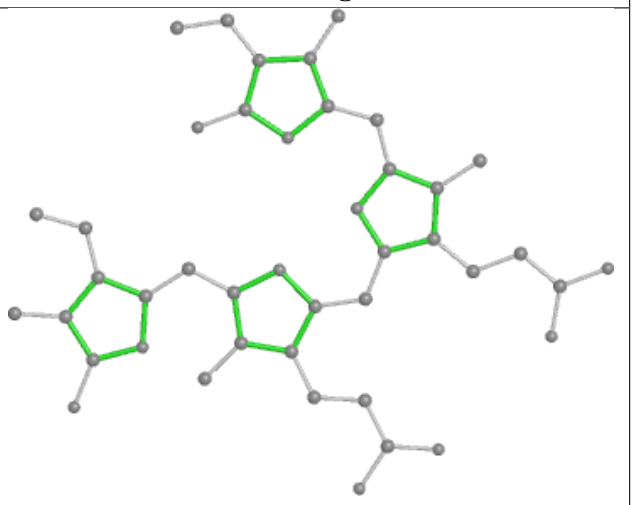
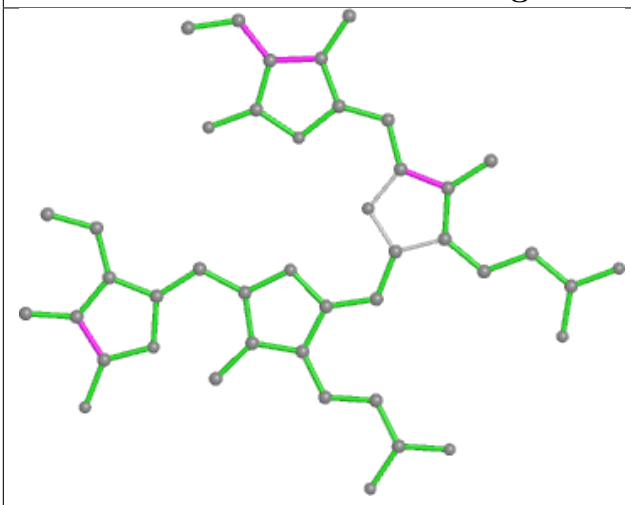


Rings

Ligand PEB ey 1001



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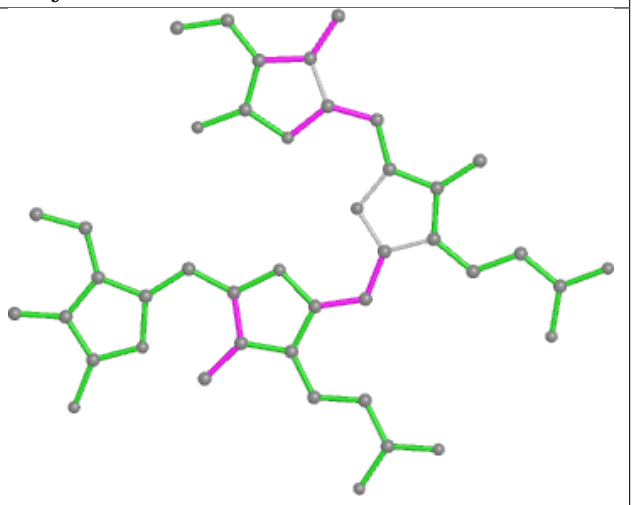

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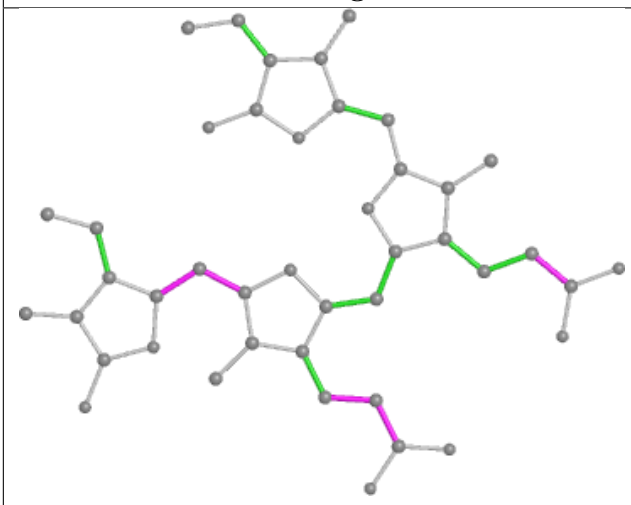

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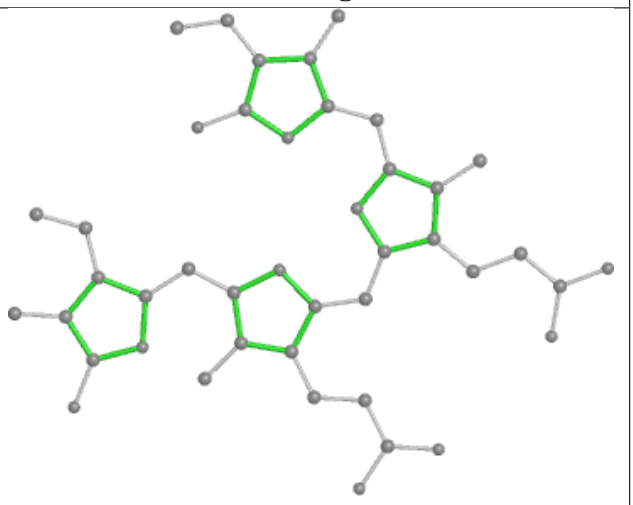
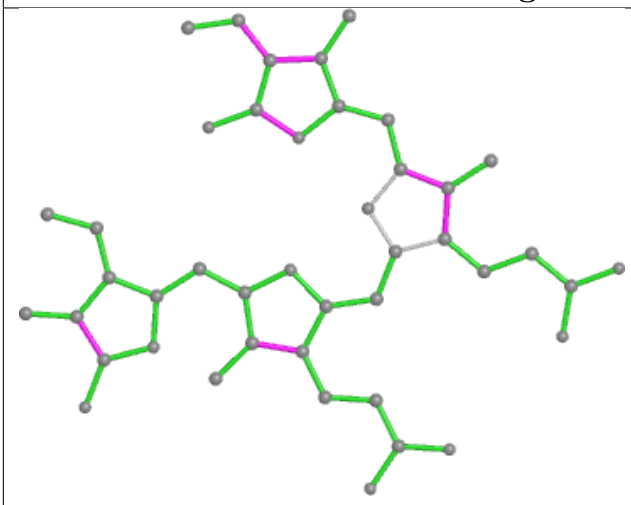


Rings

Ligand PEB gp 202



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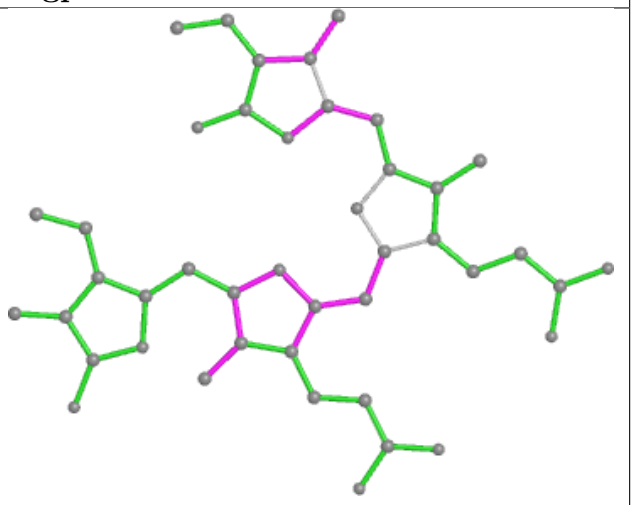

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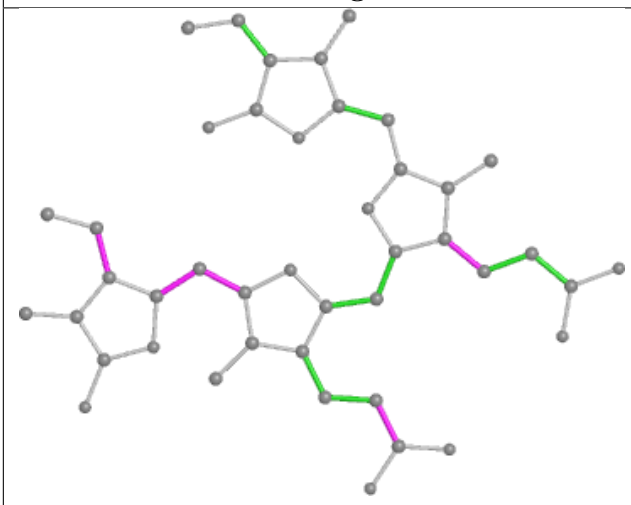

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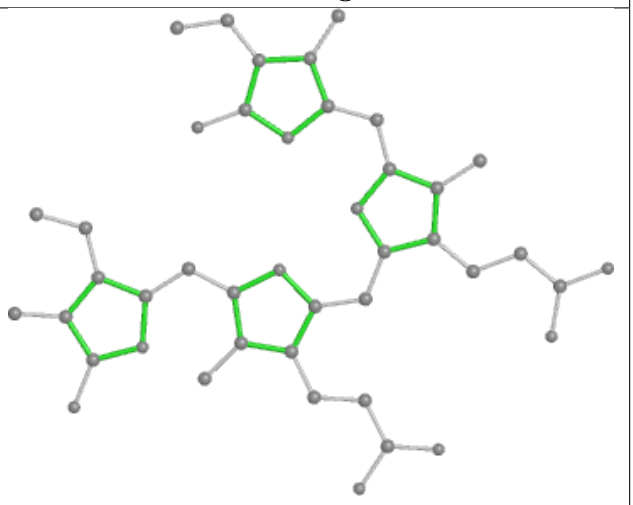
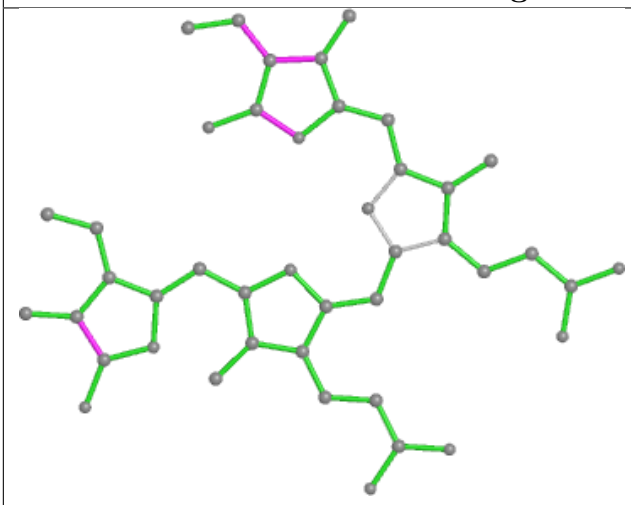


Rings

Ligand PEB y5 1001



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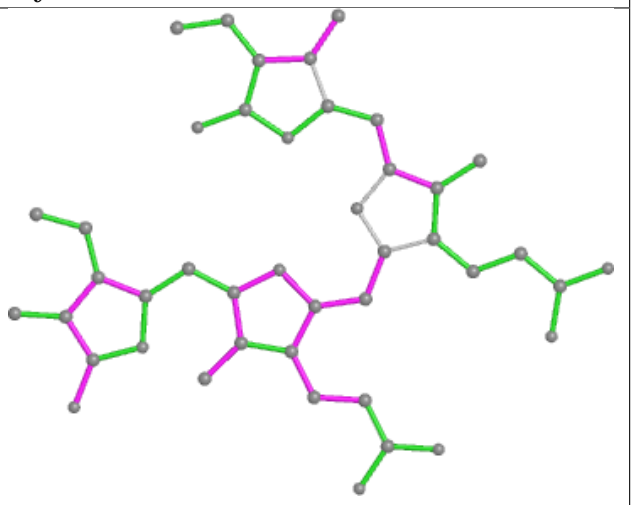
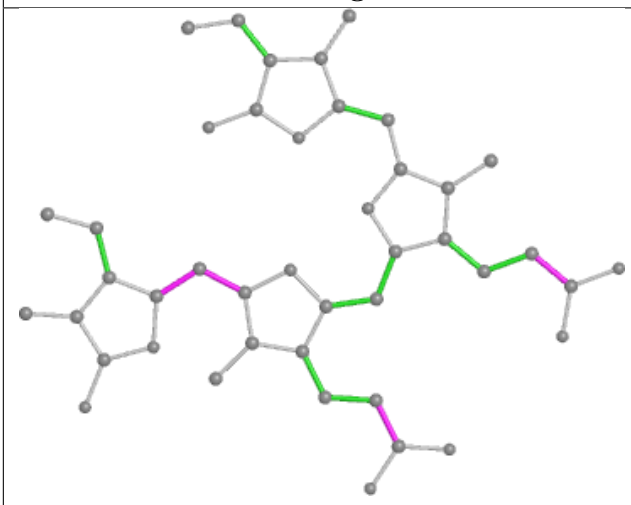


Bond angles



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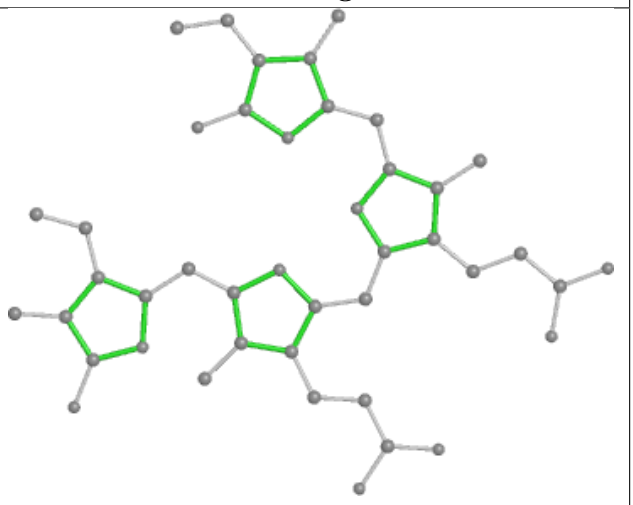
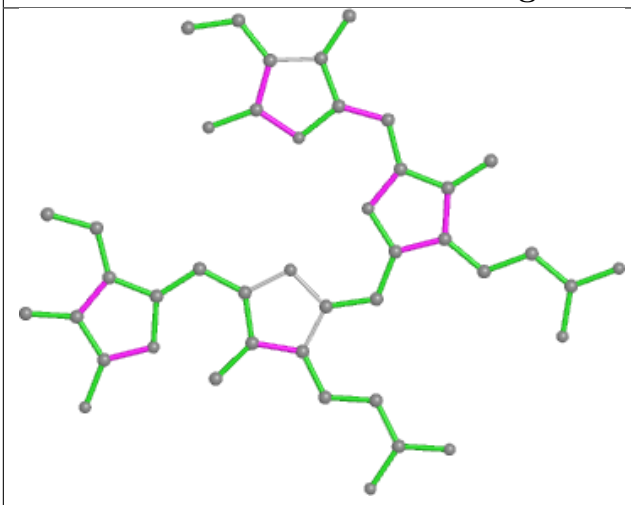


Rings

Ligand PUB c8 304



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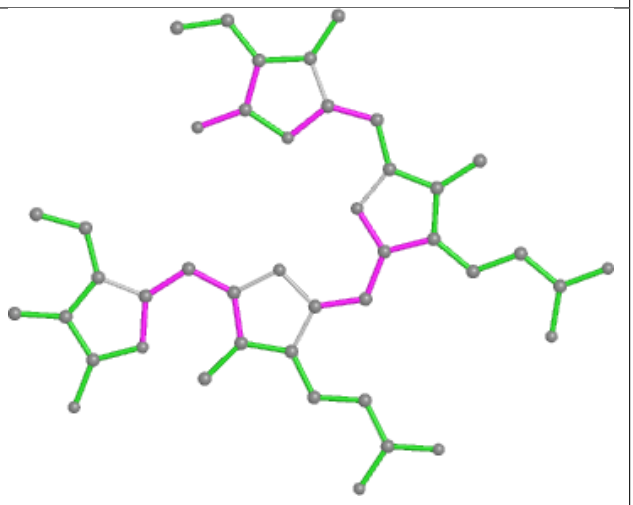

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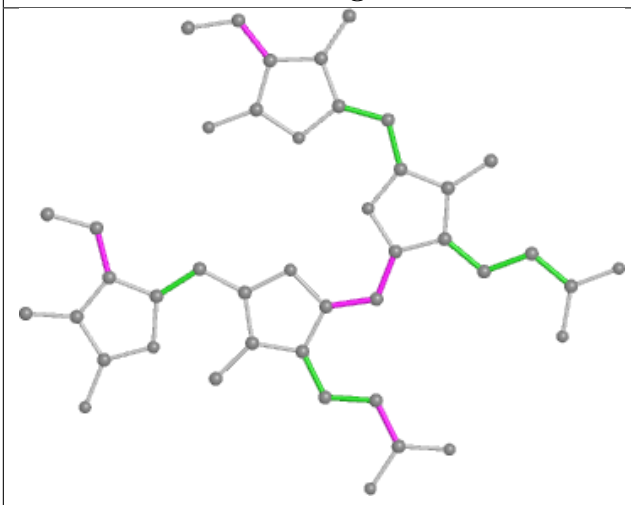
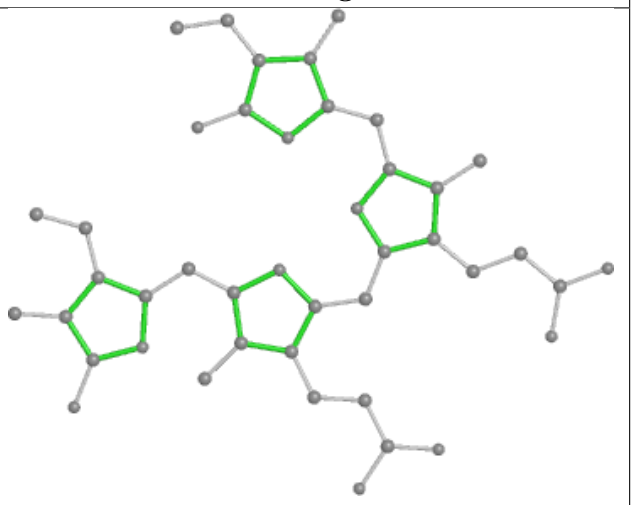
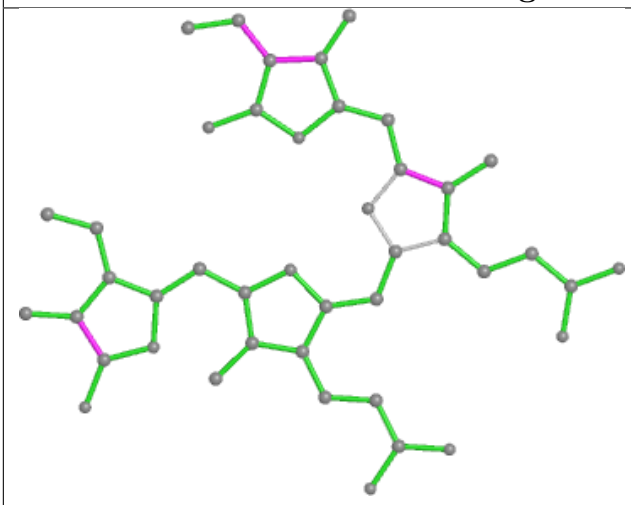


Torsions



Rings

Ligand PEB h5 202



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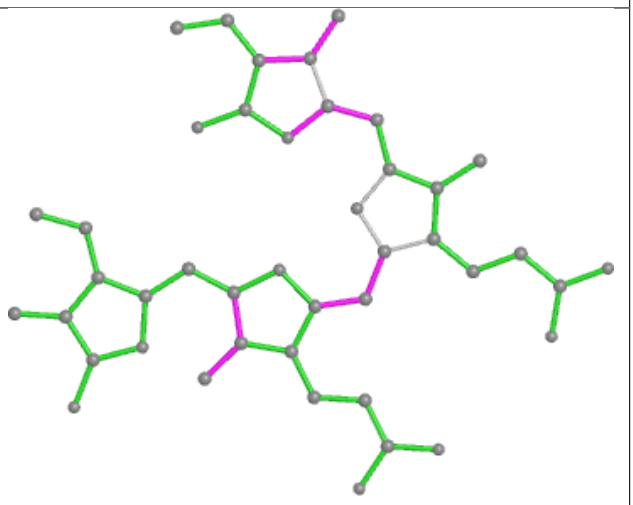

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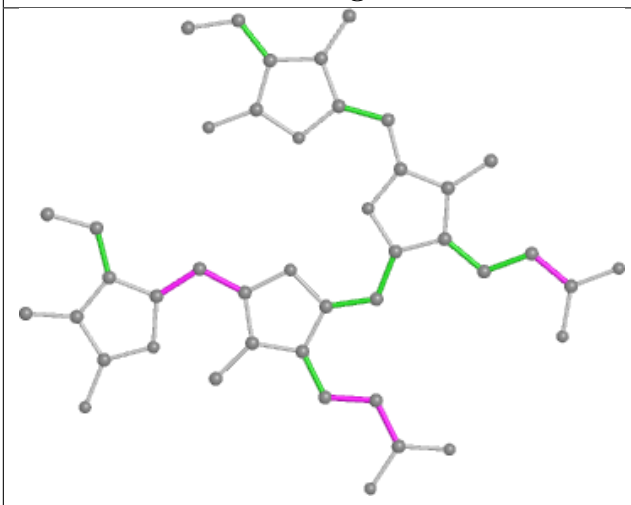

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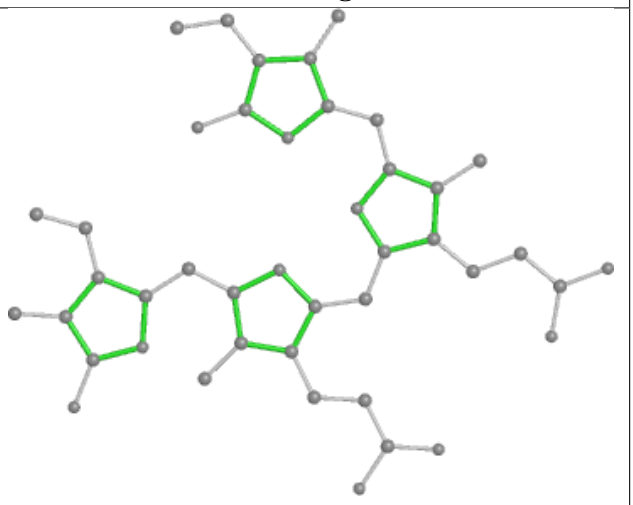
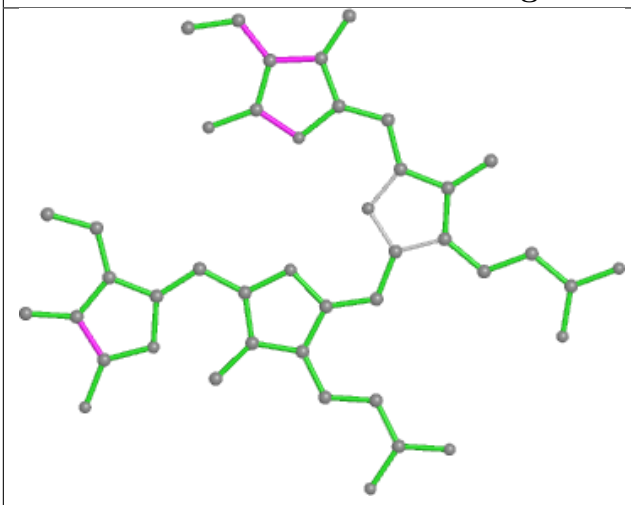


Rings

Ligand PEB e9 302



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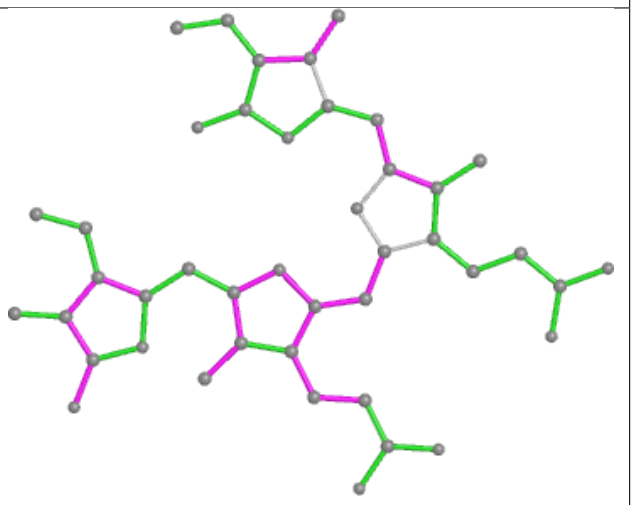

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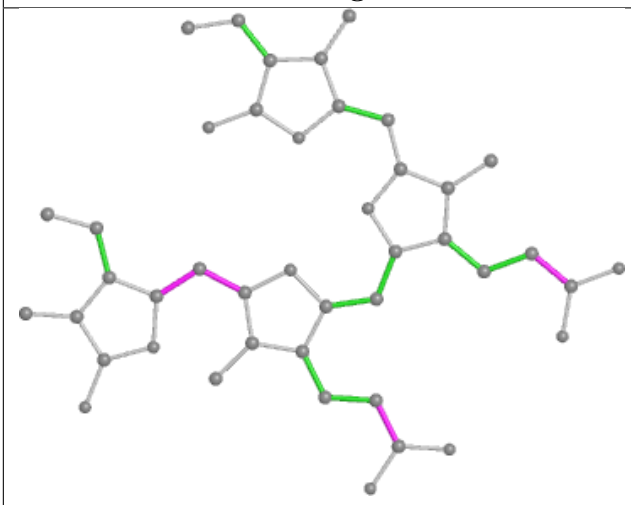

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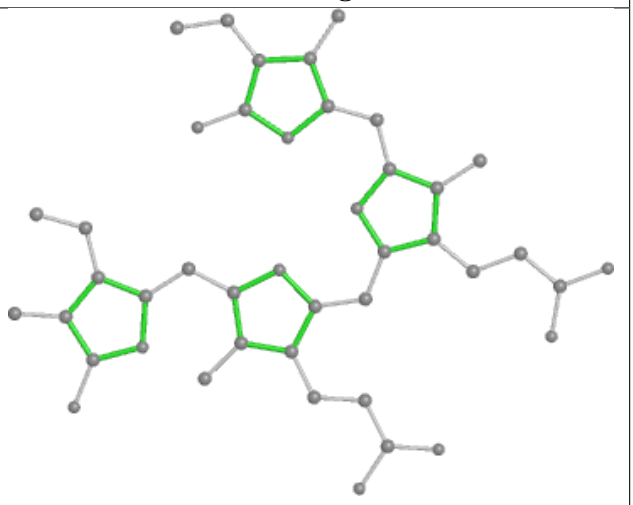
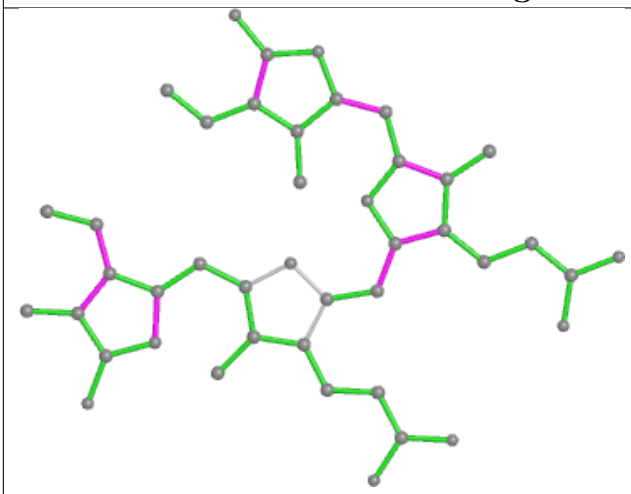


Rings

Ligand PVN T8 303



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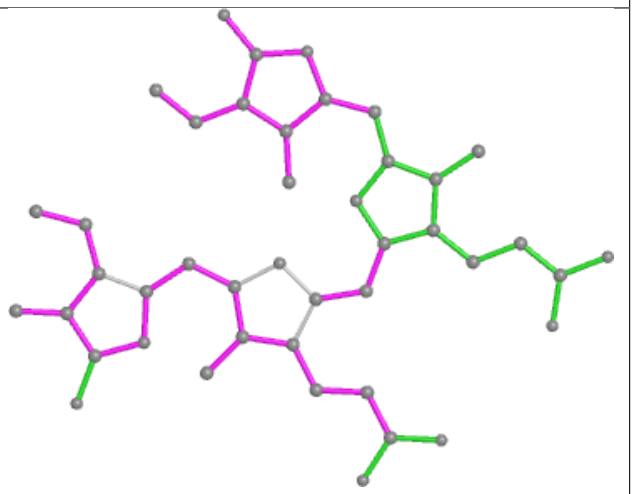

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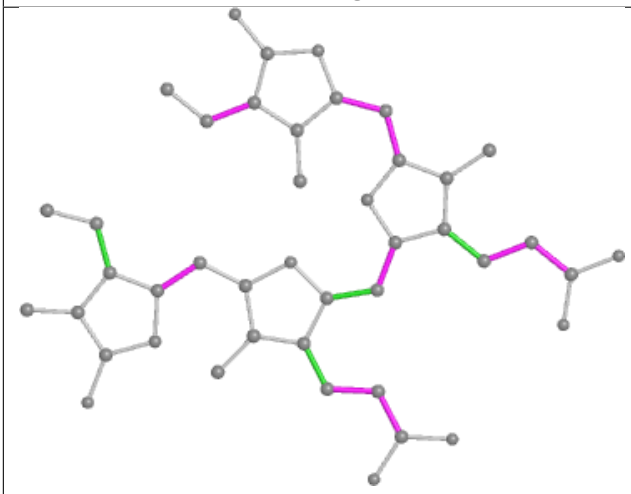

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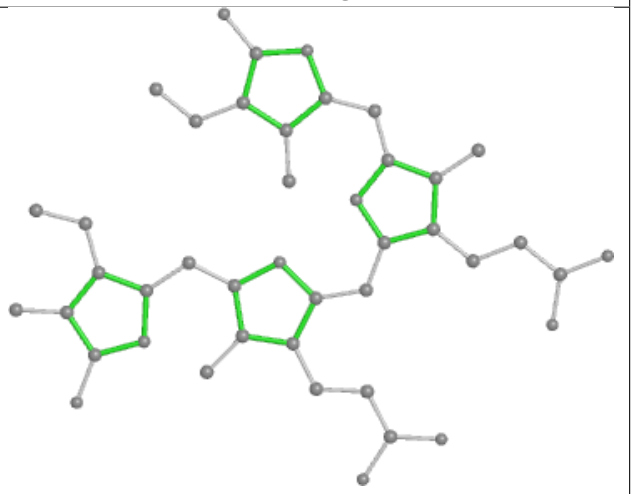
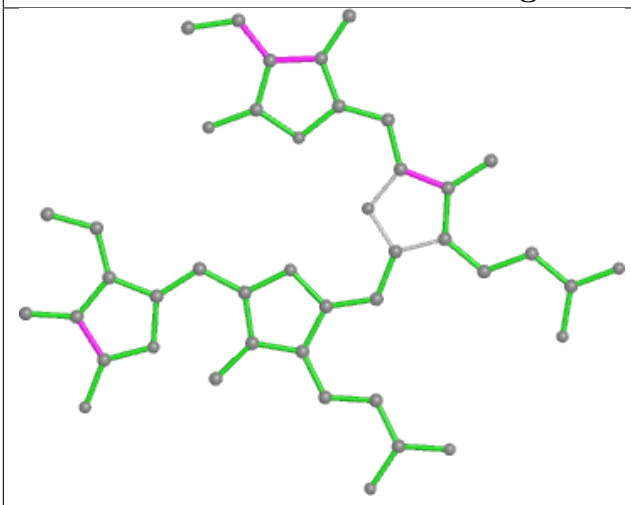


Rings

Ligand PEB o7 202



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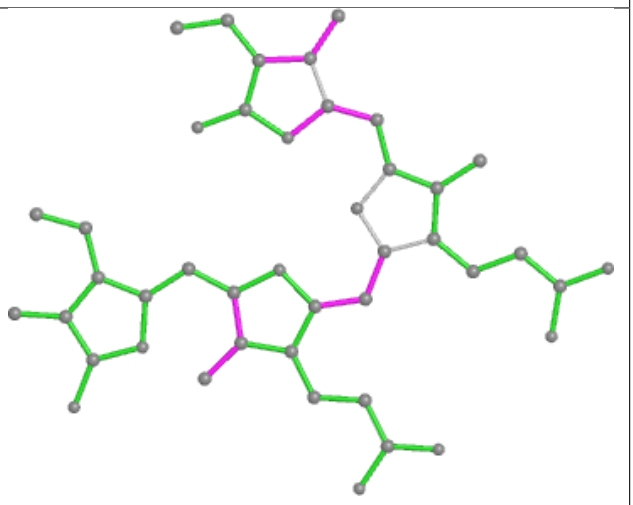

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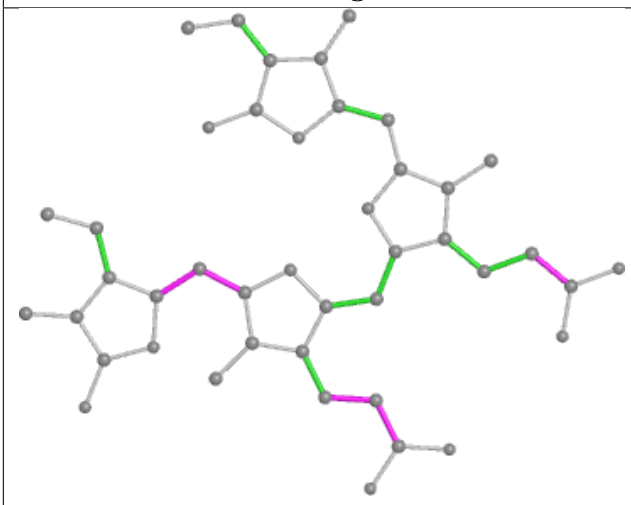

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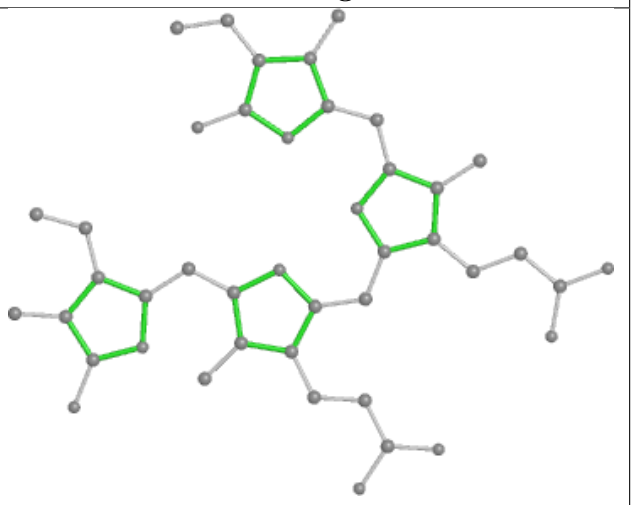

Rings

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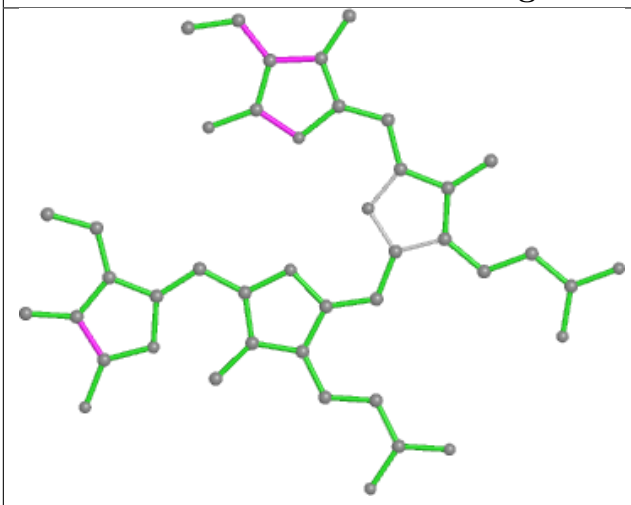

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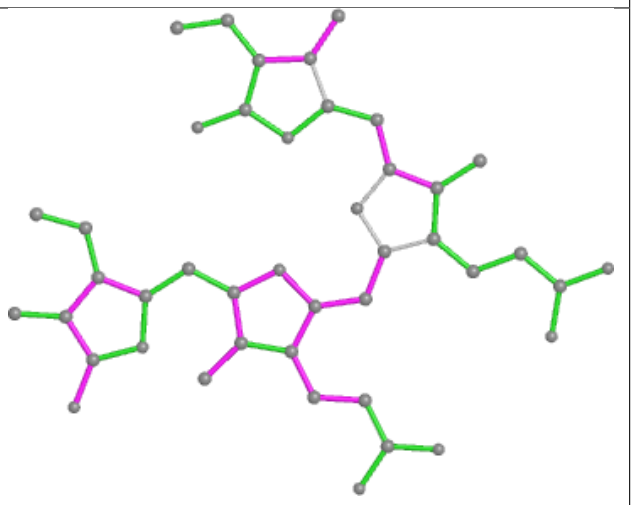

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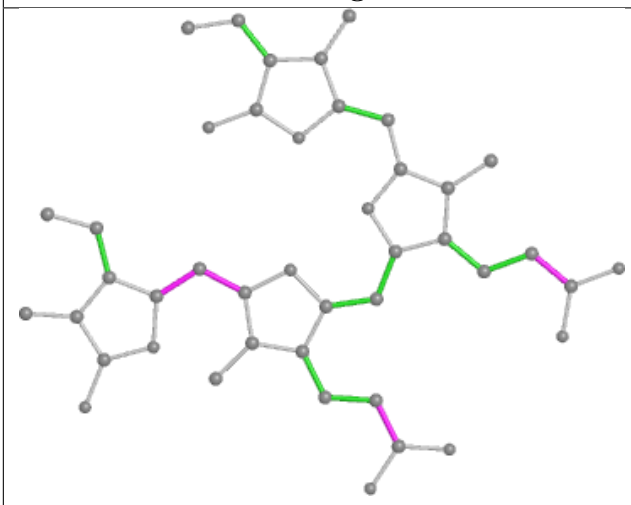

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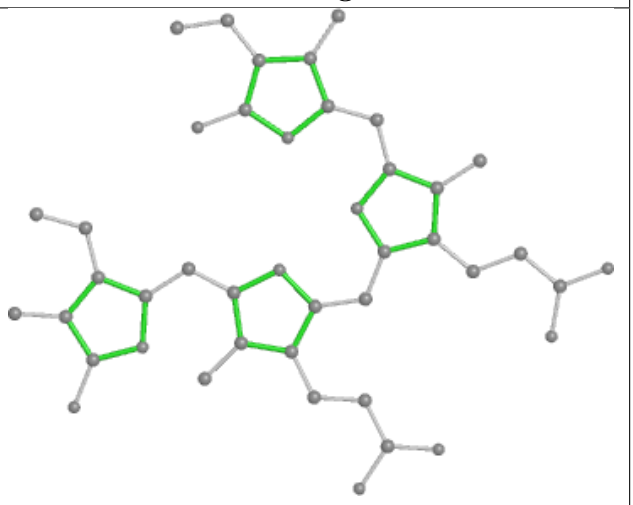
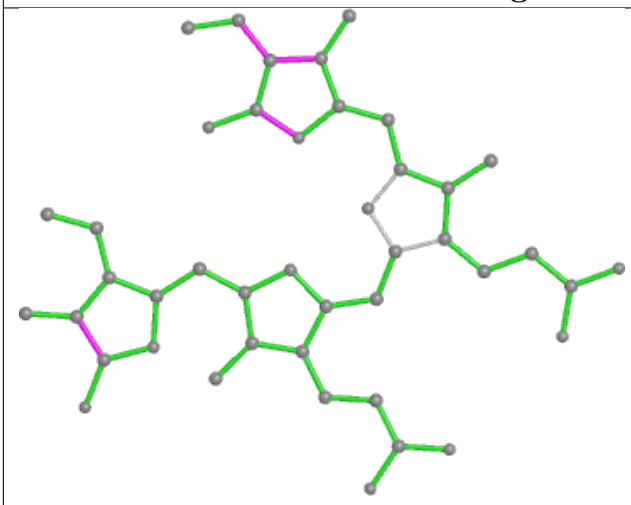


Rings

Ligand PEB k6 1002



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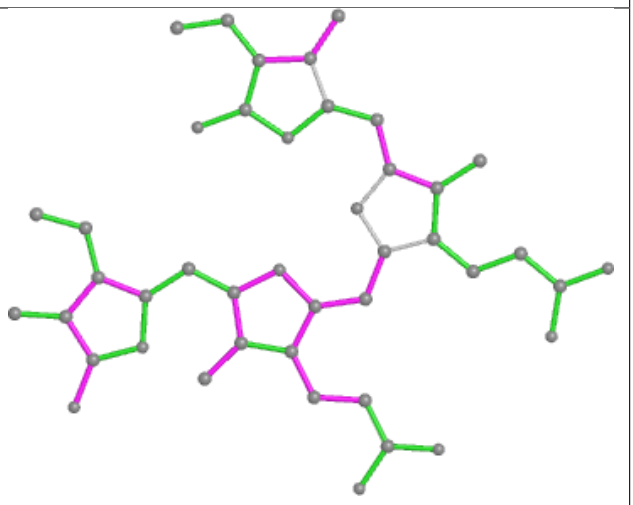

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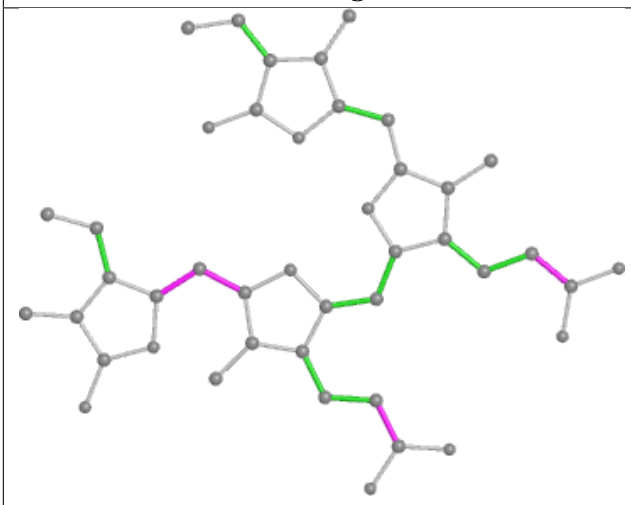

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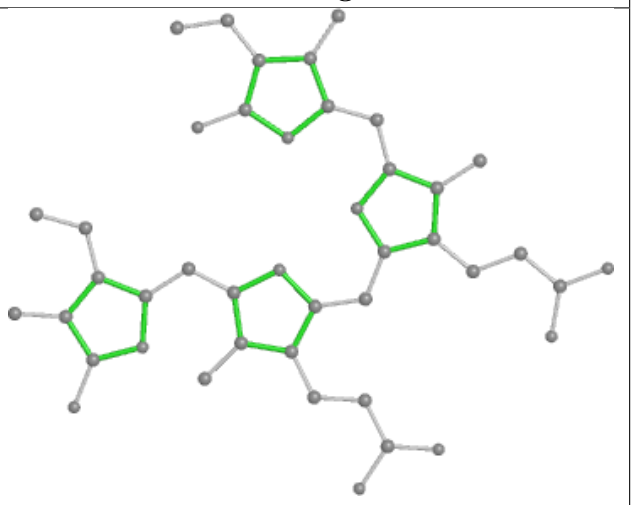

Rings

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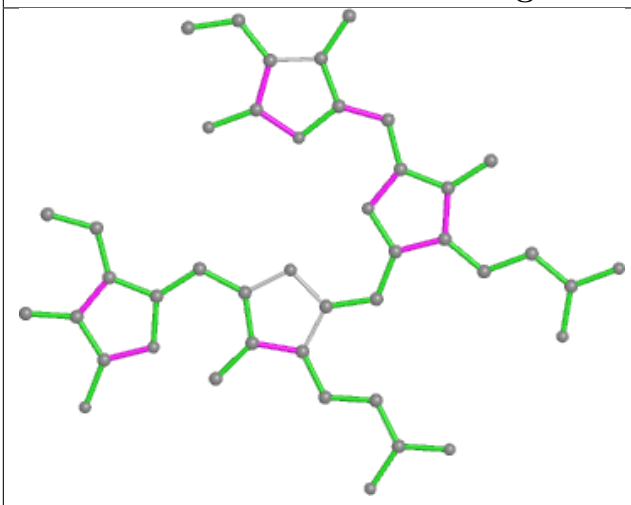

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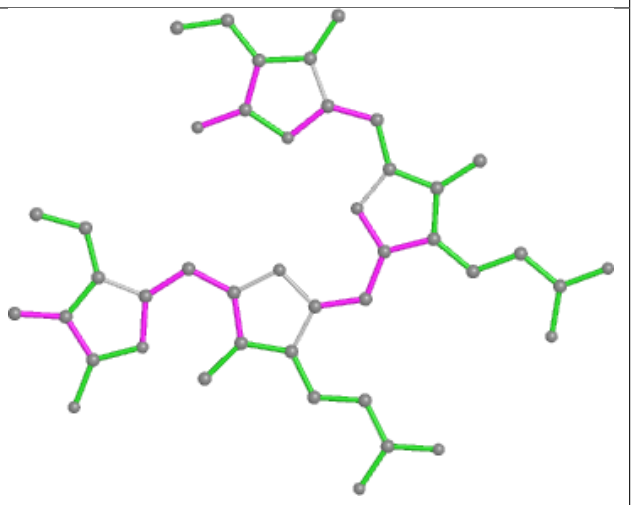

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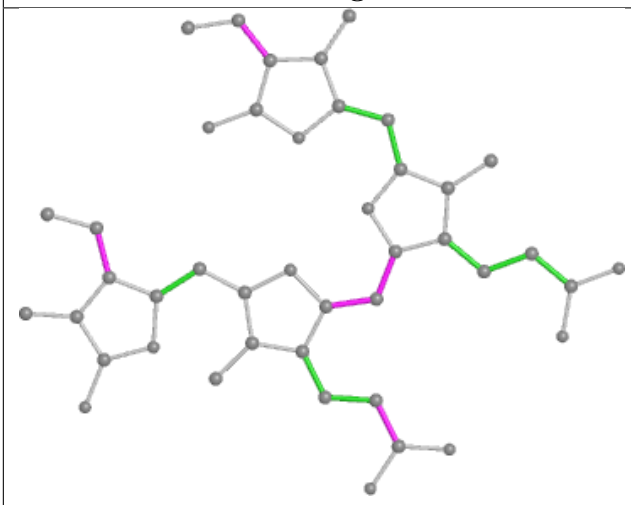

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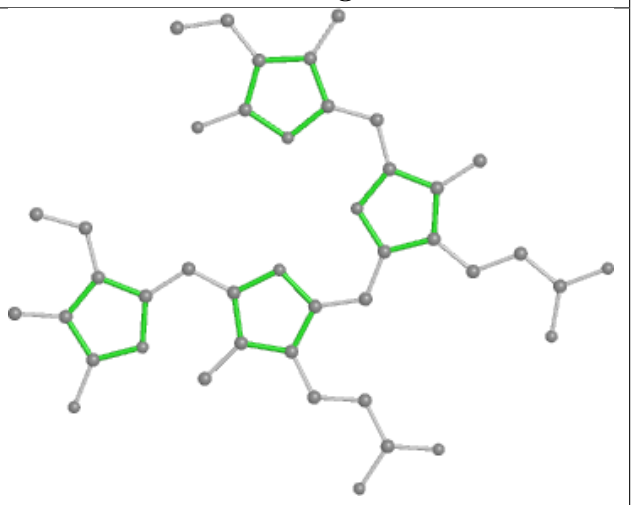

Rings

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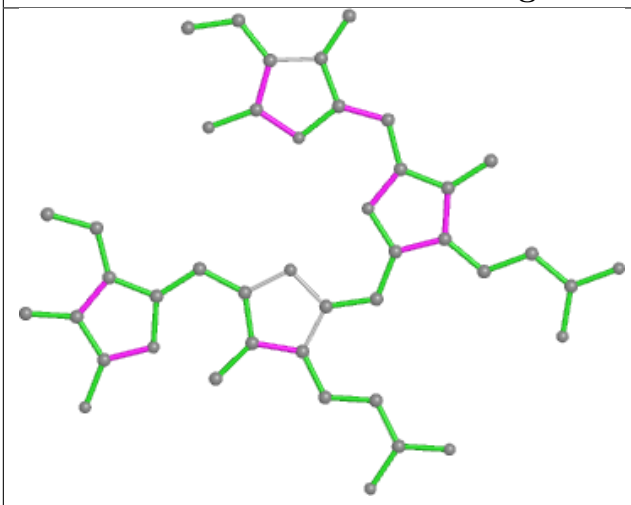

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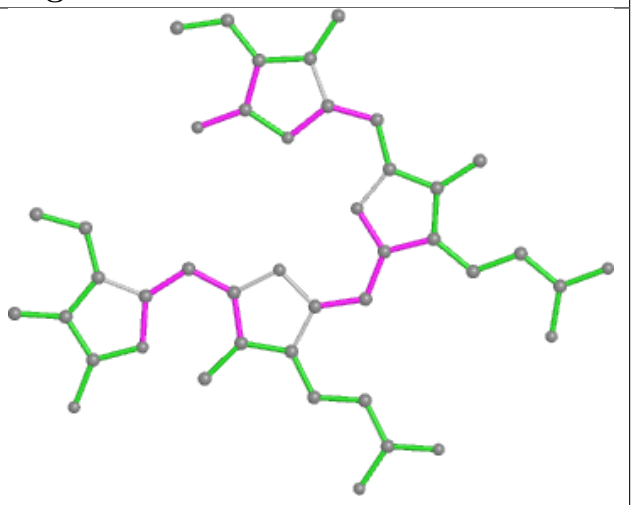

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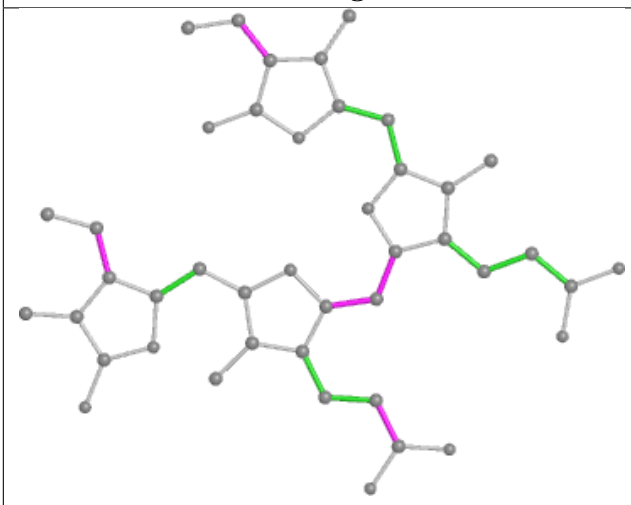

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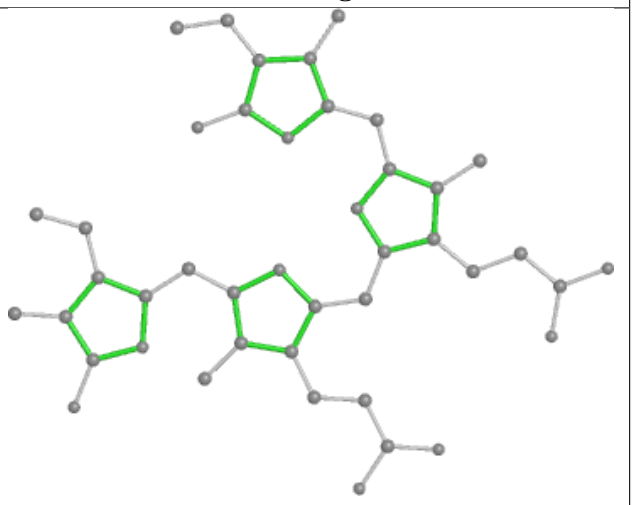
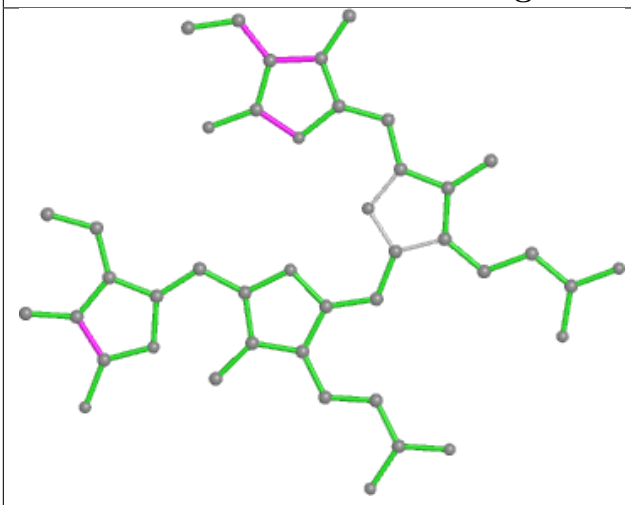


Rings

Ligand PEB K4 201



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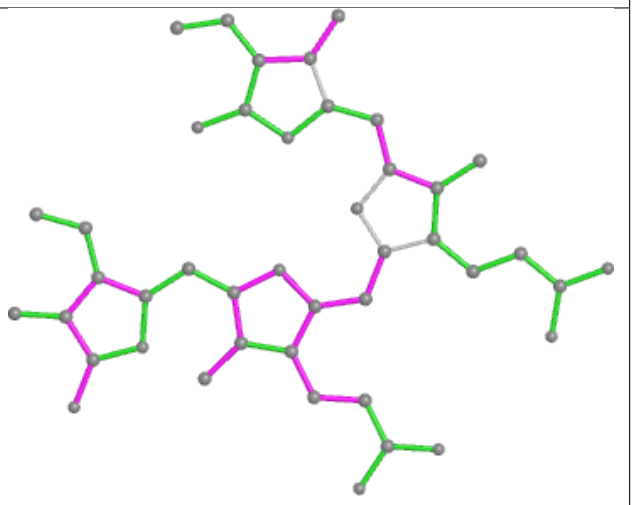

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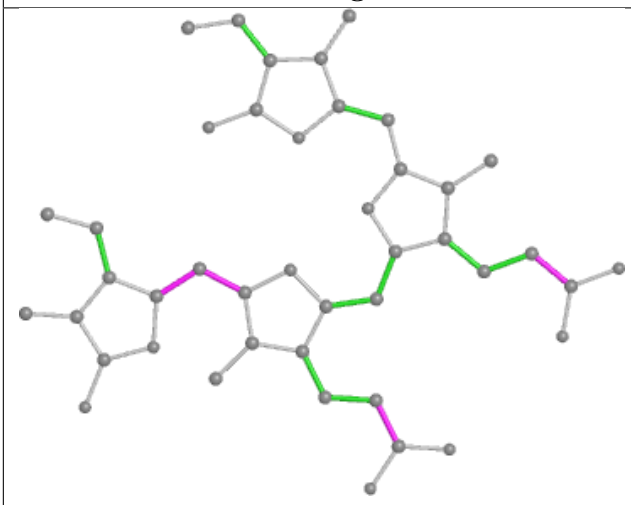

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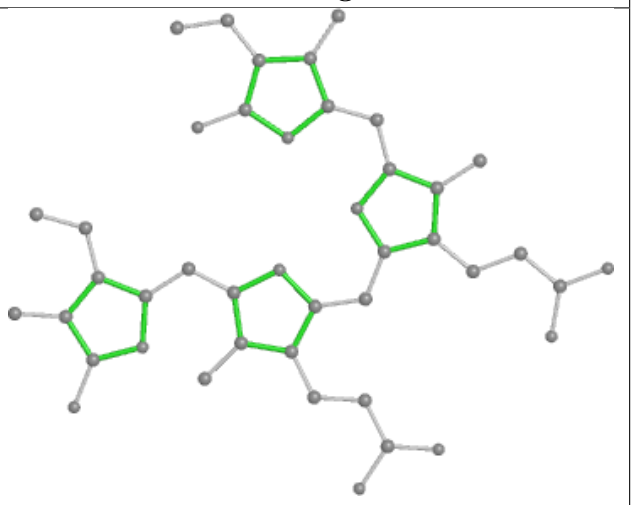

Rings

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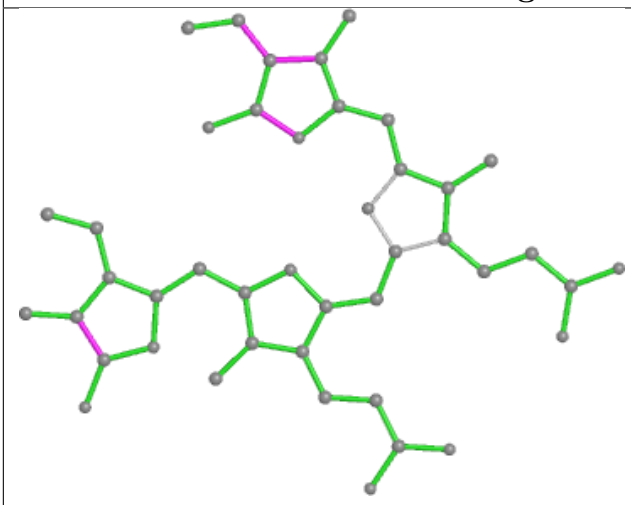

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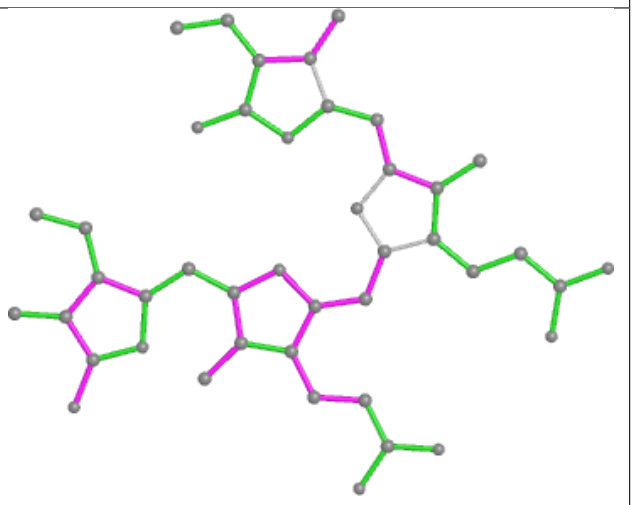

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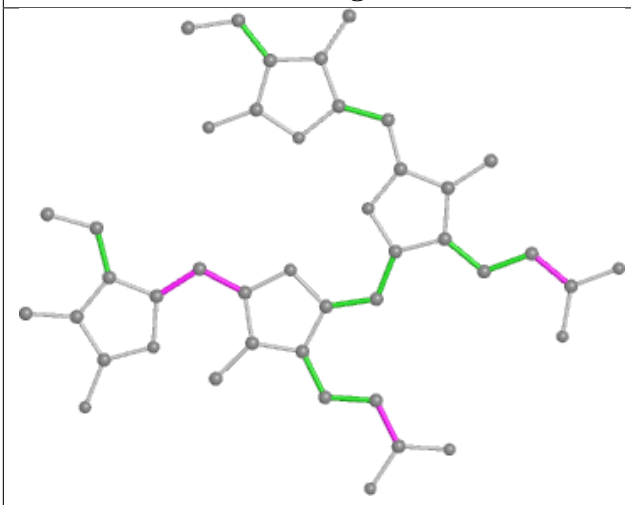

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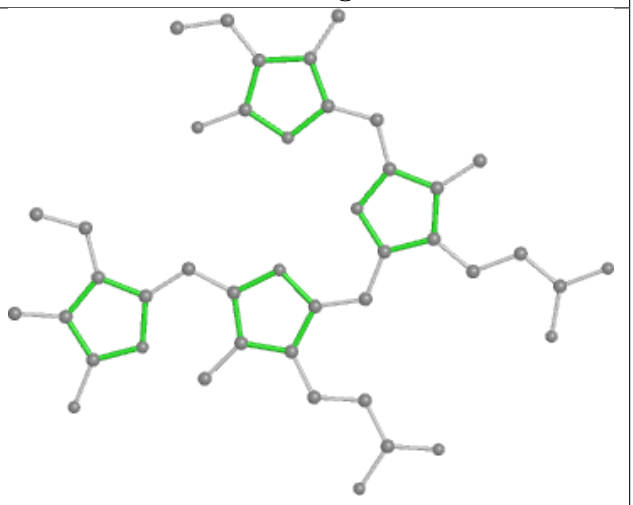

Rings

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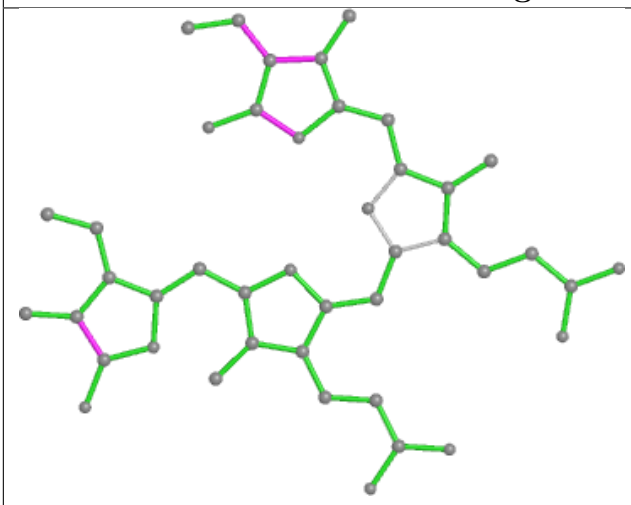

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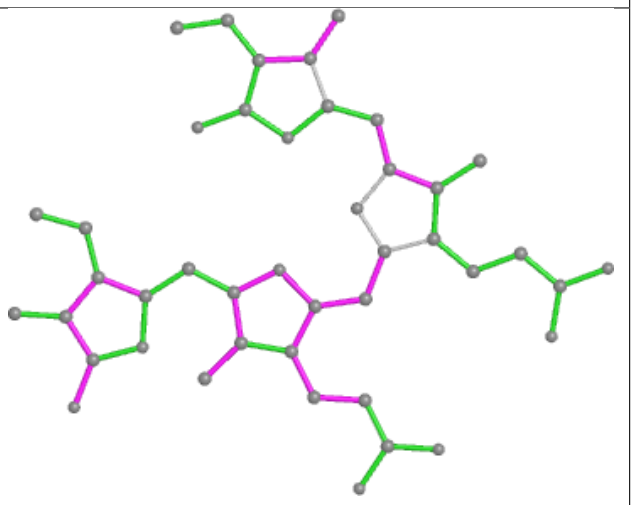

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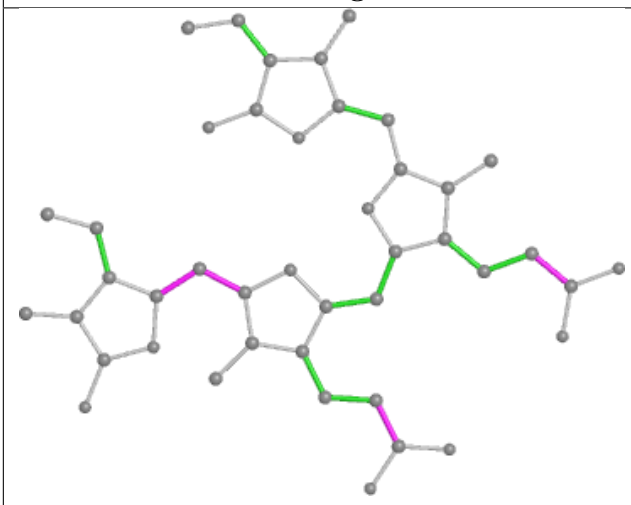

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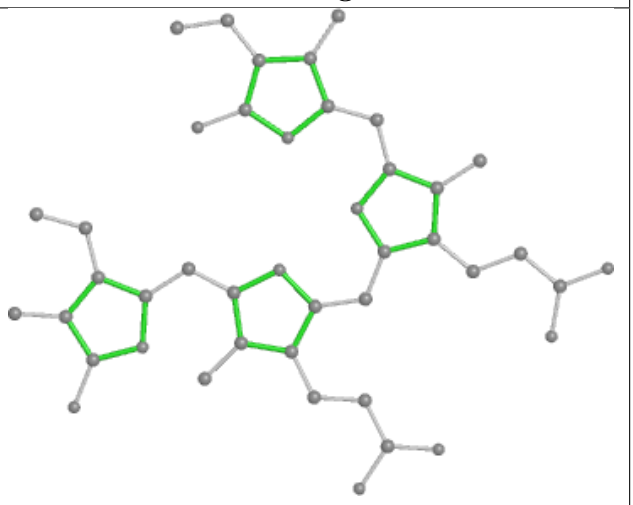
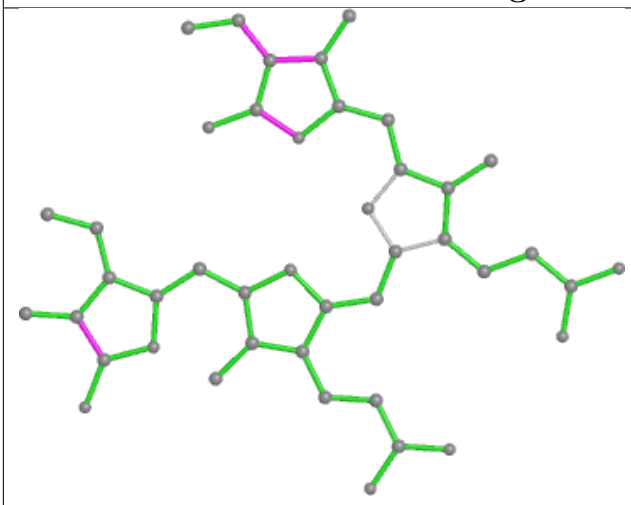


Rings

Ligand PEB jK 1001



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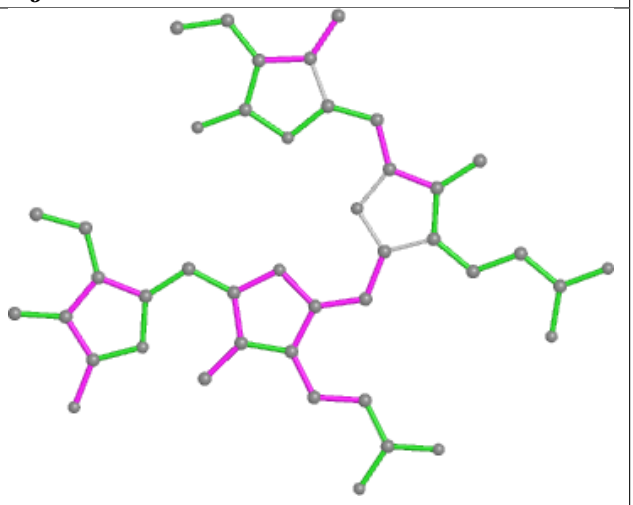

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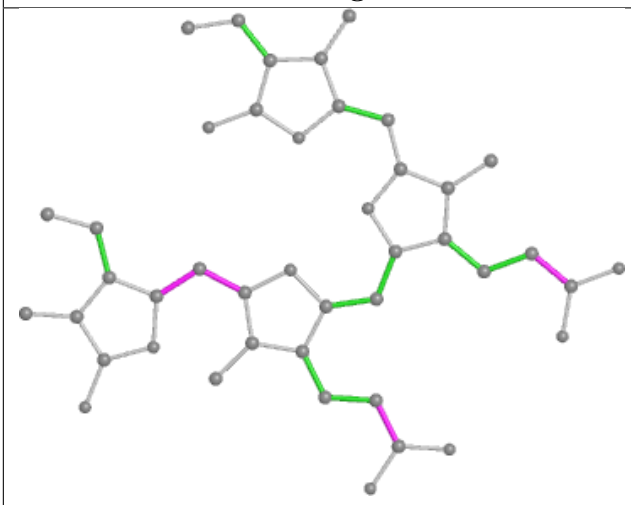

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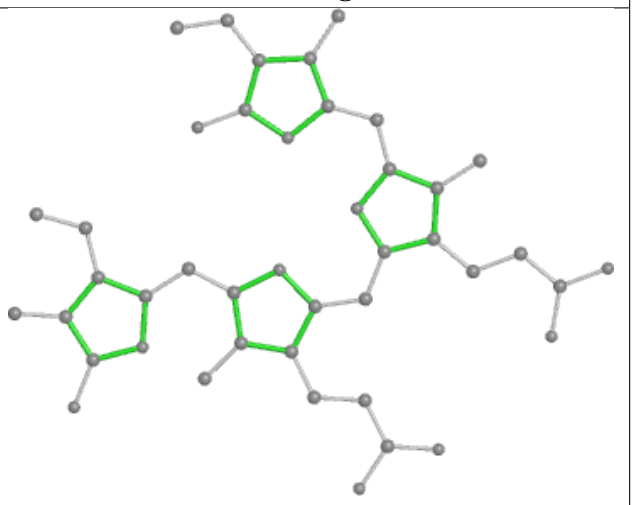

Rings

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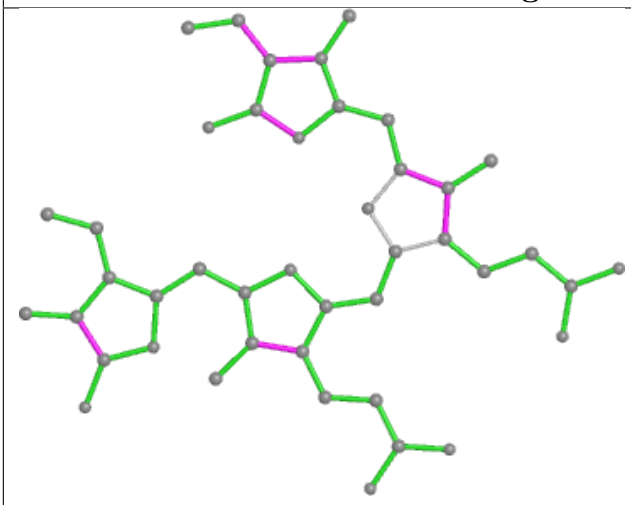

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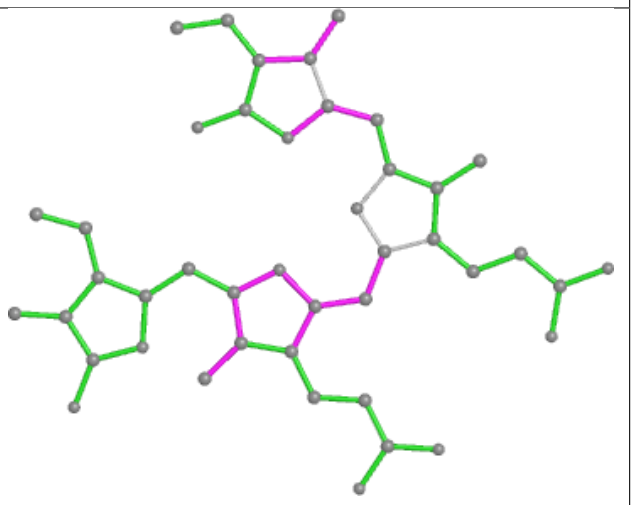
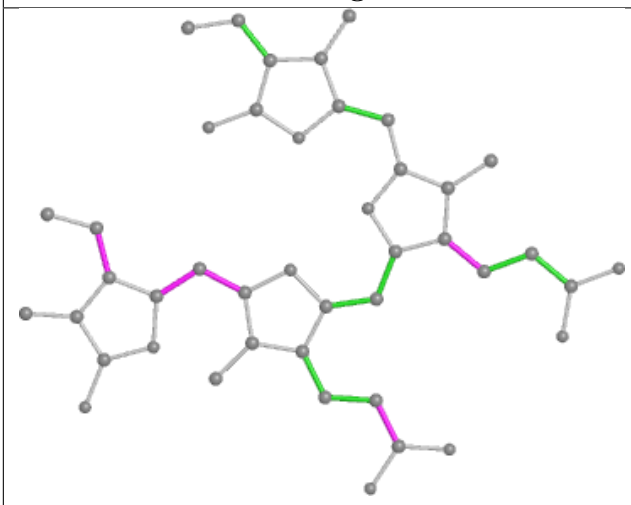
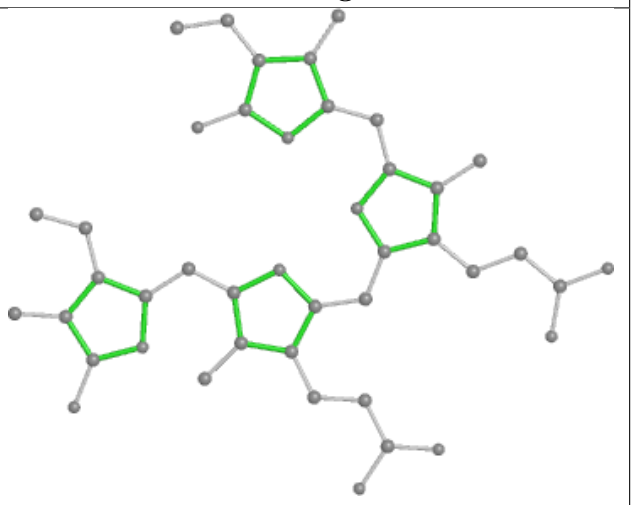


Bond angles

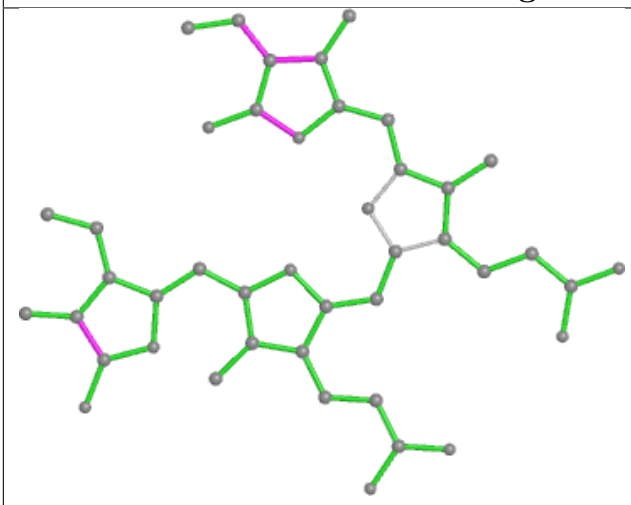


Torsions



Rings

Ligand PEB b7 201



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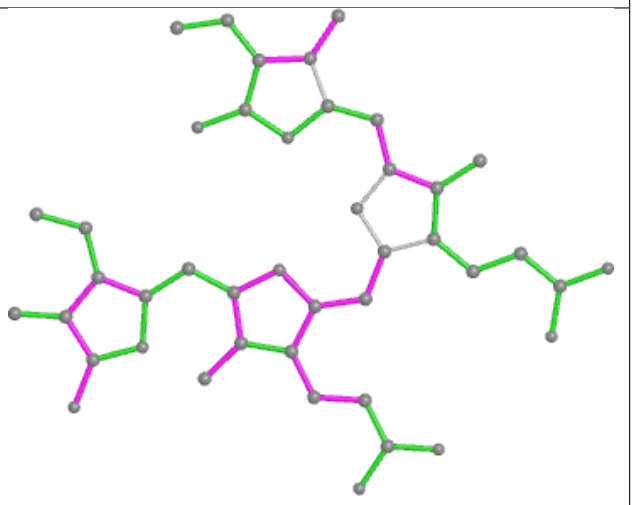

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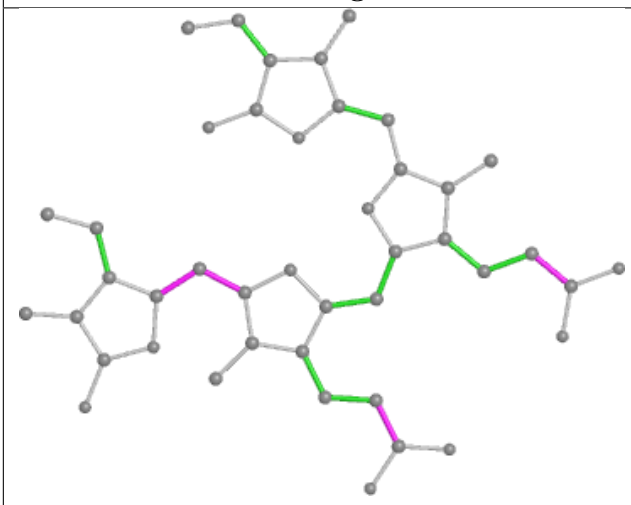

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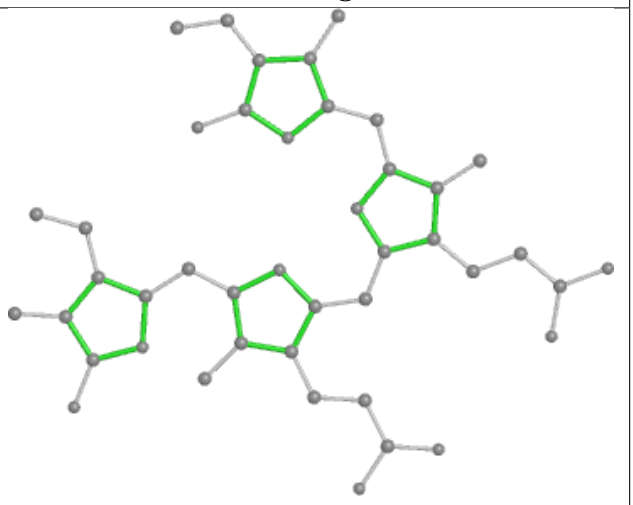
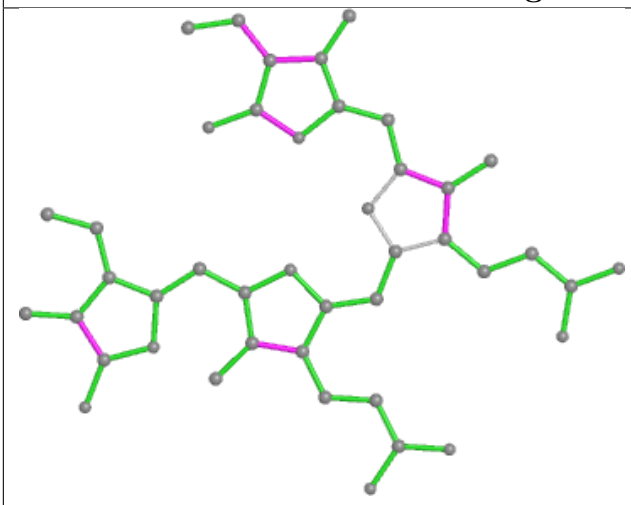


Rings

Ligand PEB fs 202



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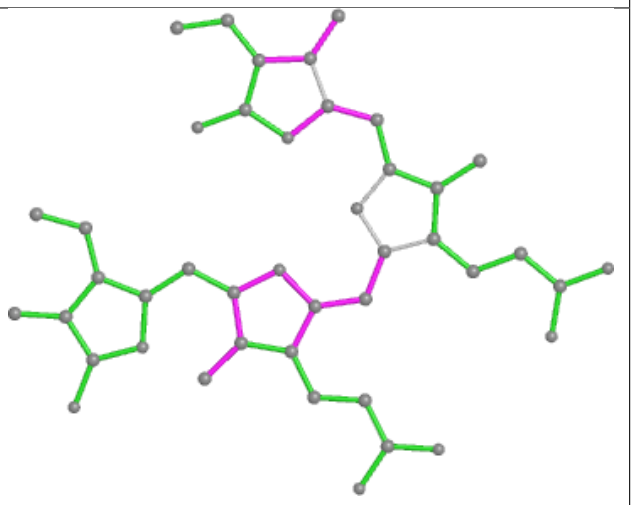

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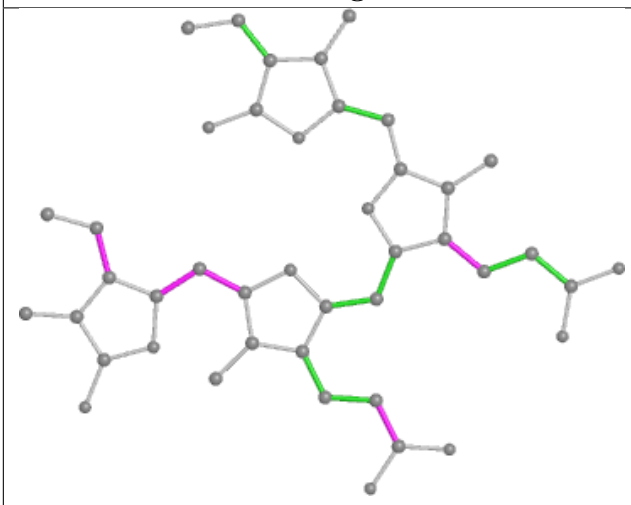

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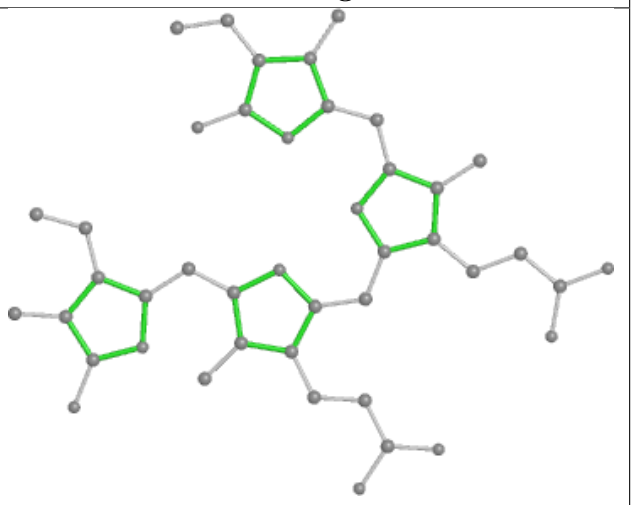
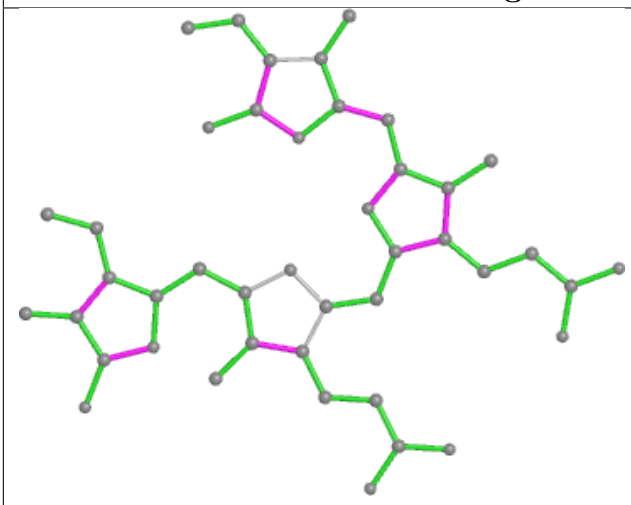


Rings

Ligand PUB A2 1005



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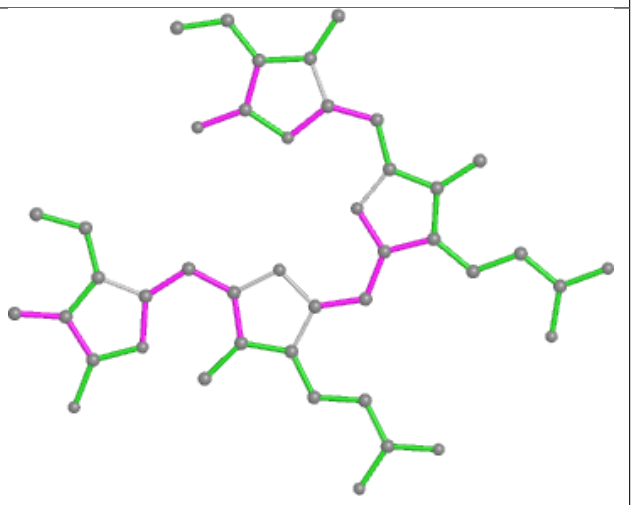

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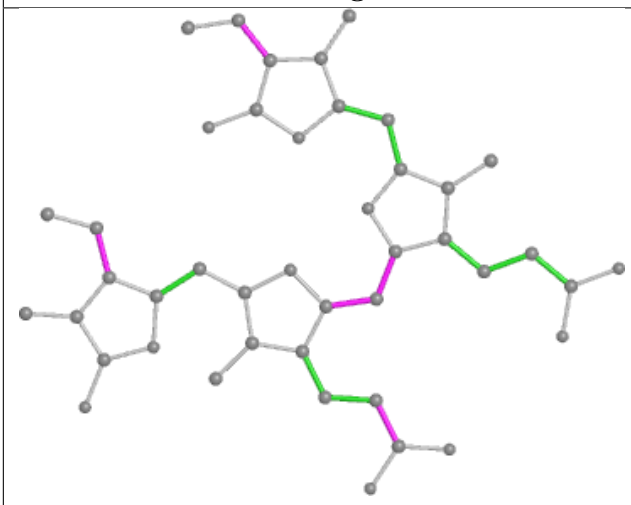

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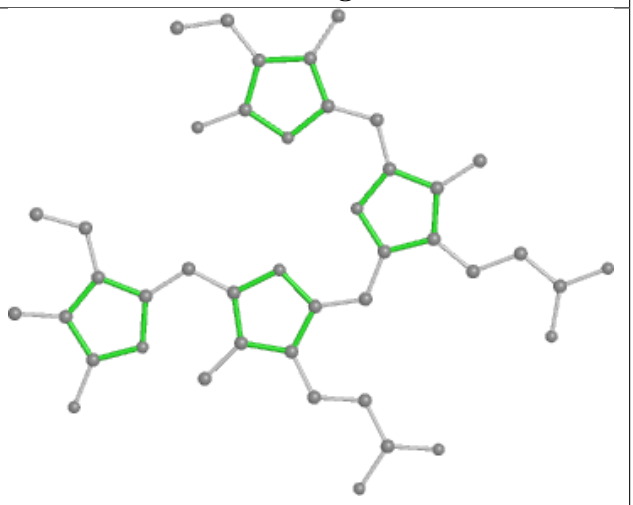
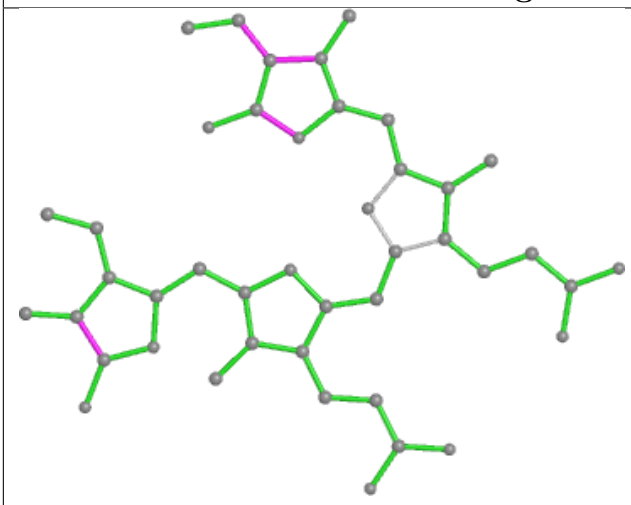


Rings

Ligand PEB X7 201



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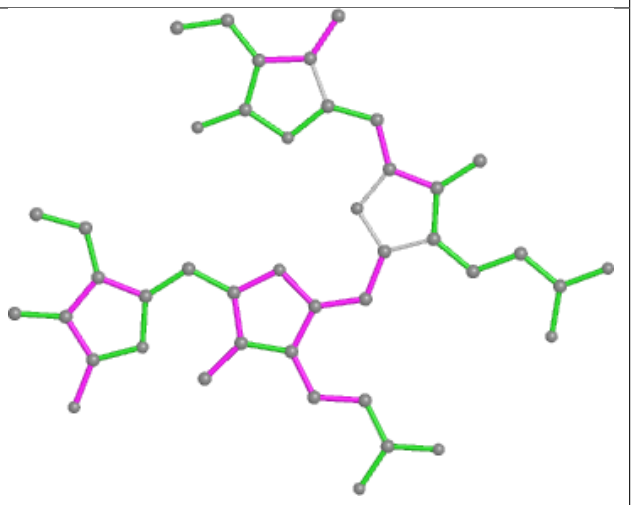

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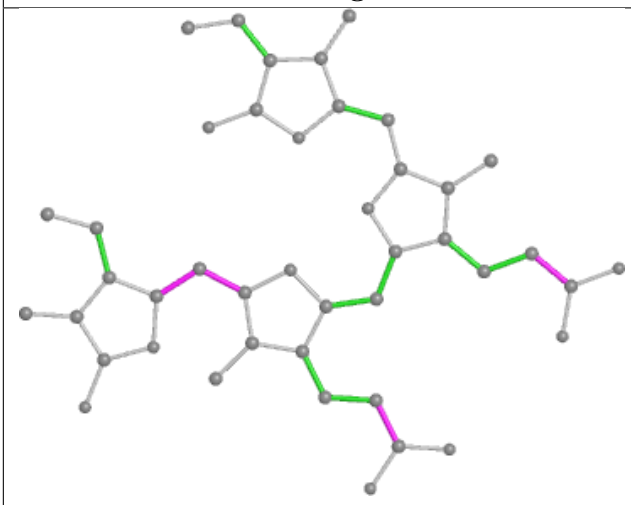

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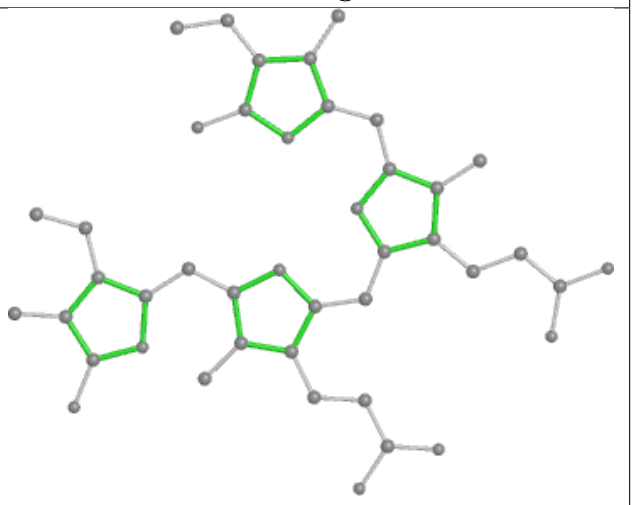
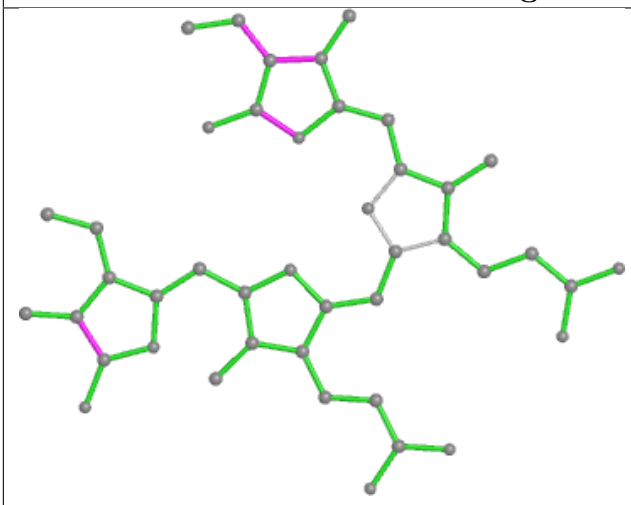


Rings

Ligand PEB br 201



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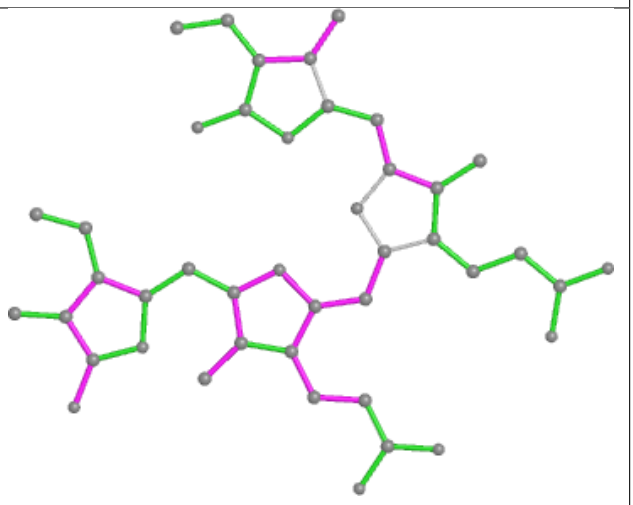

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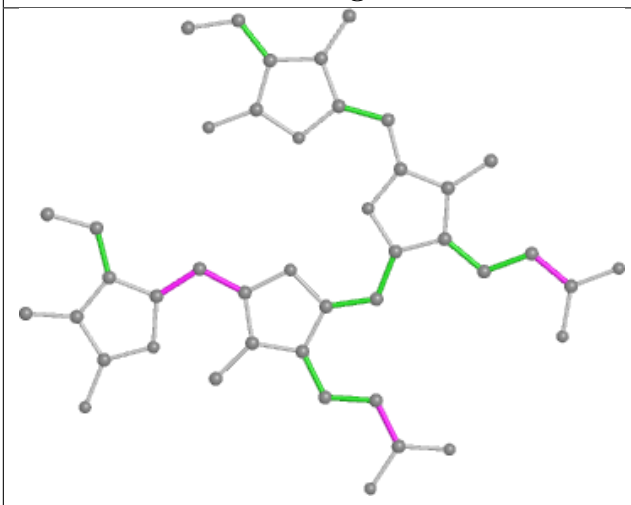

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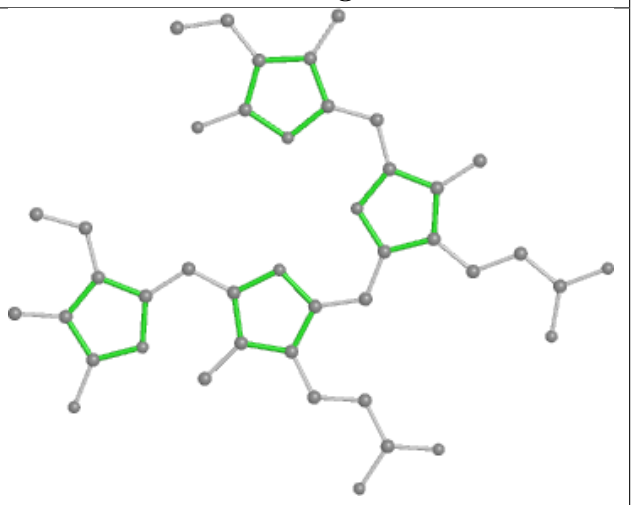
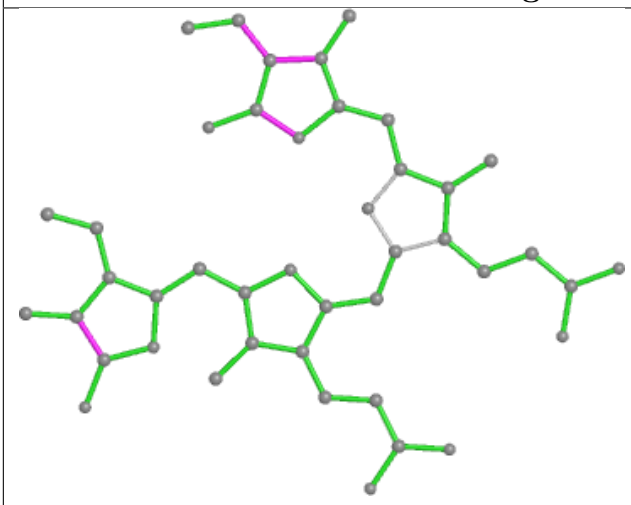


Rings

Ligand PEB fd 302



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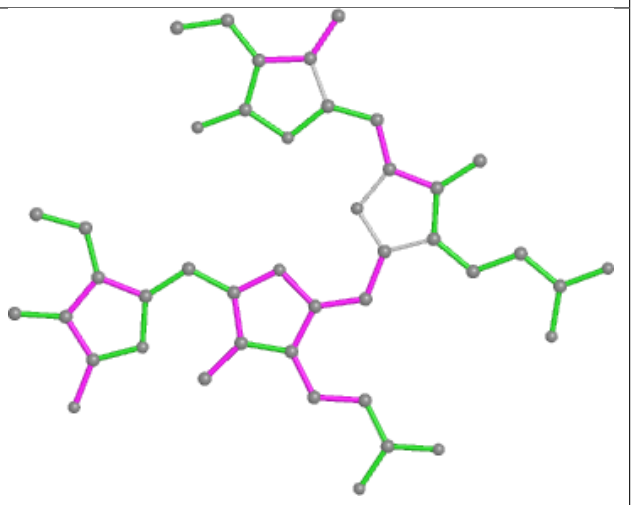

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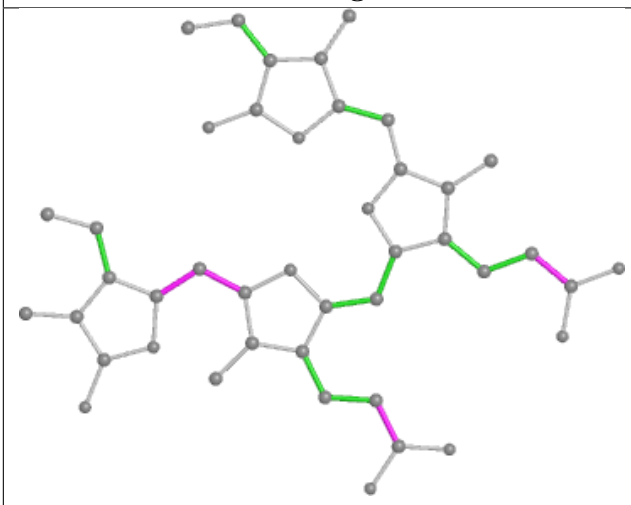

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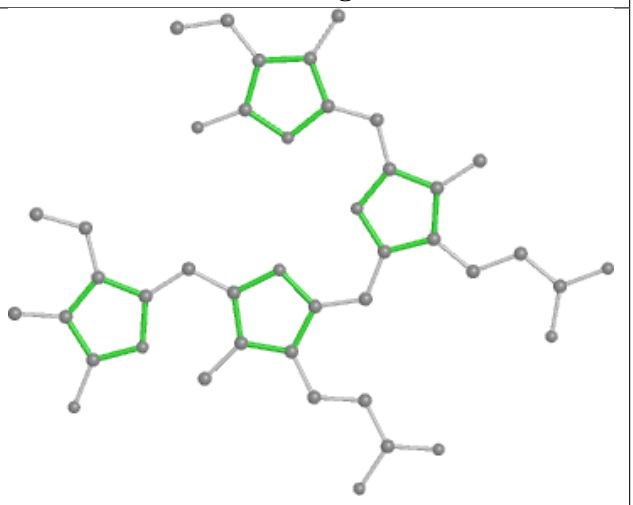
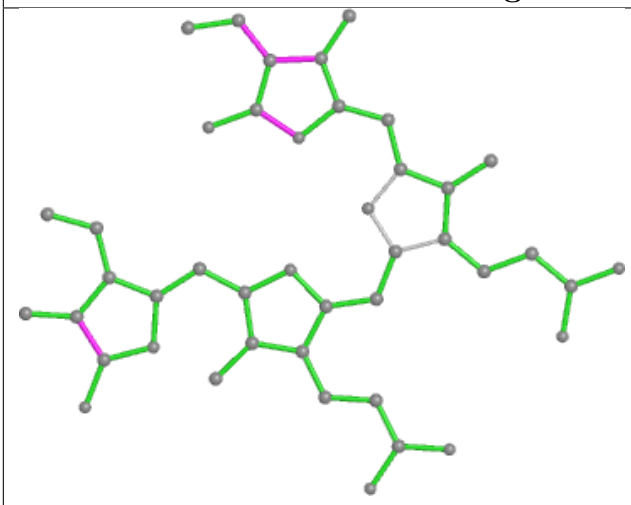


Rings

Ligand PEB bm 1002



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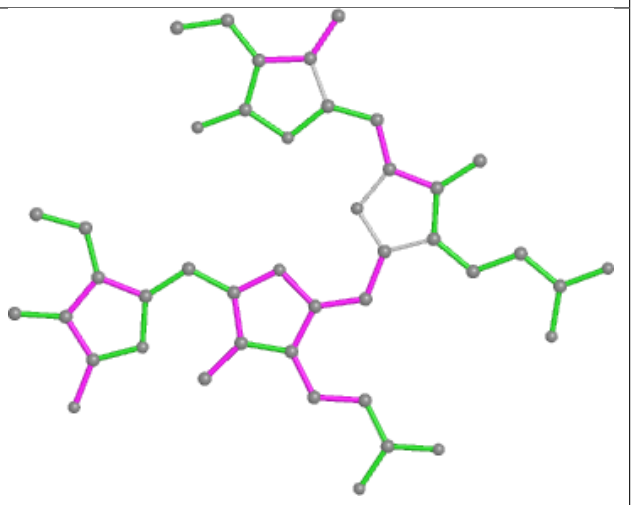
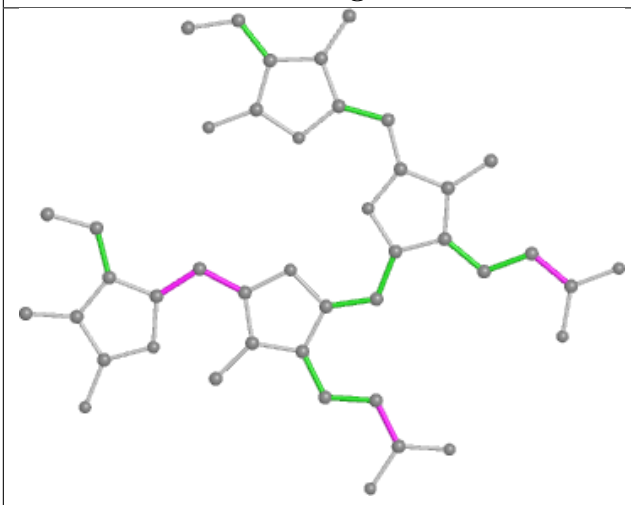


Bond angles



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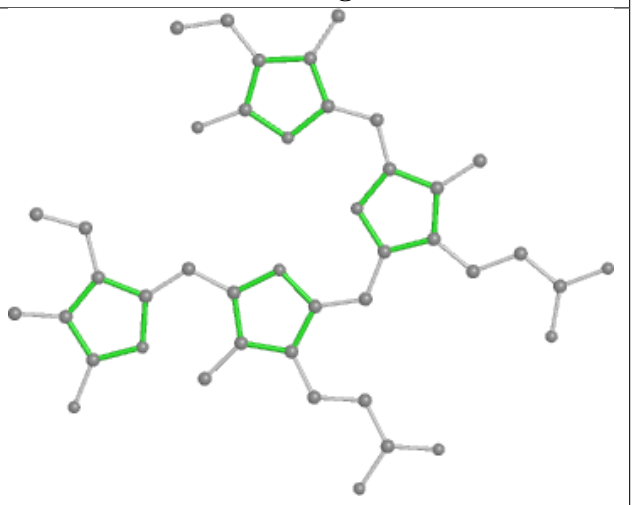
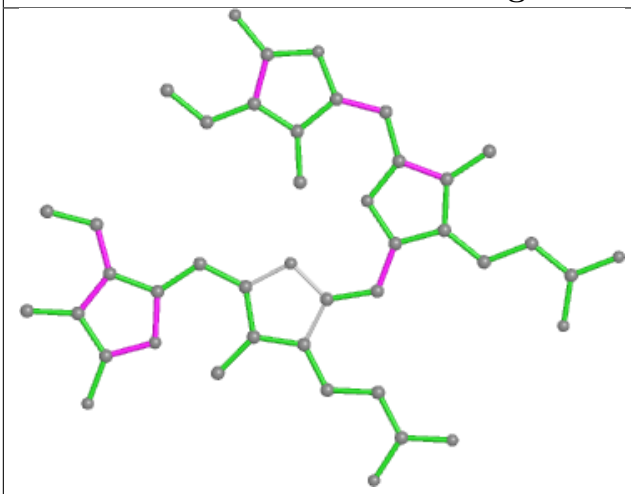


Rings

Ligand PVN a3 1004



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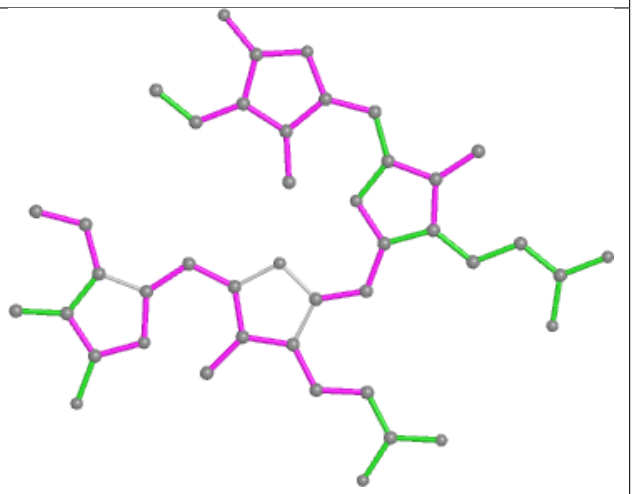
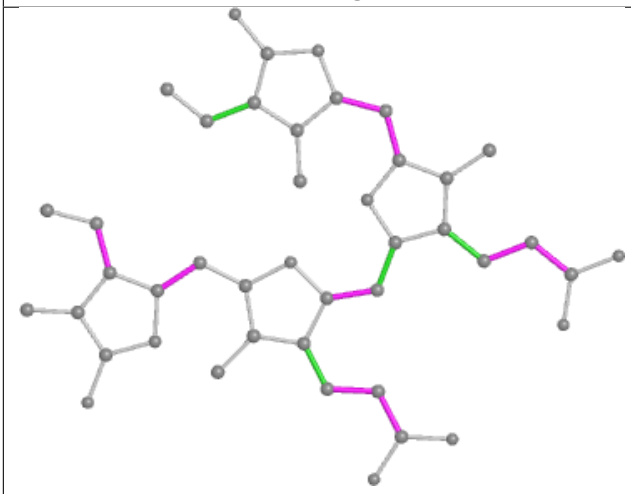


Bond angles



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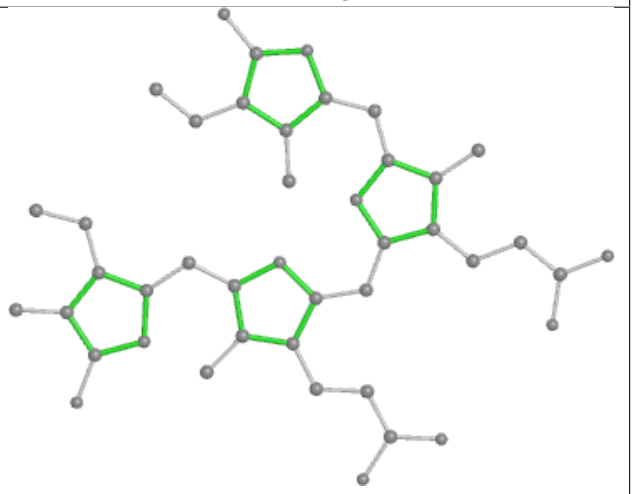
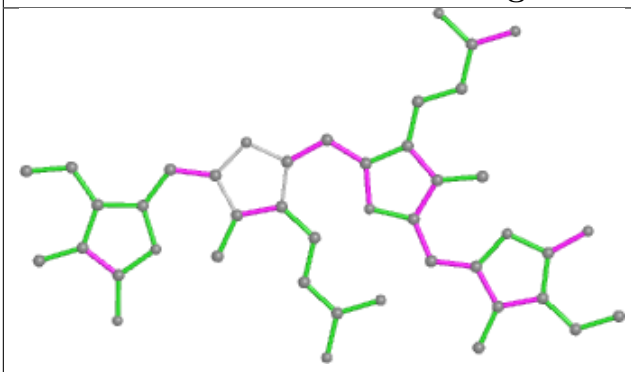


Rings

Ligand CYC W1 201



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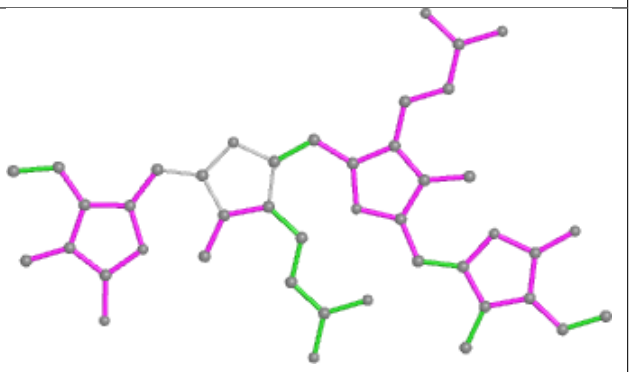

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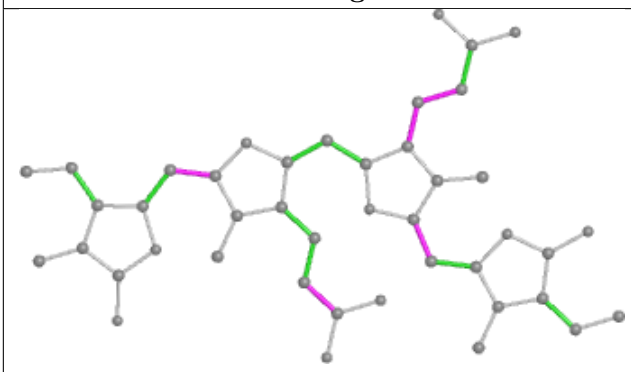

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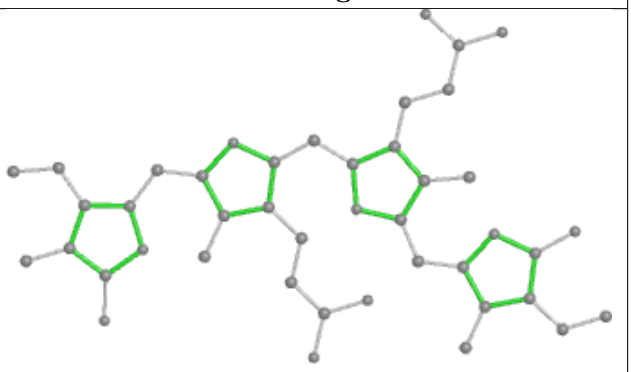
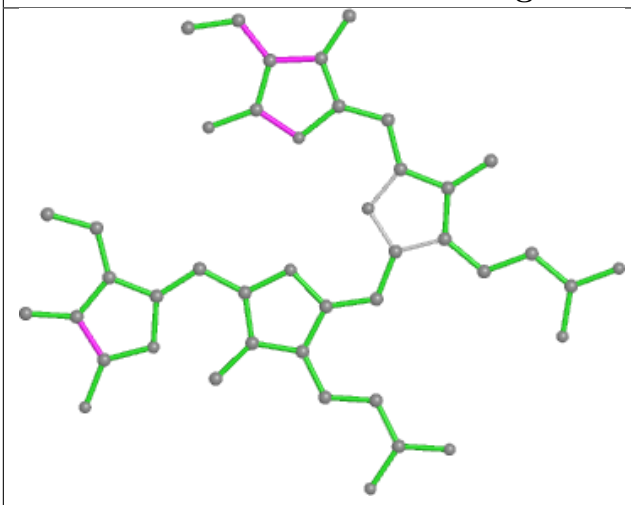


Rings

Ligand PEB C7 201



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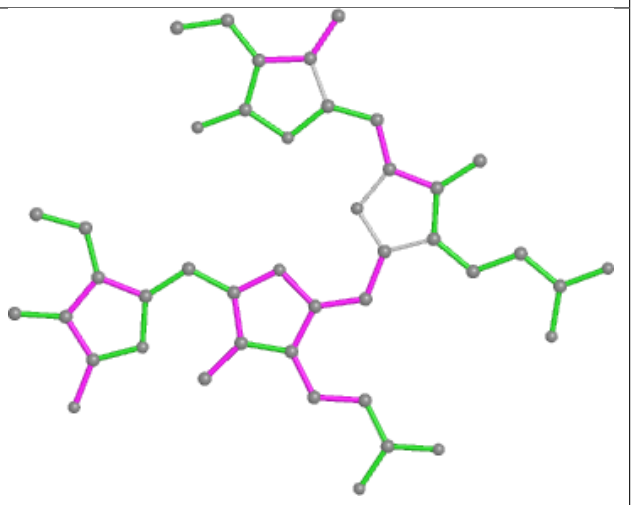

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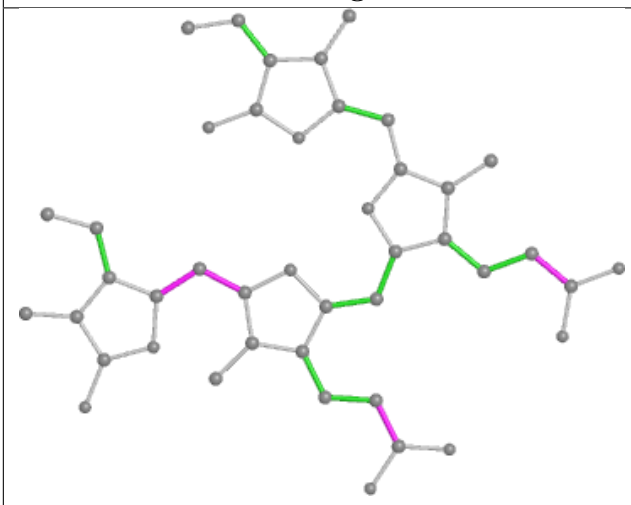

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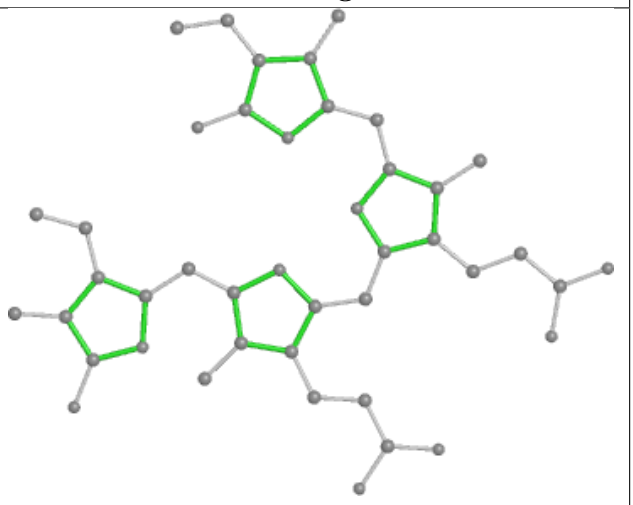
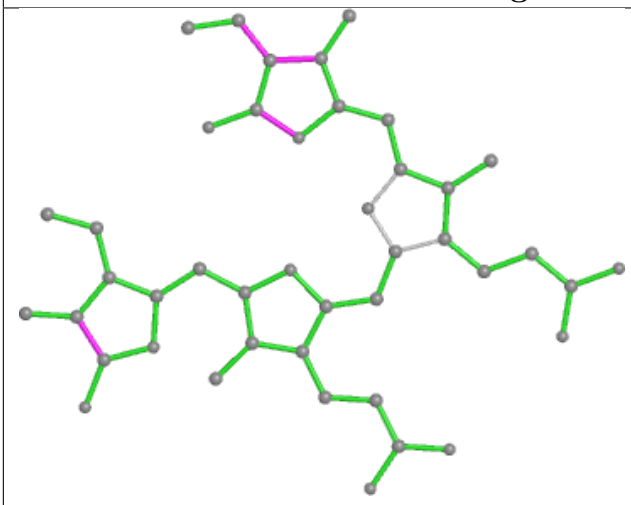


Rings

Ligand PEB iA 1001



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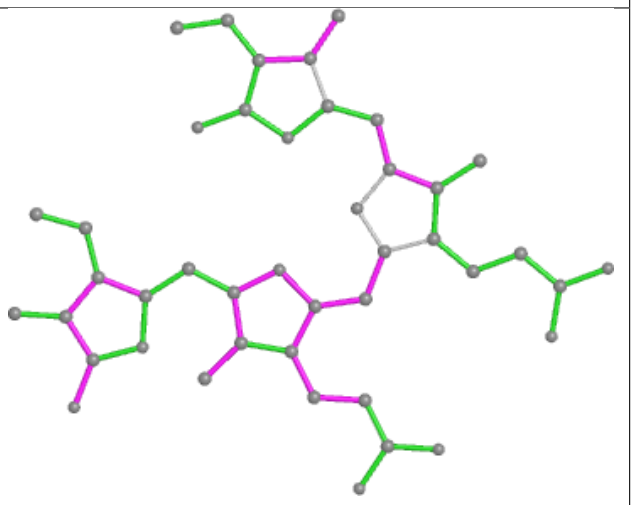

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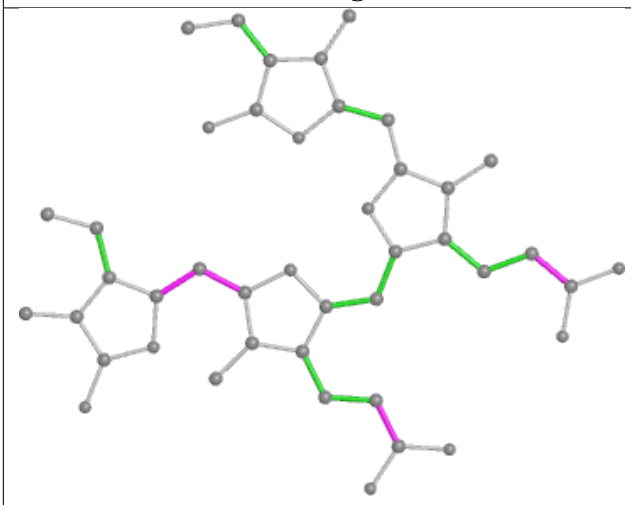

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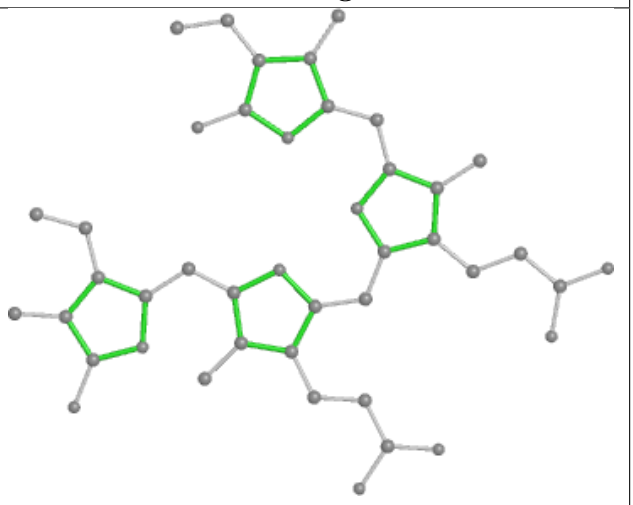

Rings

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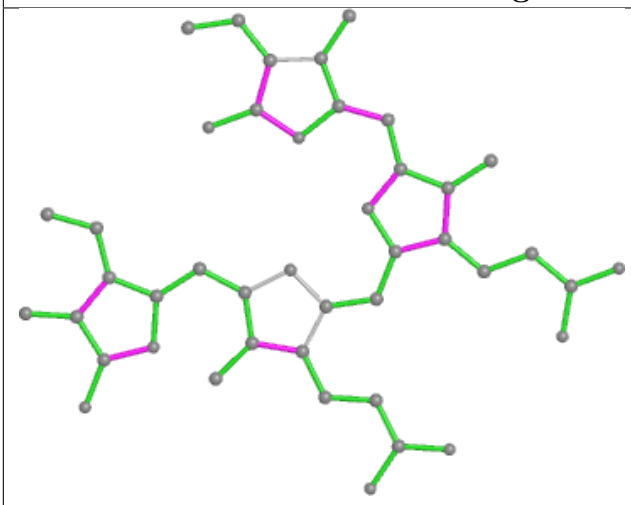

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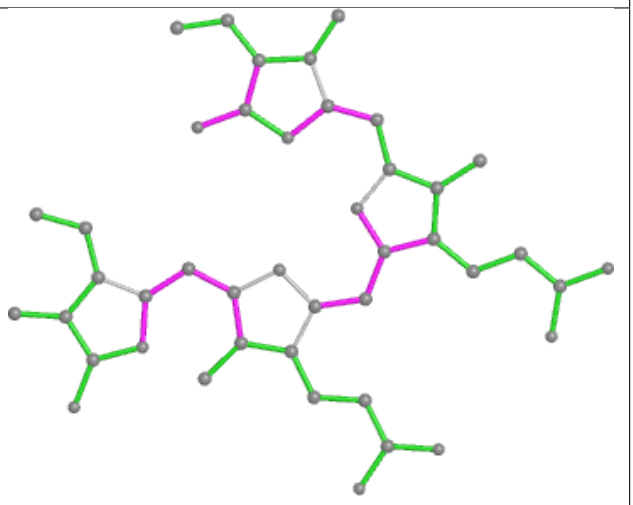

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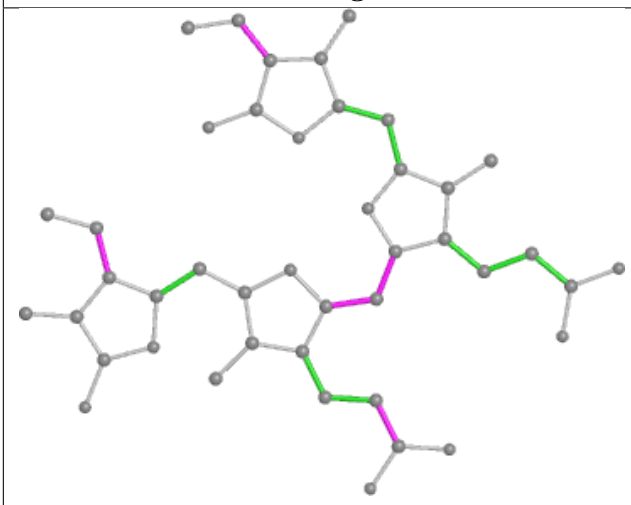

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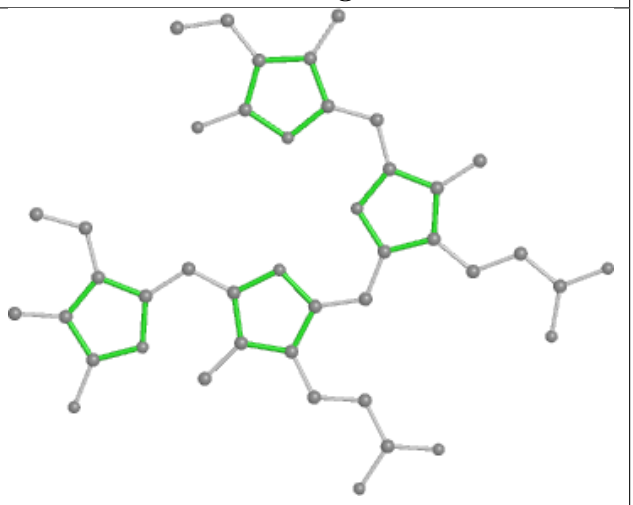
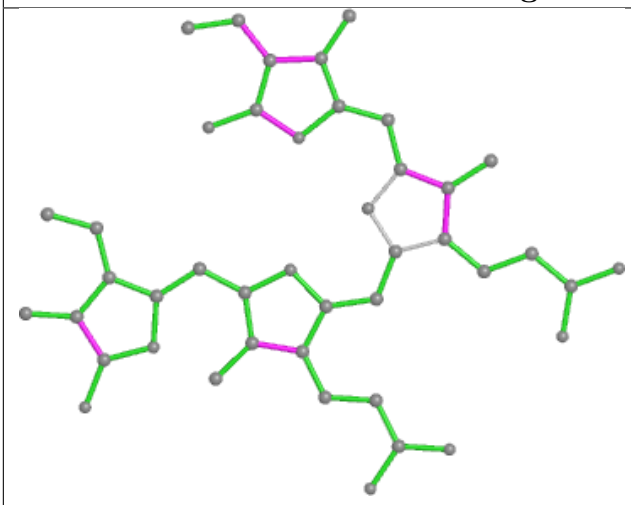


Rings

Ligand PEB cJ 202



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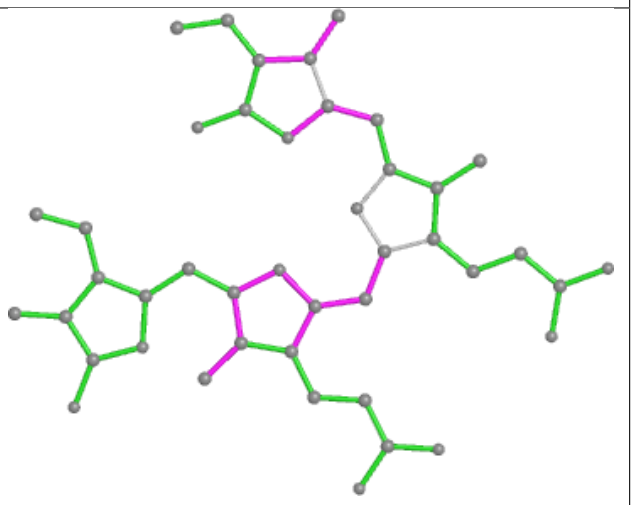
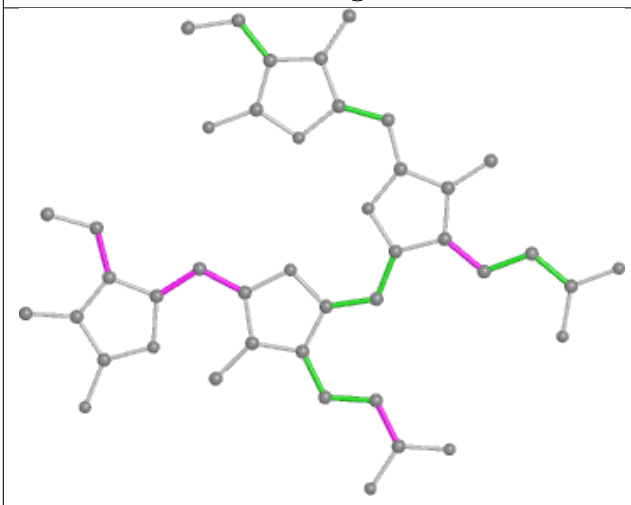
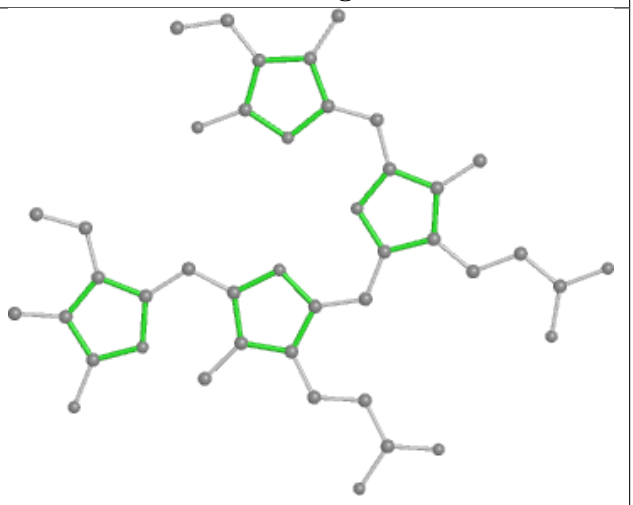


Bond angles

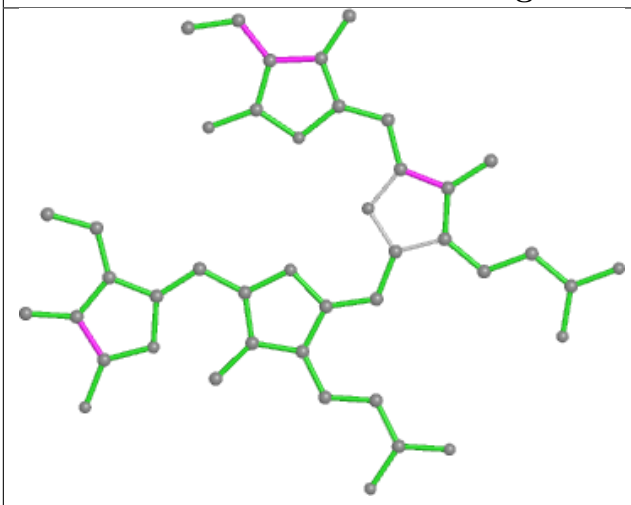


Torsions



Rings

Ligand PEB w4 202



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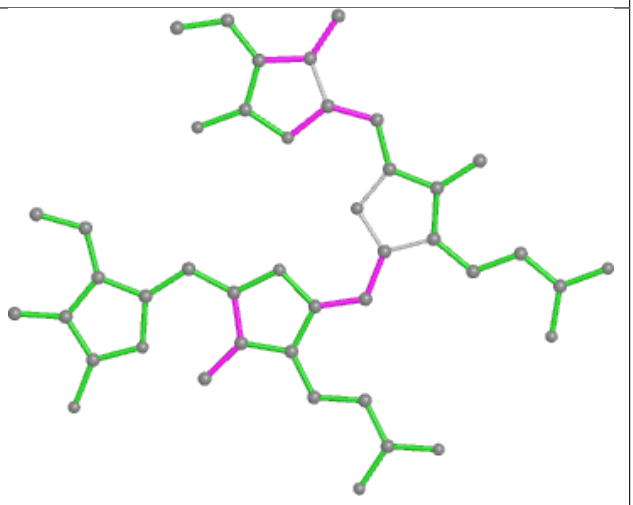

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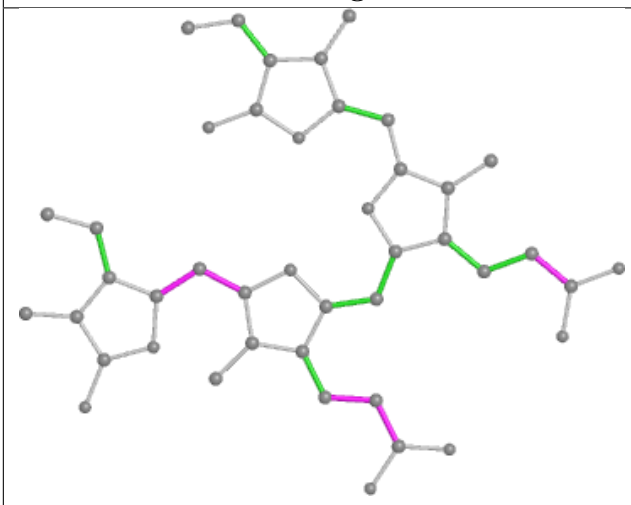

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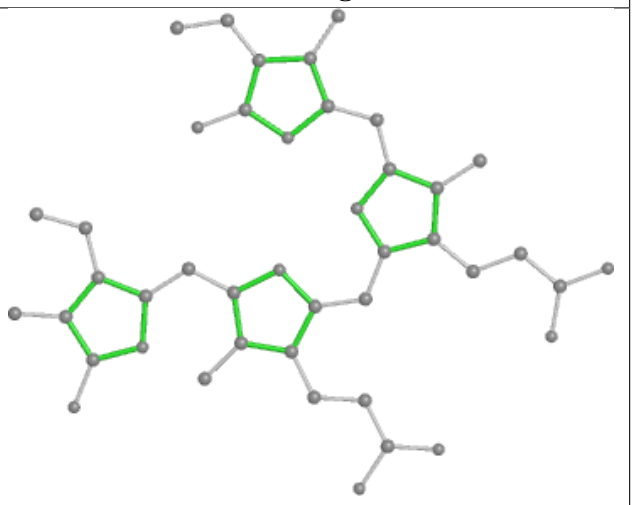
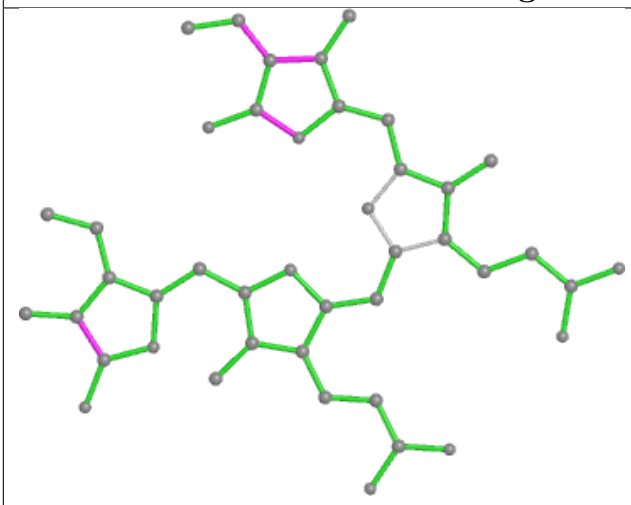


Rings

Ligand PEB dx 401



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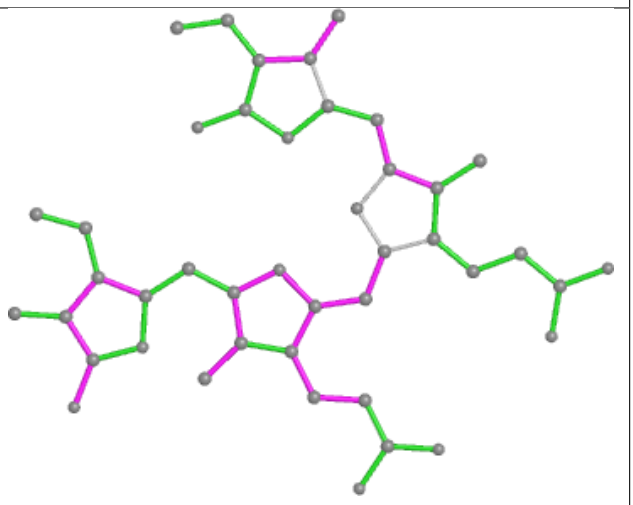

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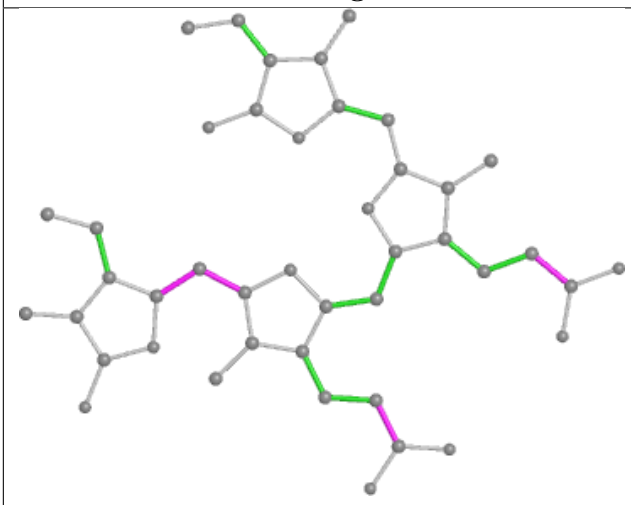

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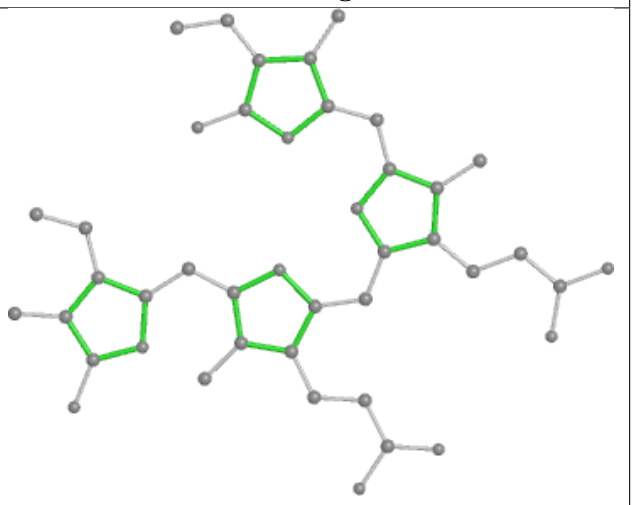
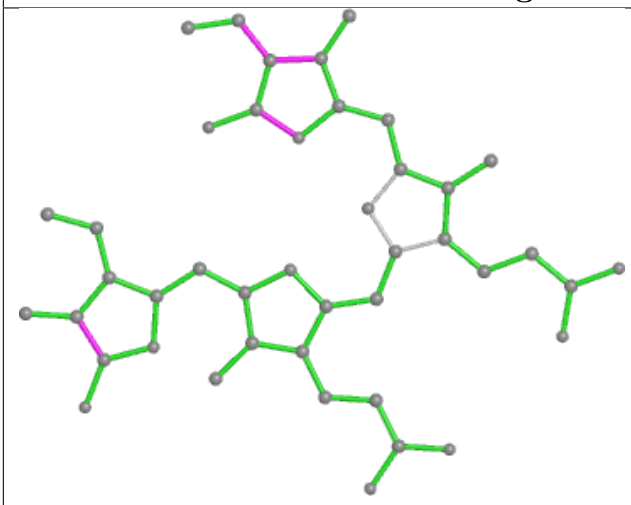


Rings

Ligand PEB aQ 201



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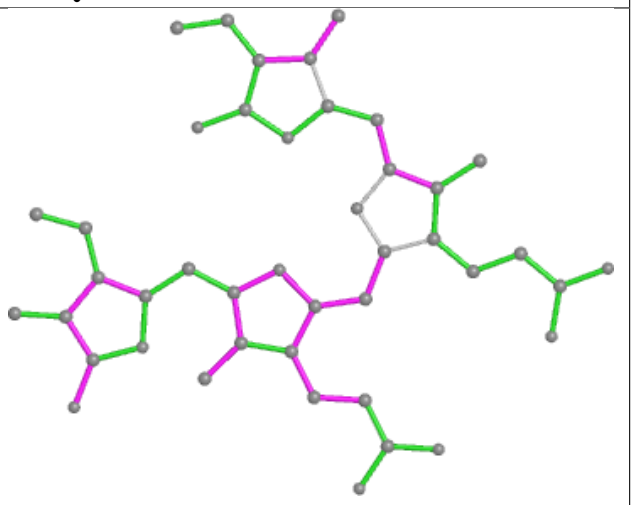

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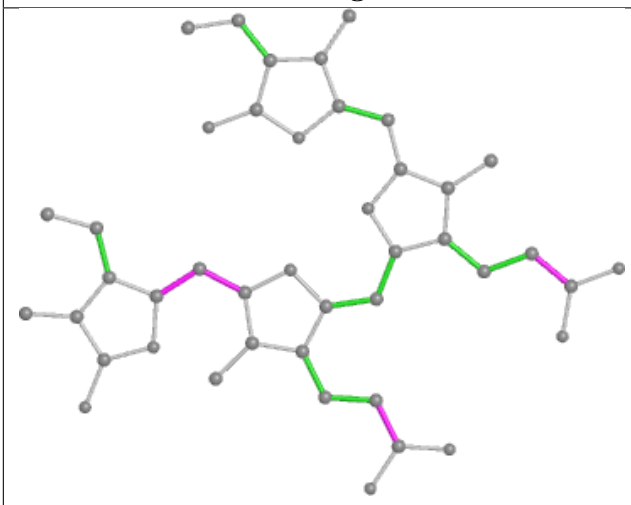

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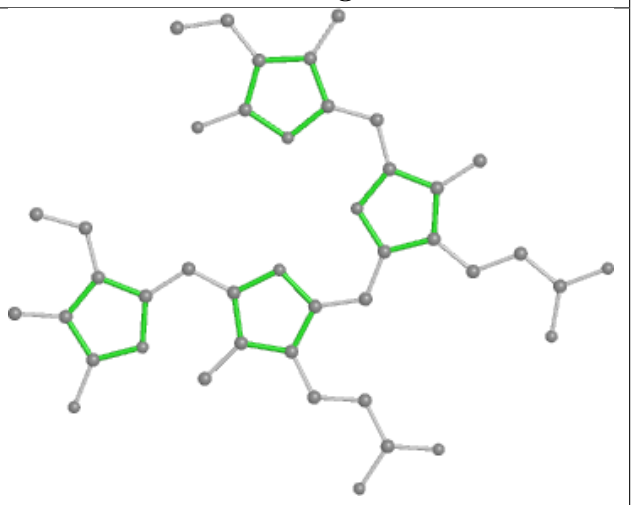
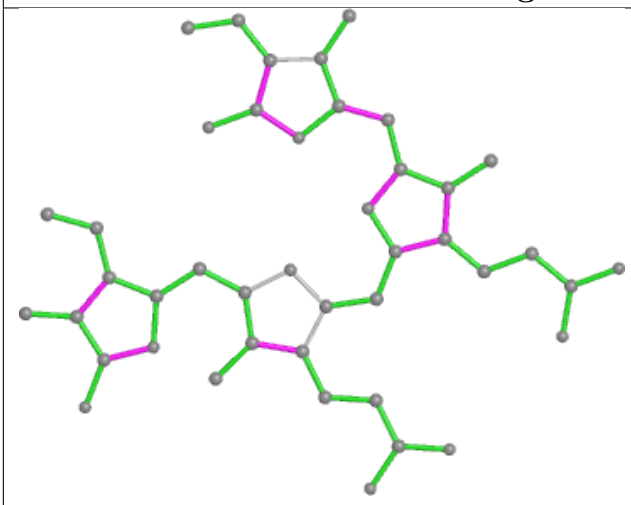


Rings

Ligand PUB v3 203



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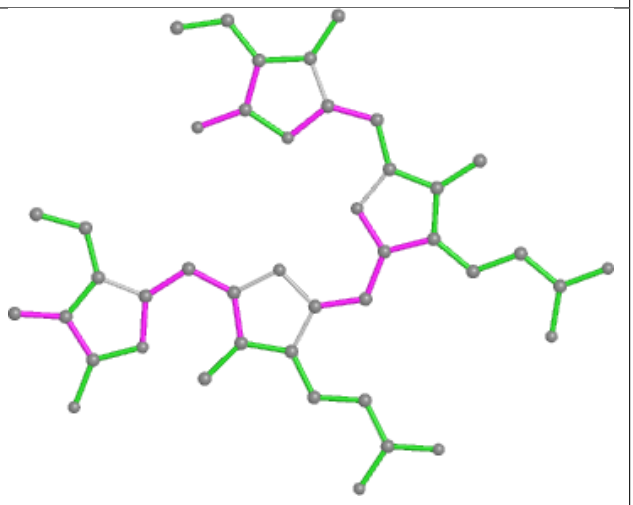

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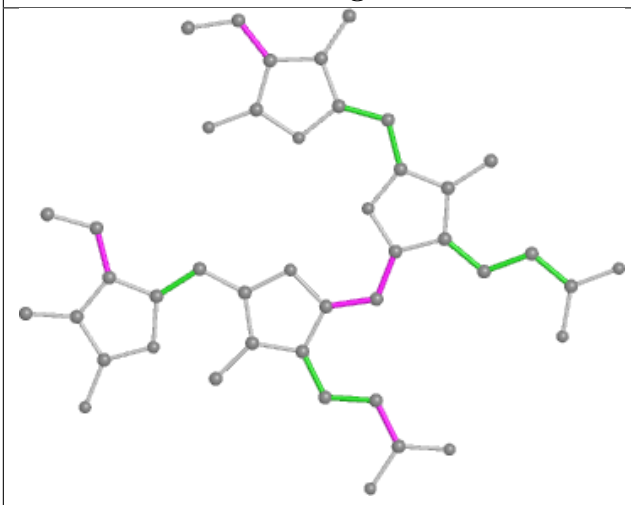

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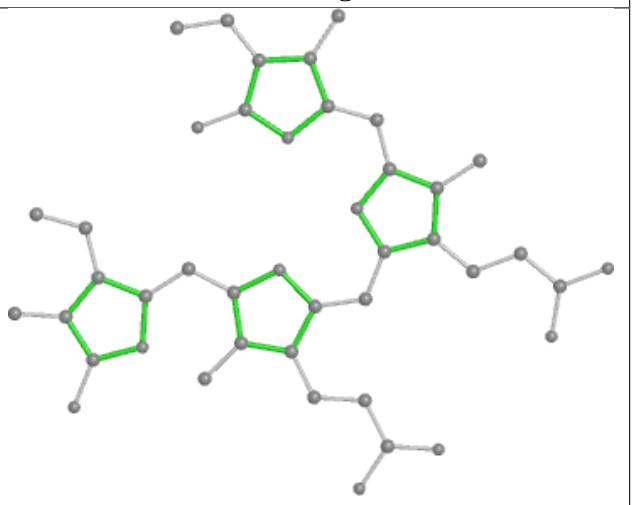
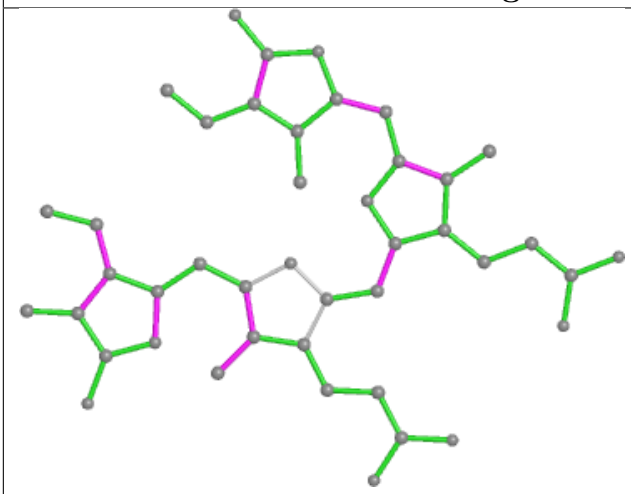


Rings

Ligand PVN bY 1004



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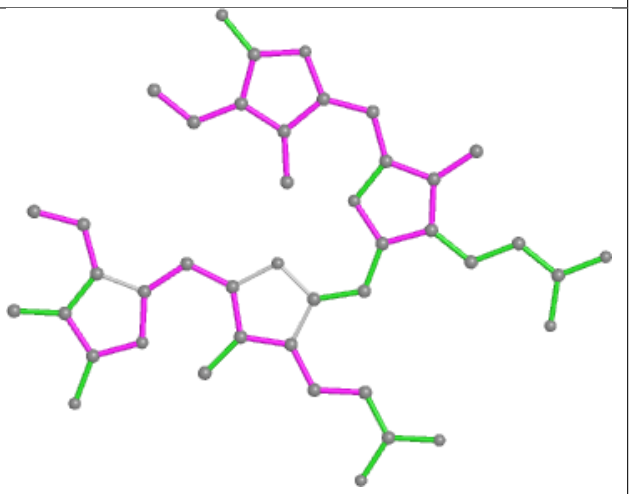

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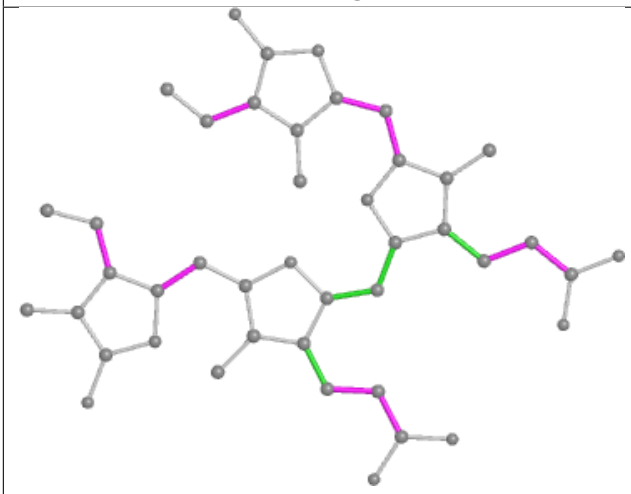

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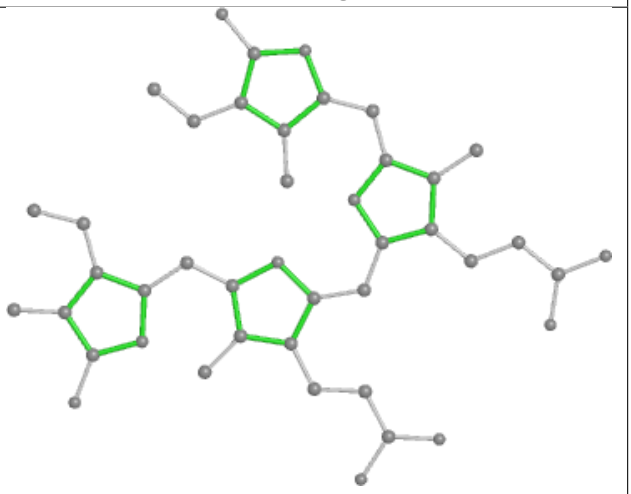
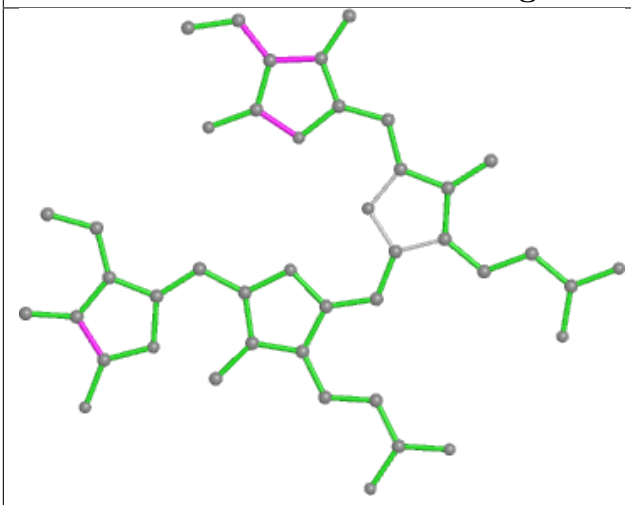


Rings

Ligand PEB ad 201



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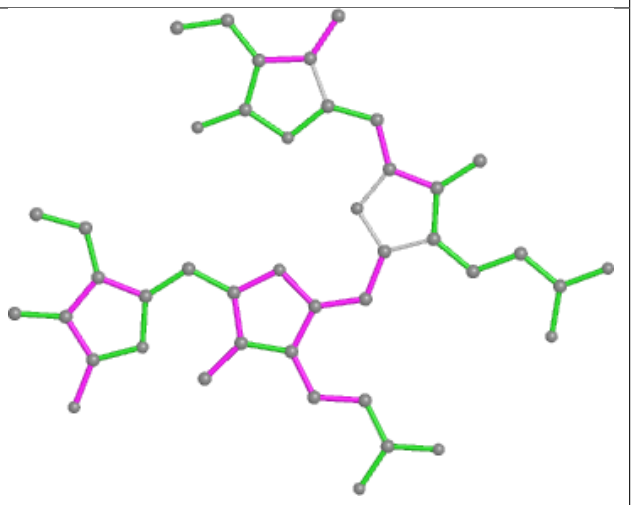

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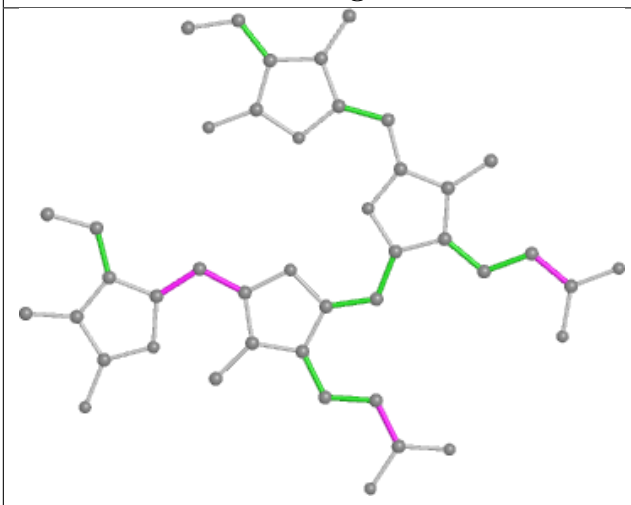

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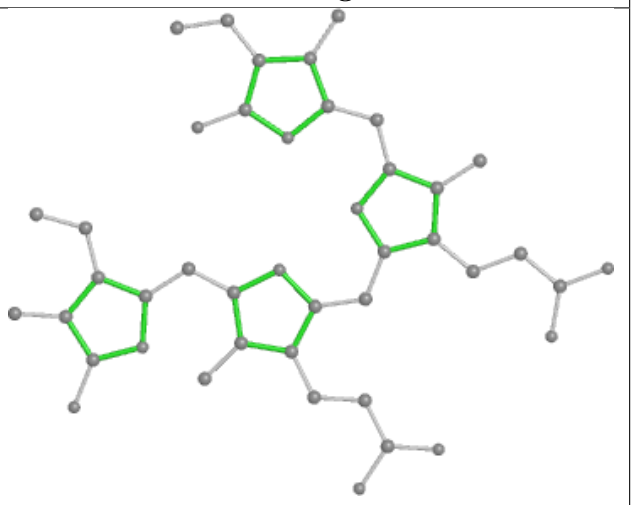

Rings

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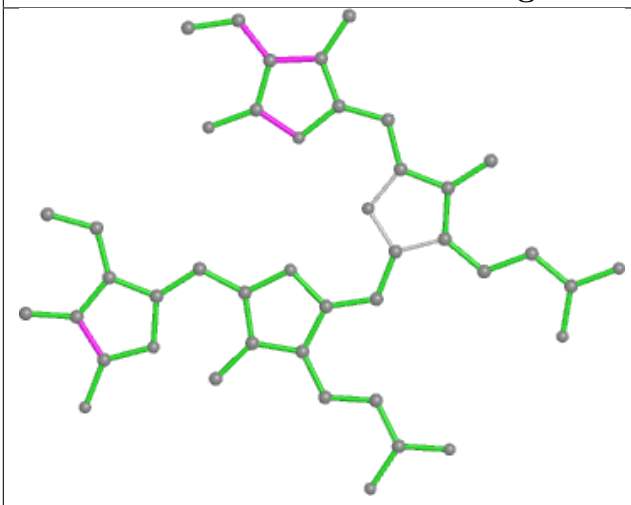

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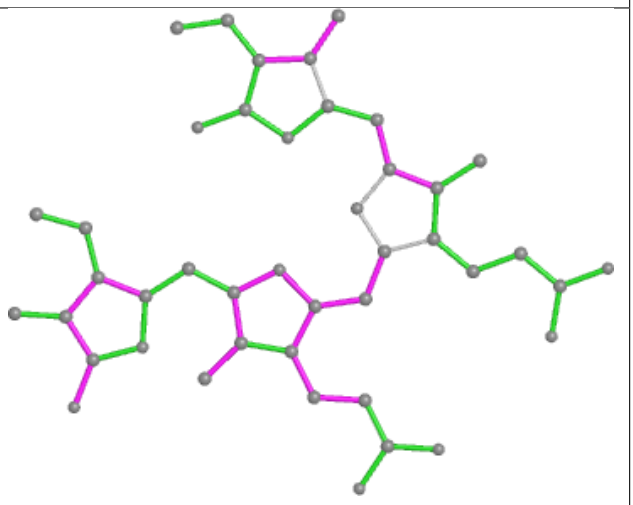

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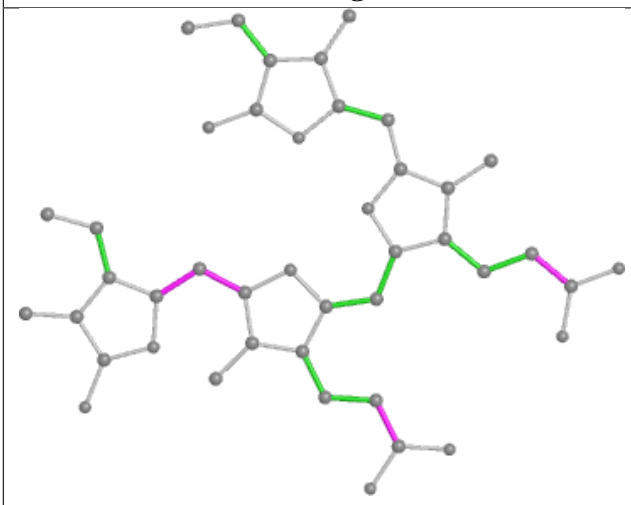

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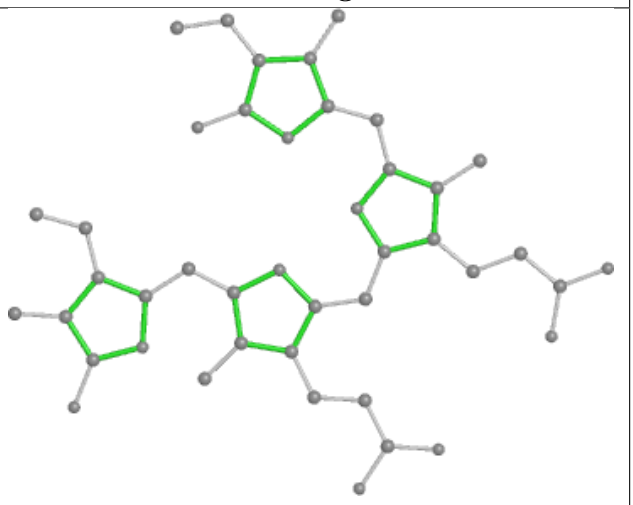
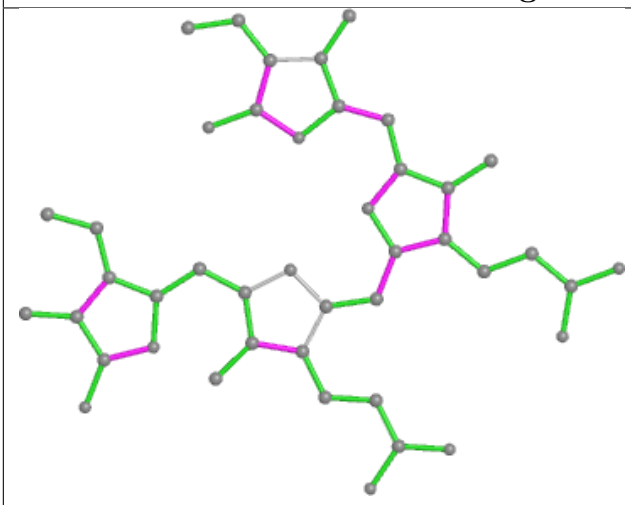


Rings

Ligand PUB gr 202



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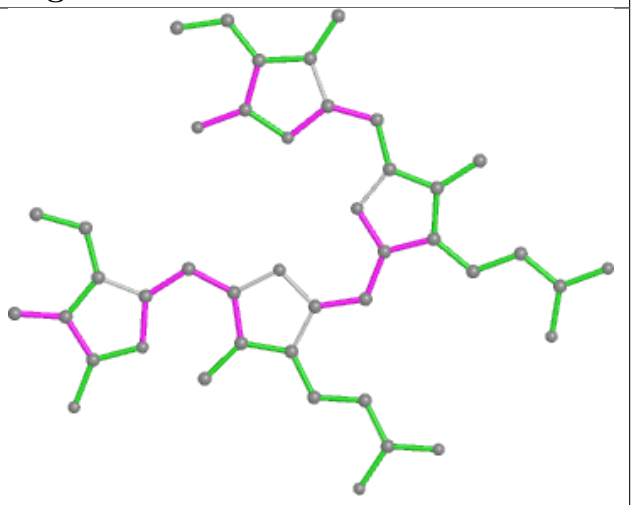

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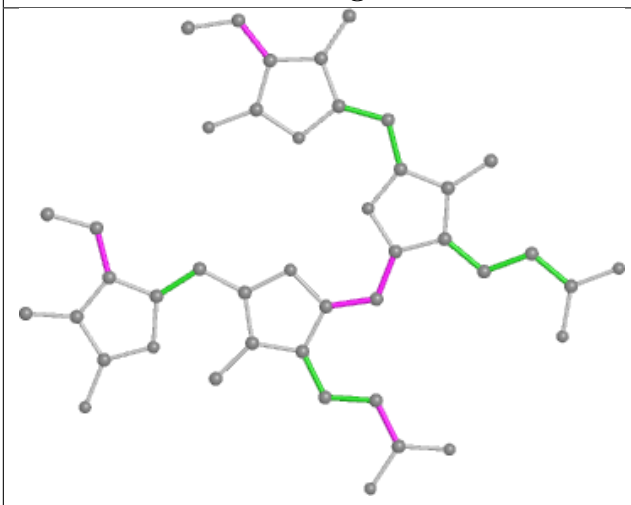

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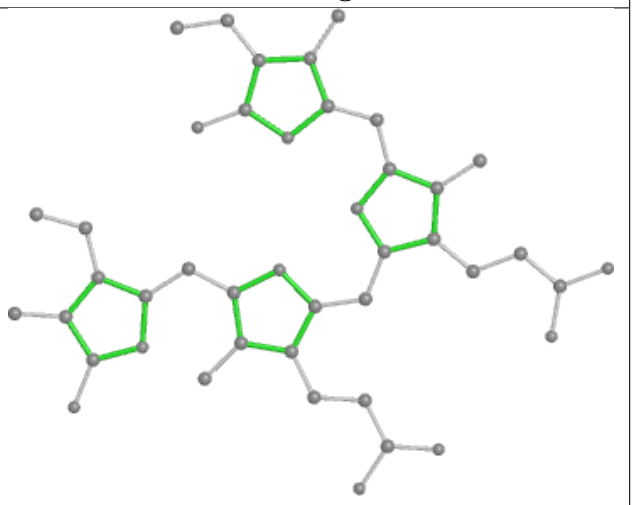
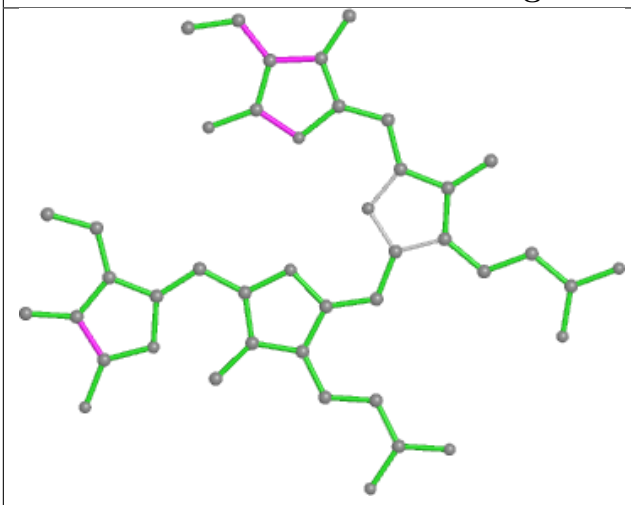


Rings

Ligand PEB i2 202



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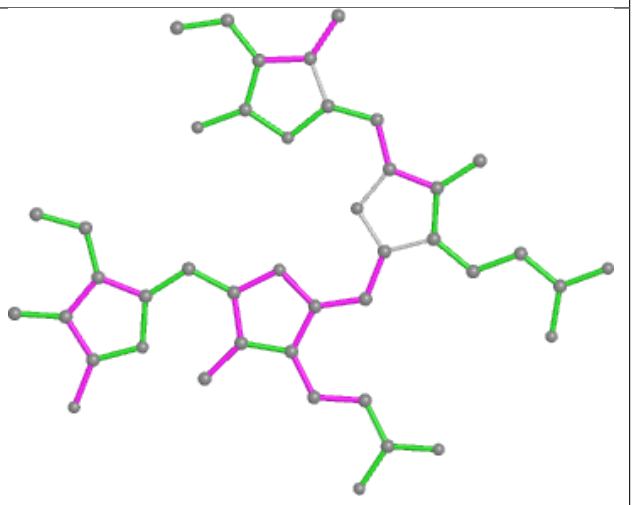

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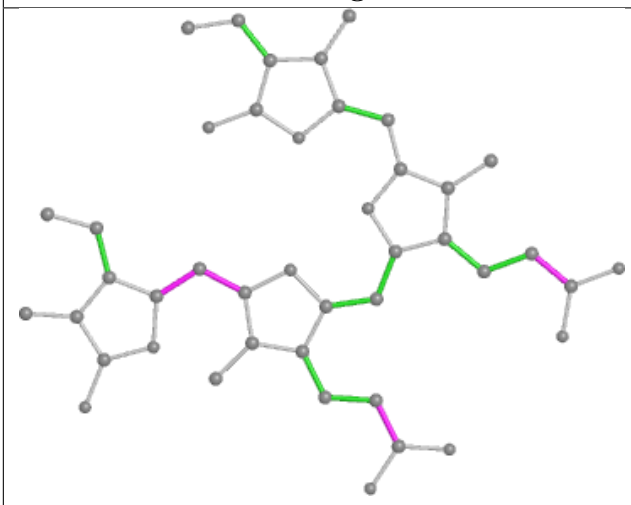

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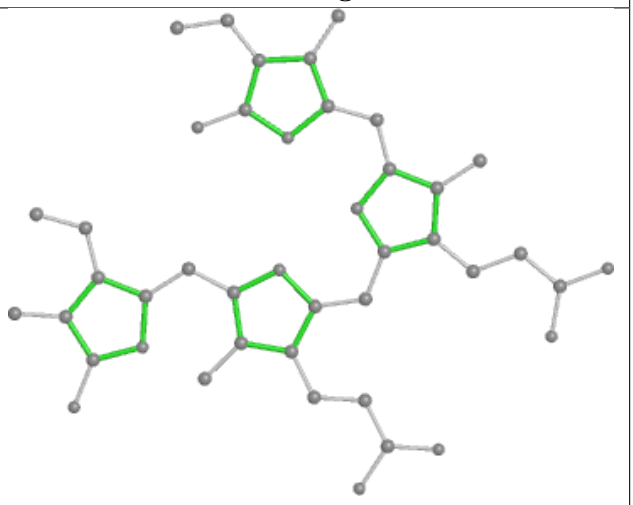
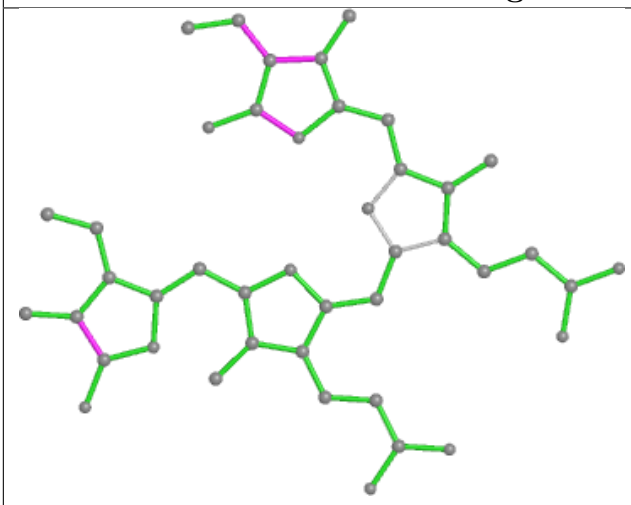


Rings

Ligand PEB A2 1002



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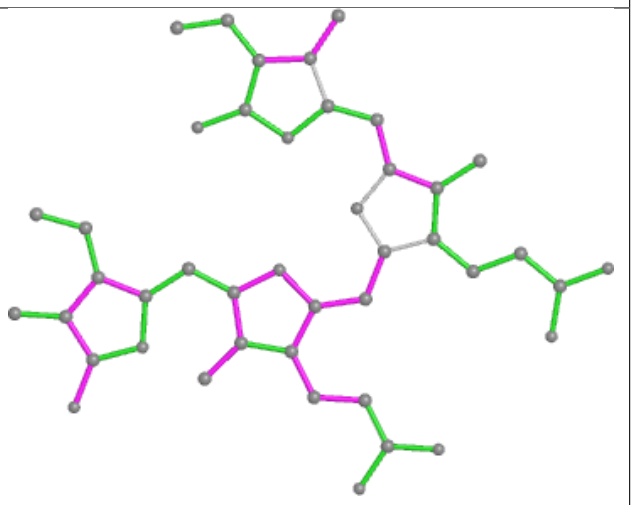

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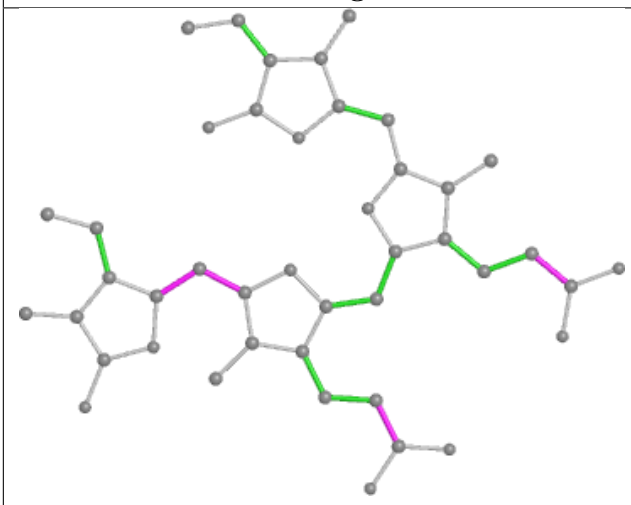

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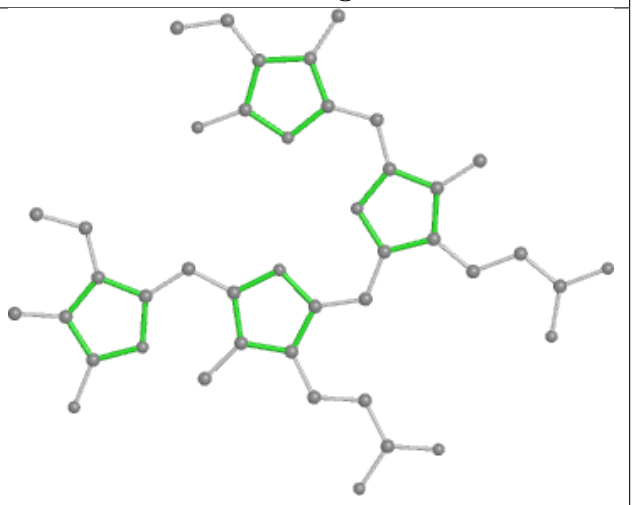
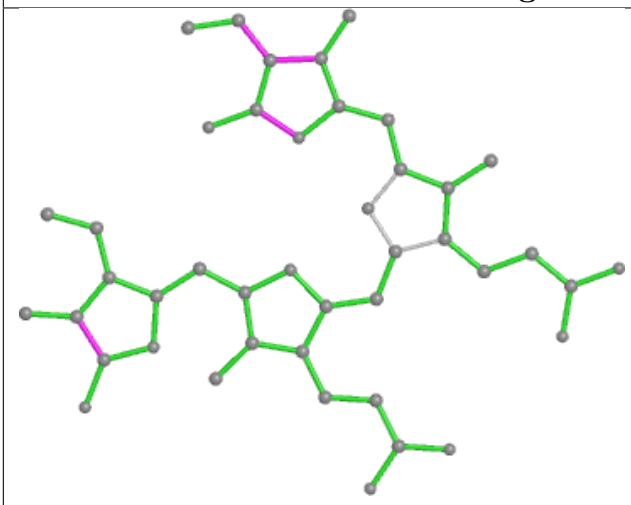


Rings

Ligand PEB d9 303



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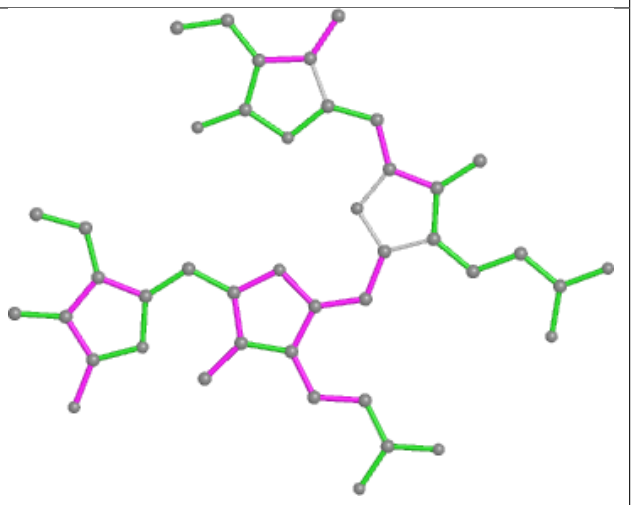

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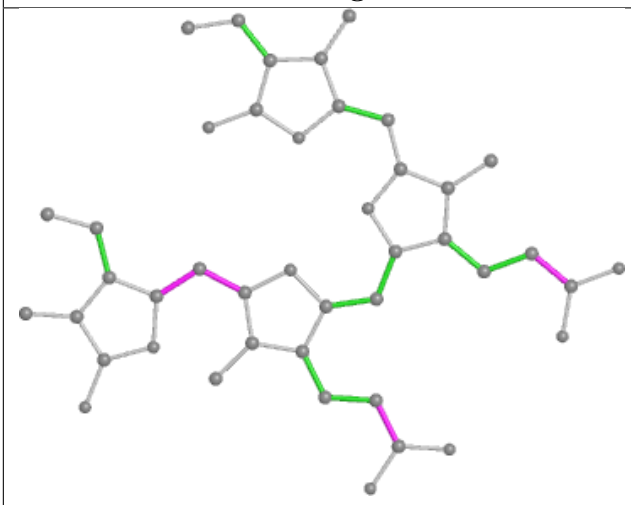

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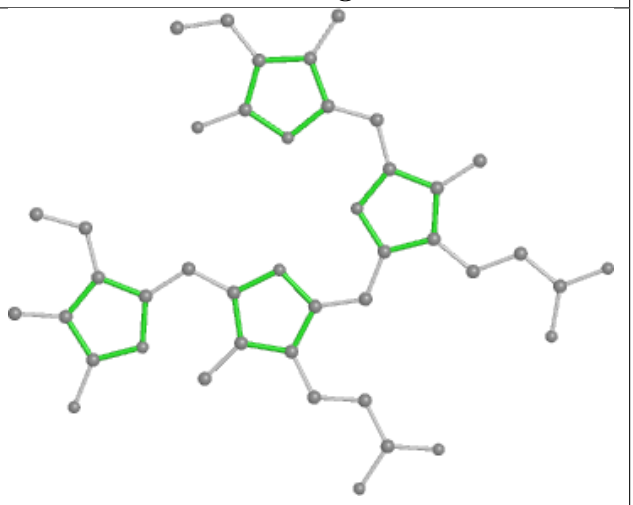
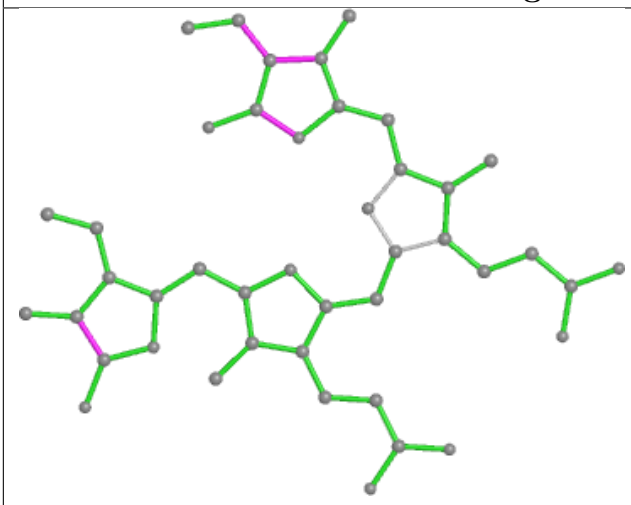


Rings

Ligand PEB i4 201



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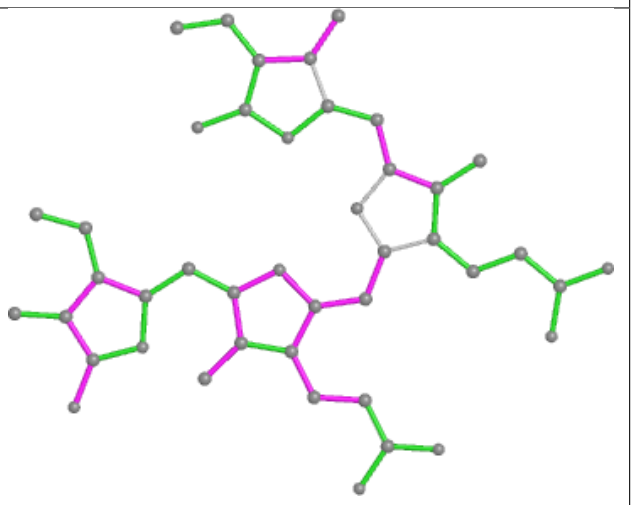

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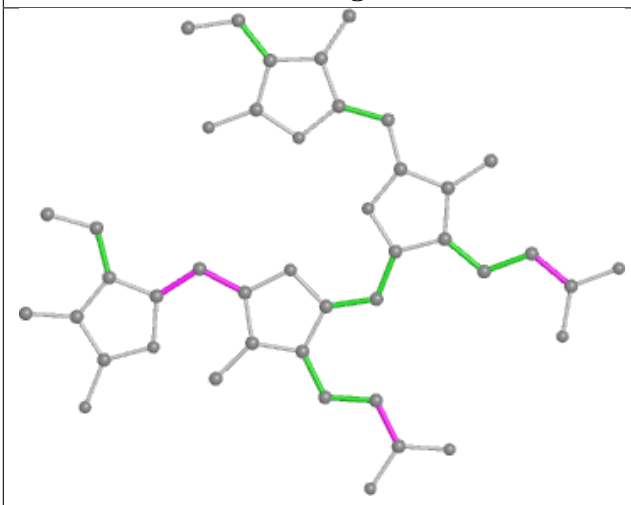

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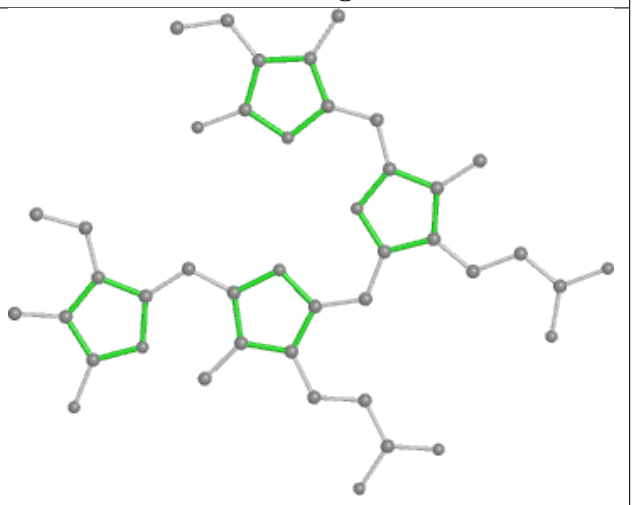
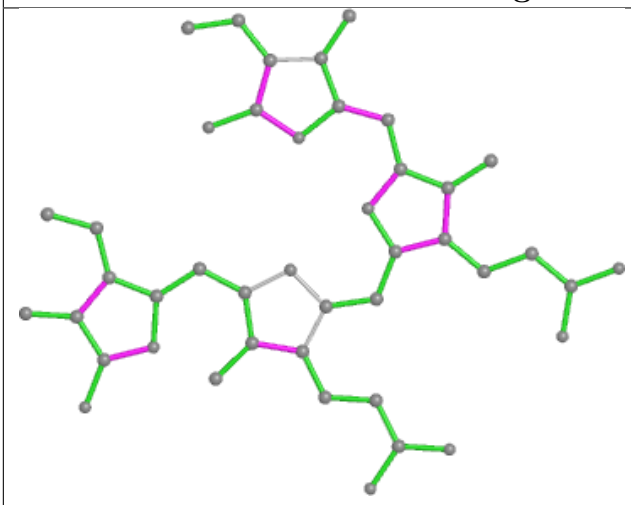


Rings

Ligand PUB aY 404



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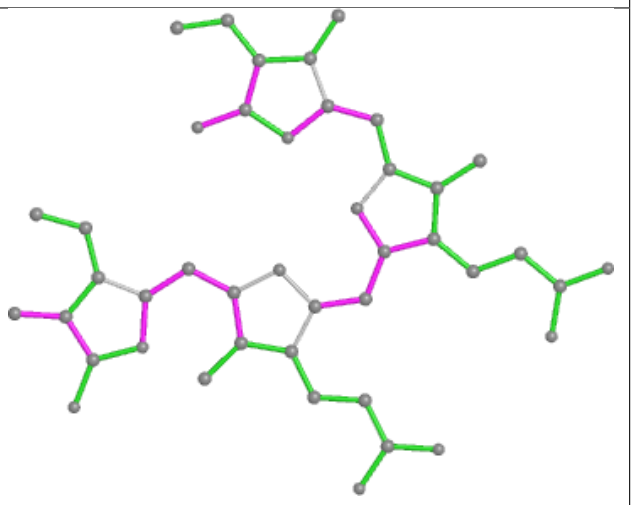
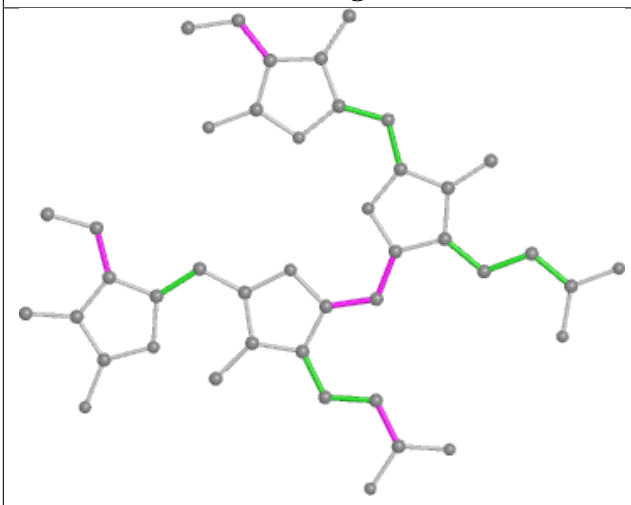


Bond angles



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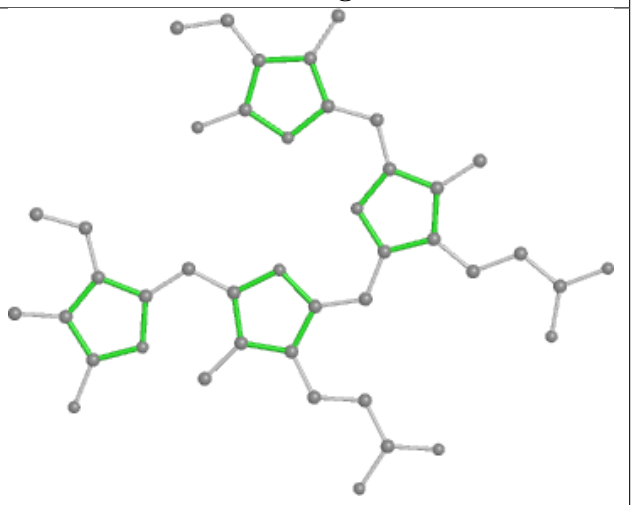
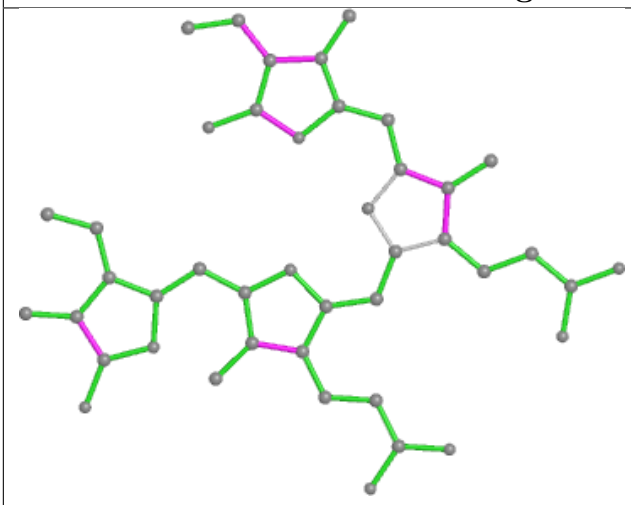
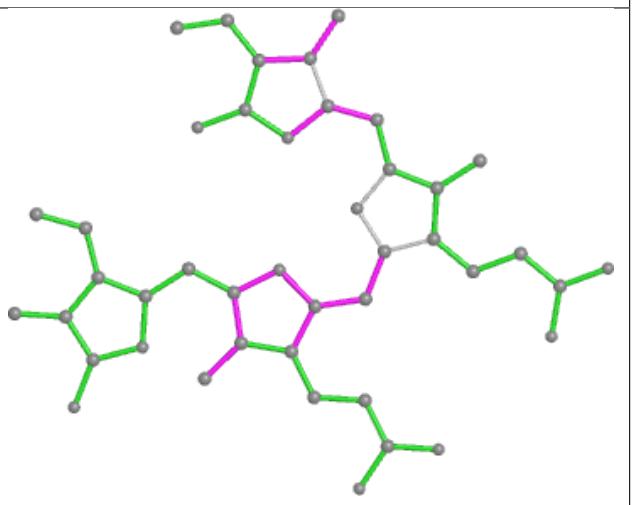


Rings

Ligand PEB eN 202



Bond lengths



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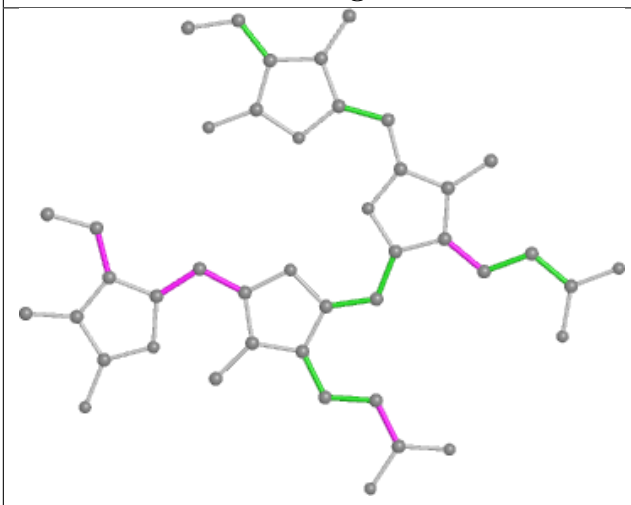
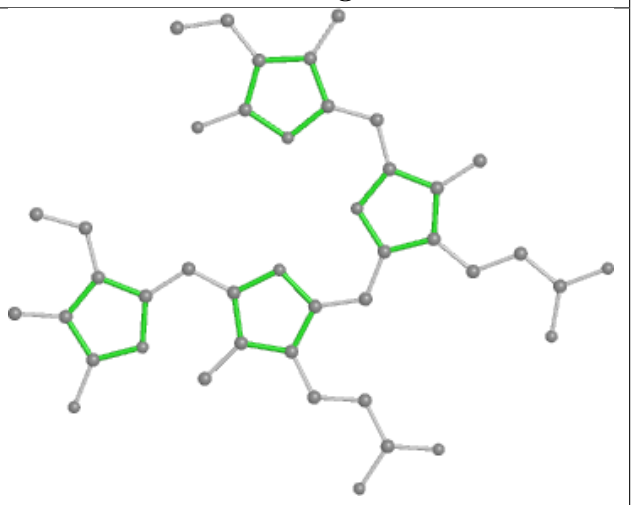
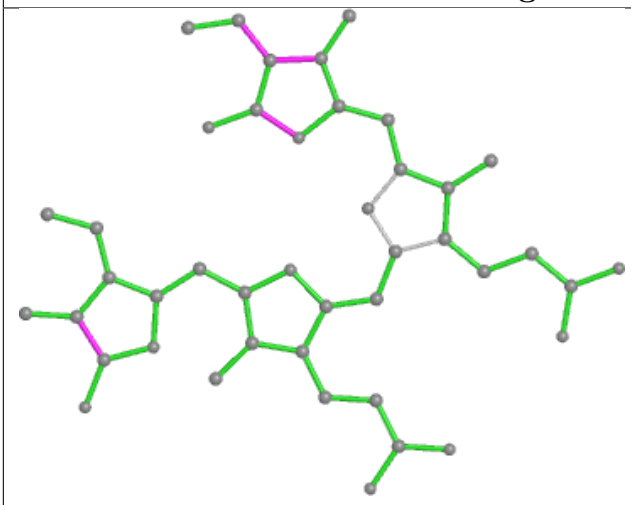


Torsions



Rings

Ligand PEB b9 404



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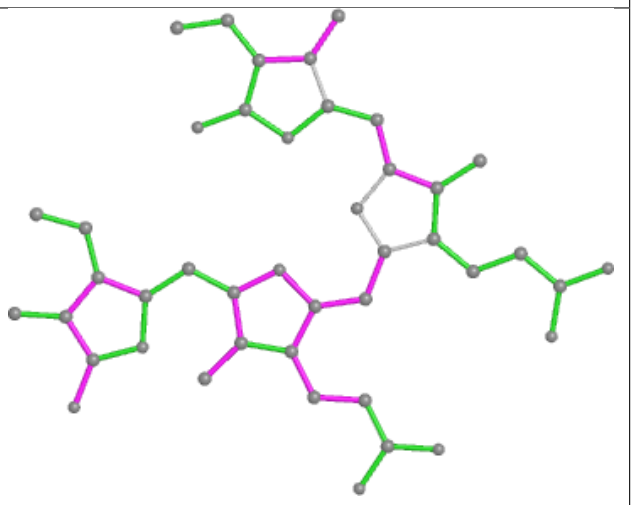

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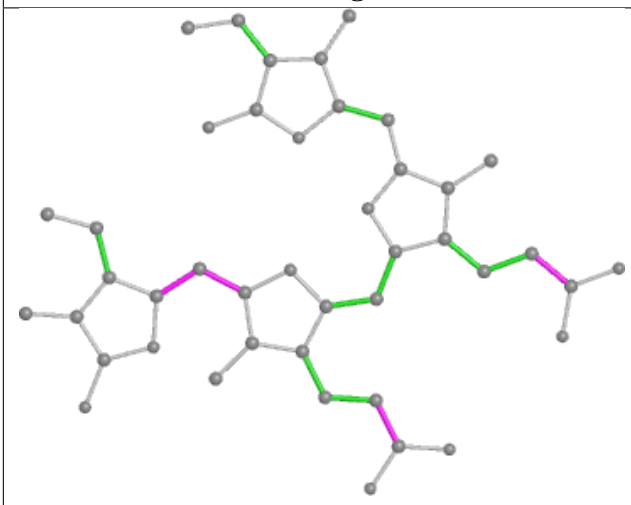

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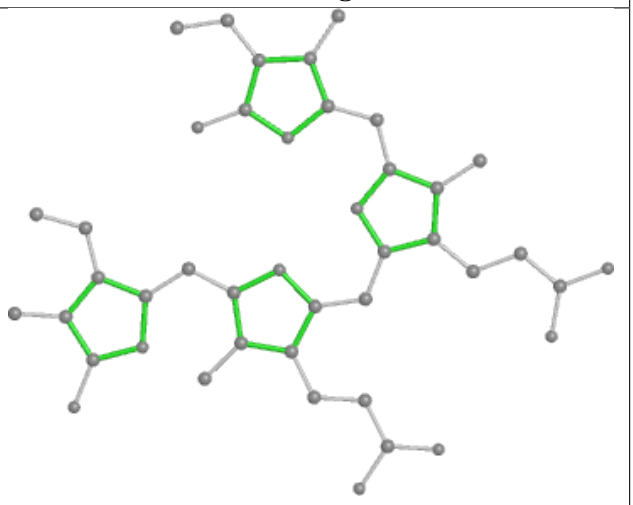
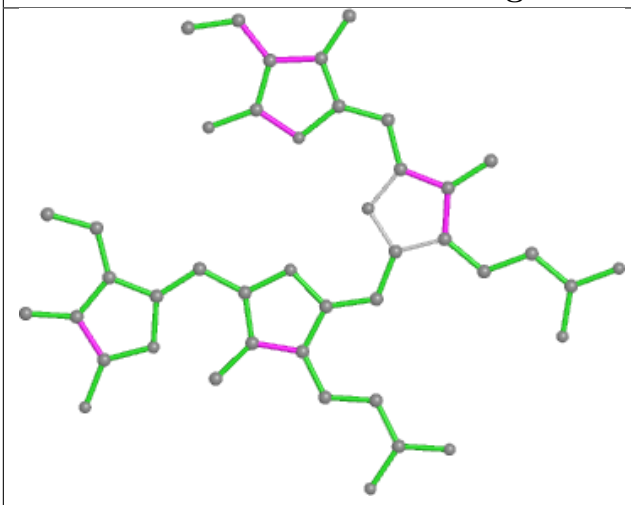


Rings

Ligand PEB kR 1002



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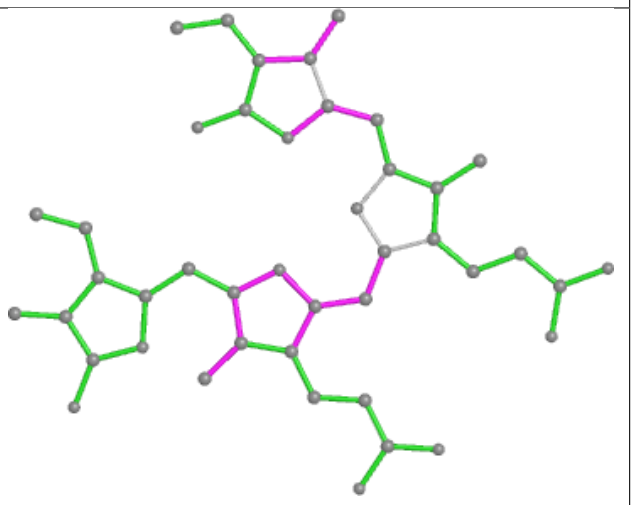

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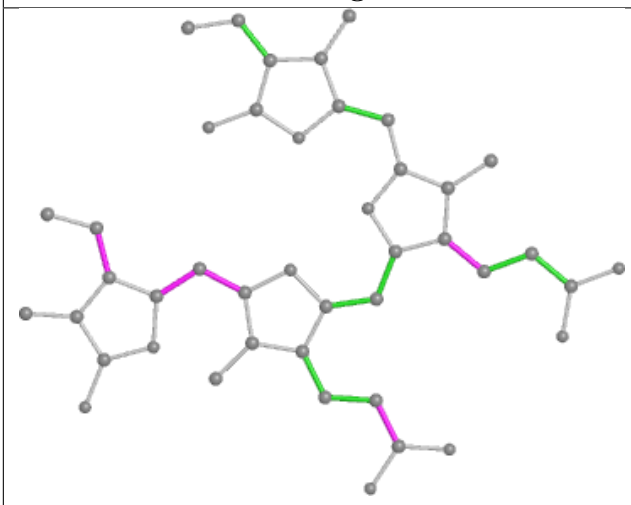

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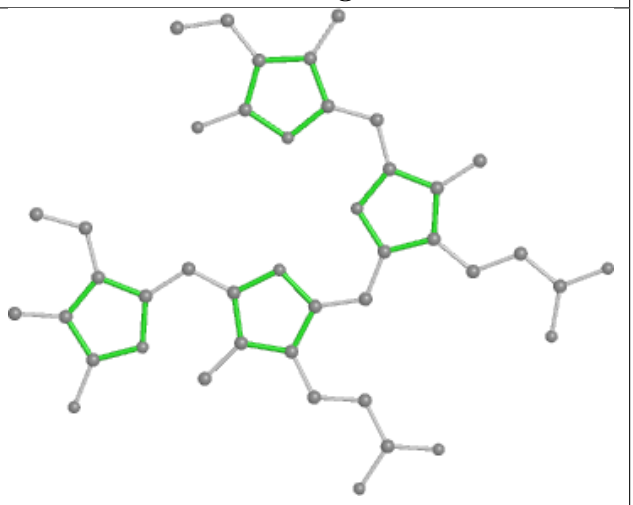
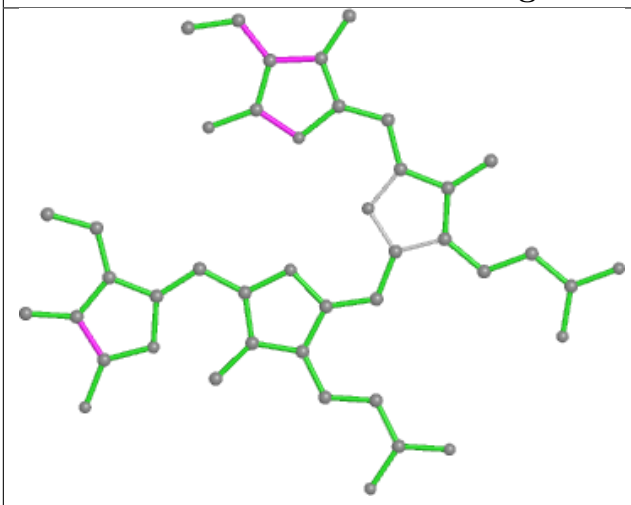


Rings

Ligand PEB eZ 401



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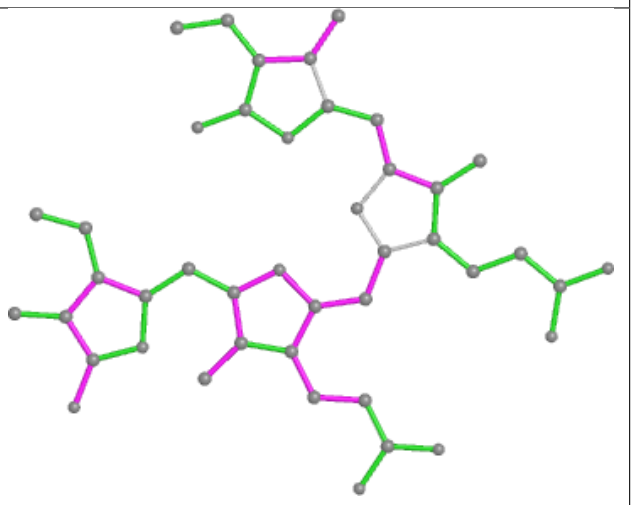

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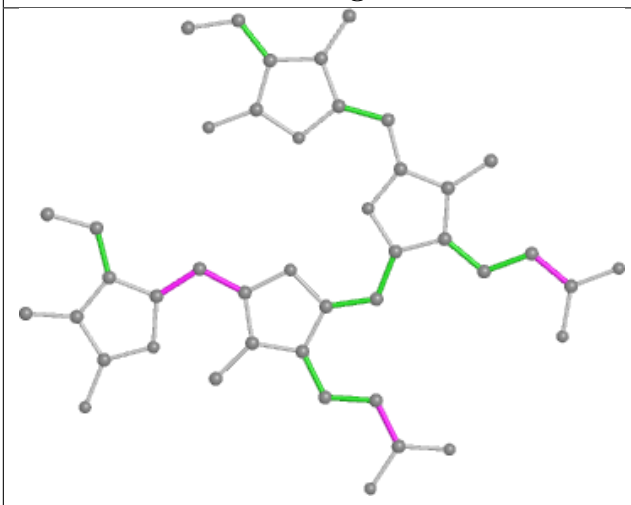

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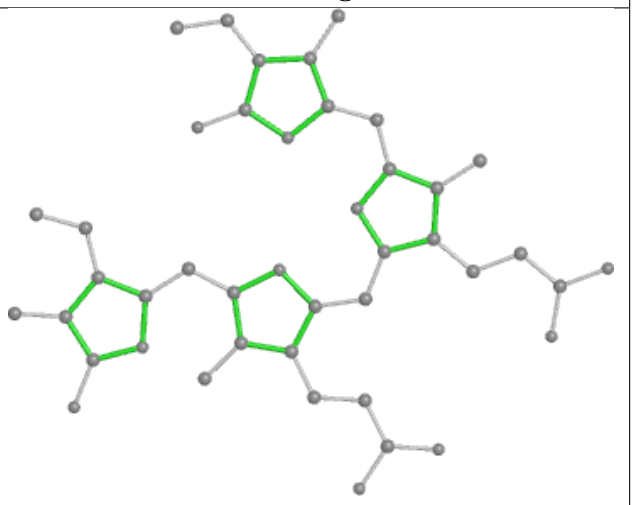
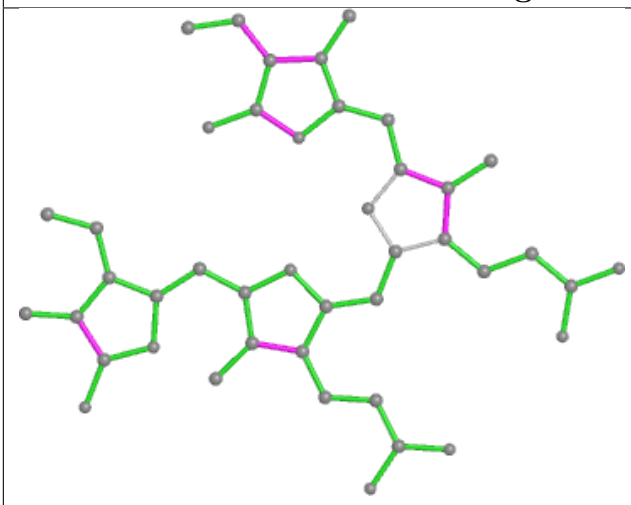


Rings

Ligand PEB H9 202



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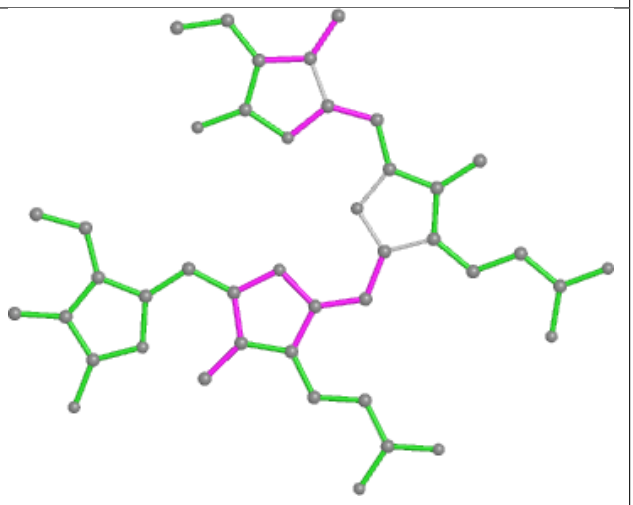

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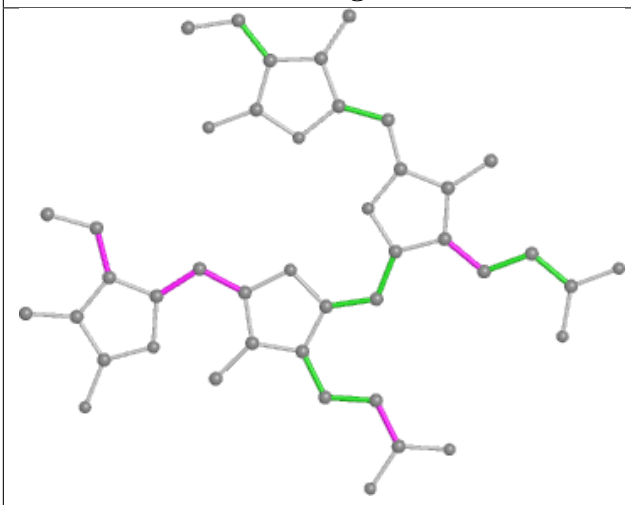

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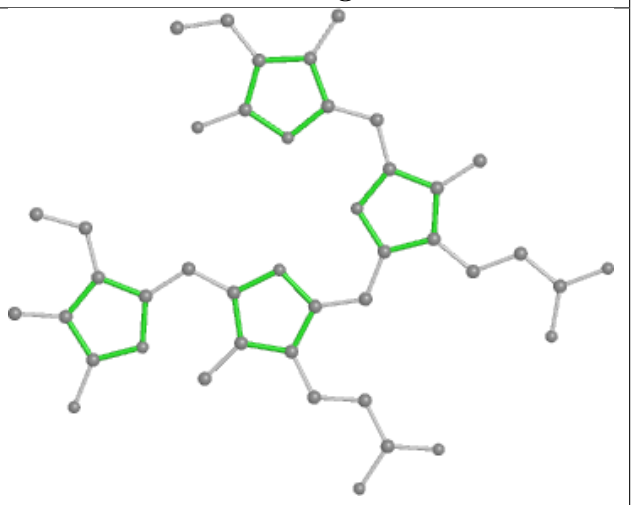
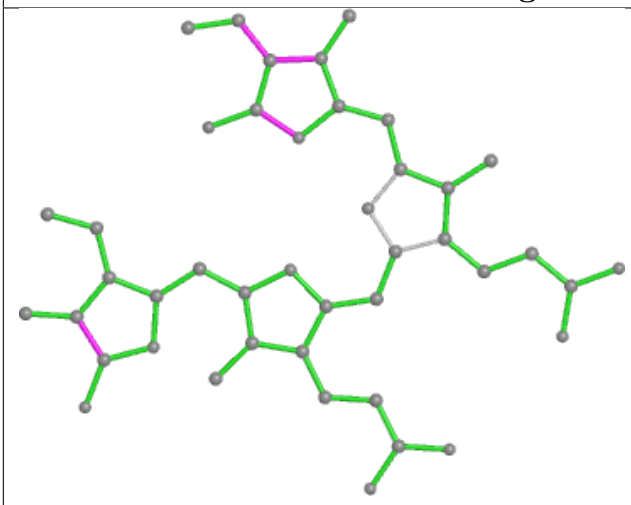


Rings

Ligand PEB n5 201



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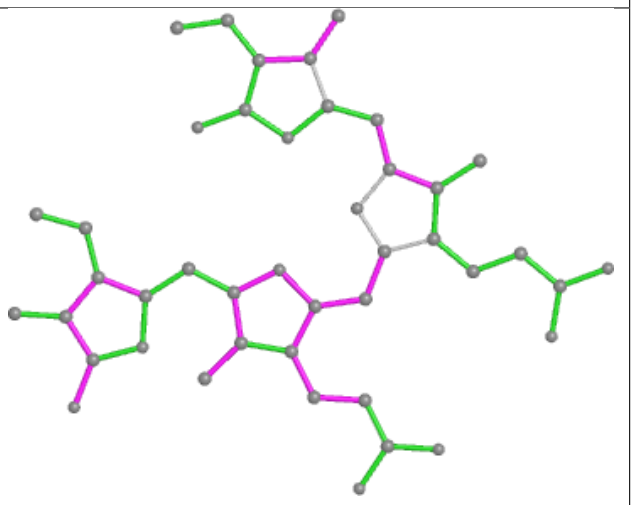

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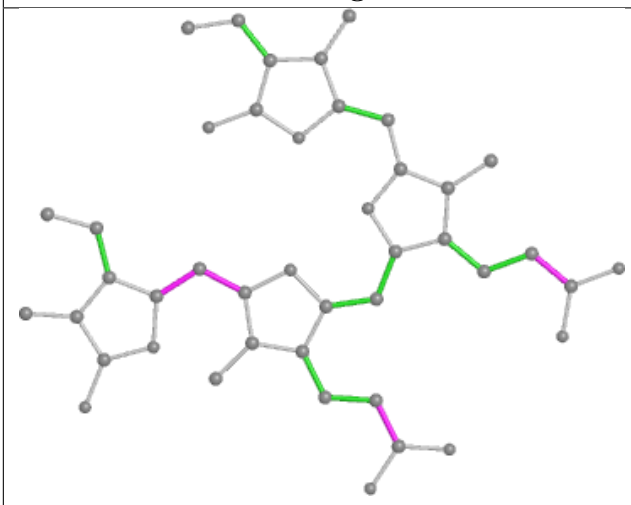

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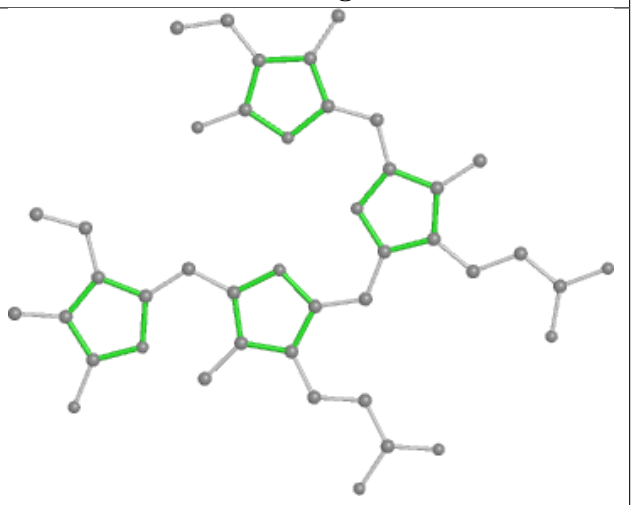

Rings

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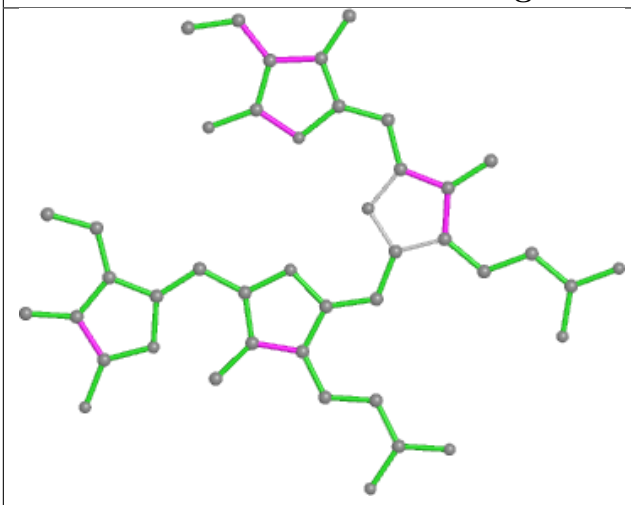

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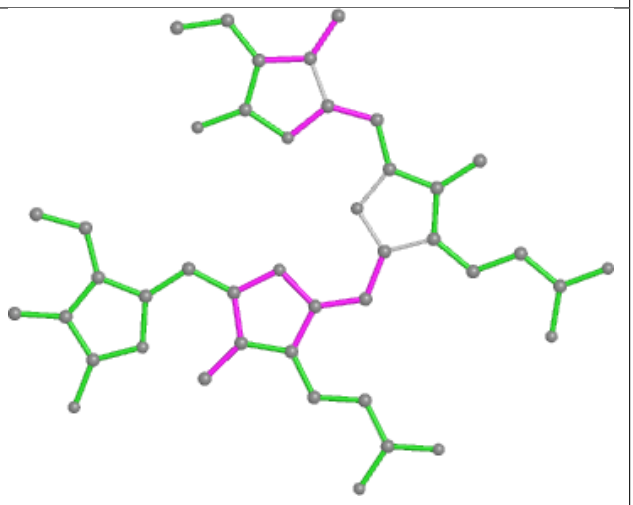

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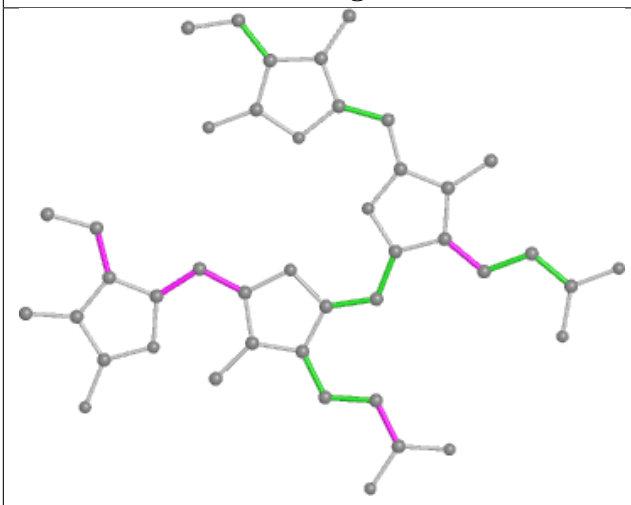

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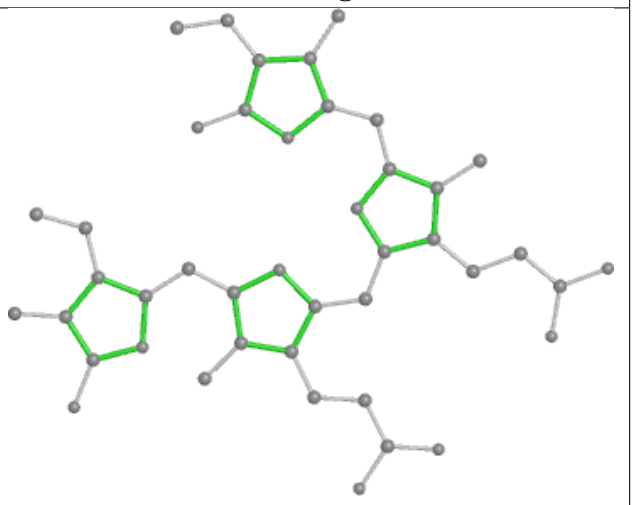
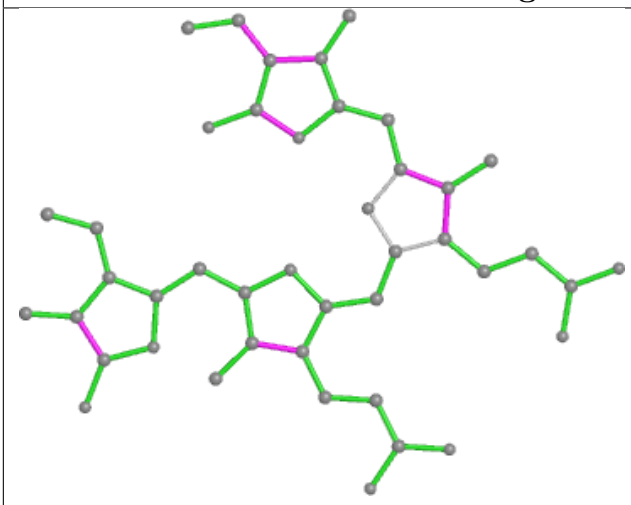


Rings

Ligand PEB p2 202



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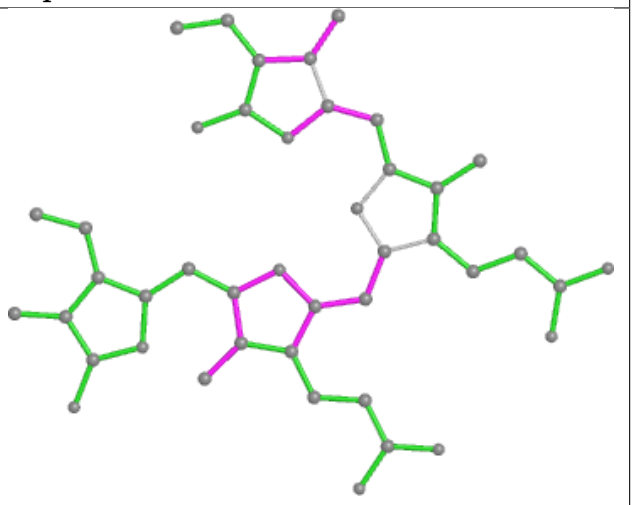

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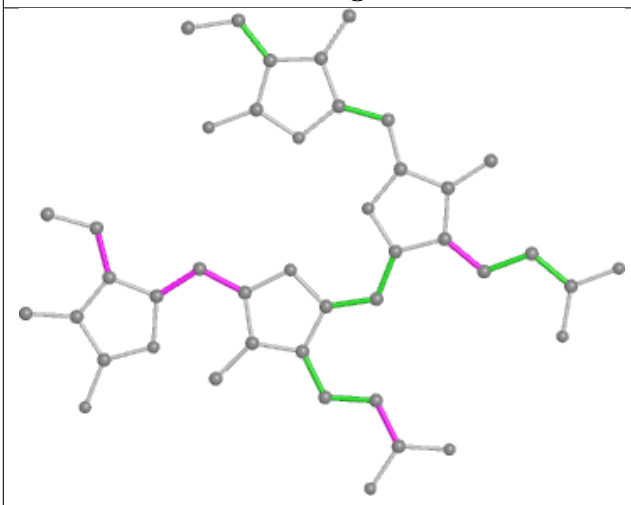

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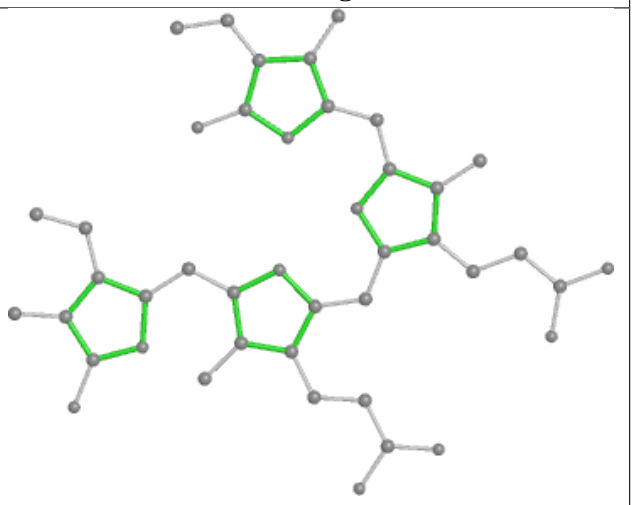
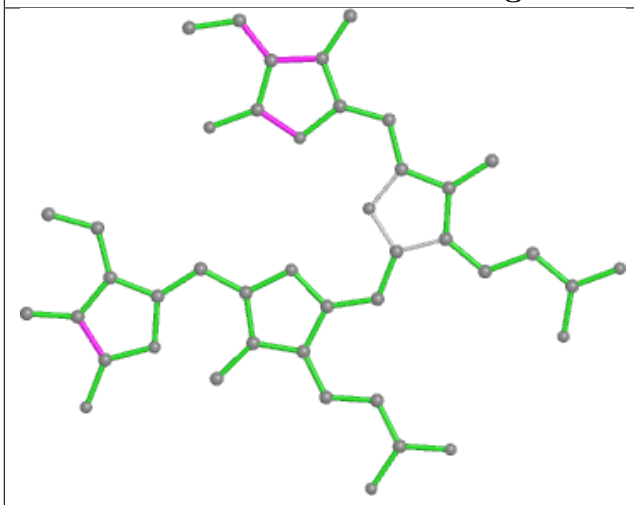


Rings

Ligand PEB eM 1001



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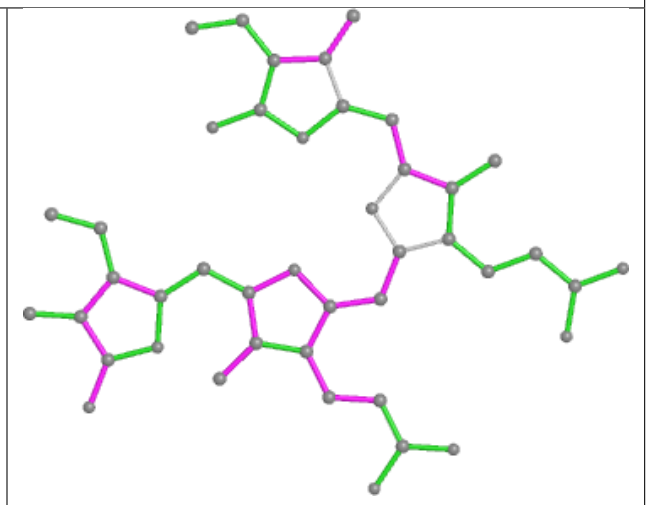

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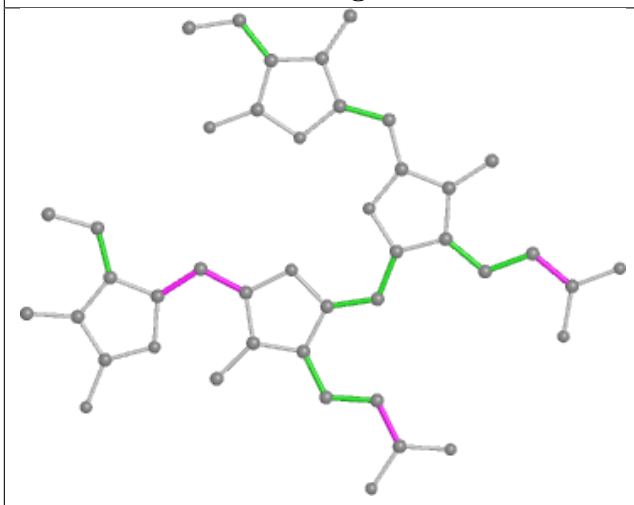

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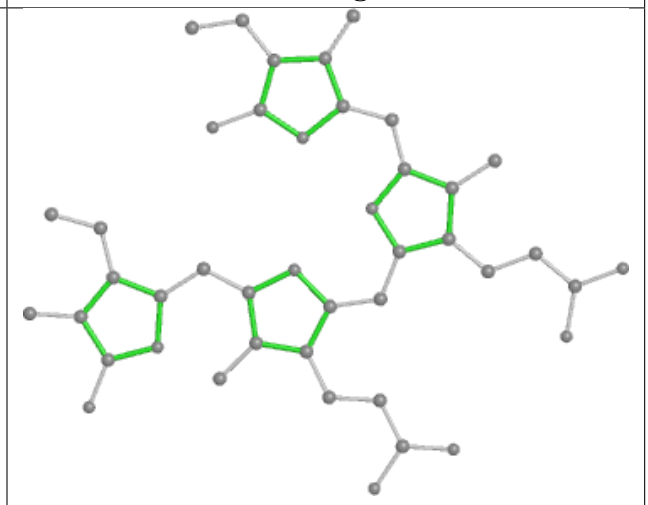
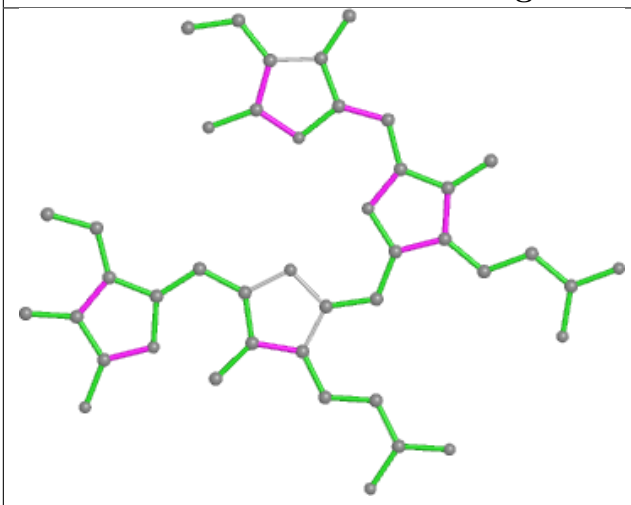


Rings

Ligand PUB F9 203



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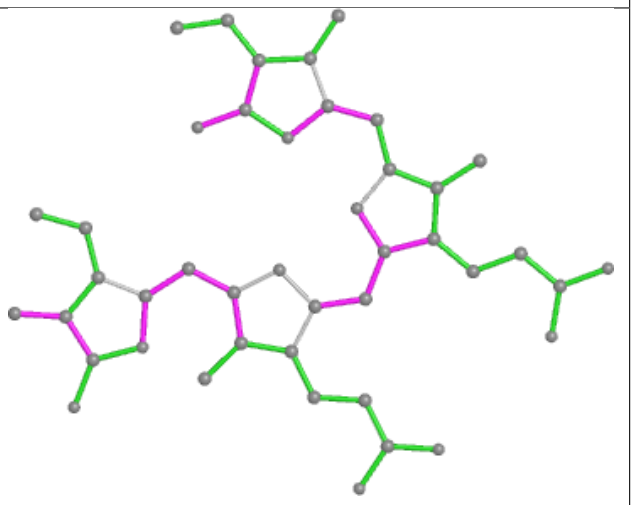

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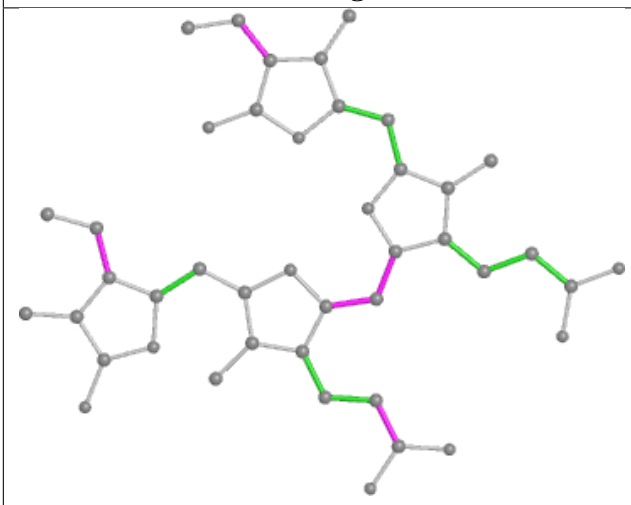

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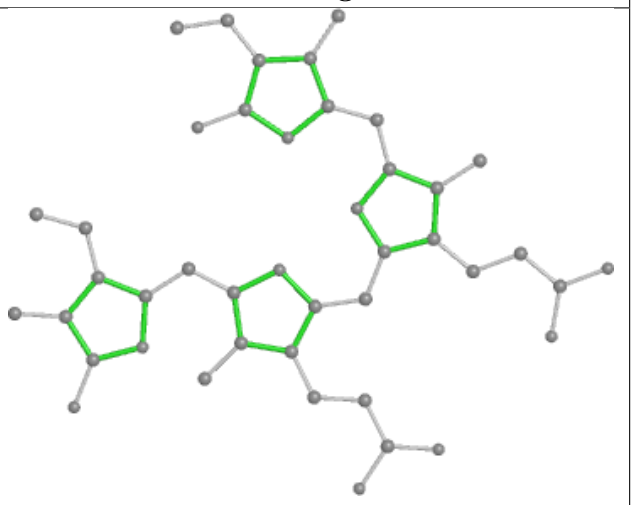

Rings

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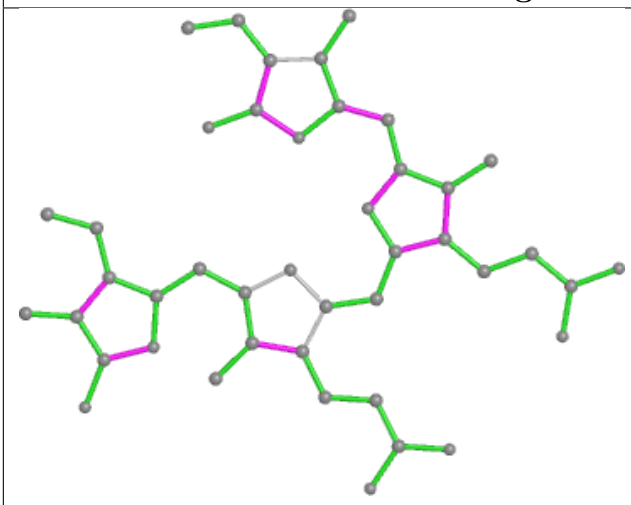

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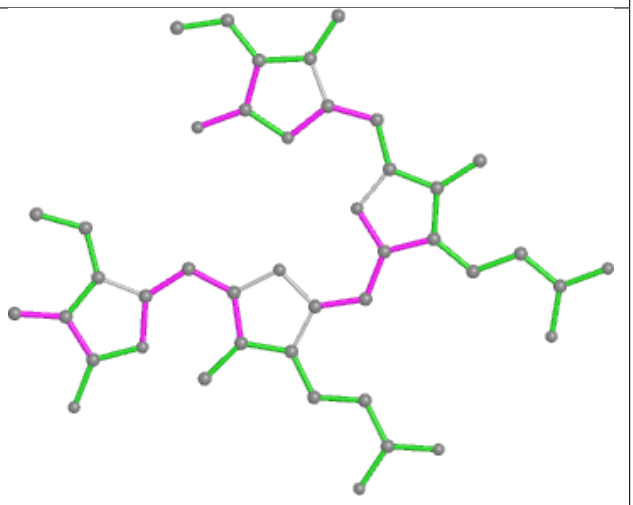

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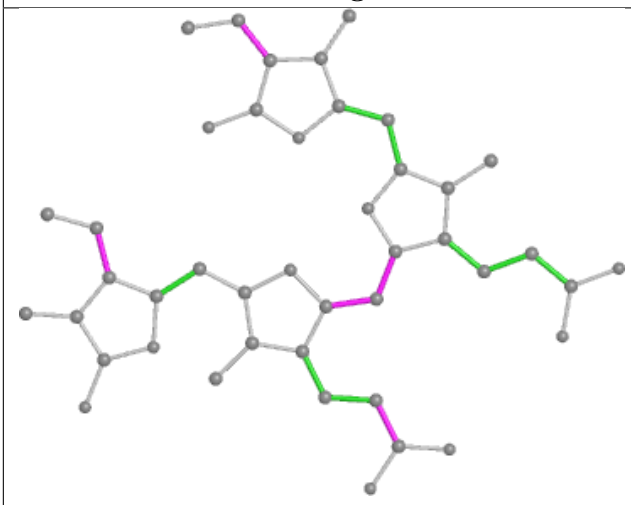

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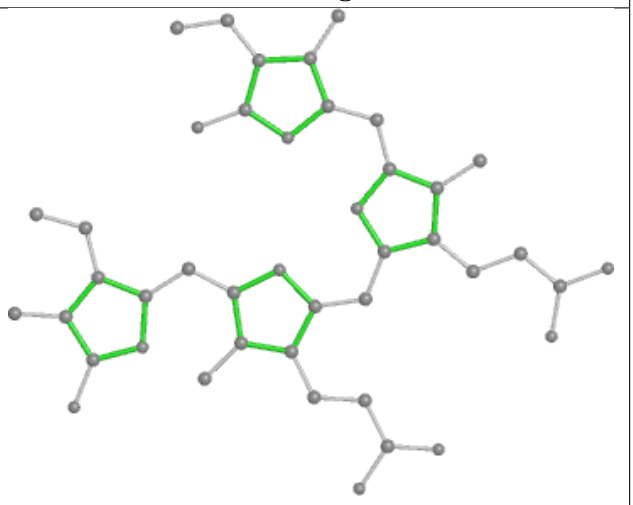
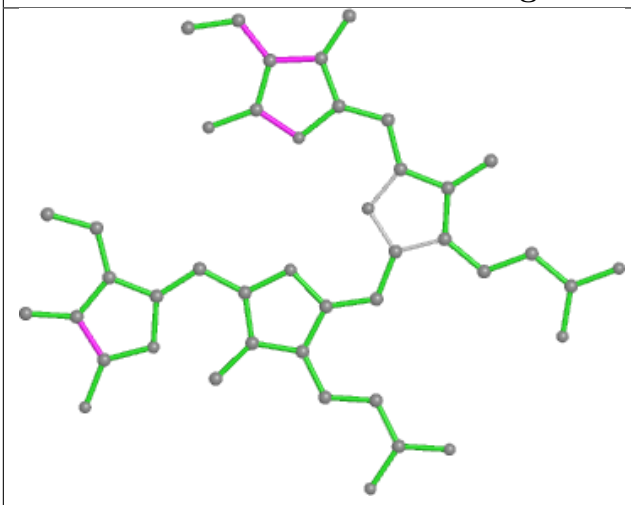


Rings

Ligand PEB g4 201



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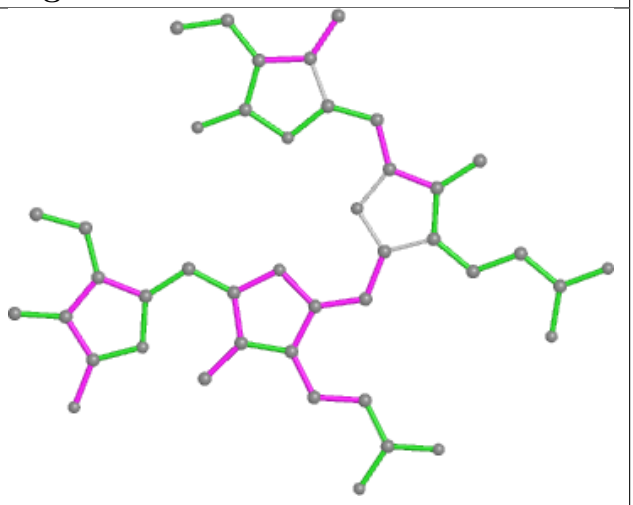

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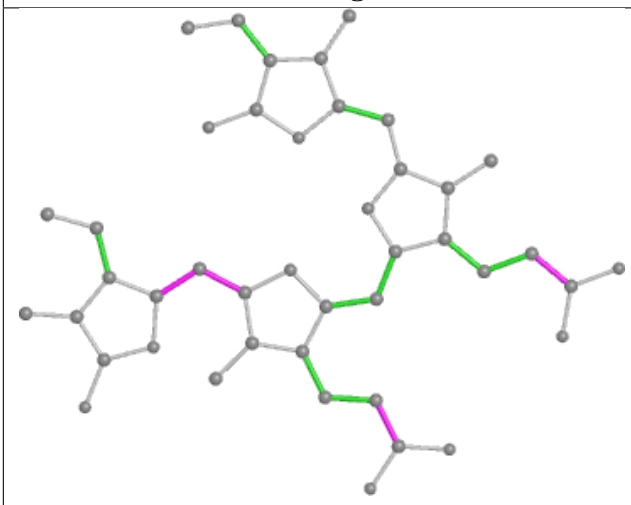

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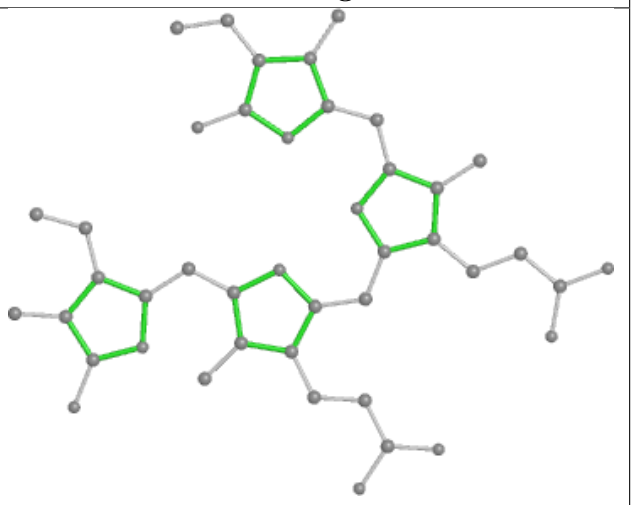
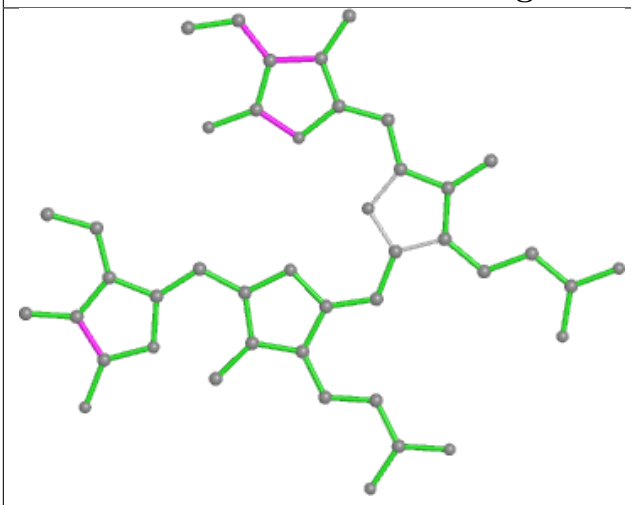


Rings

Ligand PEB B8 202



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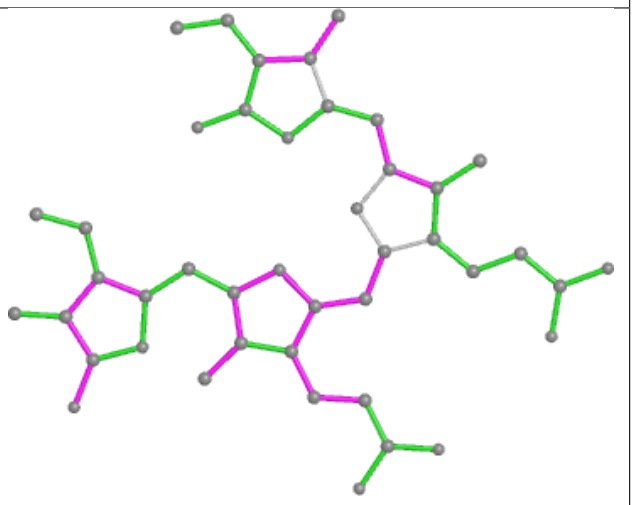

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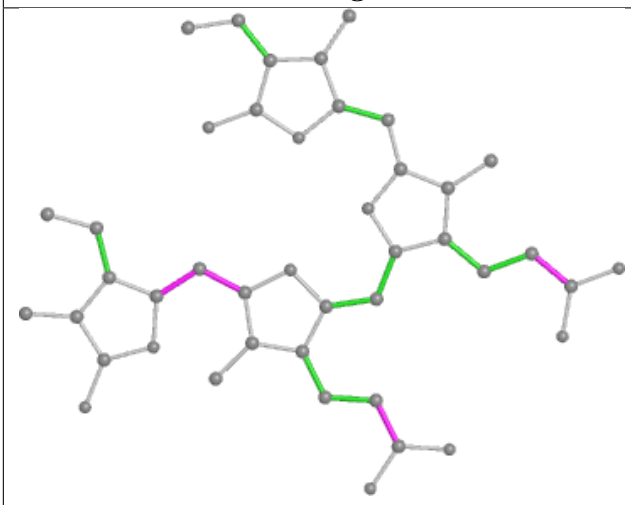

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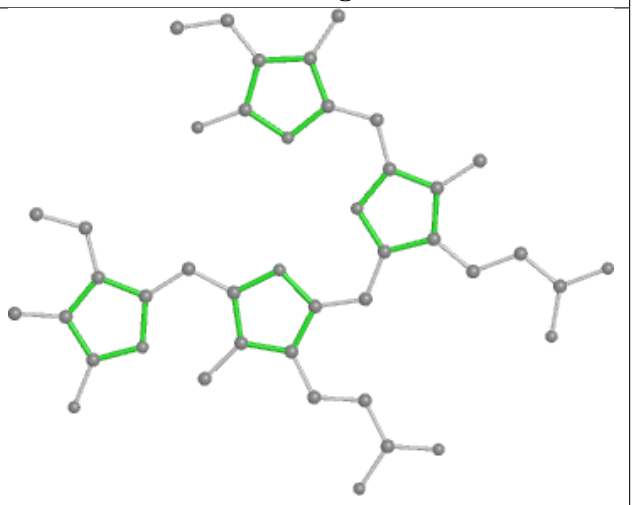
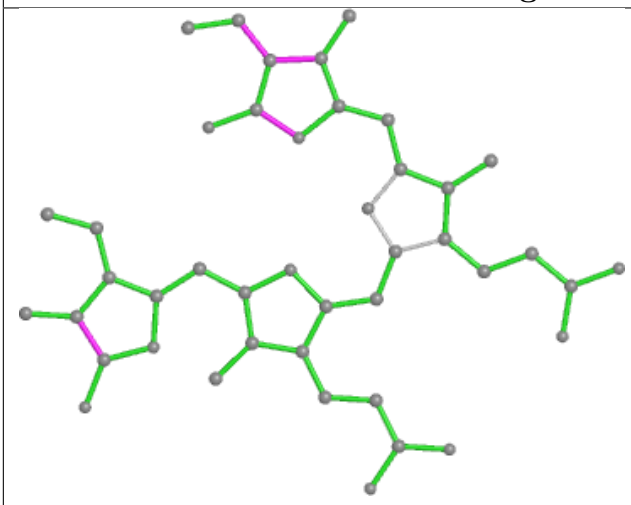
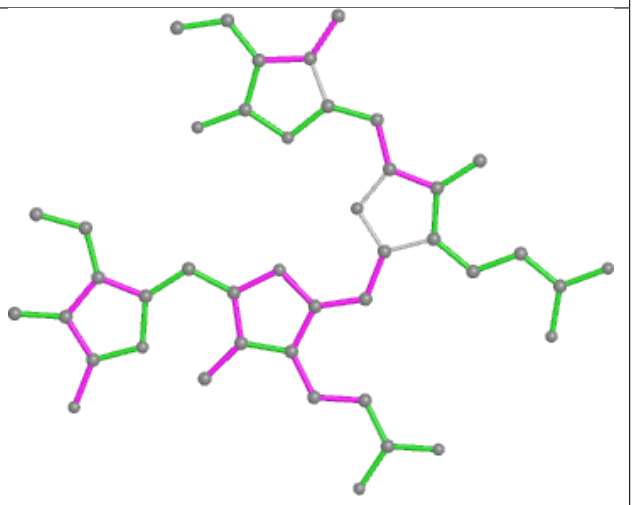


Rings

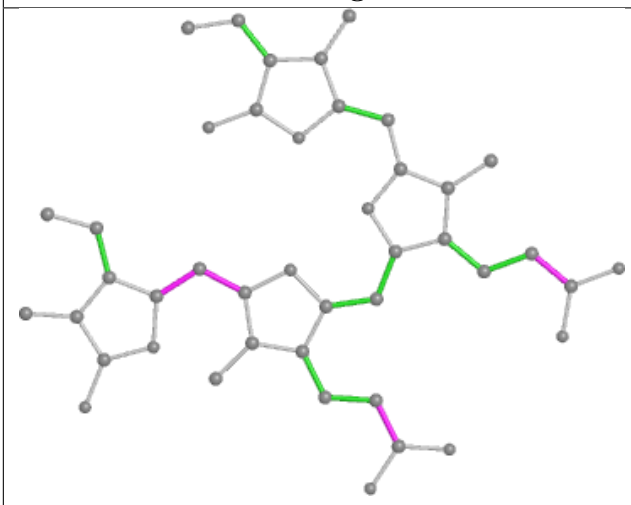
Ligand PEB ed 202



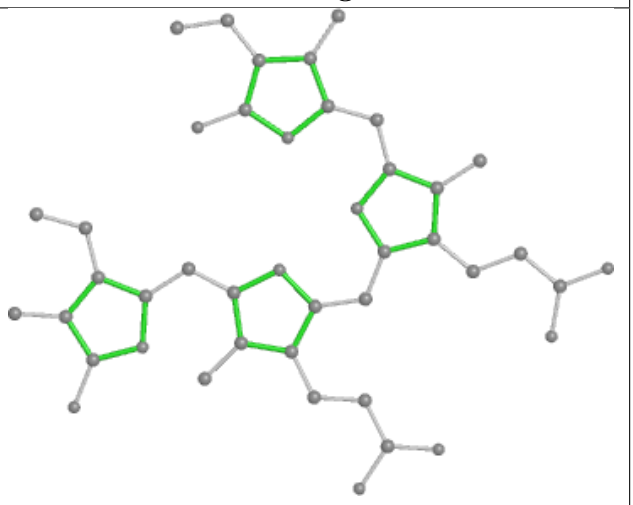
Bond lengths



Bond angles

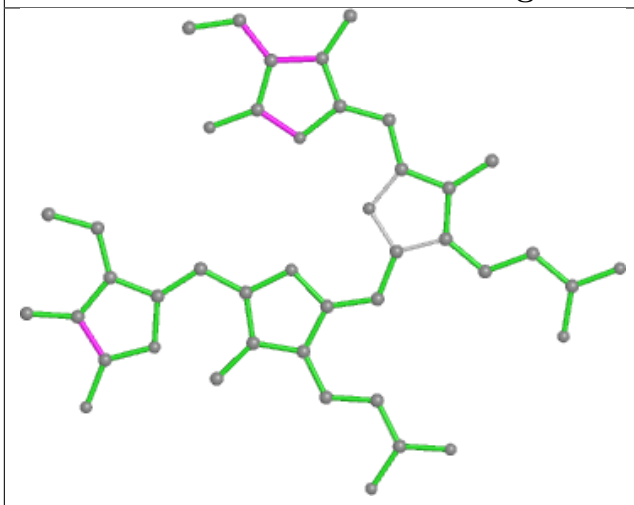


Torsions



Rings

Ligand PEB C2 301



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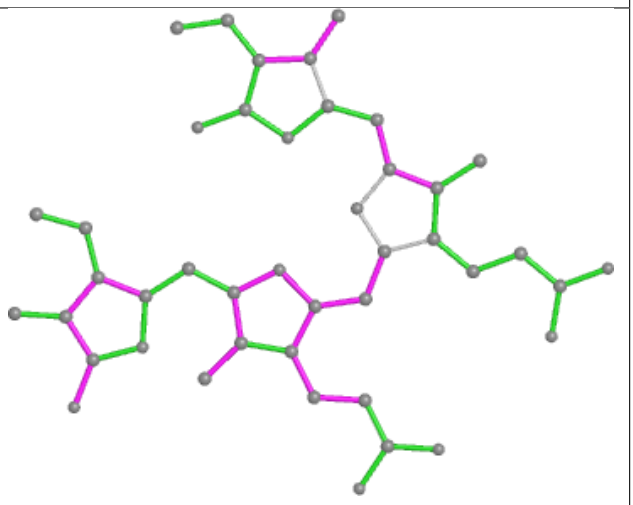

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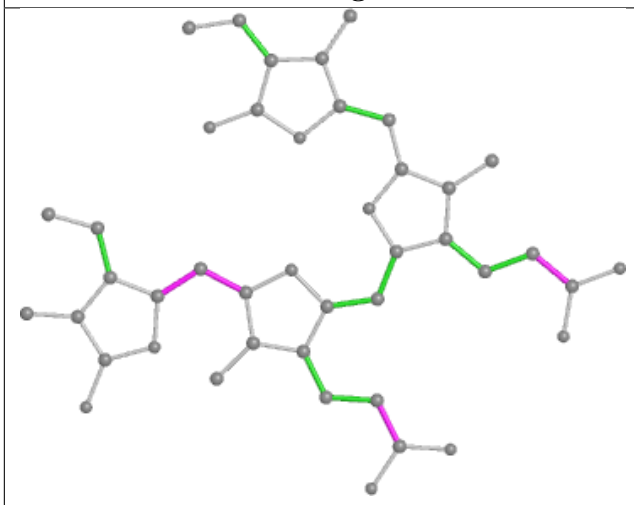

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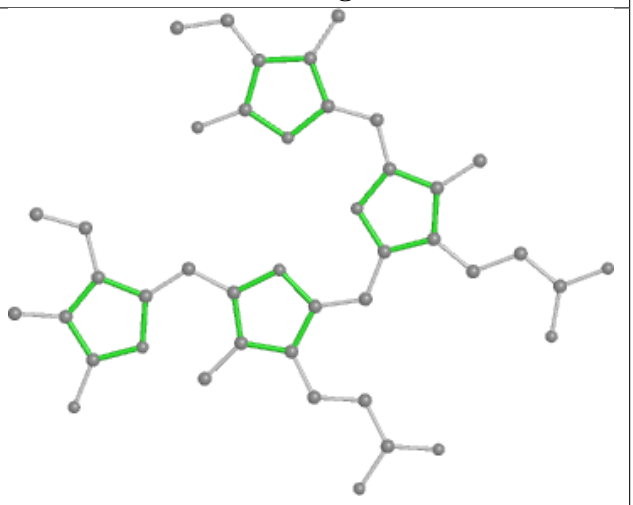
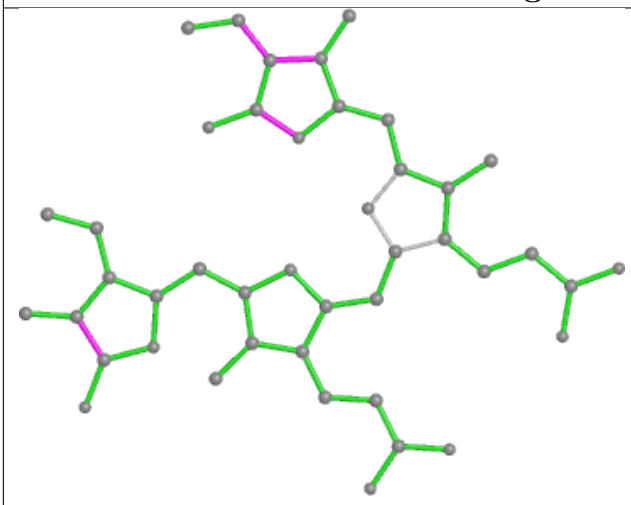


Rings

Ligand PEB fe 201



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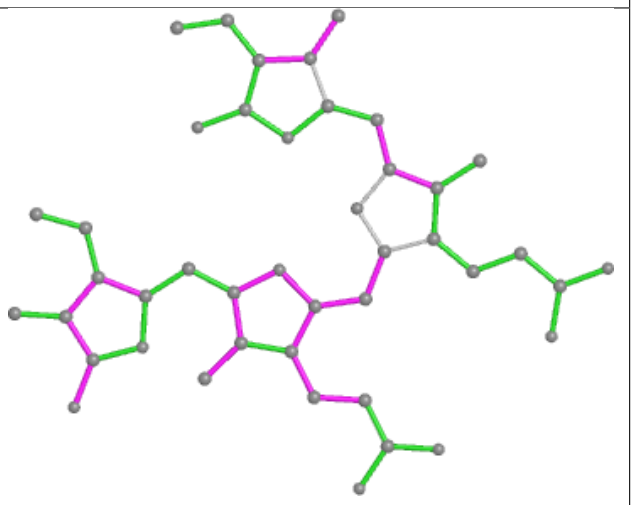

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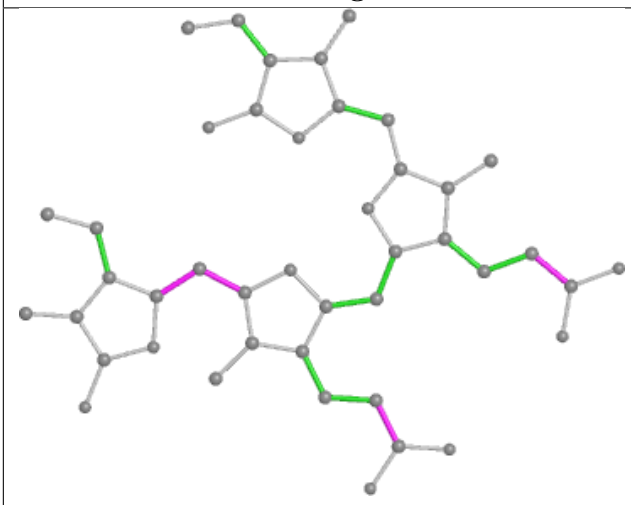

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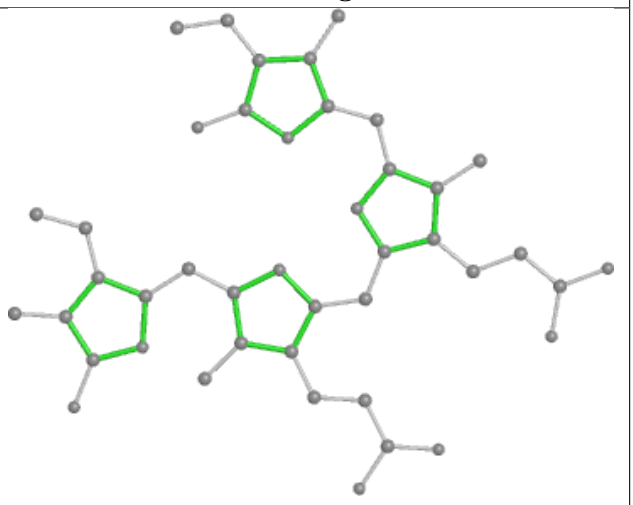
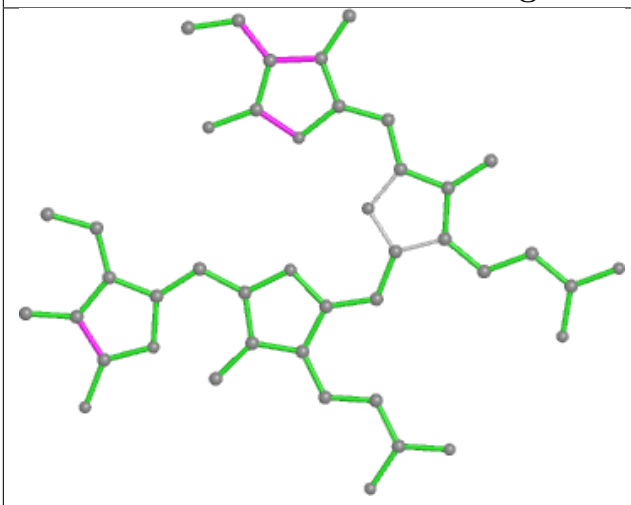


Rings

Ligand PEB x7 201



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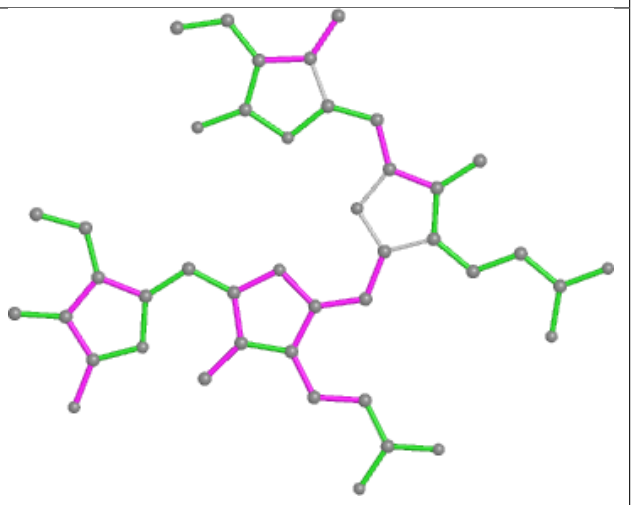

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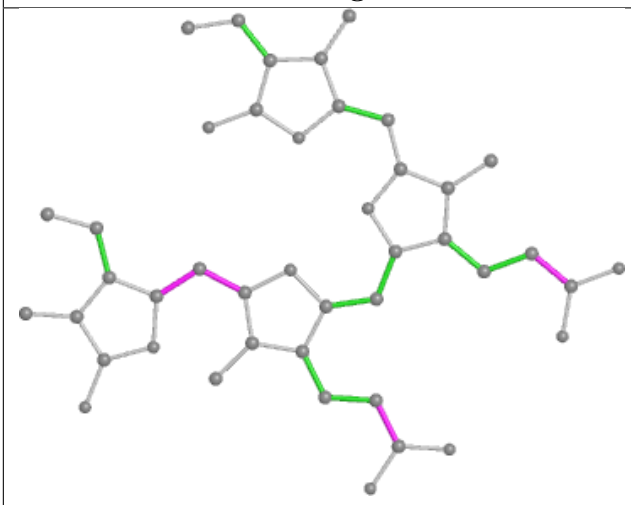

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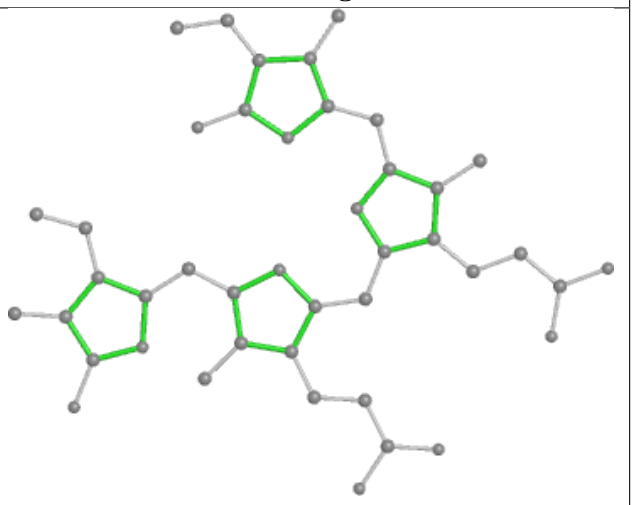
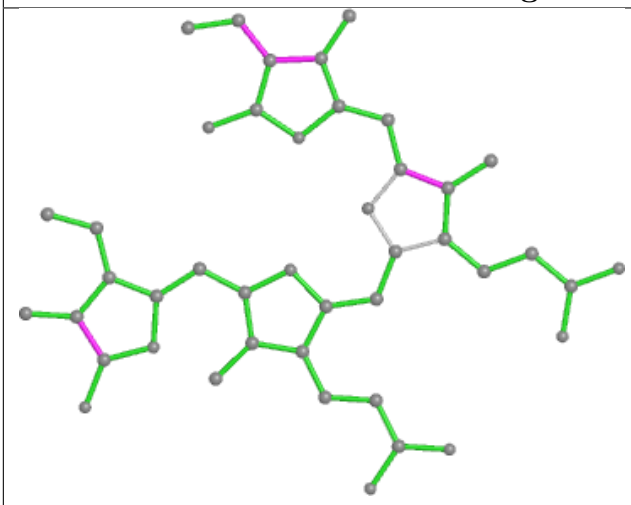


Rings

Ligand PEB gz 302



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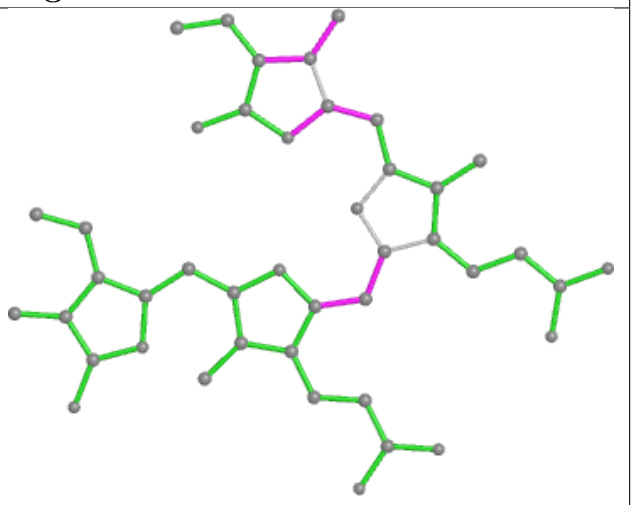
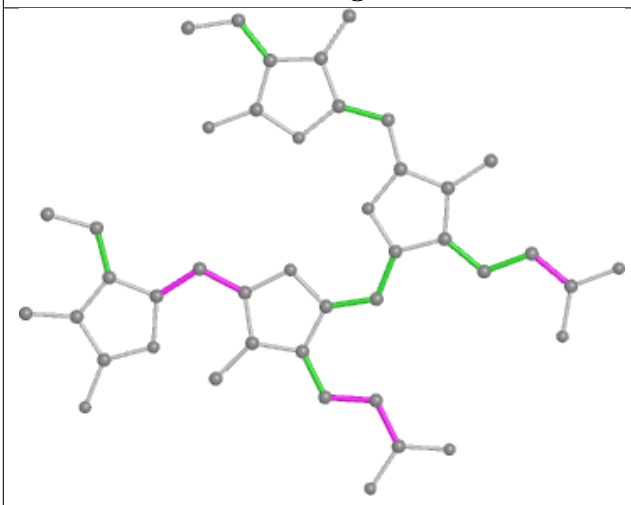


Bond angles



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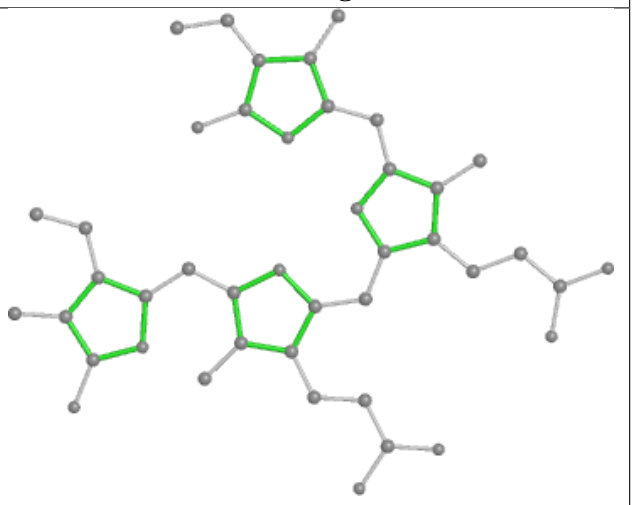

Rings

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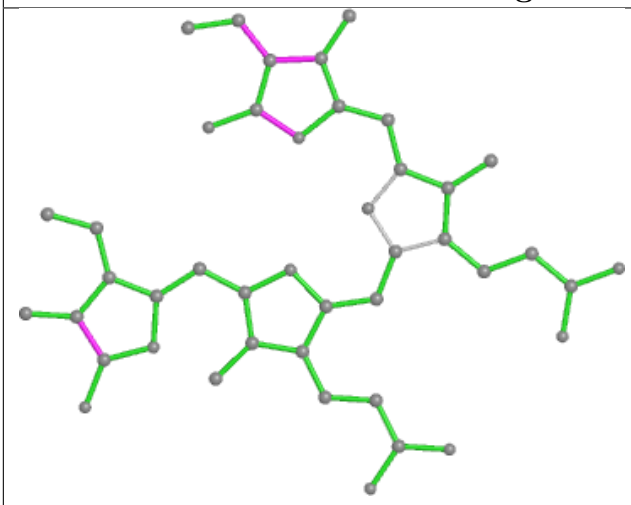

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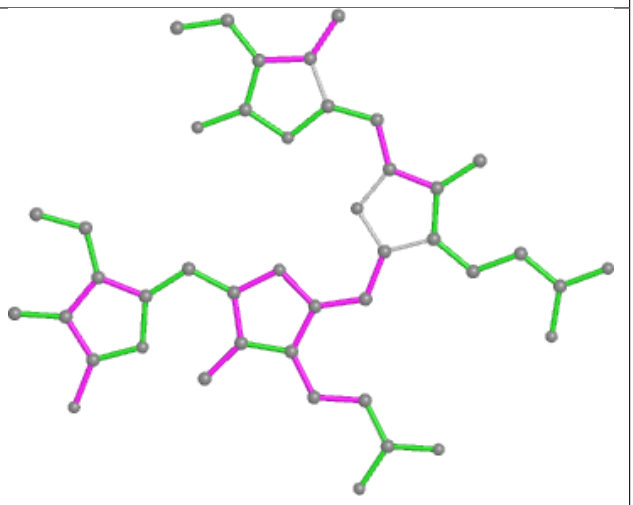

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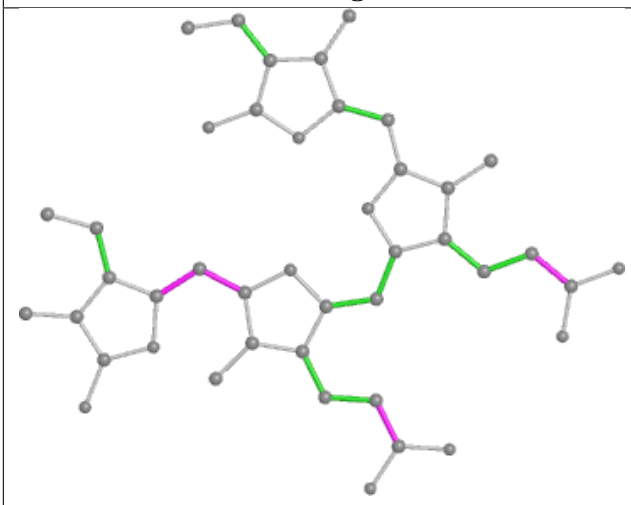

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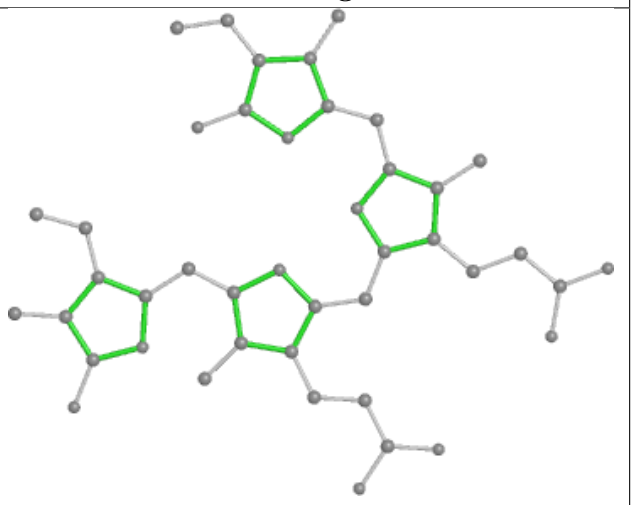
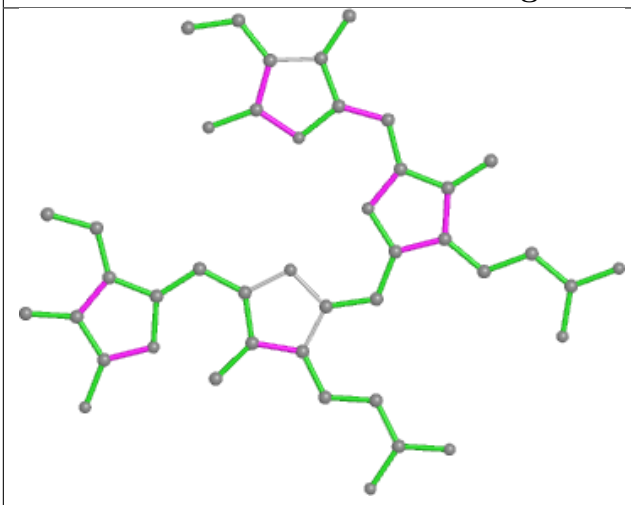


Rings

Ligand PUB di 203



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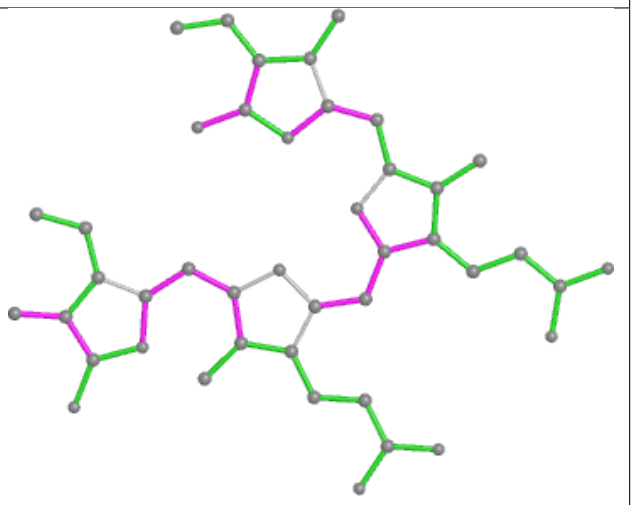

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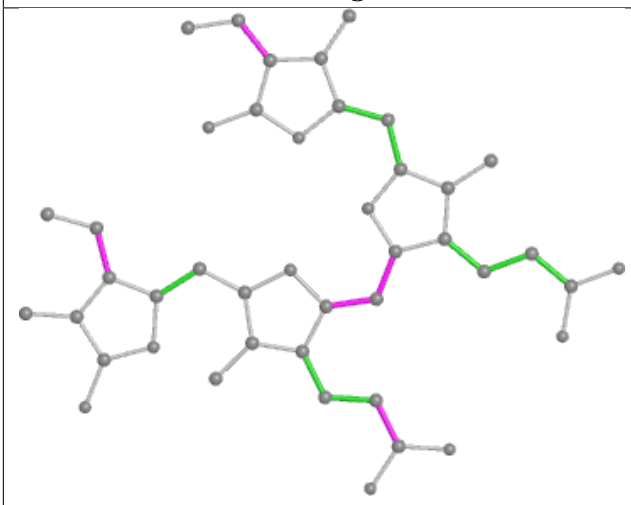

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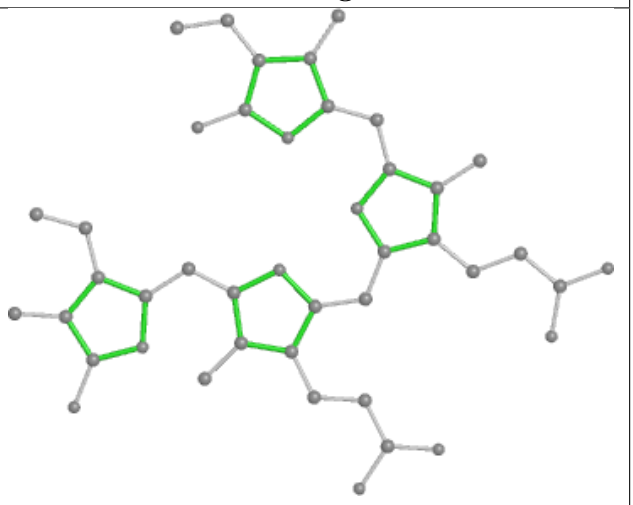
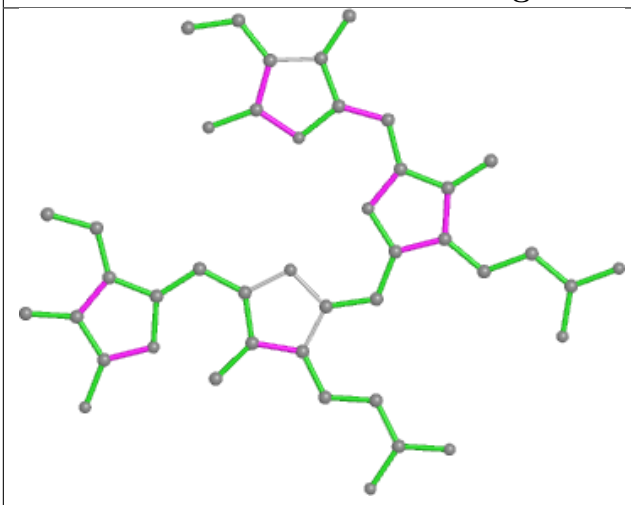


Rings

Ligand PUB H6 203



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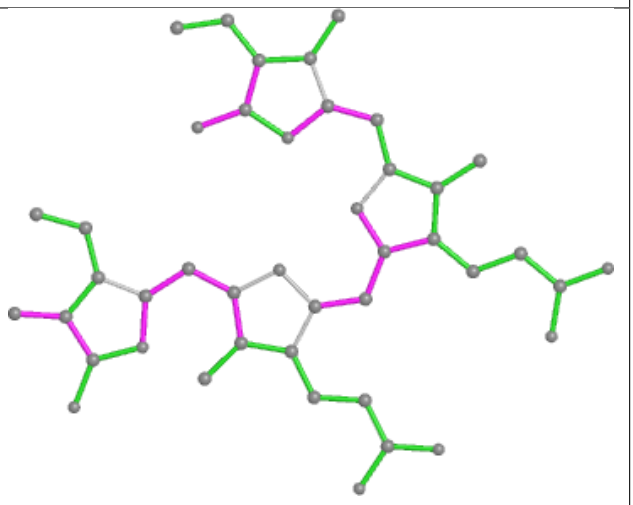

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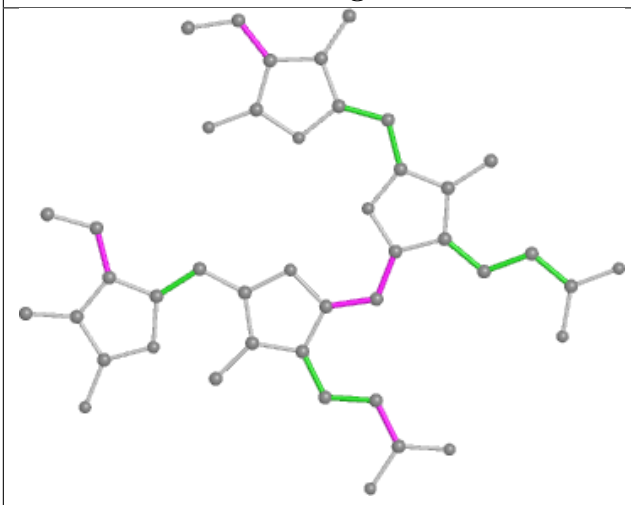

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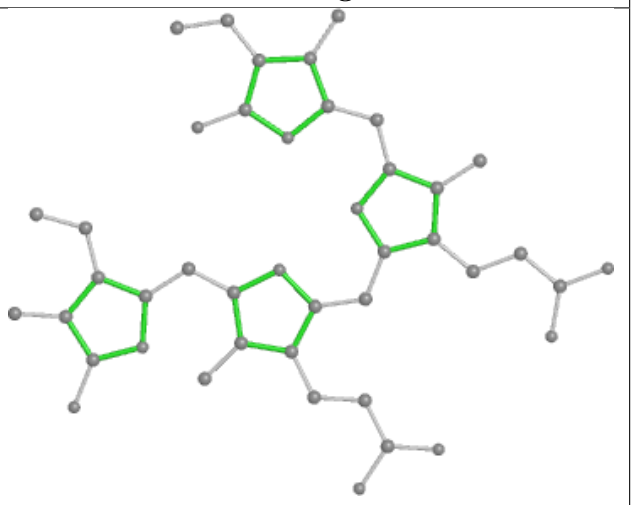
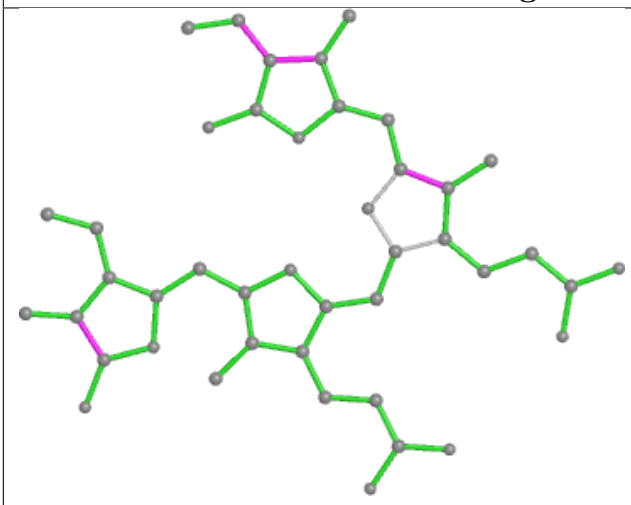


Rings

Ligand PEB k3 202



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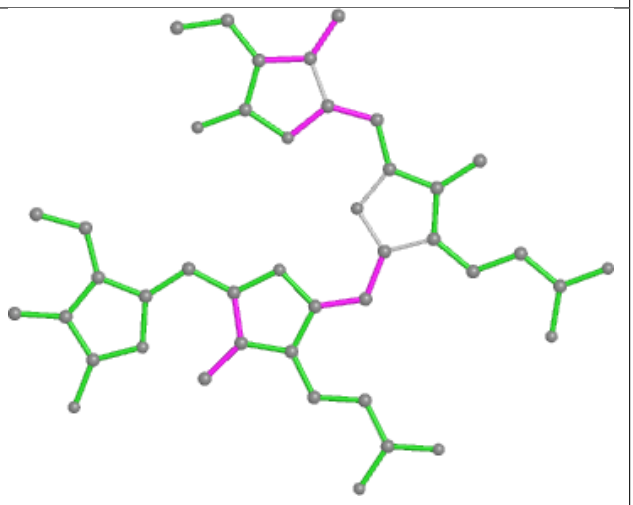
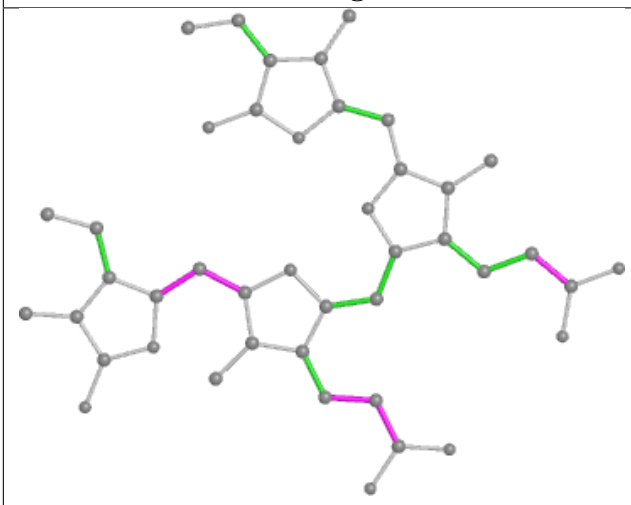


Bond angles



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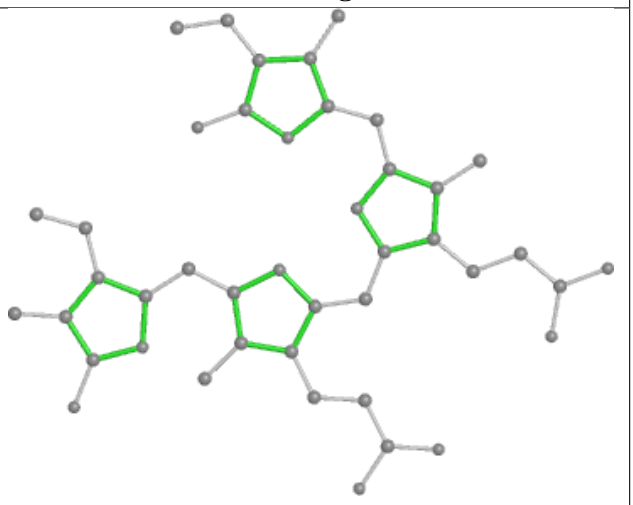
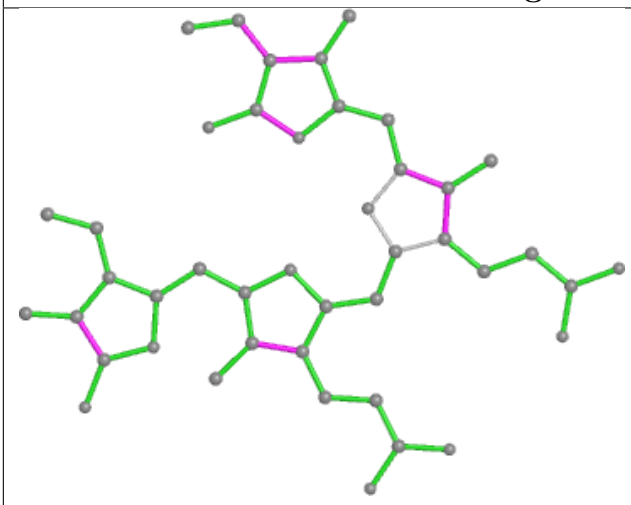


Rings

Ligand PEB cl 202



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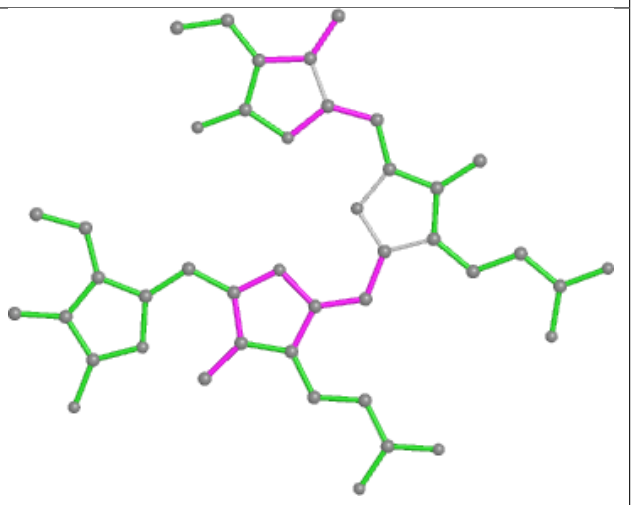

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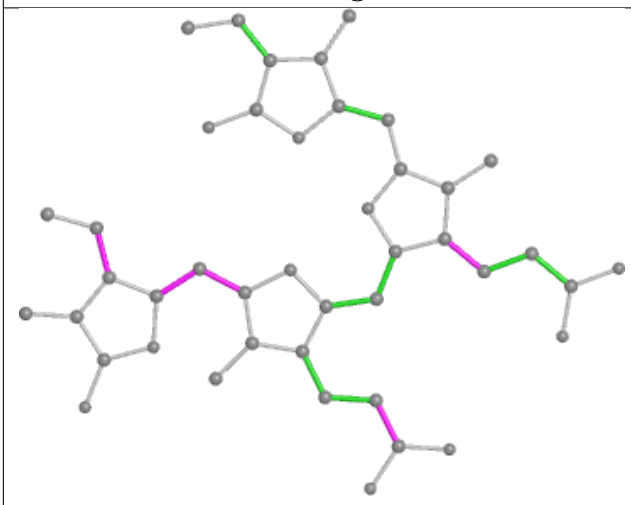

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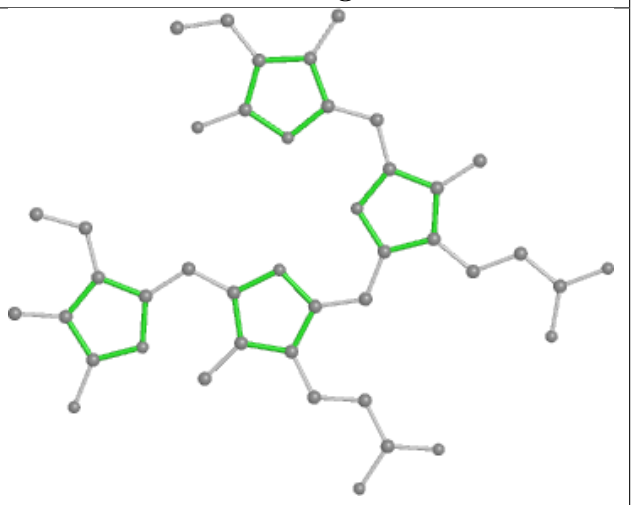
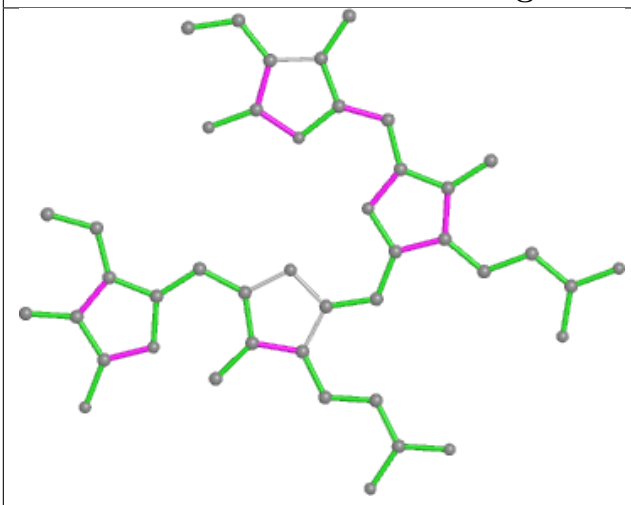


Rings

Ligand PUB dv 202



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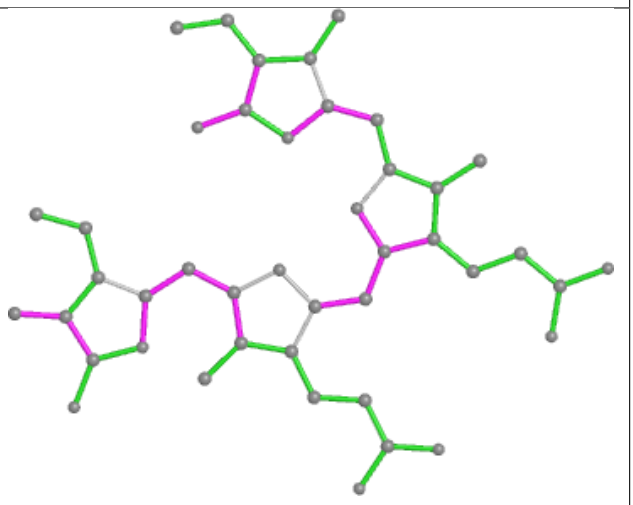

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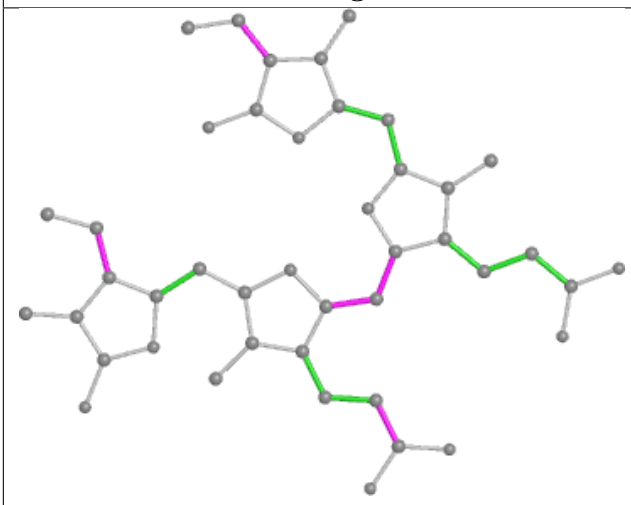

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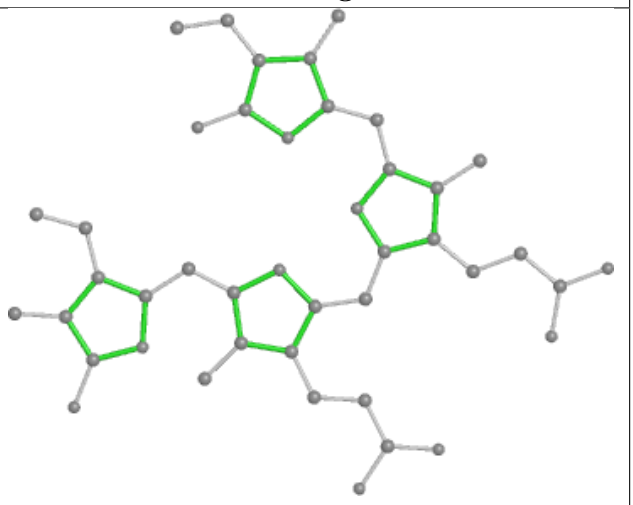
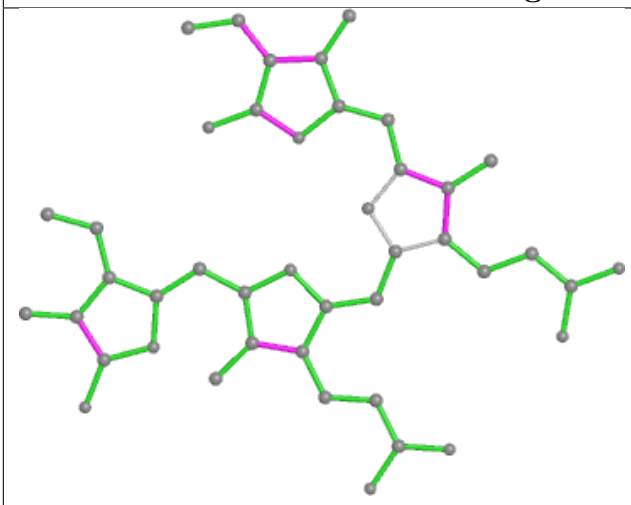


Rings

Ligand PEB cf 201



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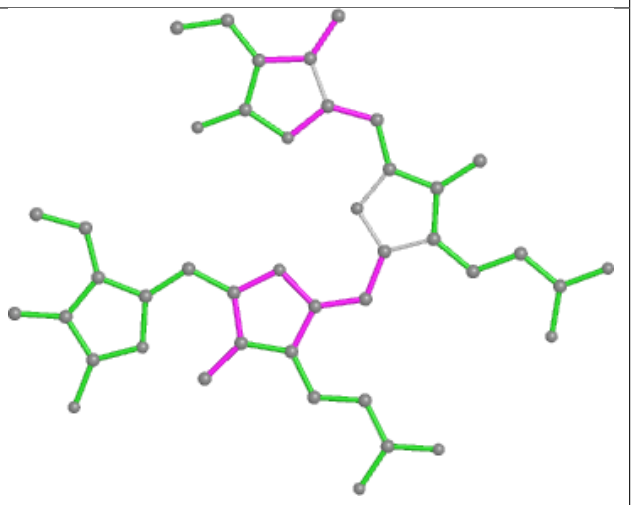
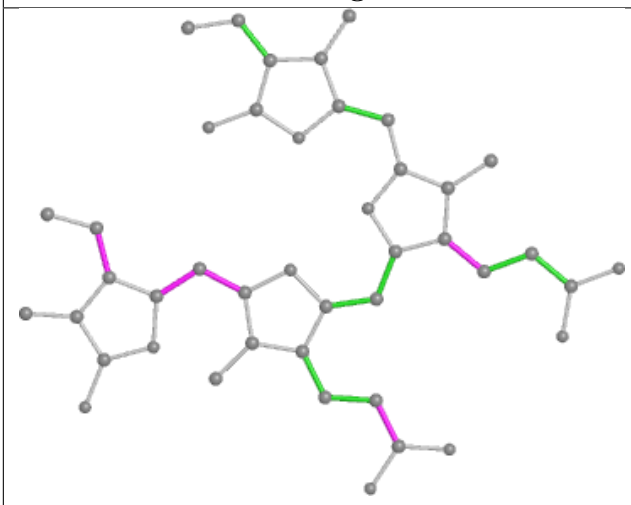


Bond angles



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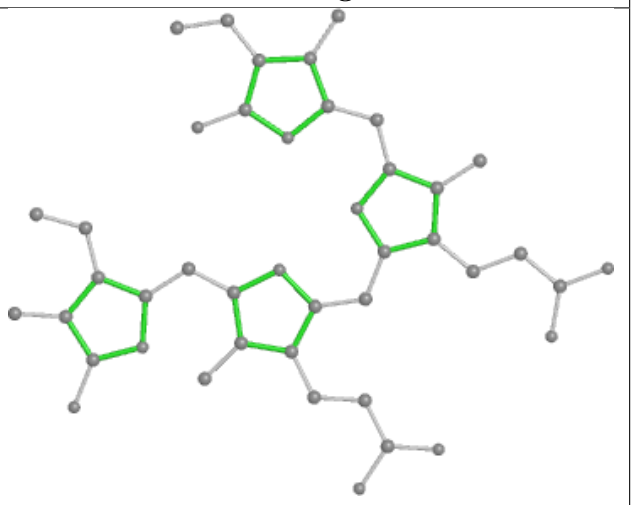

Rings

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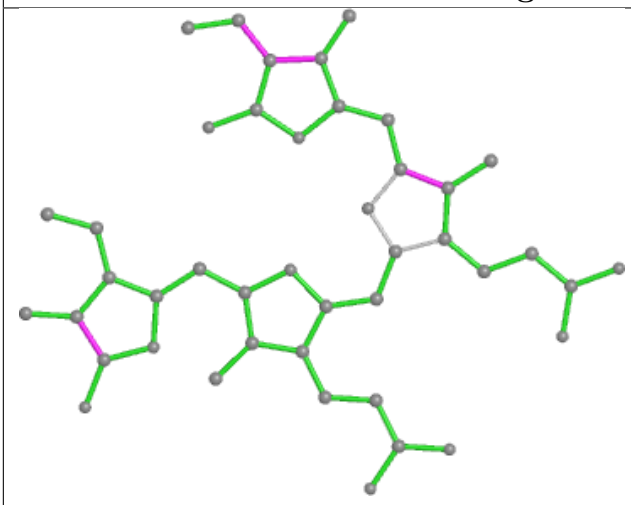

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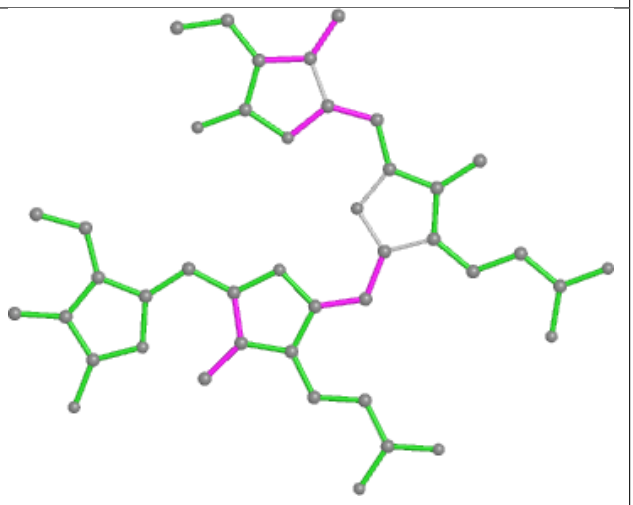
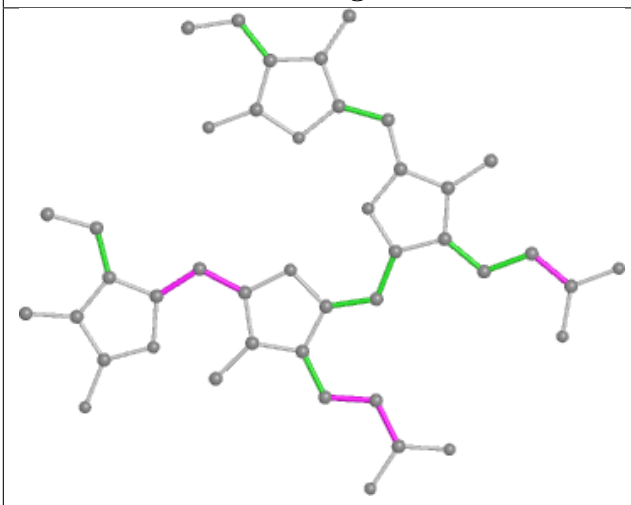


Bond angles



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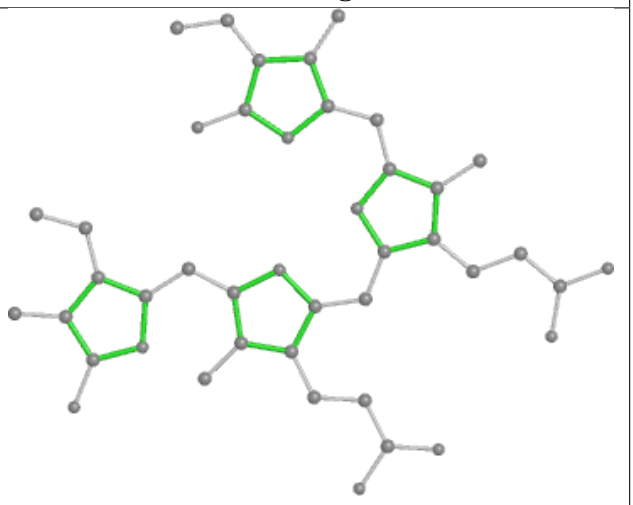
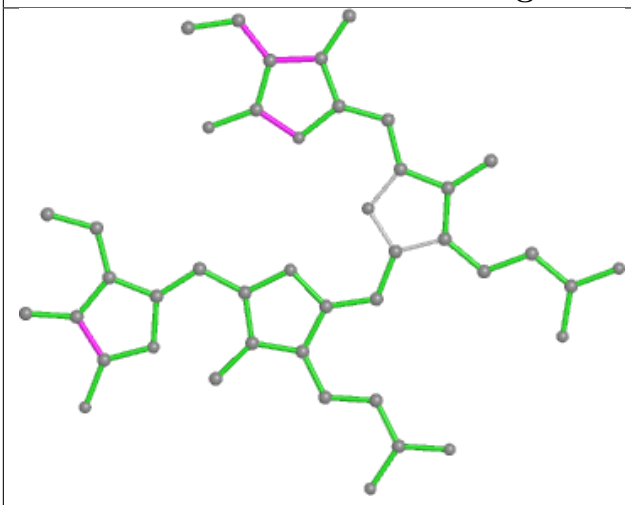


Rings

Ligand PEB T7 201



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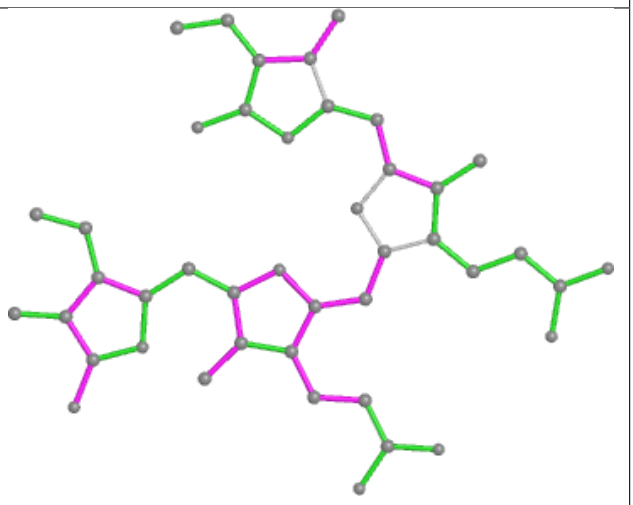
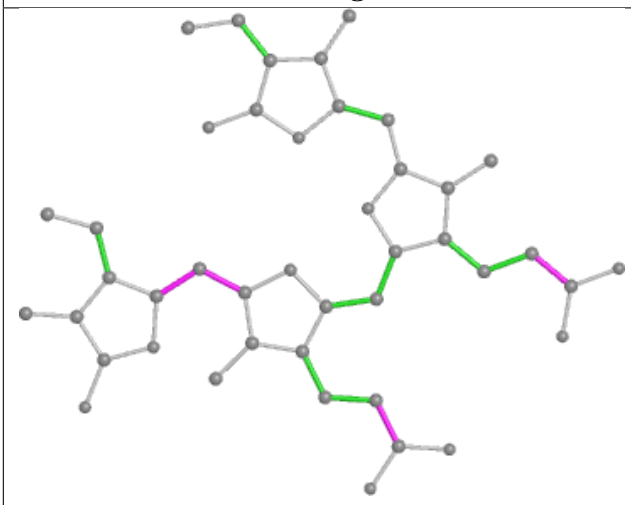
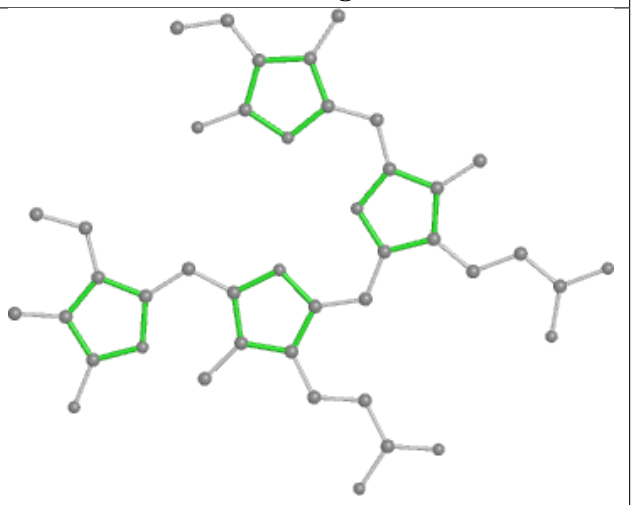


Bond angles

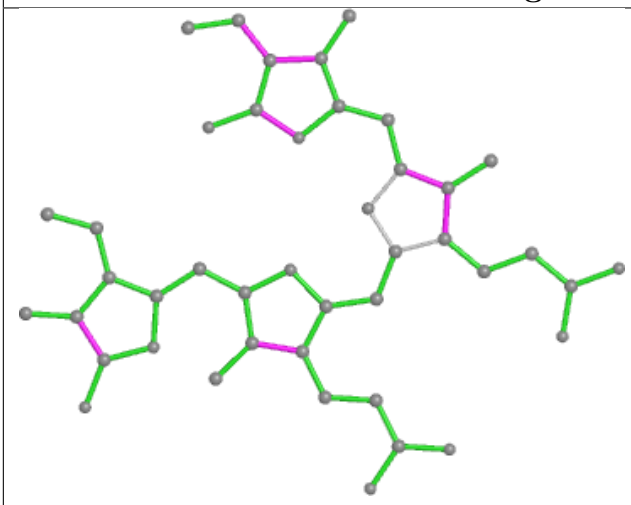


Torsions



Rings

Ligand PEB el 202



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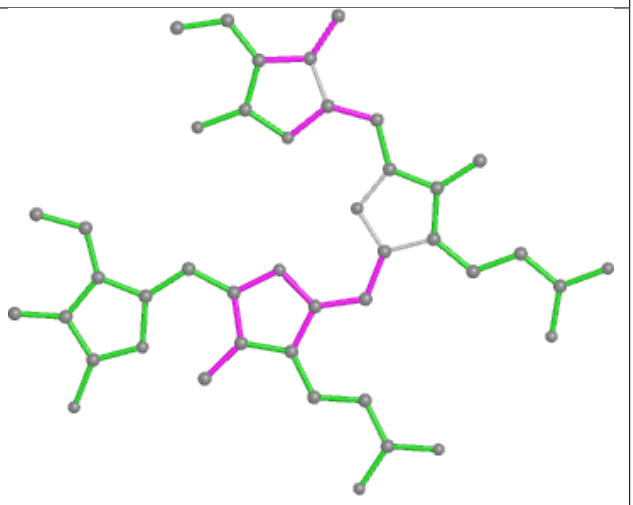

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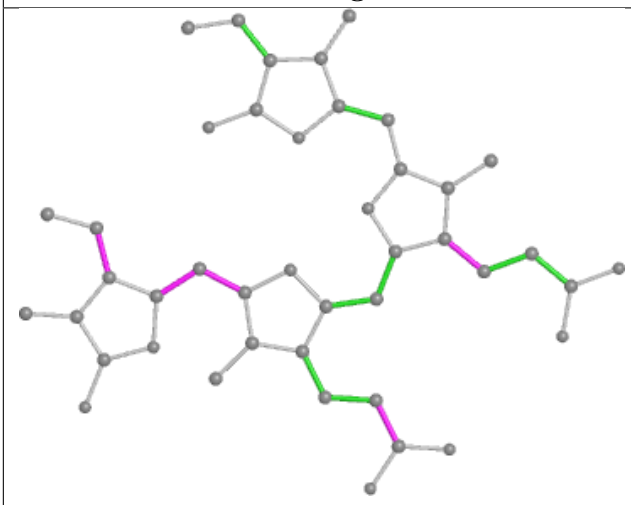

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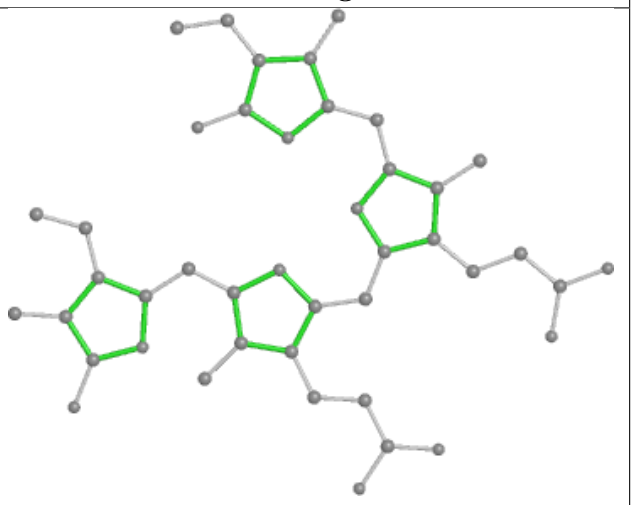
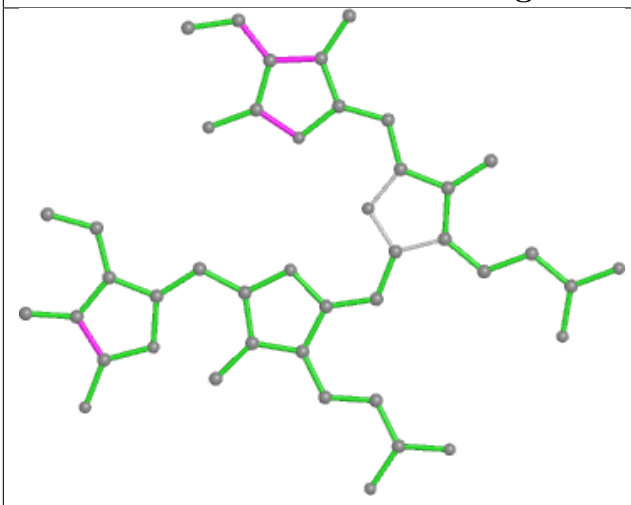


Rings

Ligand PEB U5 201



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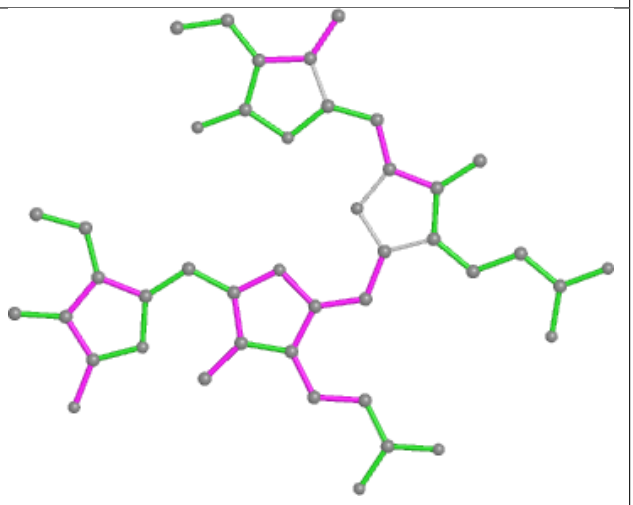

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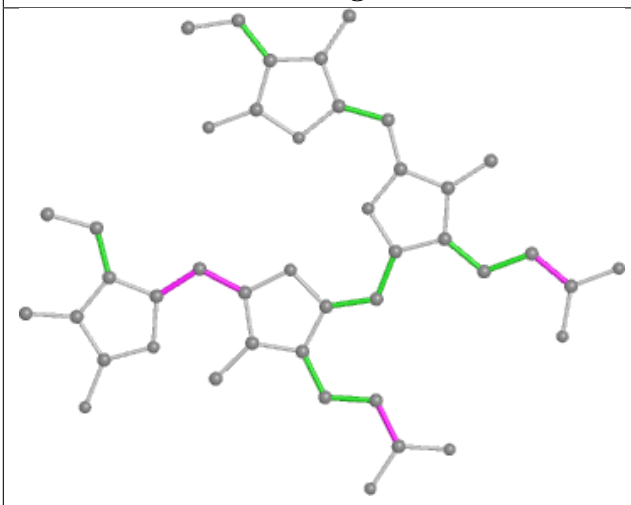

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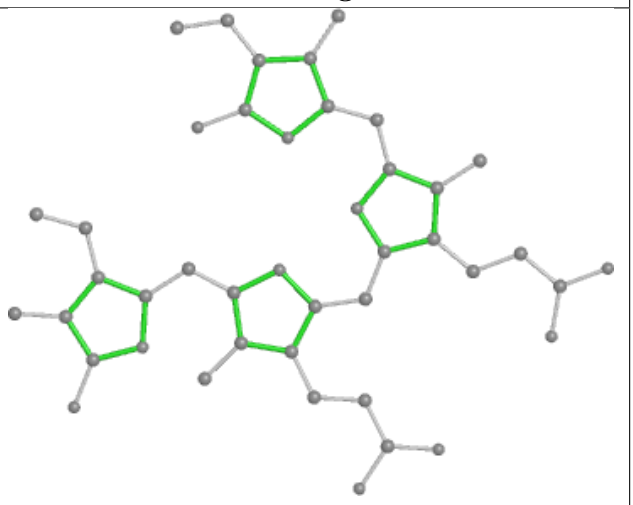
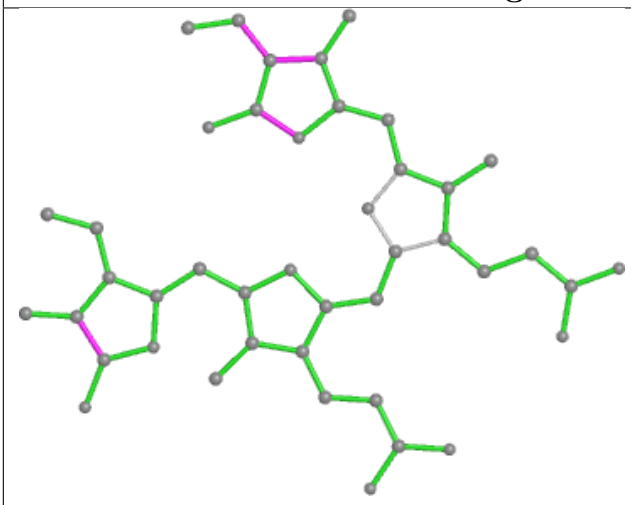


Rings

Ligand PEB K9 1001



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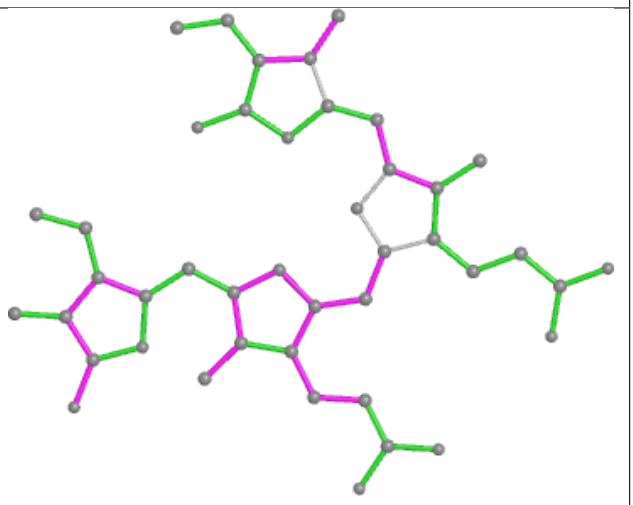

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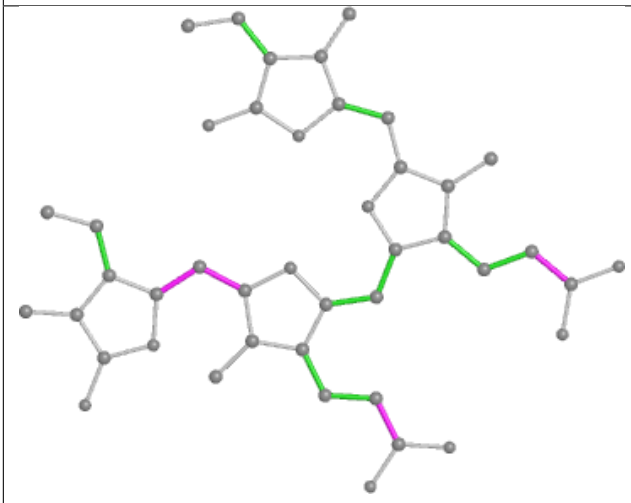

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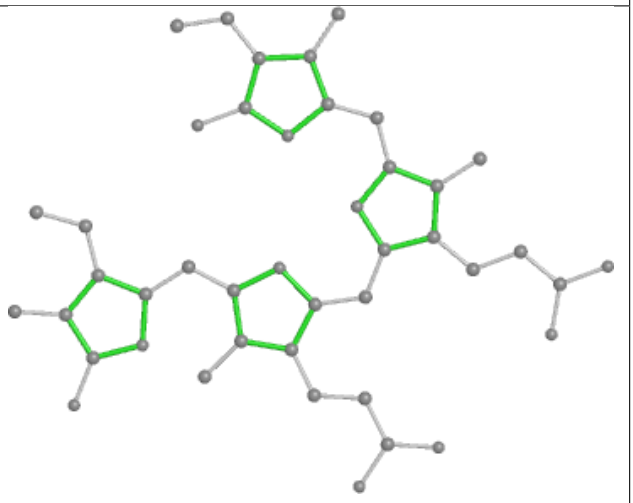

Rings

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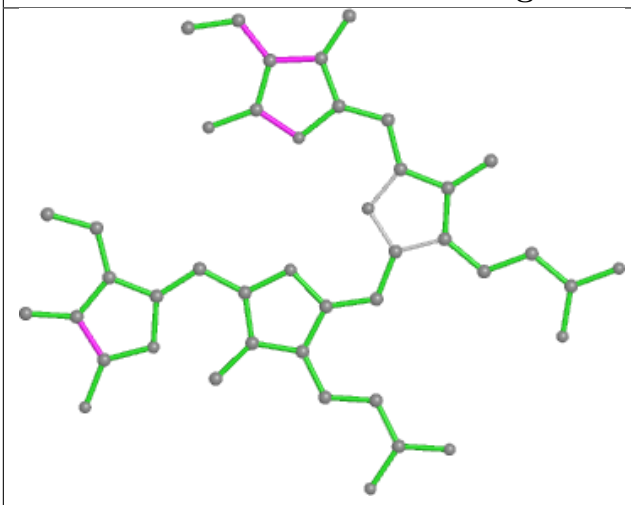

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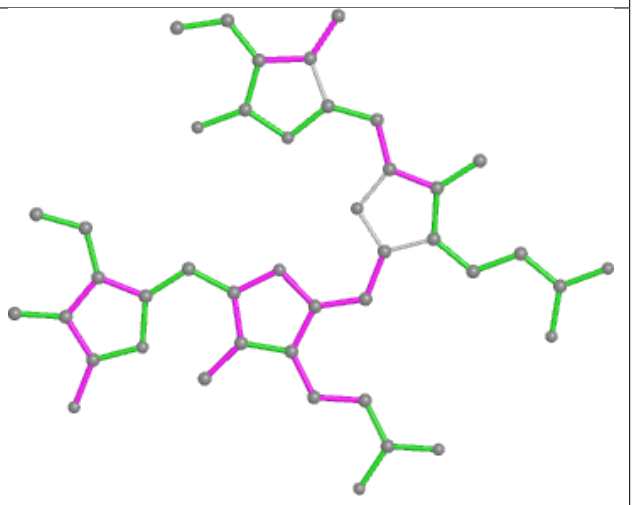

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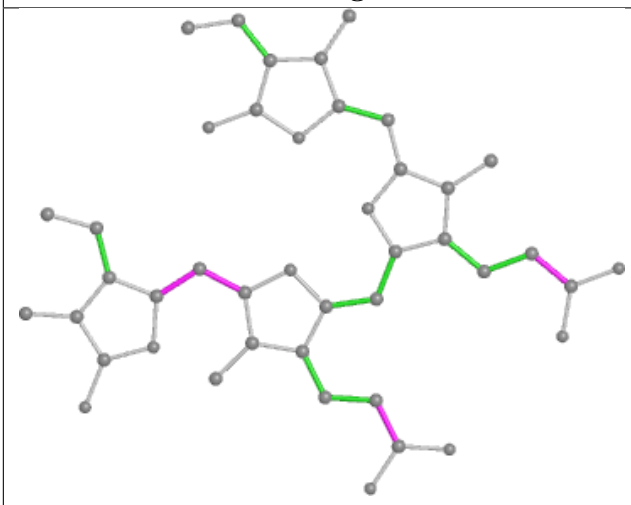

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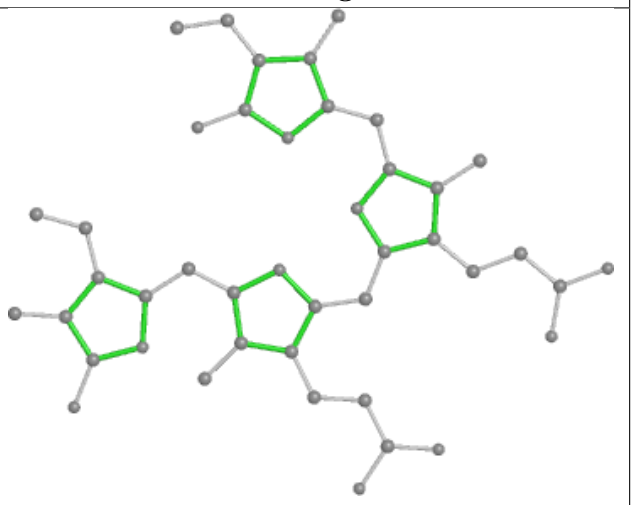

Rings

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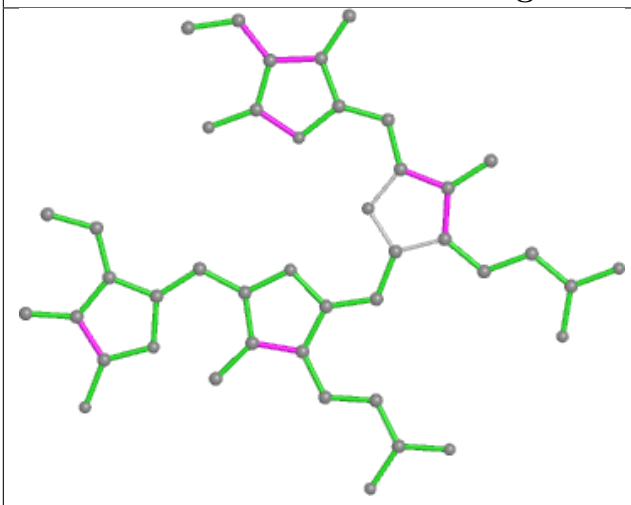

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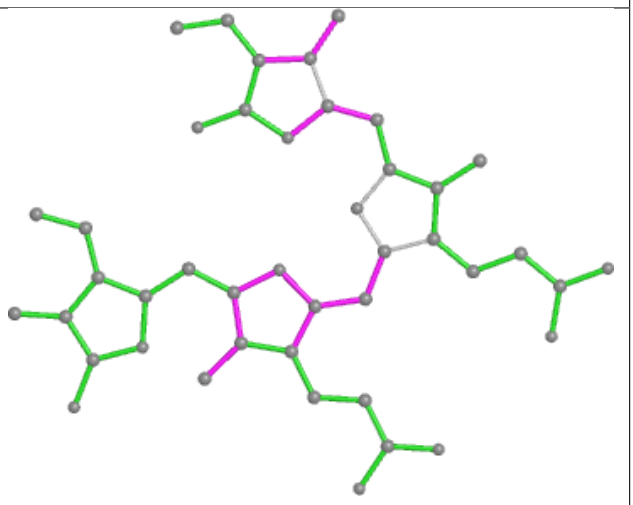

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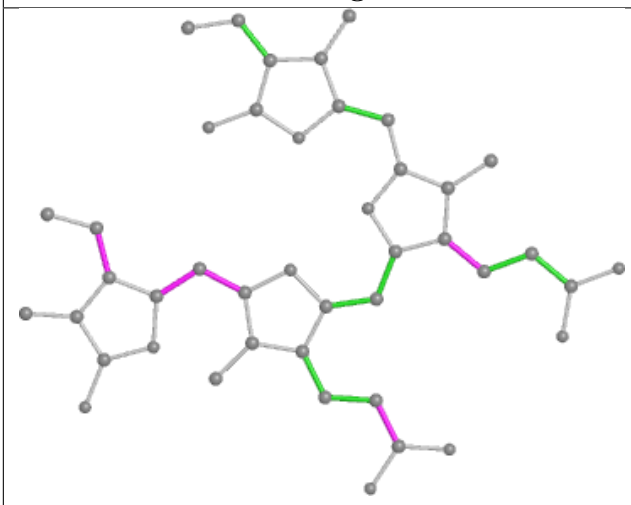

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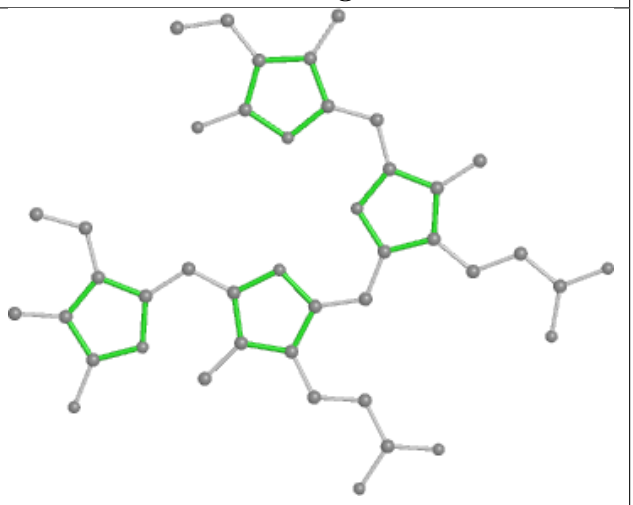
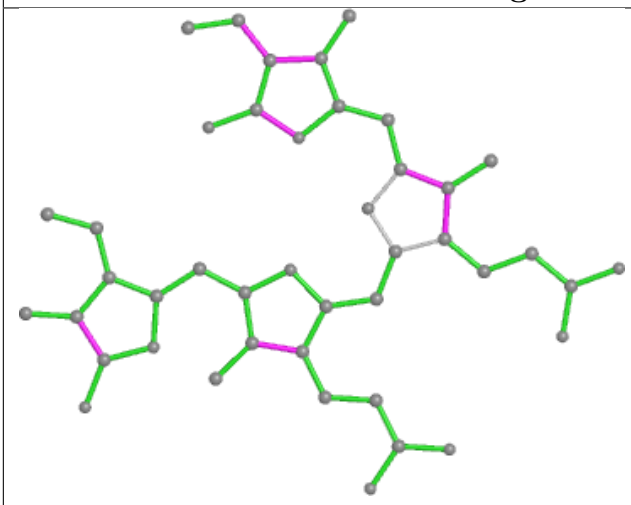


Rings

Ligand PEB iD 1002



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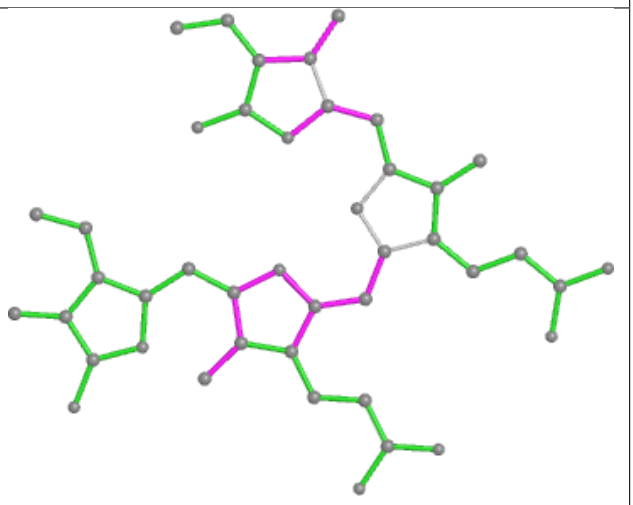

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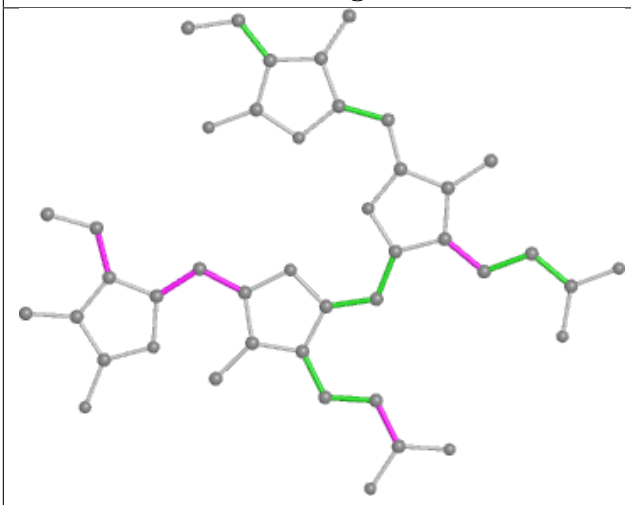

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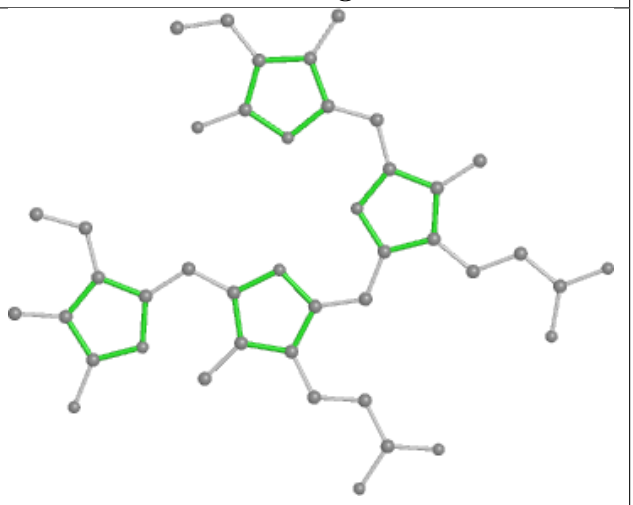

Rings

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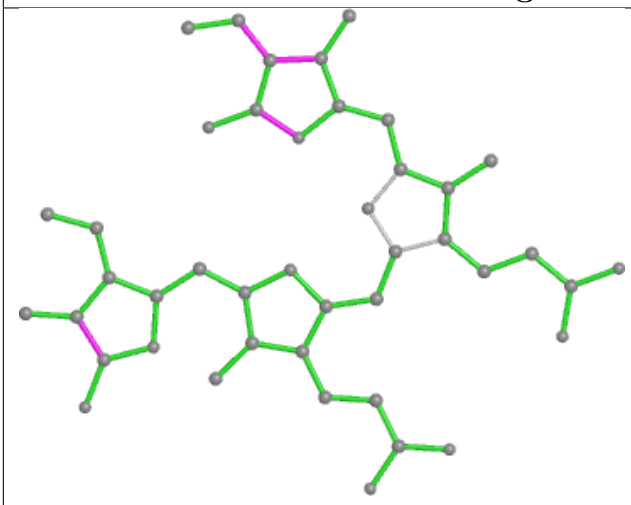

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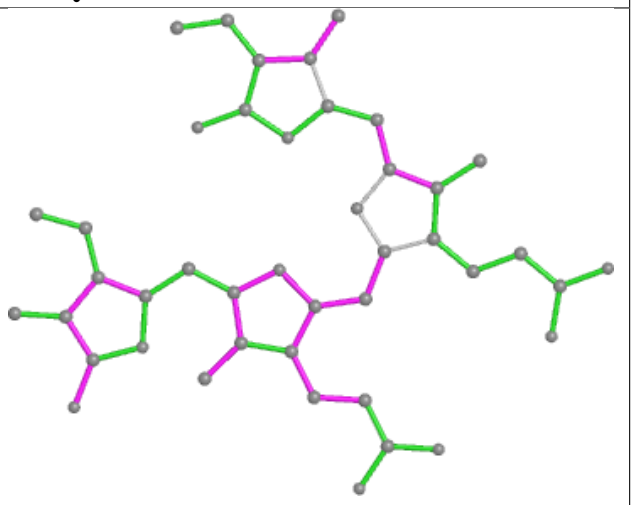

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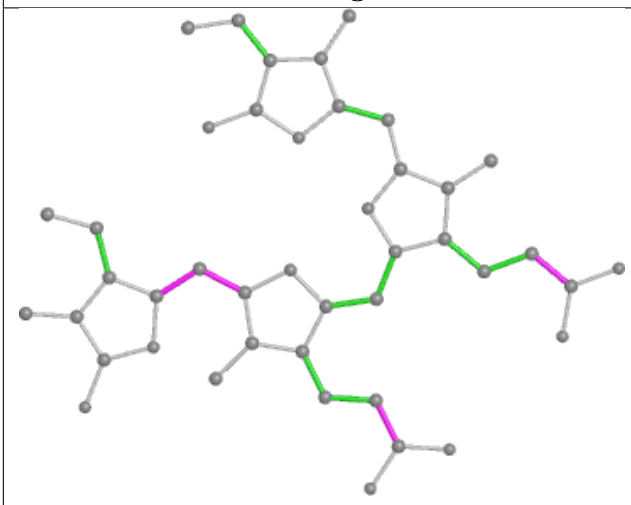

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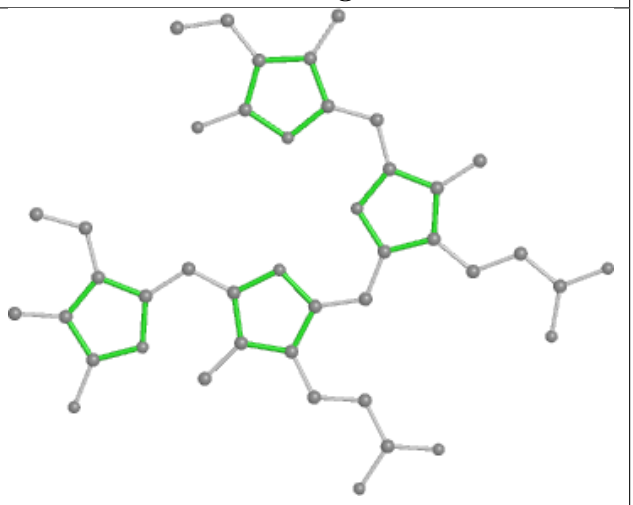

Rings

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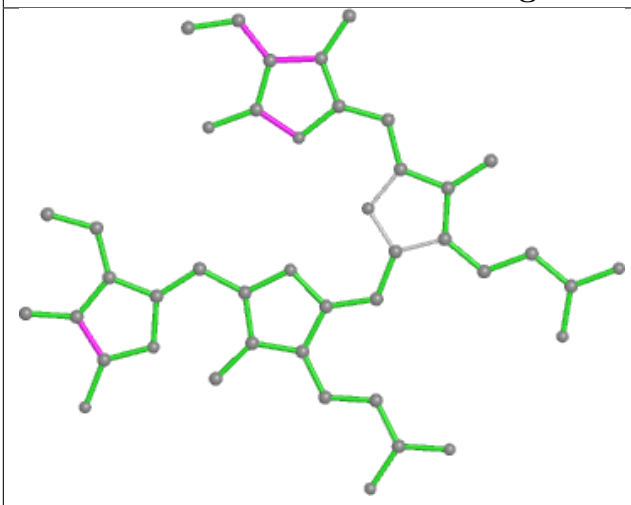

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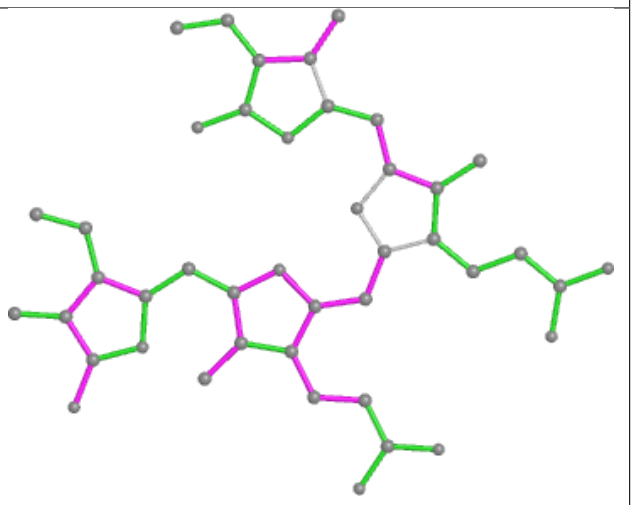

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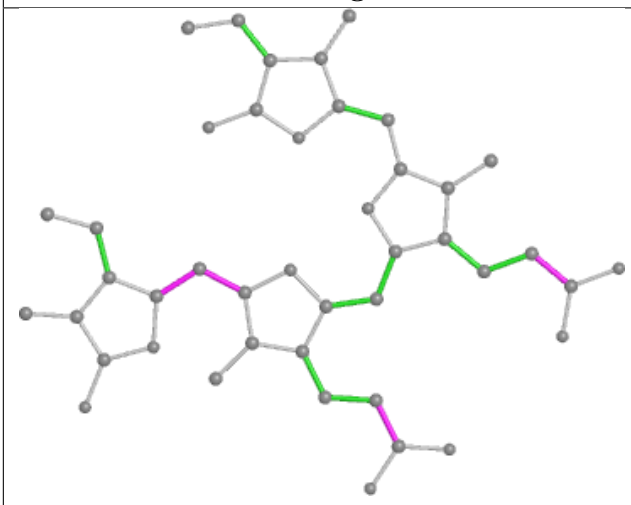

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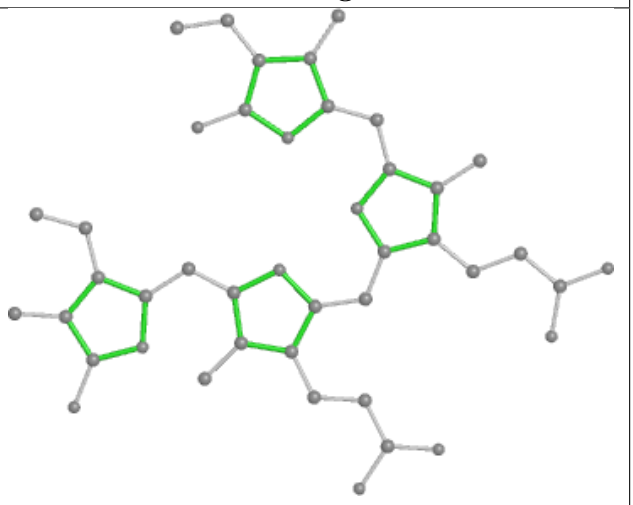
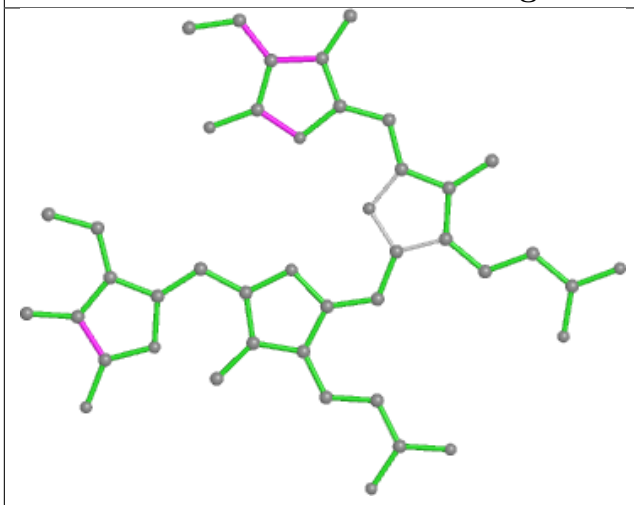


Rings

Ligand PEB bx 202



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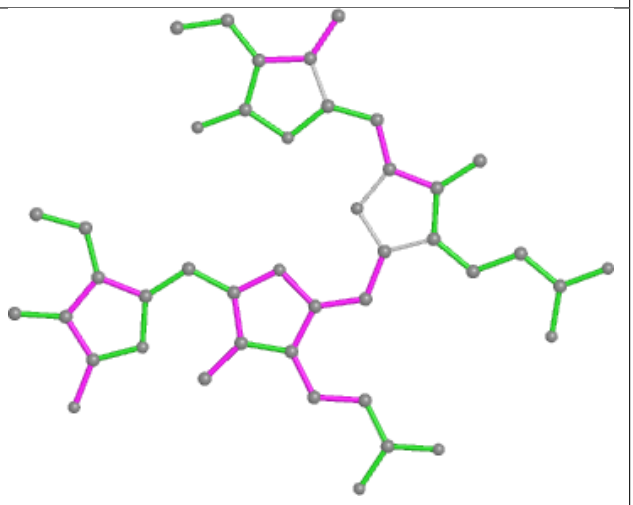

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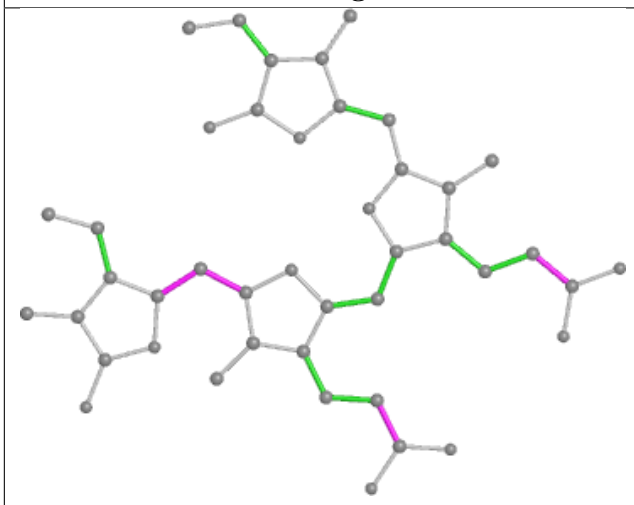

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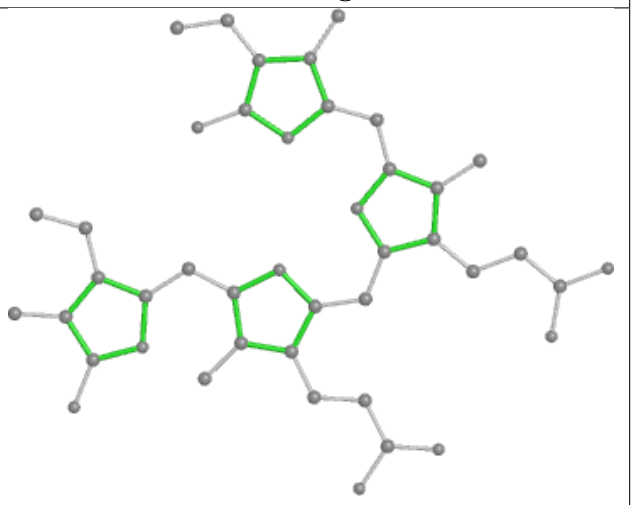
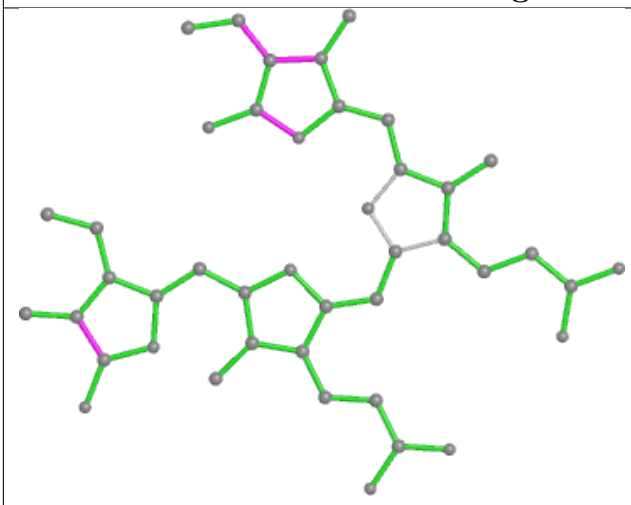


Rings

Ligand PEB M8 202



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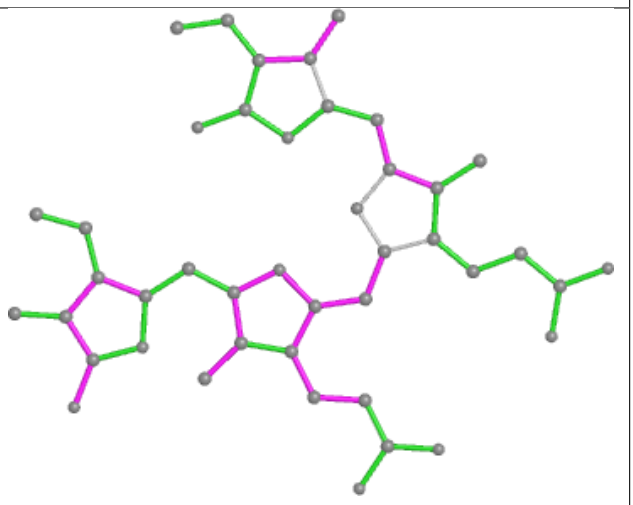

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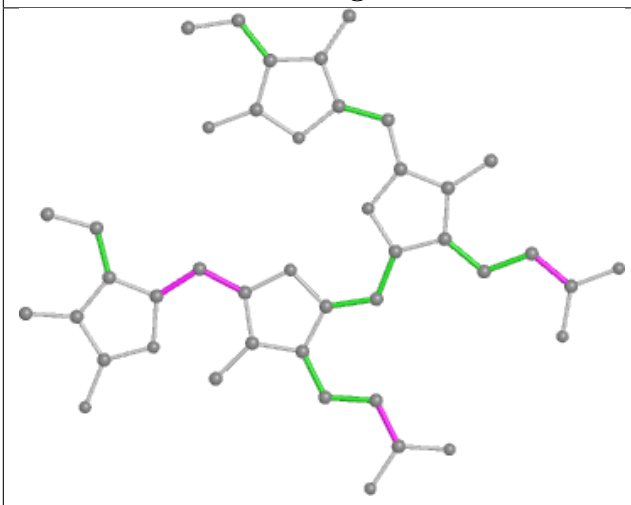

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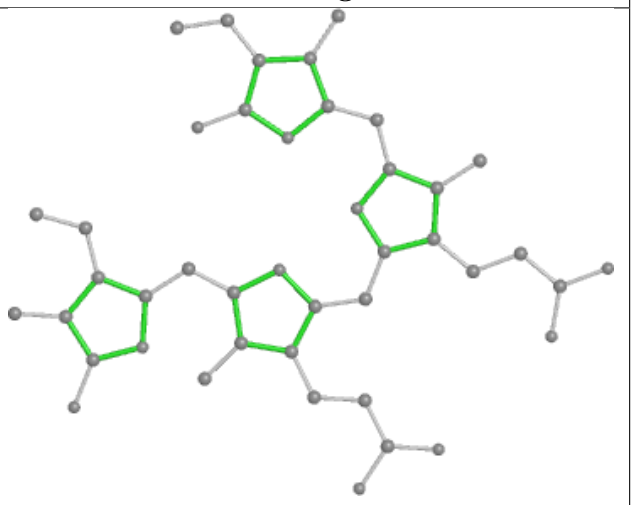

Rings

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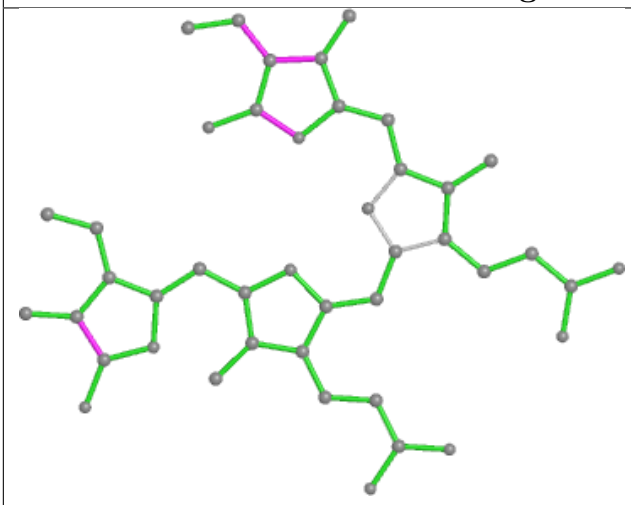

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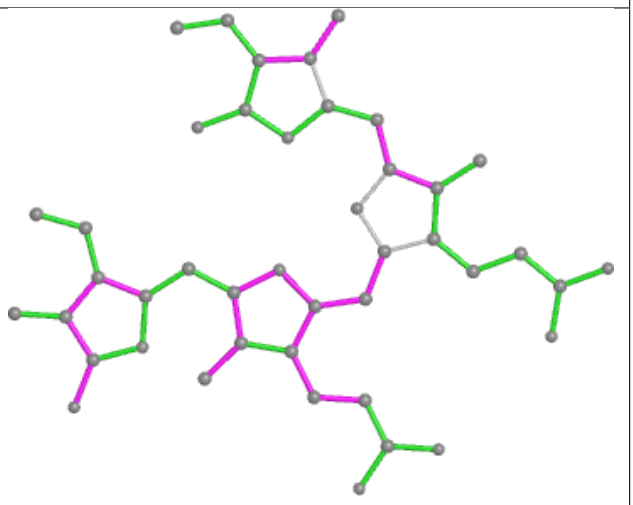

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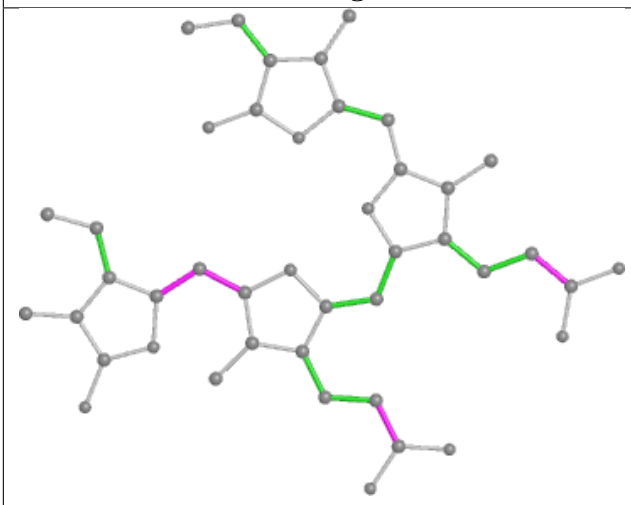

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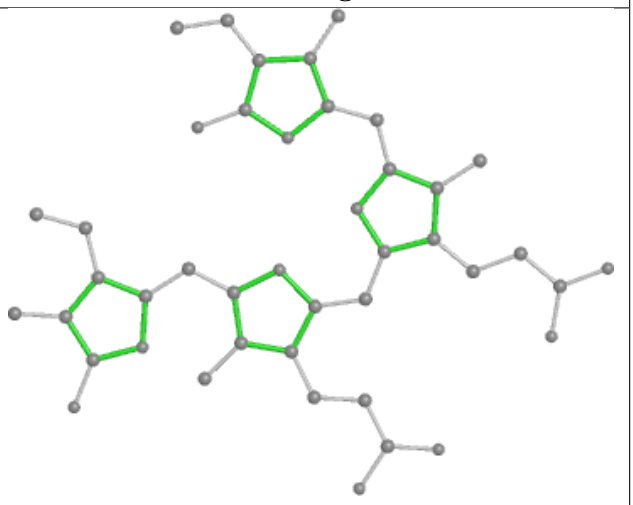
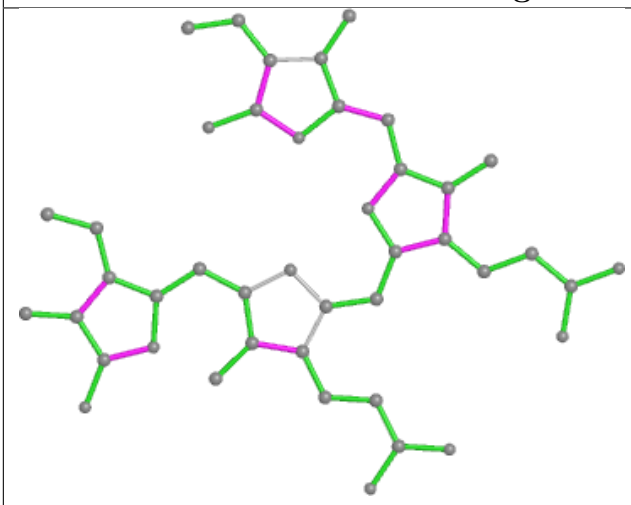


Rings

Ligand PUB bT 202



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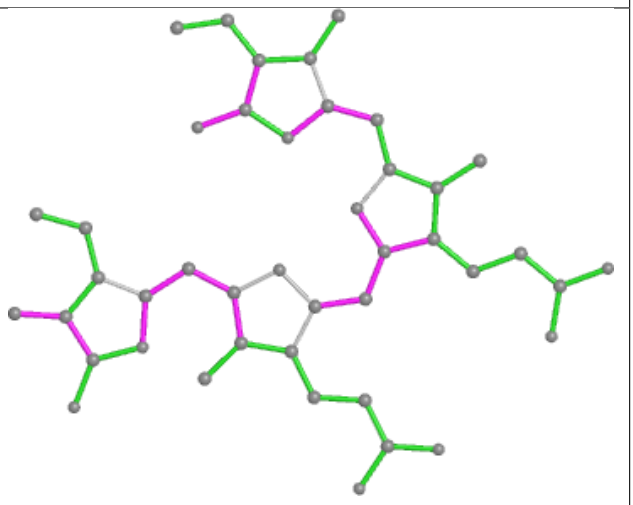

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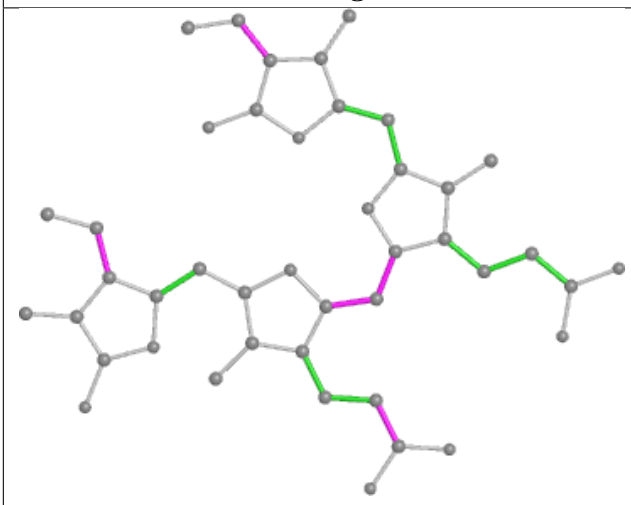

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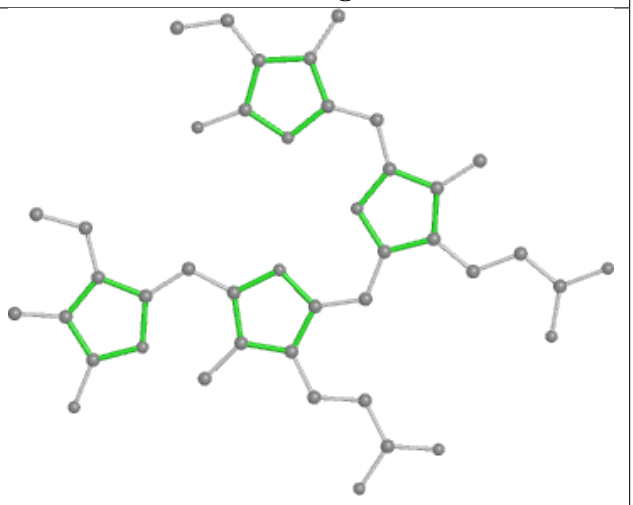

Rings

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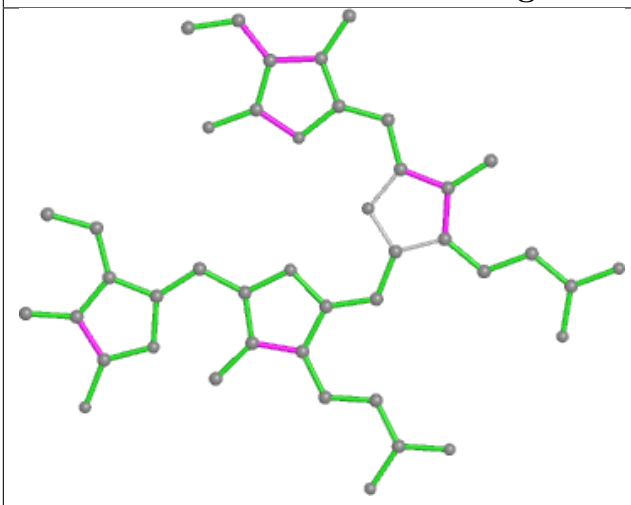

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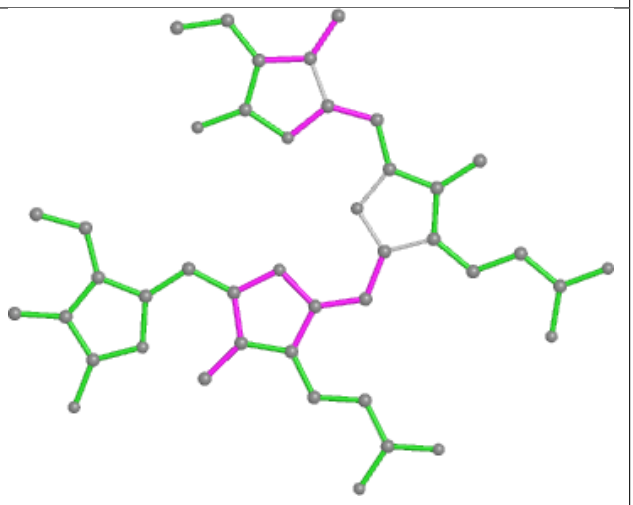

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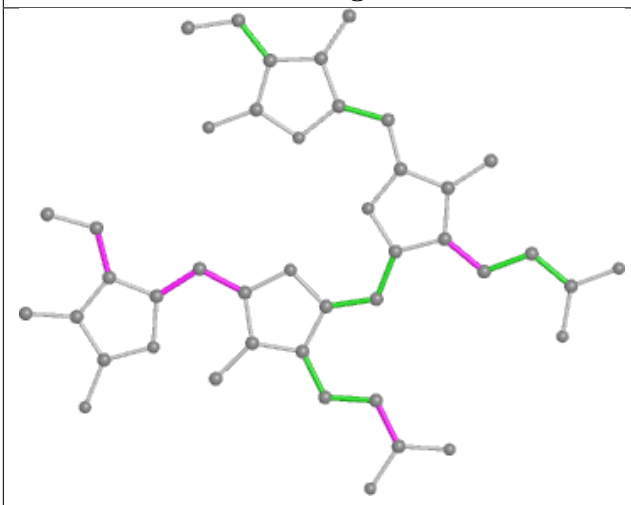
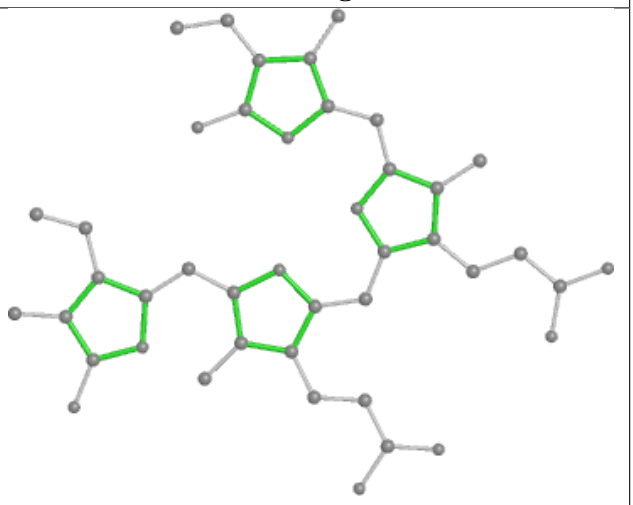
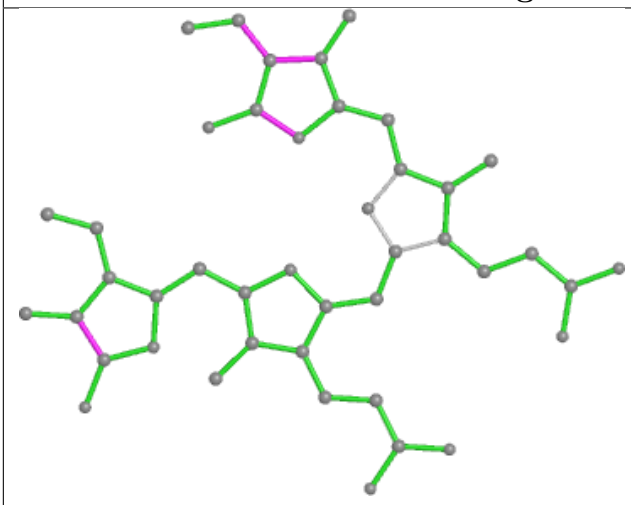


Torsions



Rings

Ligand PEB P6 201



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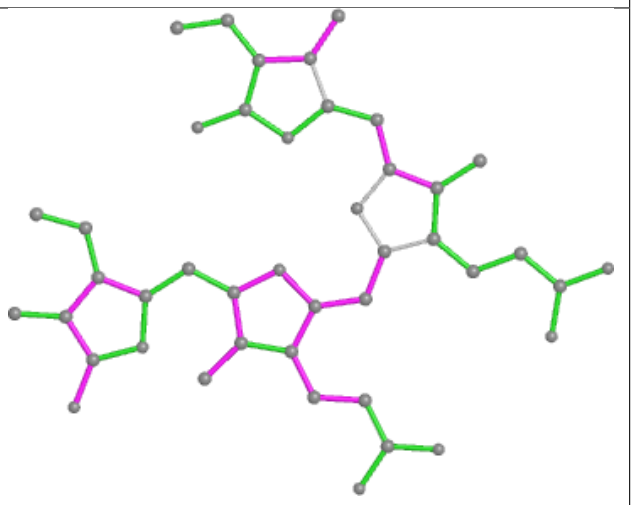

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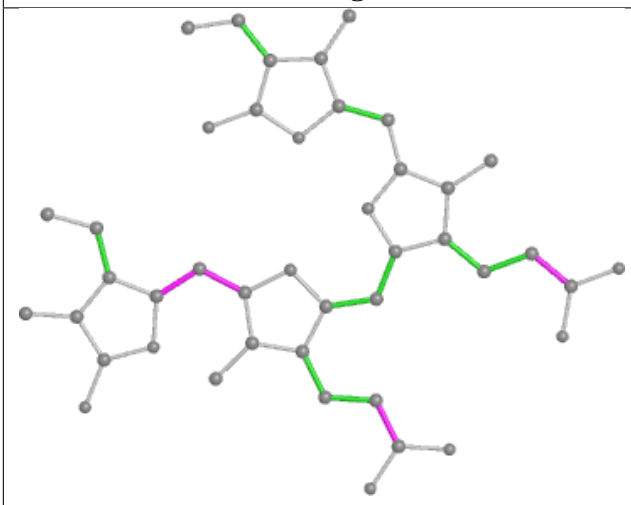

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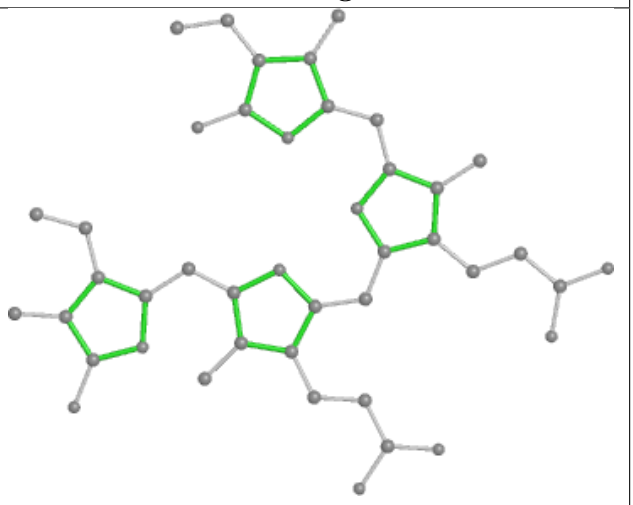
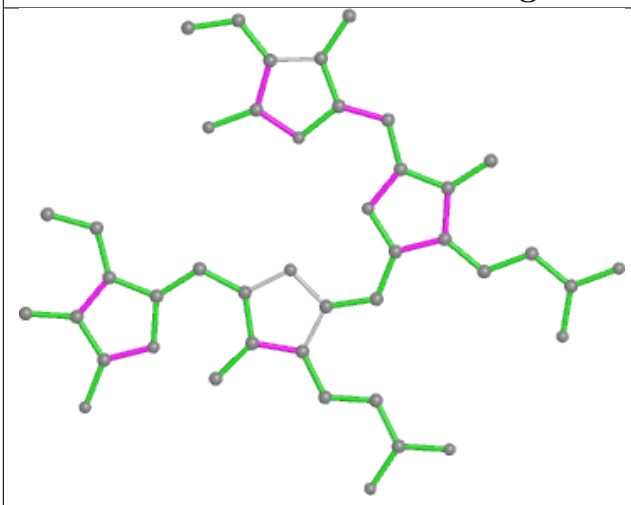


Rings

Ligand PUB r9 203



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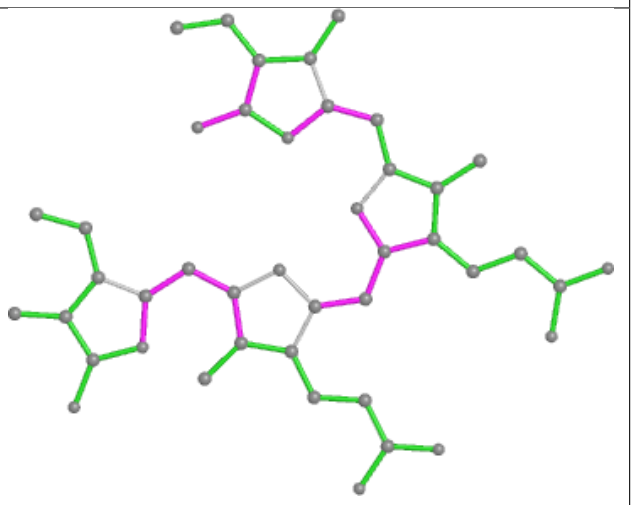

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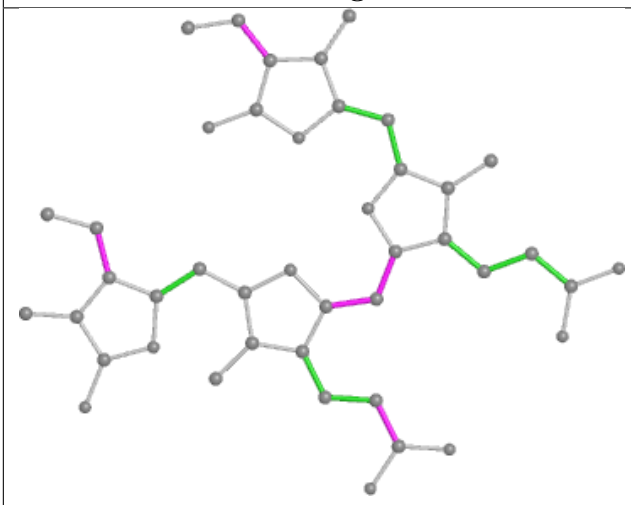

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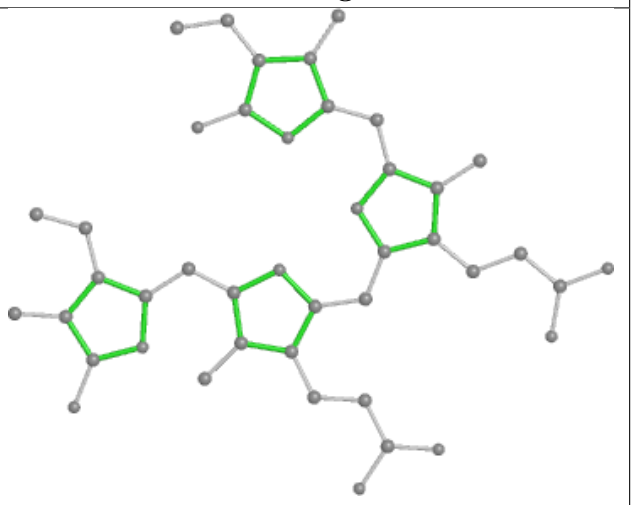
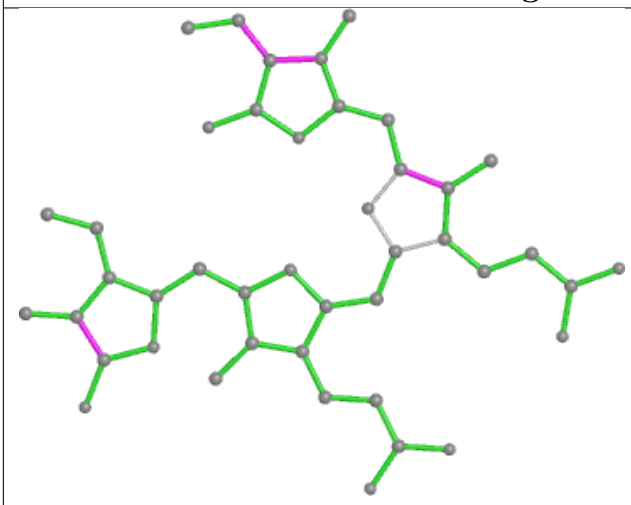


Rings

Ligand PEB s5 202



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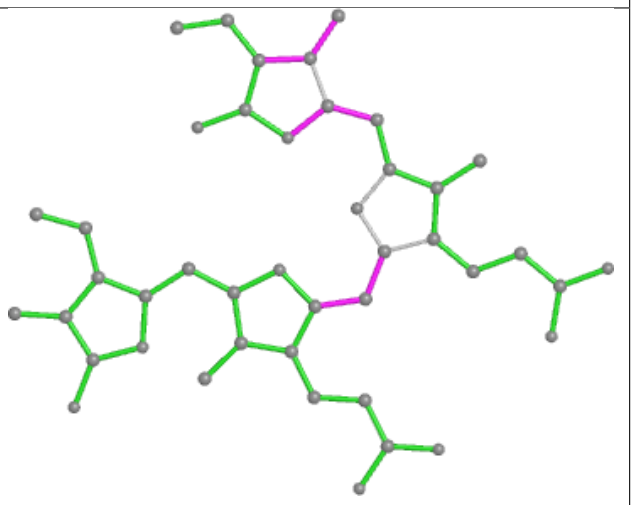

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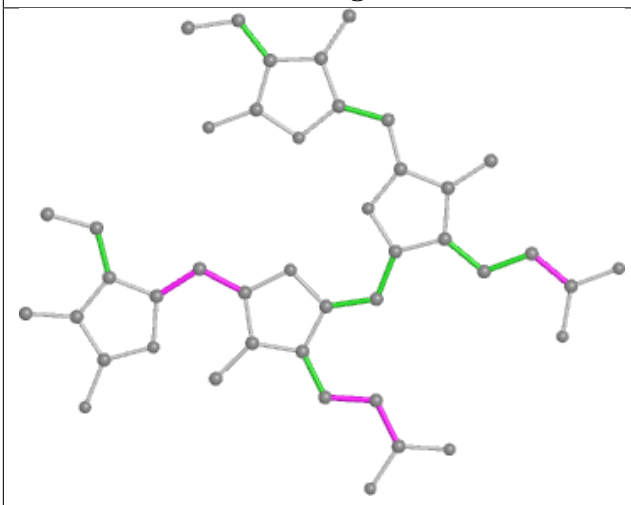

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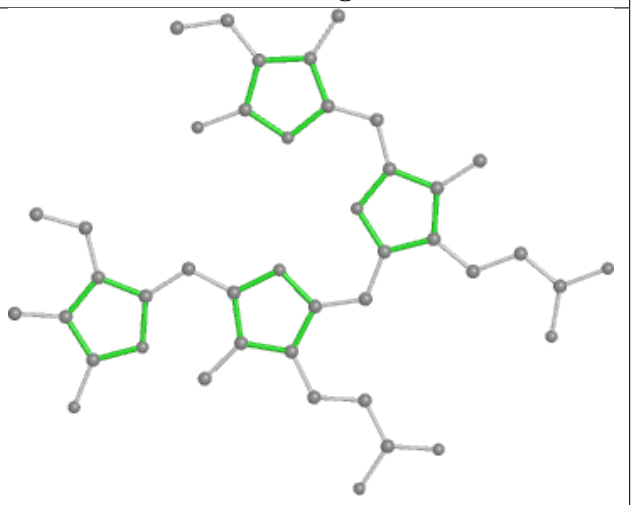
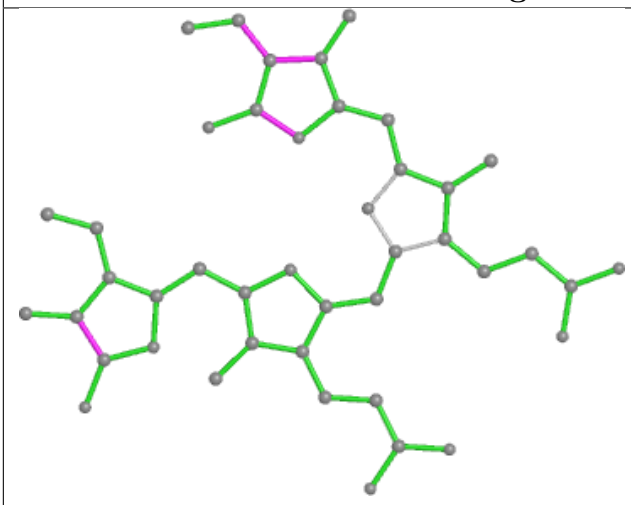


Rings

Ligand PEB dk 1001



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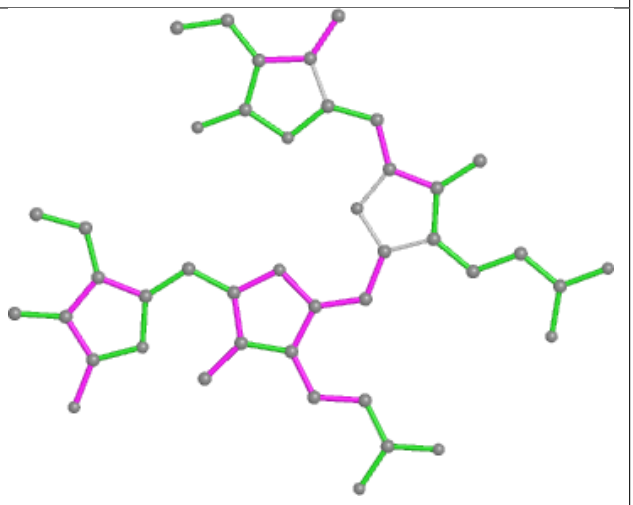

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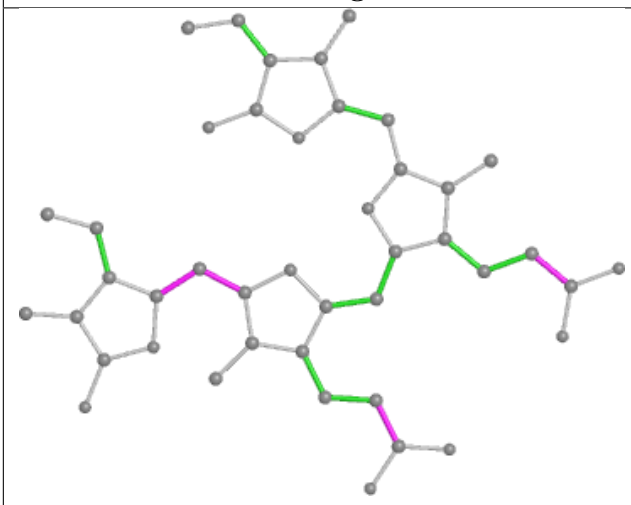

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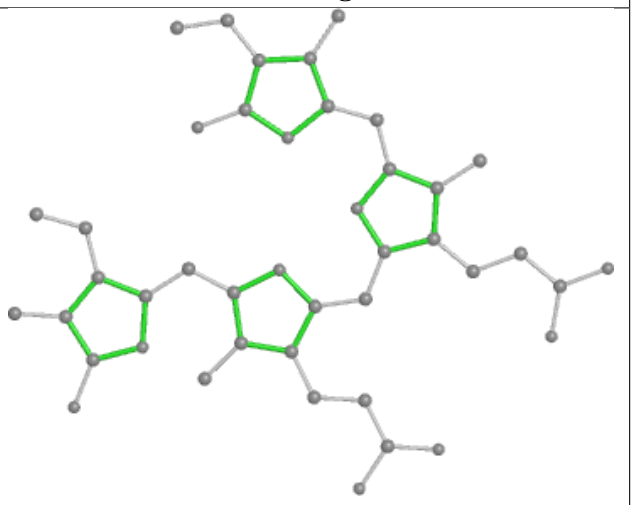
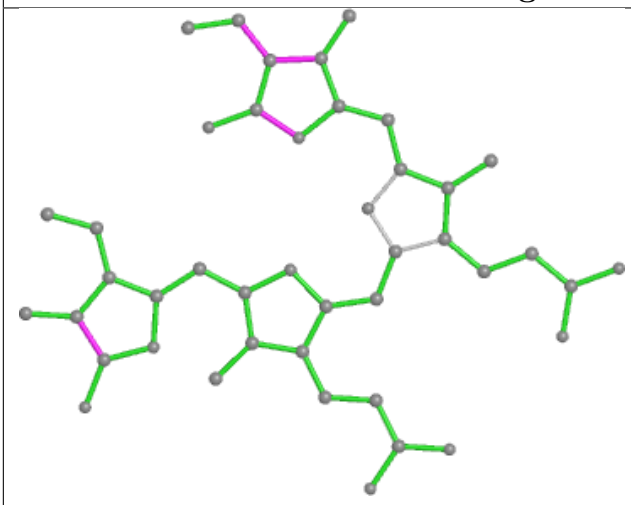


Rings

Ligand PEB S9 201



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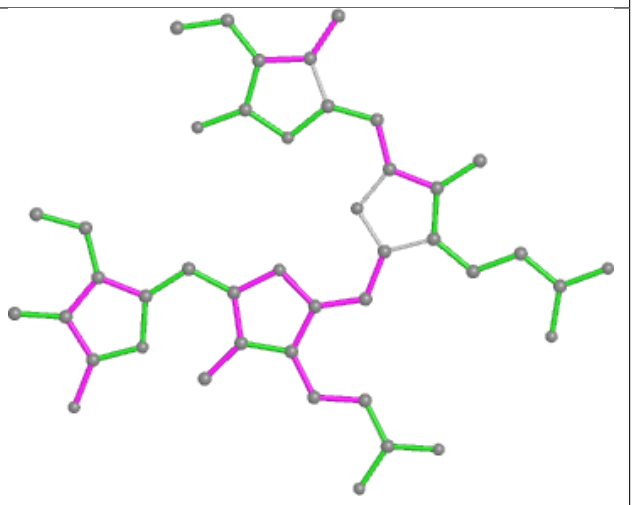

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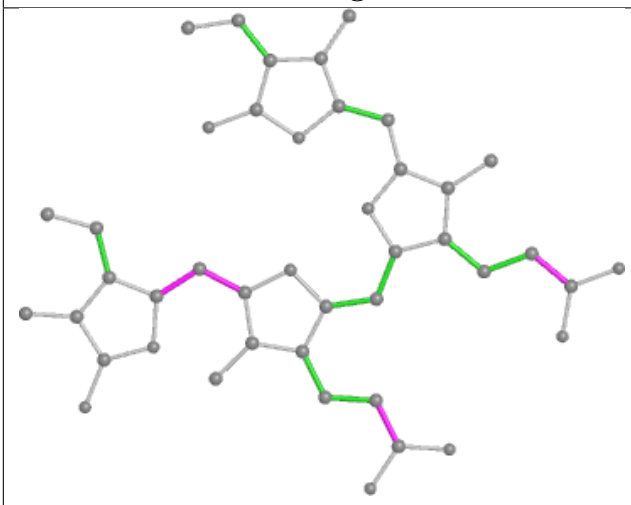

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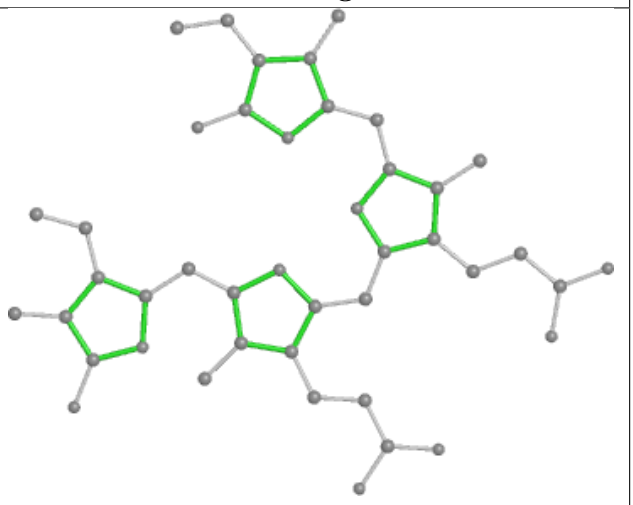

Rings

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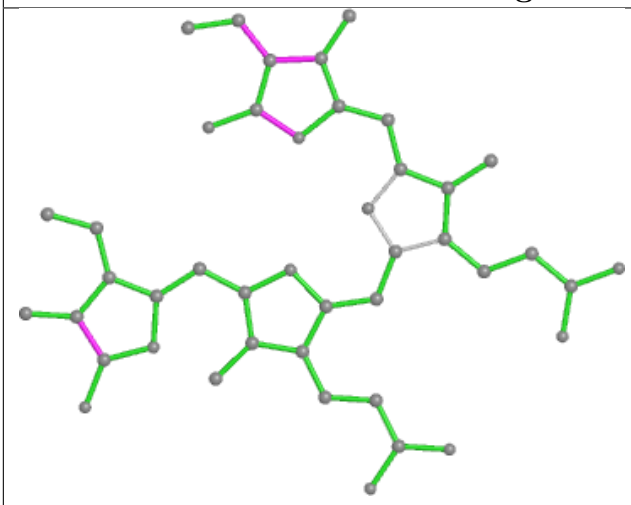

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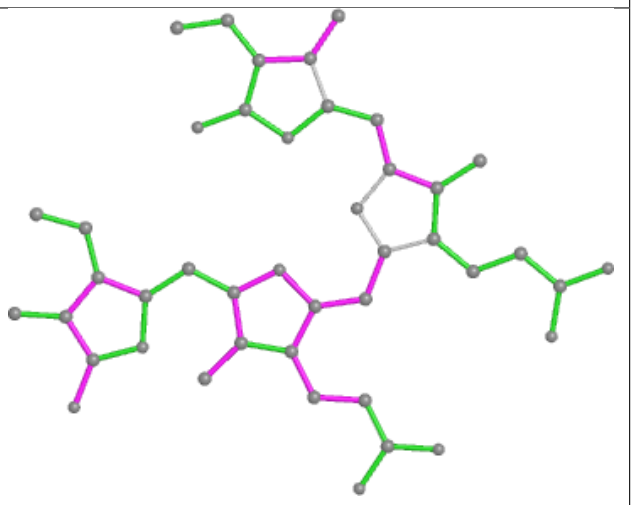

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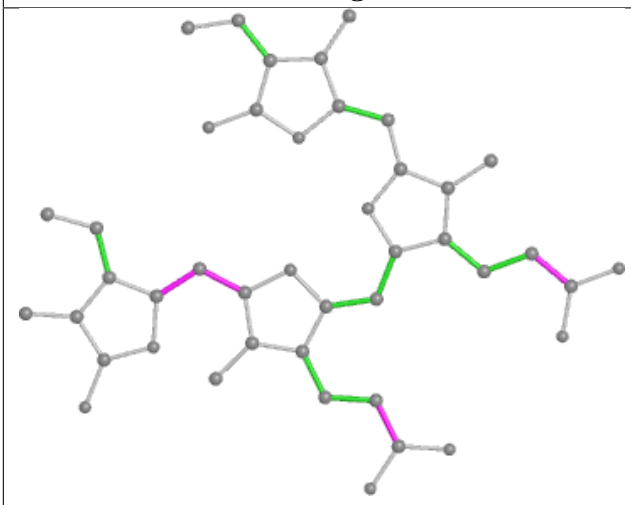

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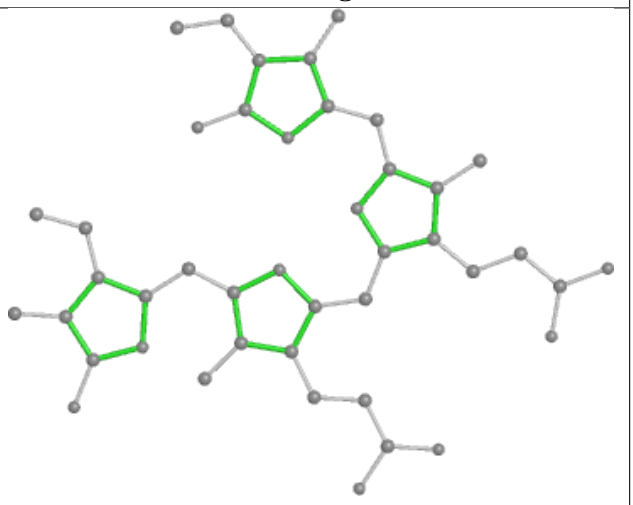

Rings

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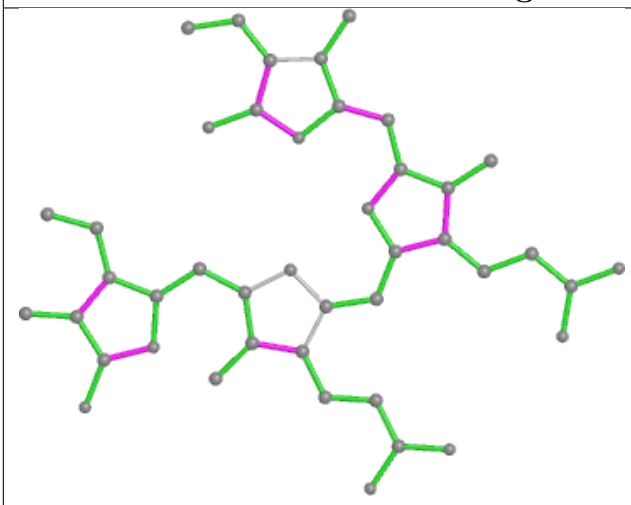

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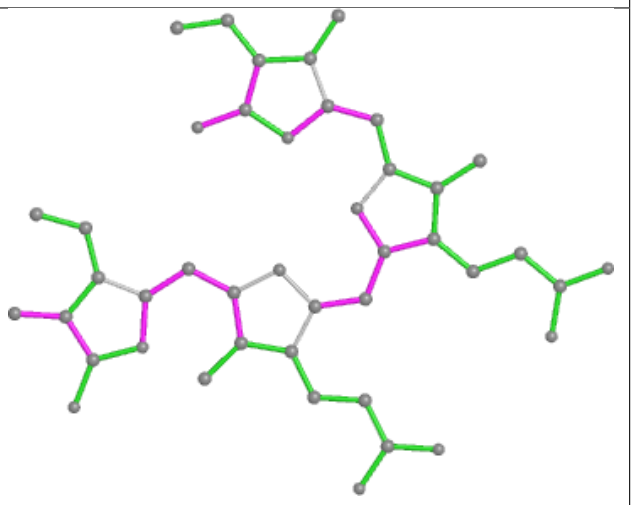

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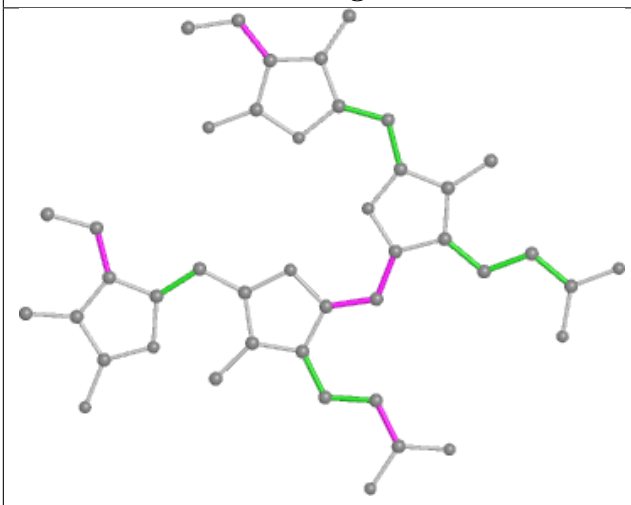

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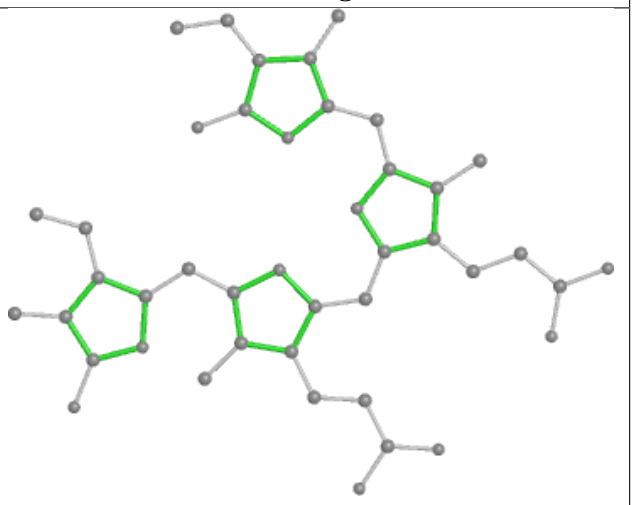
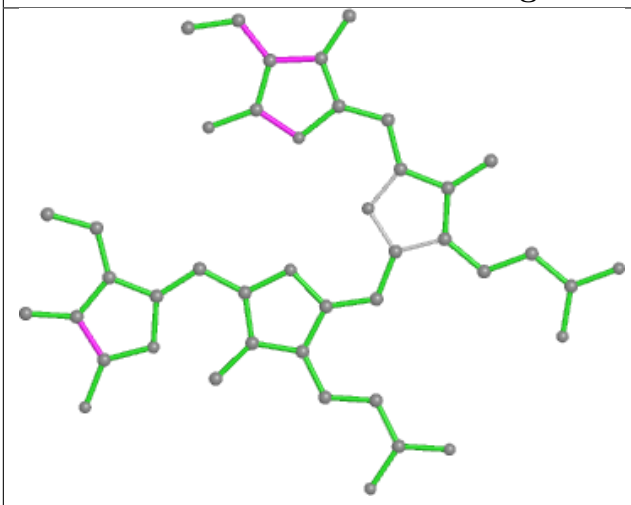


Rings

Ligand PEB g8 201



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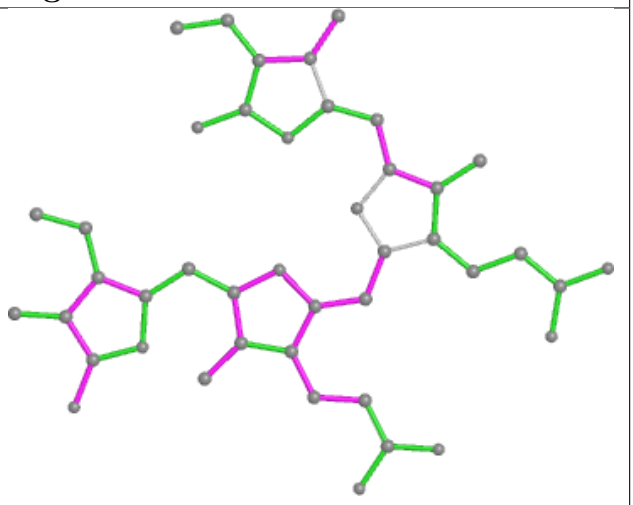

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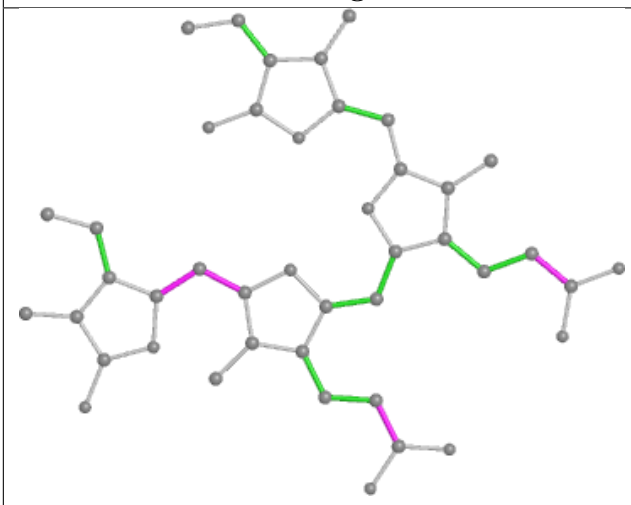

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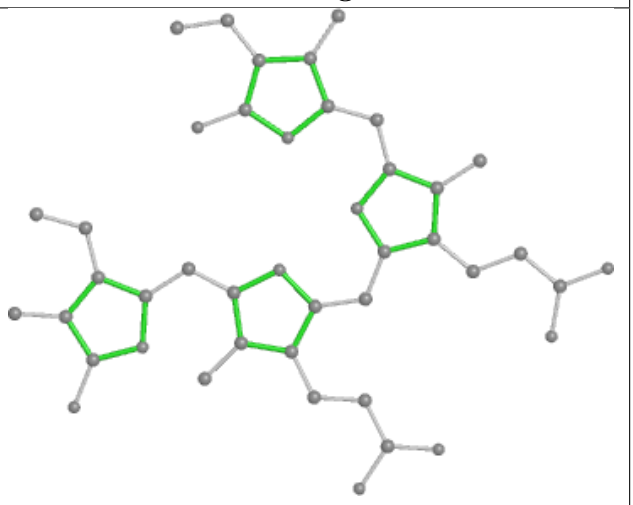
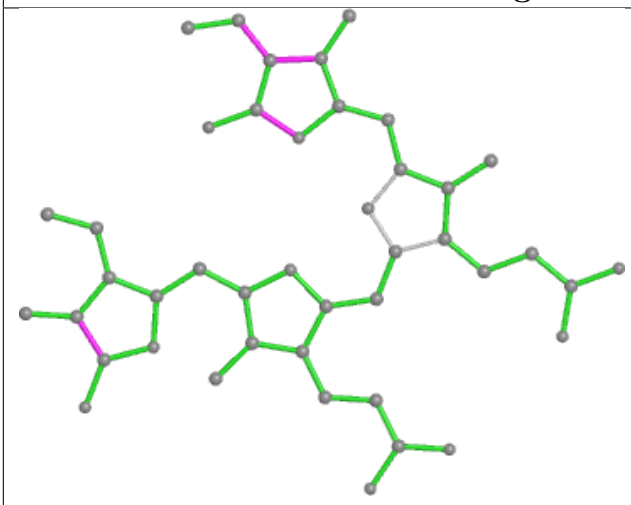


Rings

Ligand PEB m6 201



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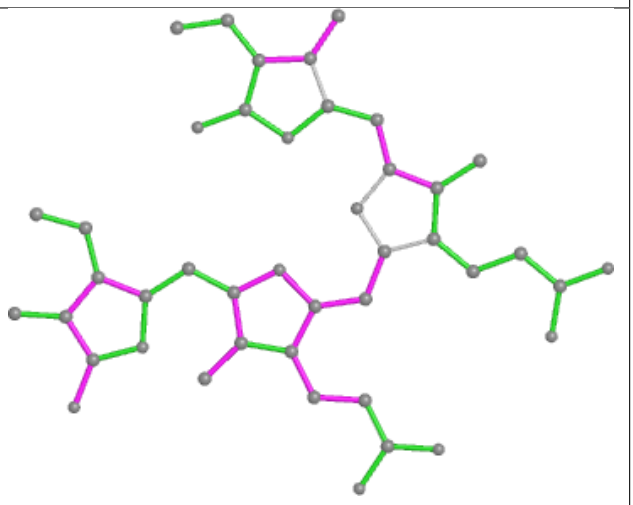

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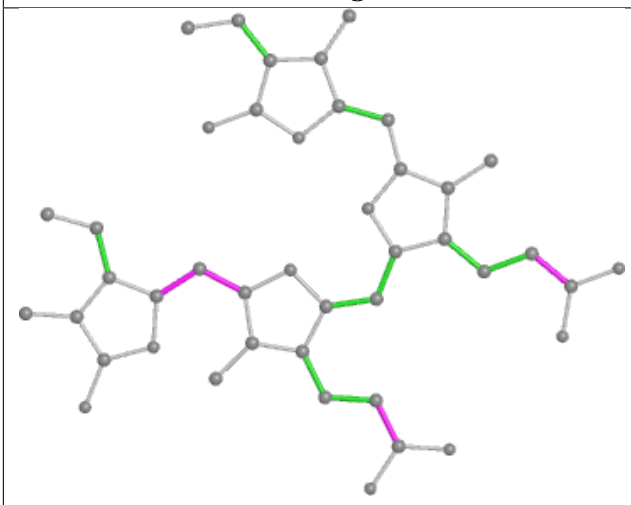

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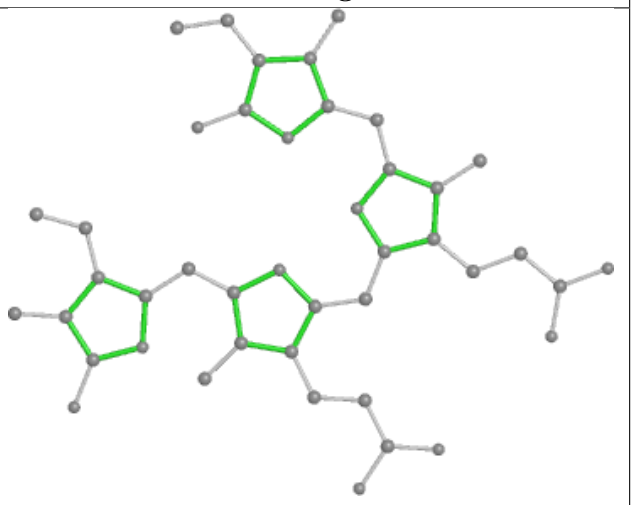
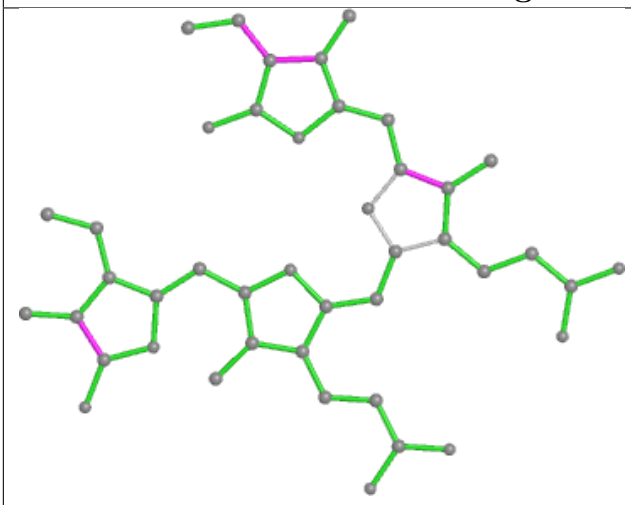


Rings

Ligand PEB K7 202



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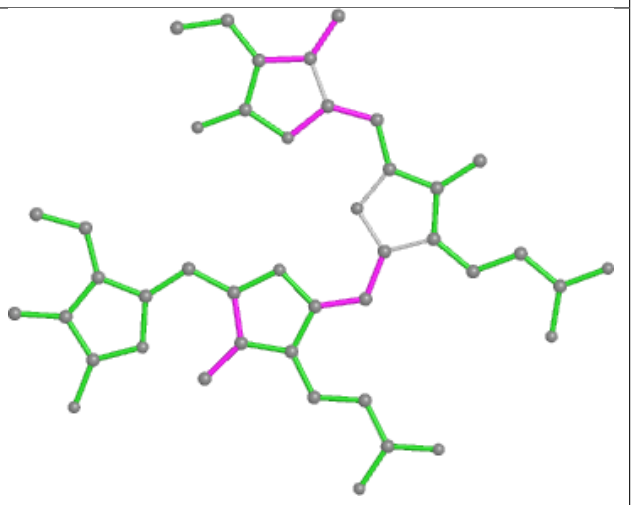

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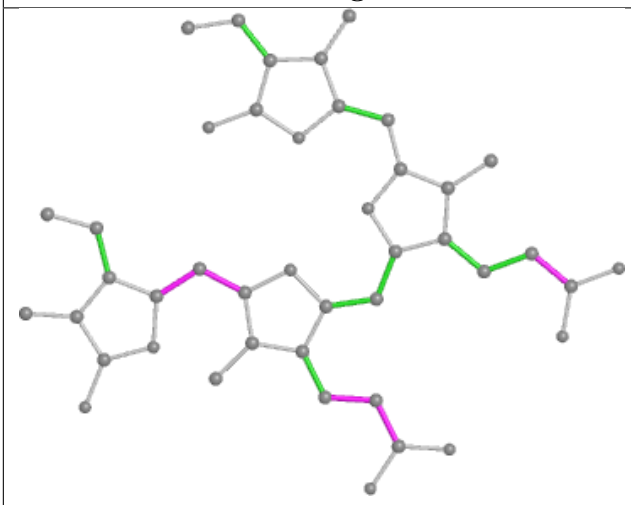

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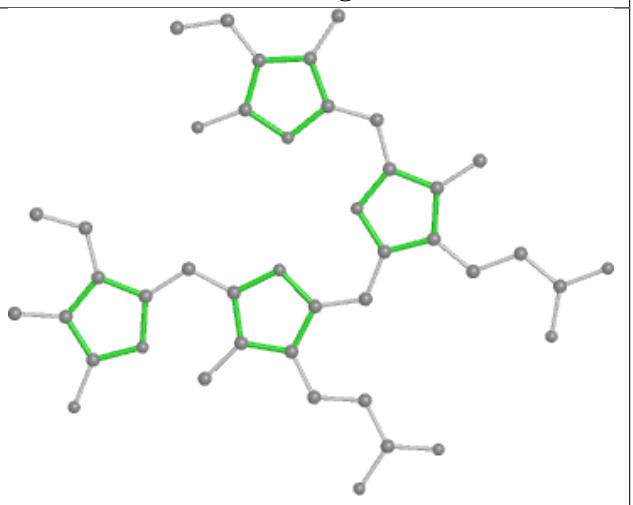

Rings

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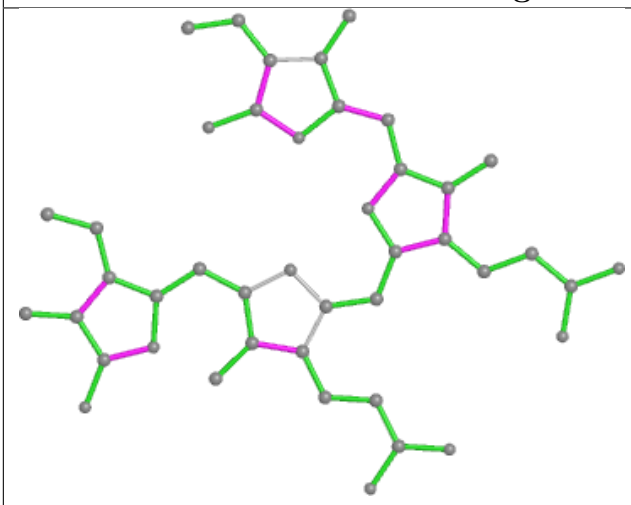

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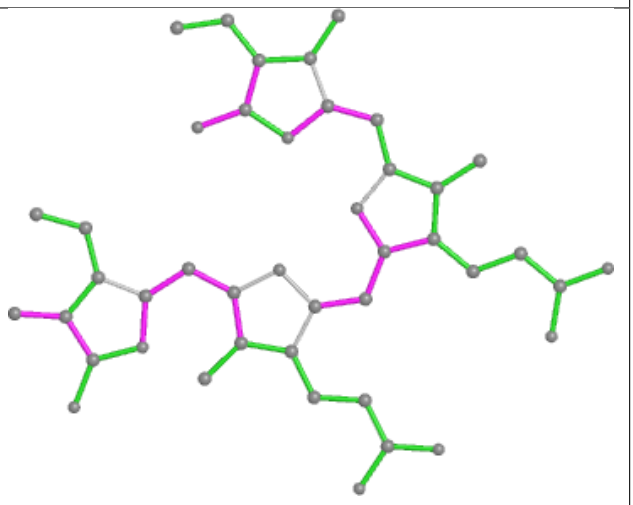

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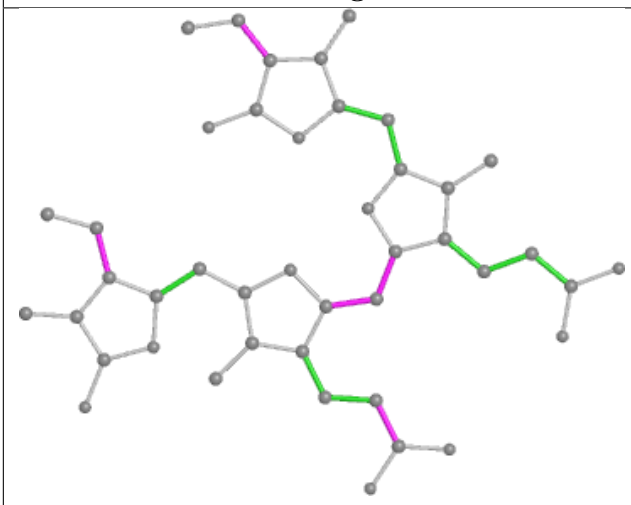

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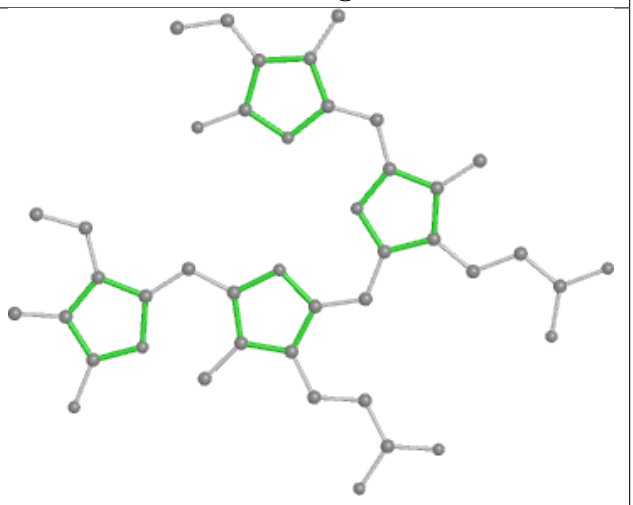
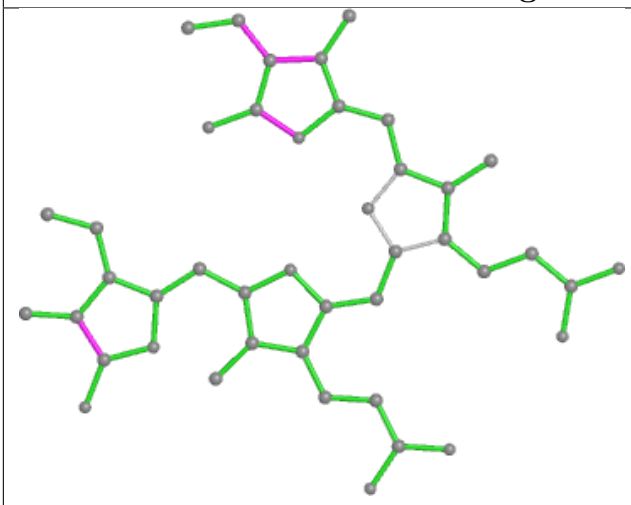


Rings

Ligand PEB k2 201



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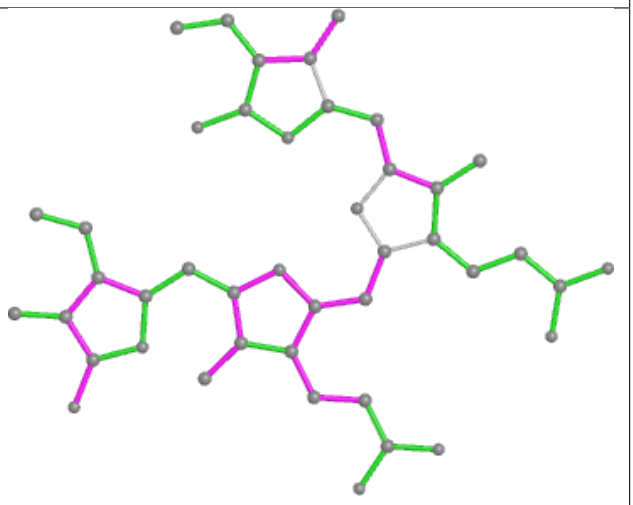

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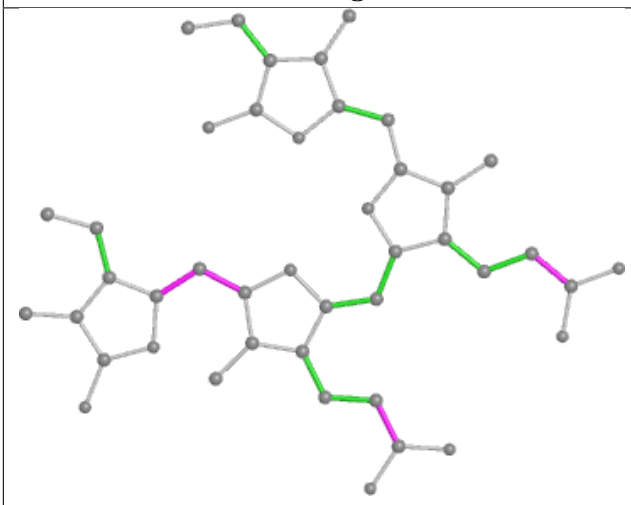

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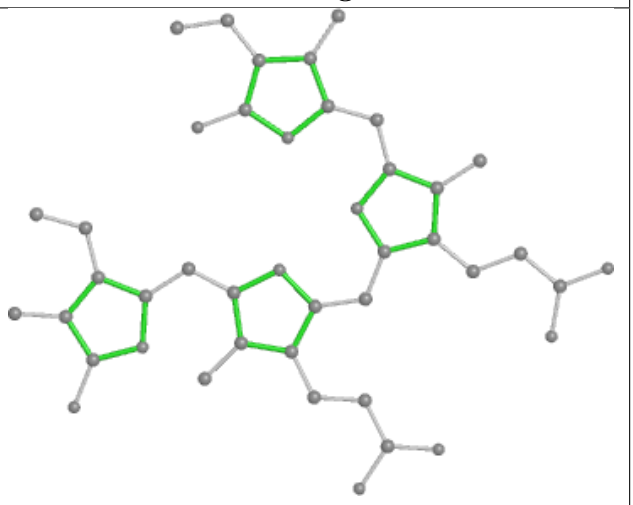

Rings

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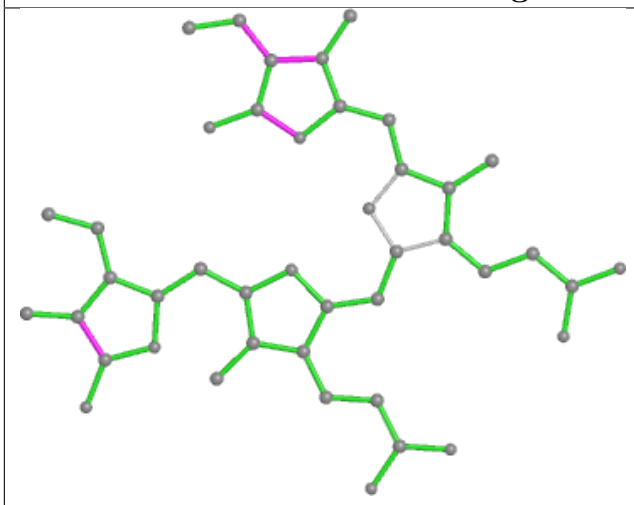

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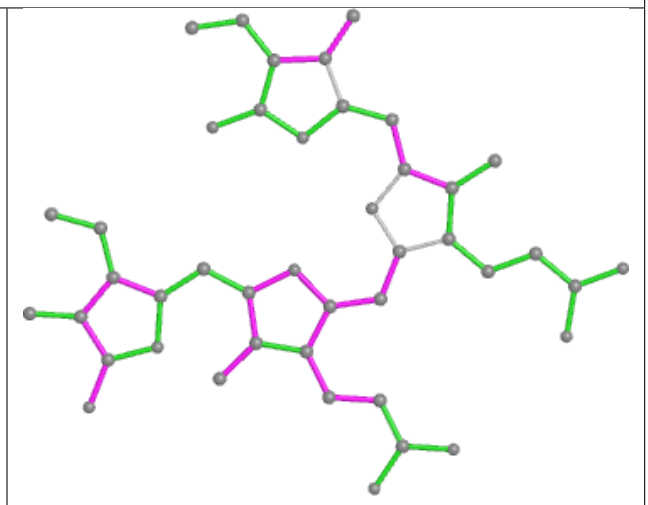
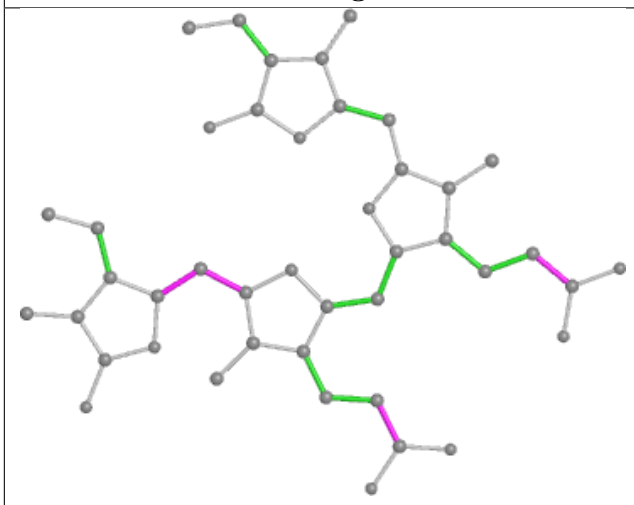


Bond angles



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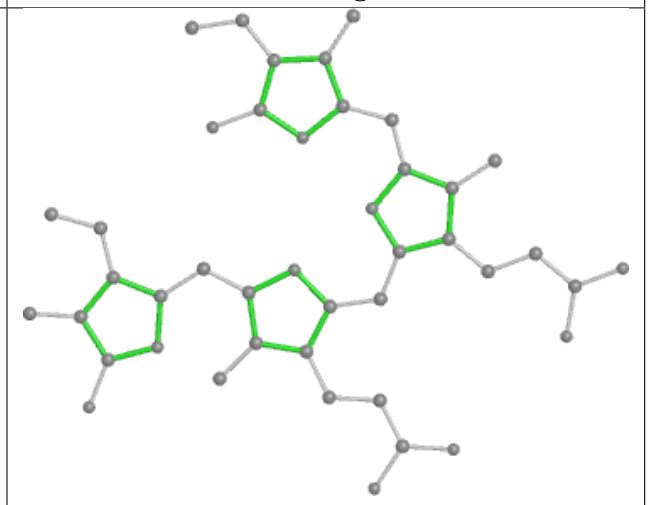
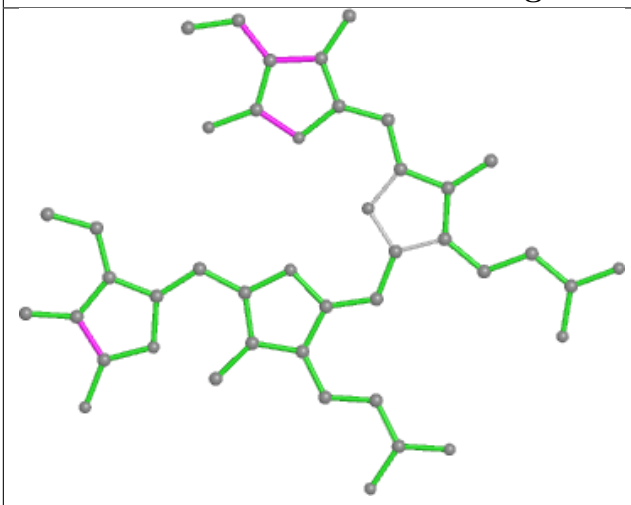
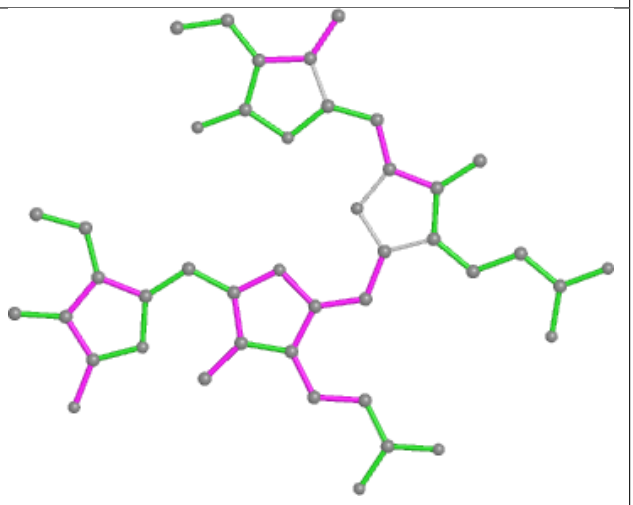


Rings

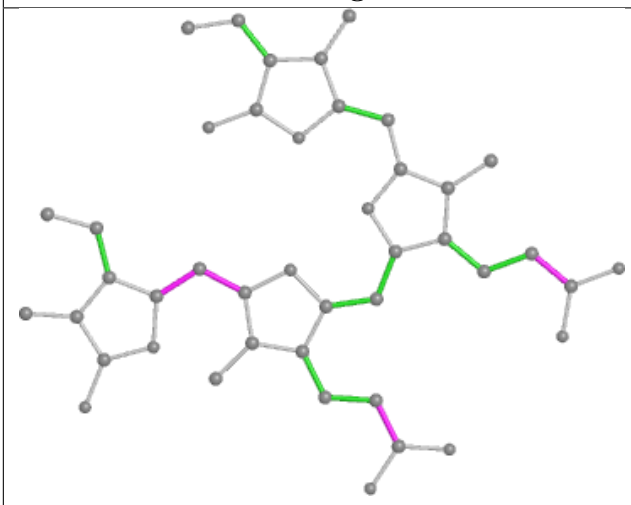
Ligand PEB ci 201



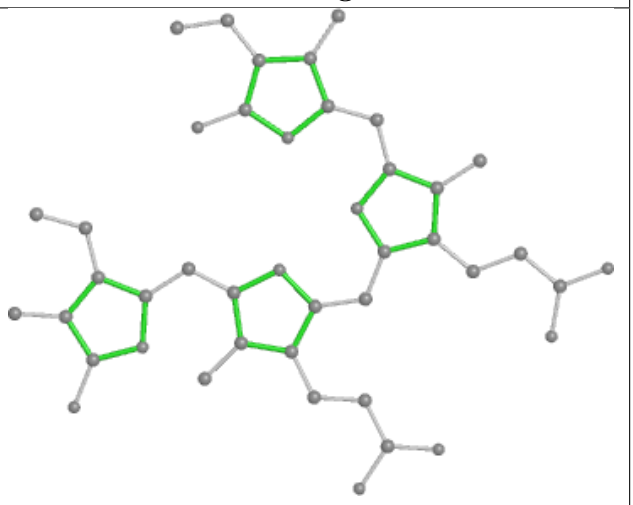
Bond lengths



Bond angles

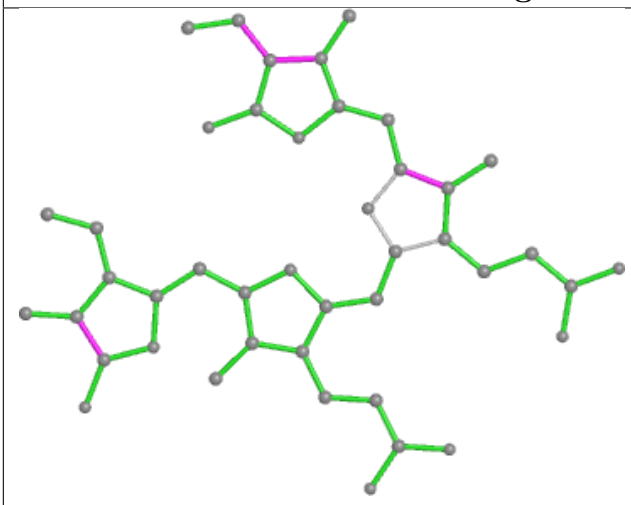


Torsions



Rings

Ligand PEB N4 202



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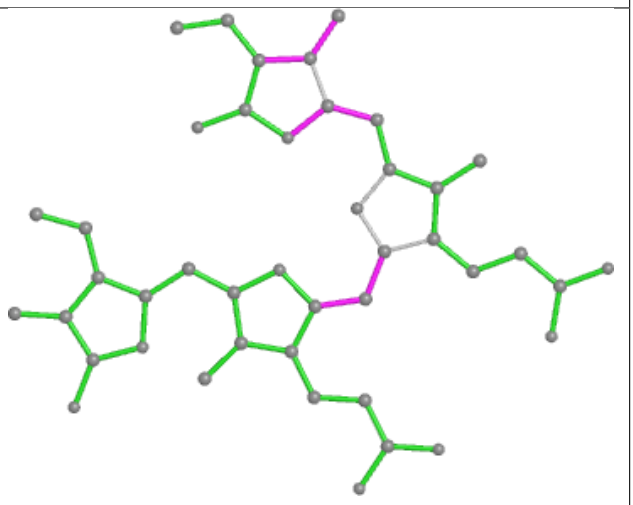

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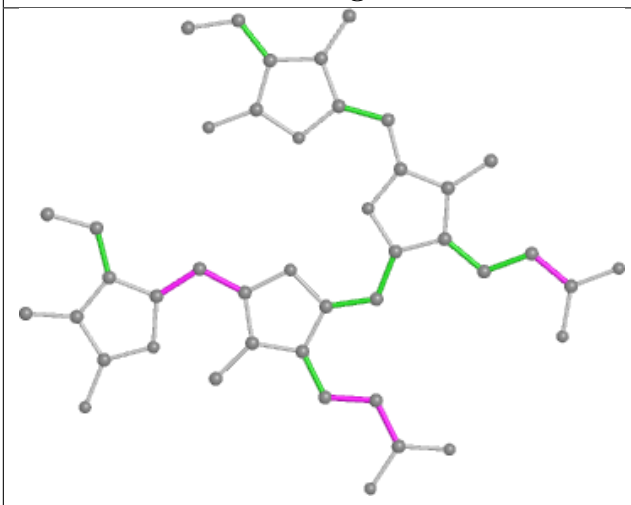

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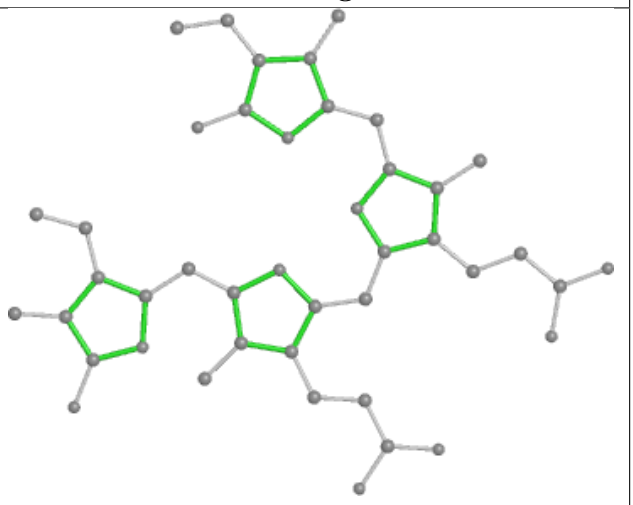
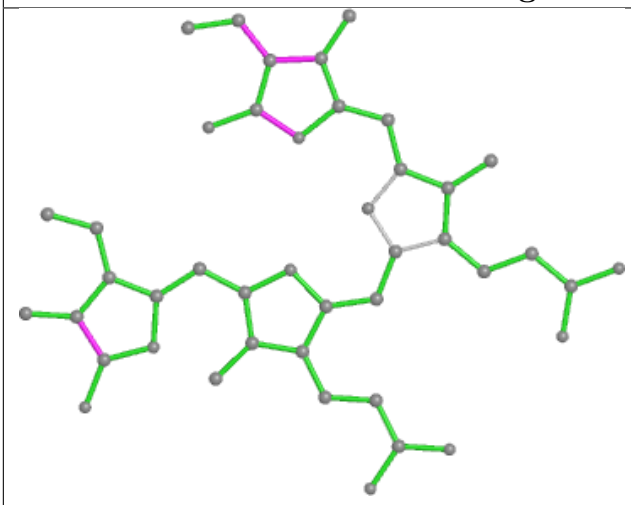


Rings

Ligand PEB h9 202



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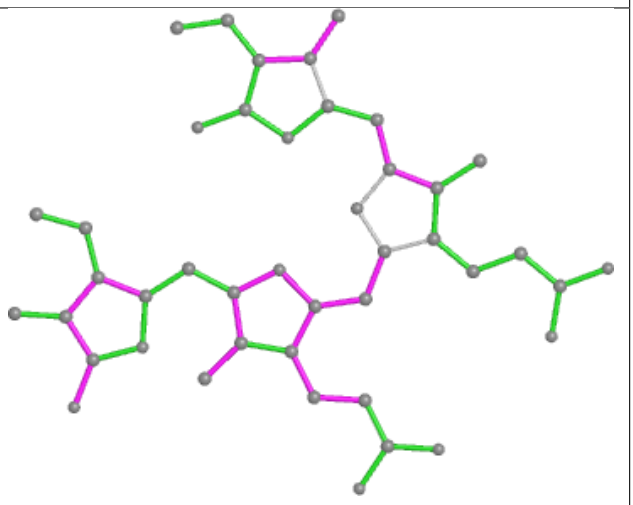

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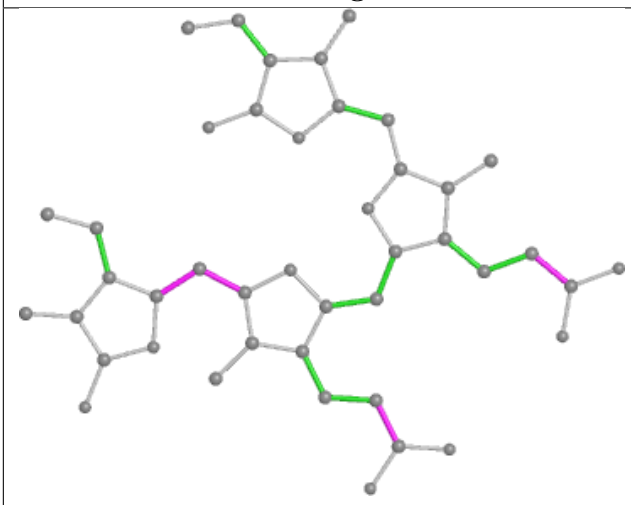

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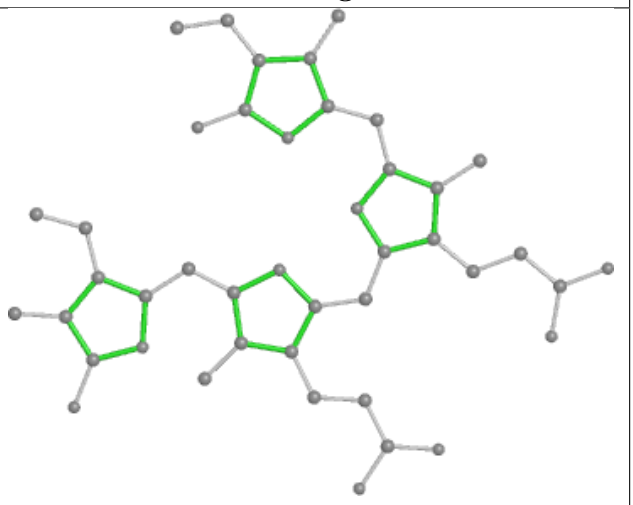
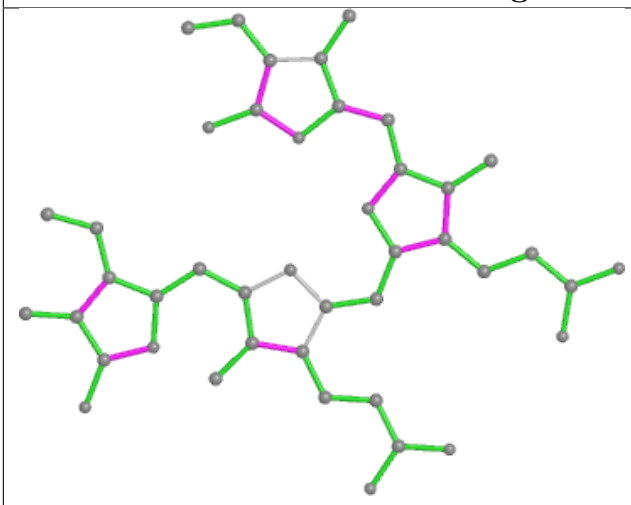


Rings

Ligand PUB ez 1005



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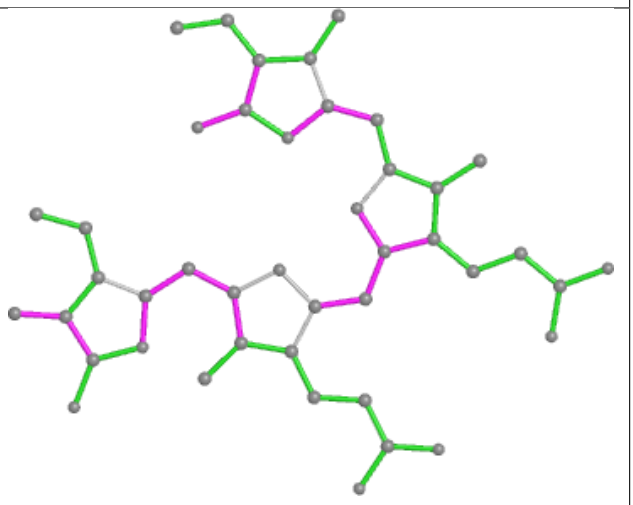

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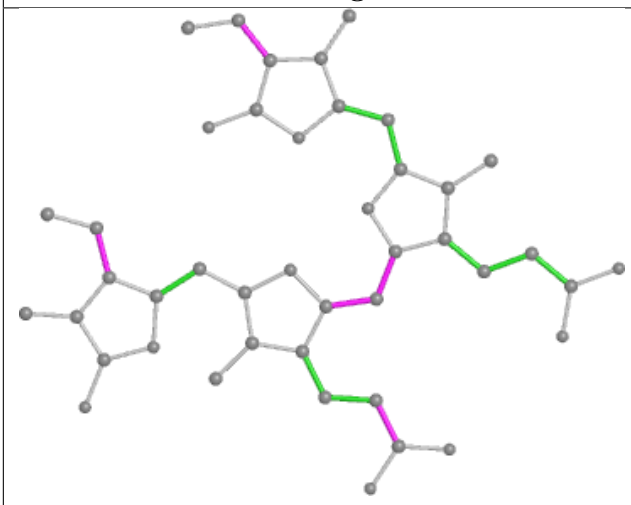

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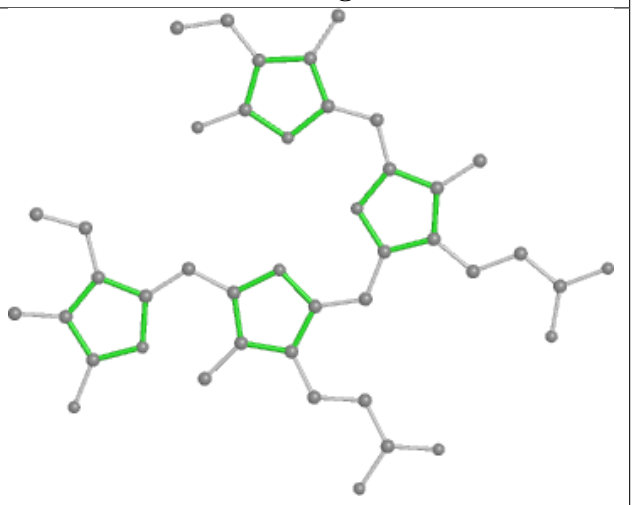

Rings

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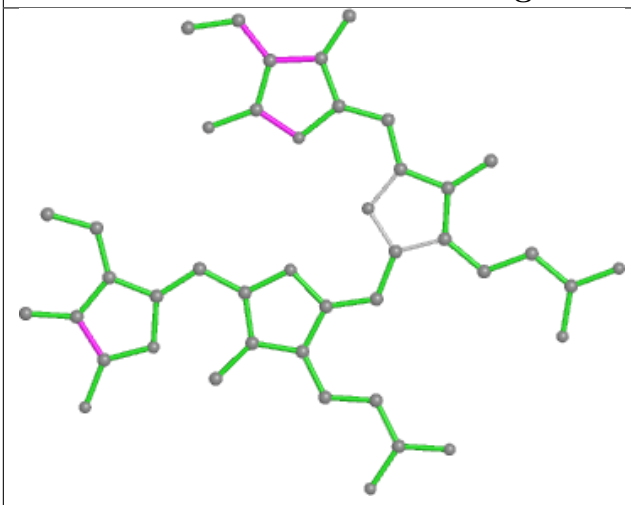

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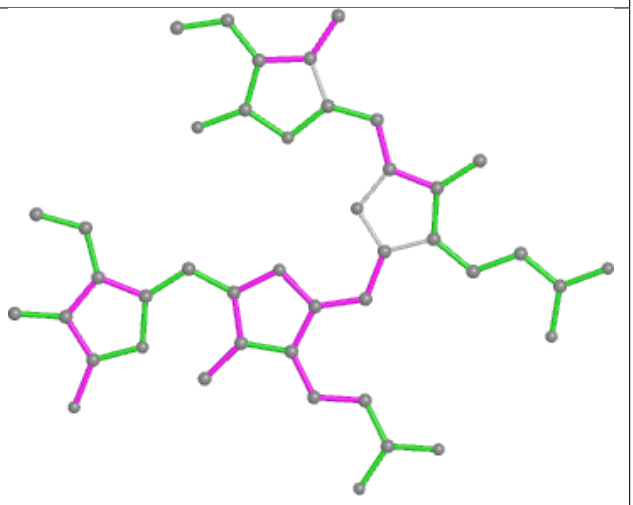

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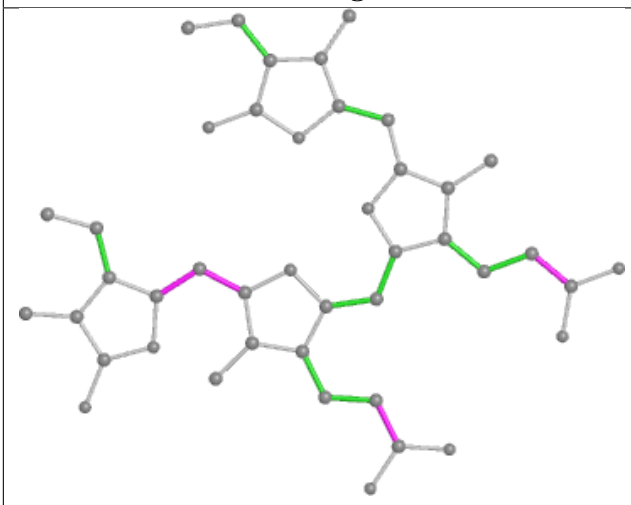

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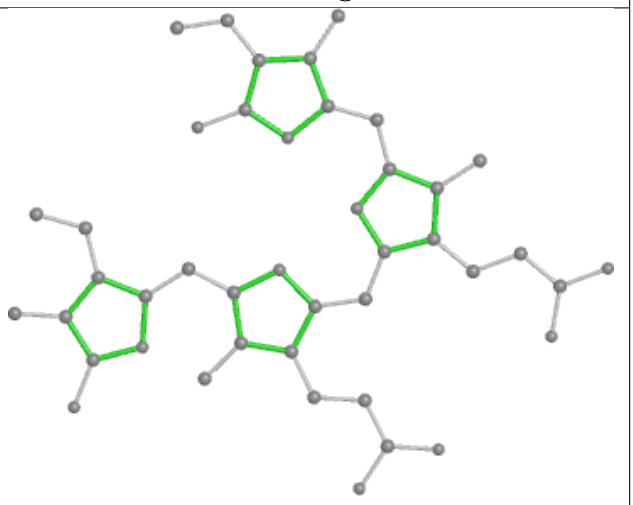

Rings

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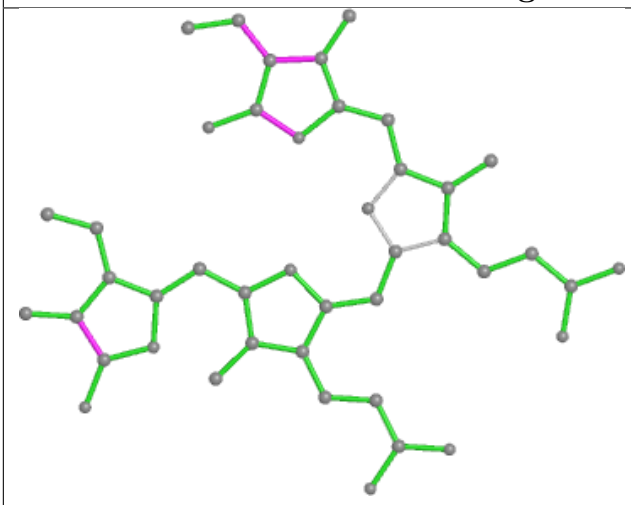

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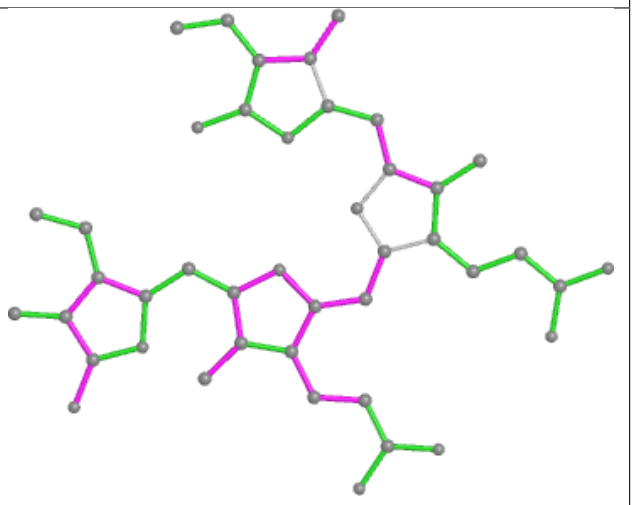

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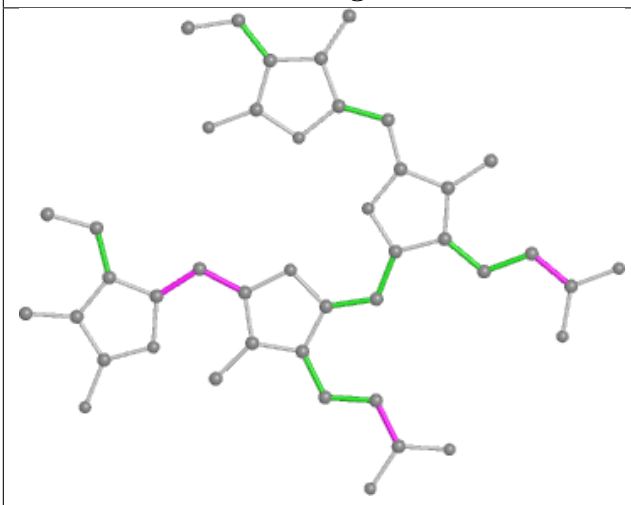

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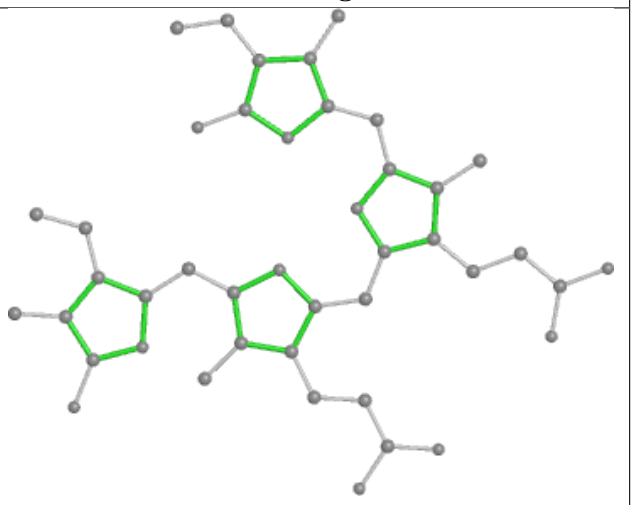

Rings

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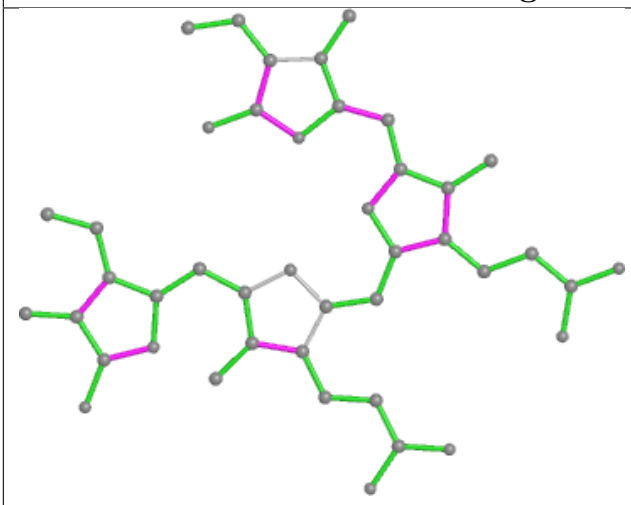

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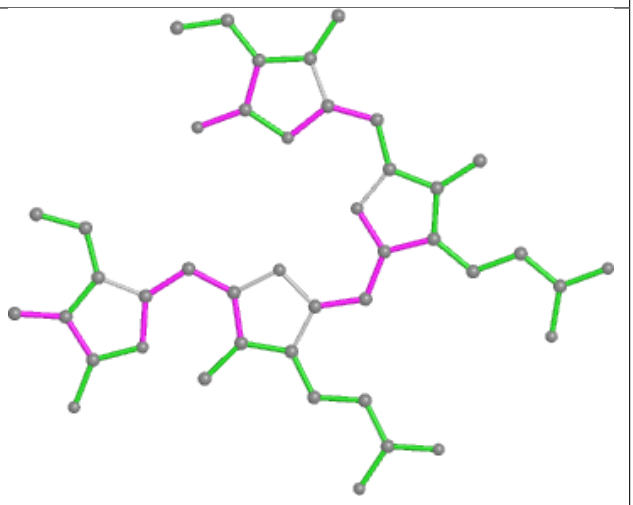

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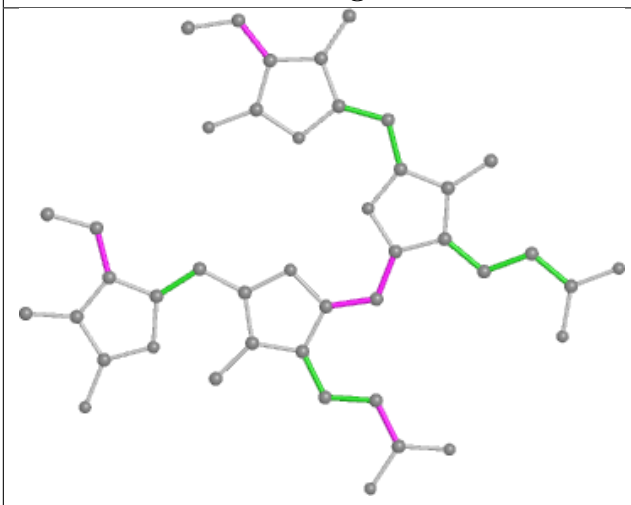

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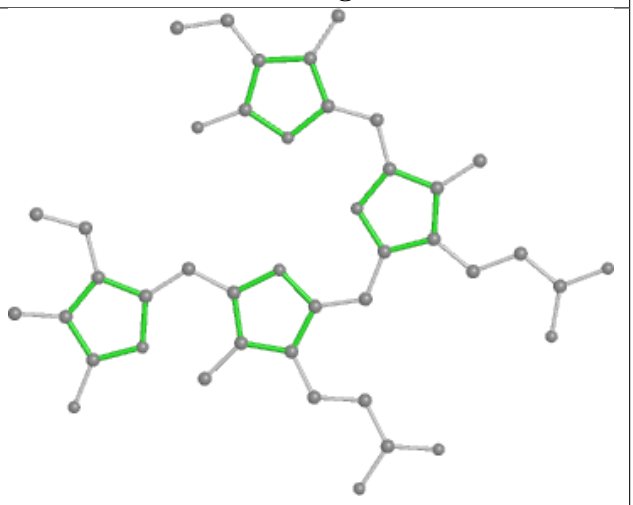

Rings

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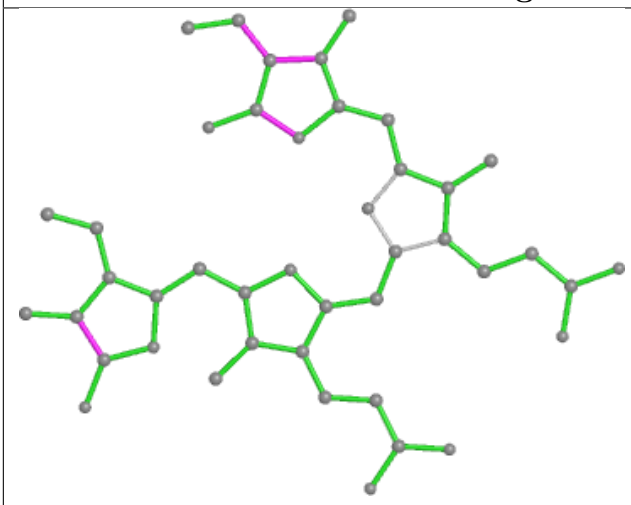

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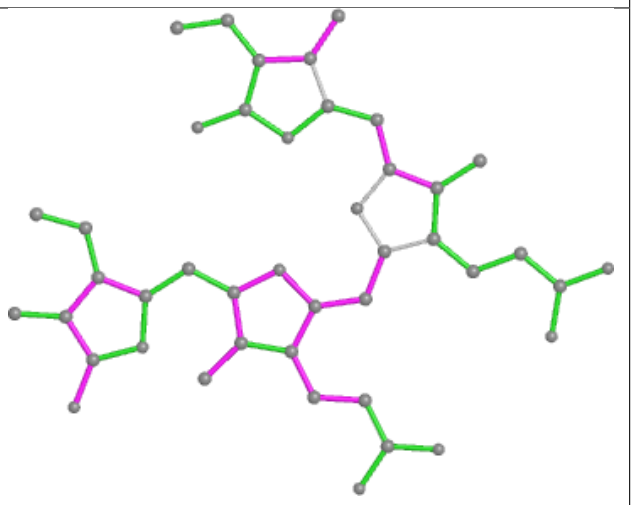

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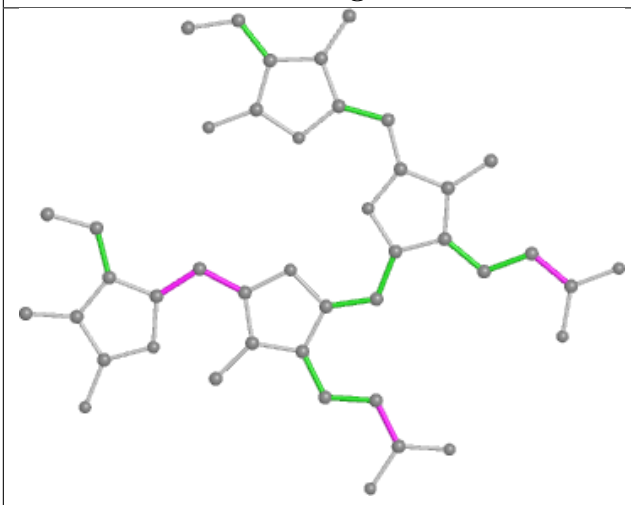

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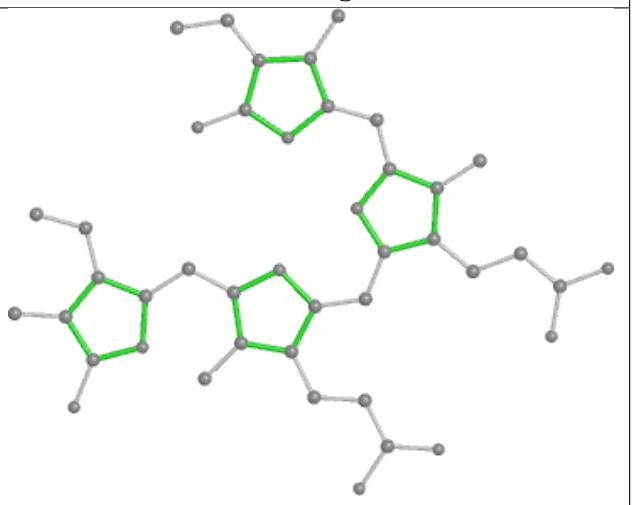

Rings

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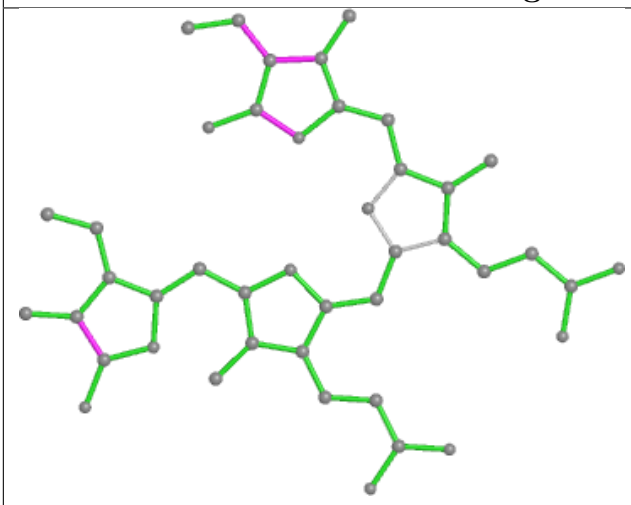

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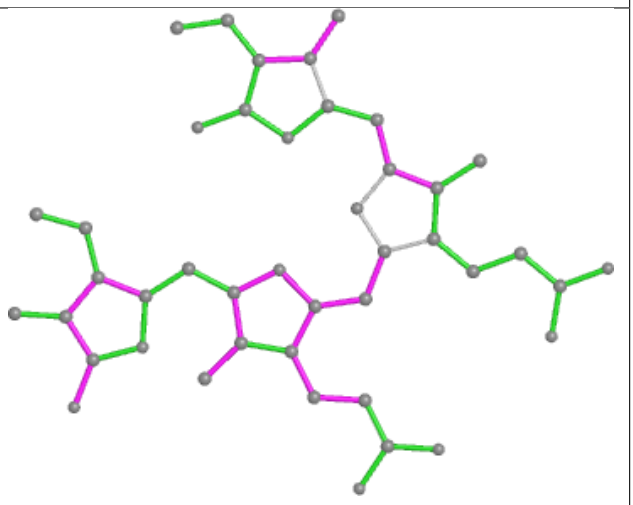

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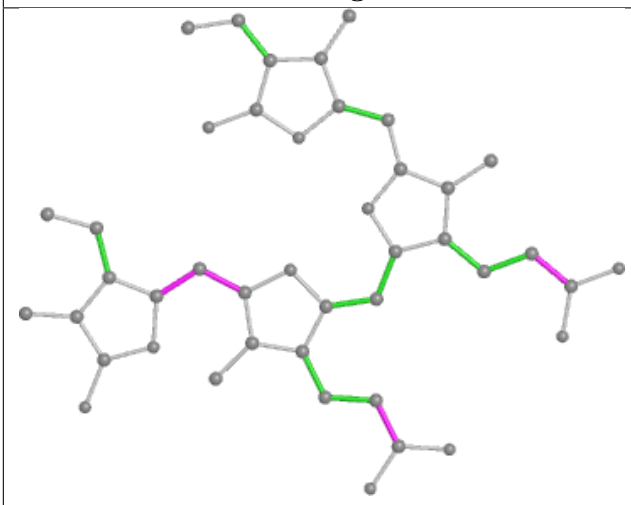

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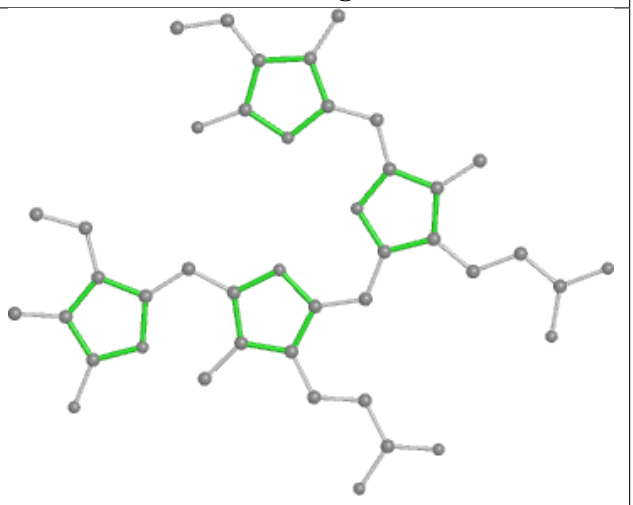

Rings

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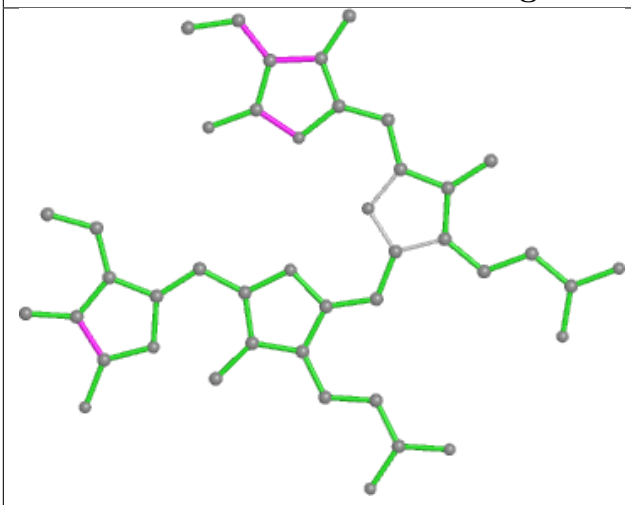

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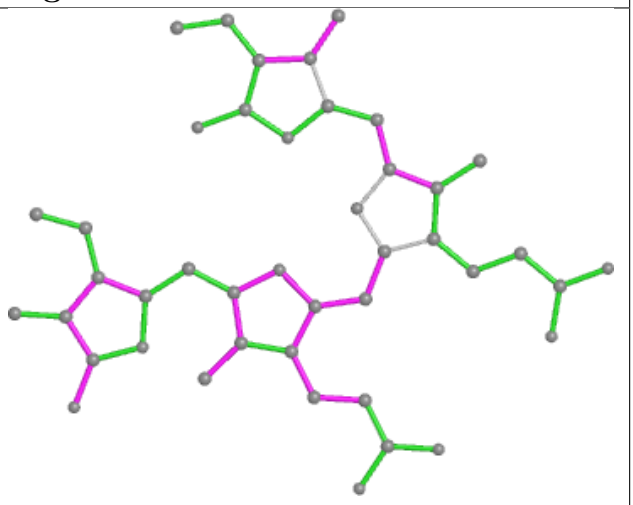

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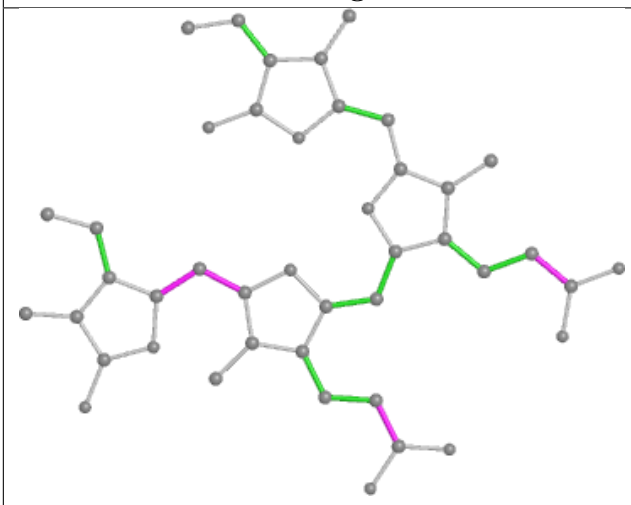

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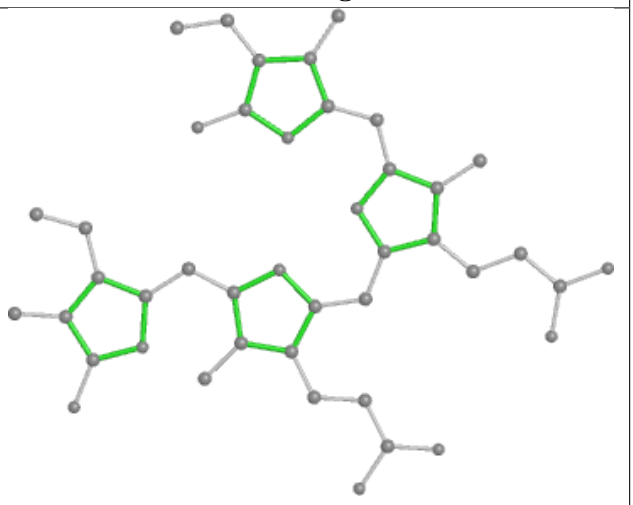
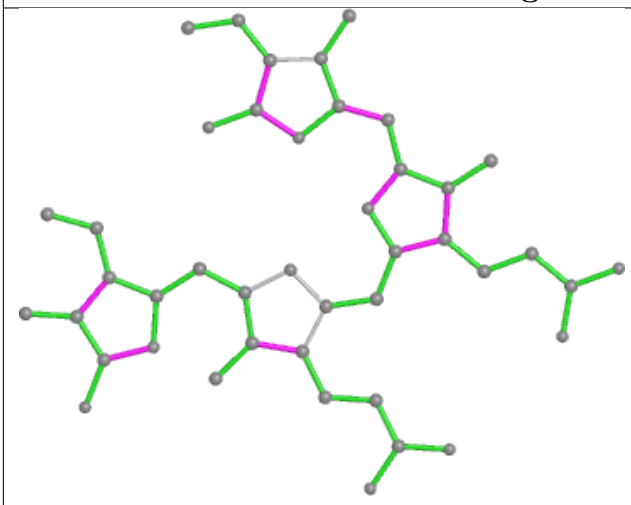


Rings

Ligand PUB ly 405



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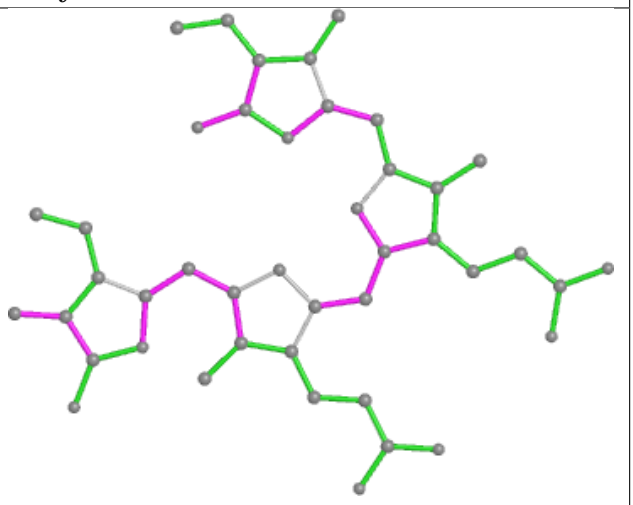

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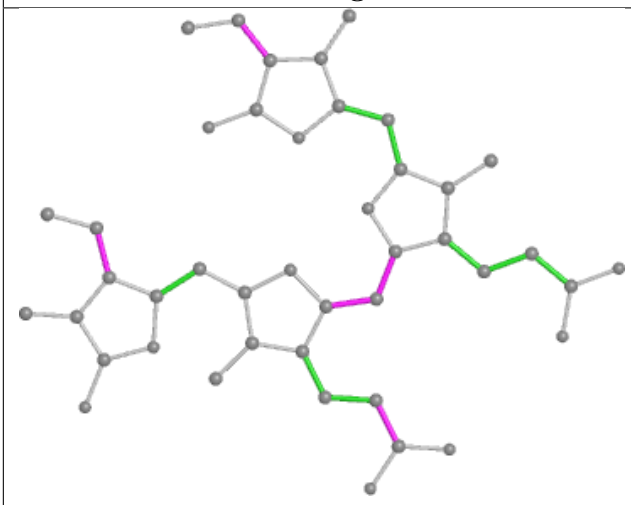

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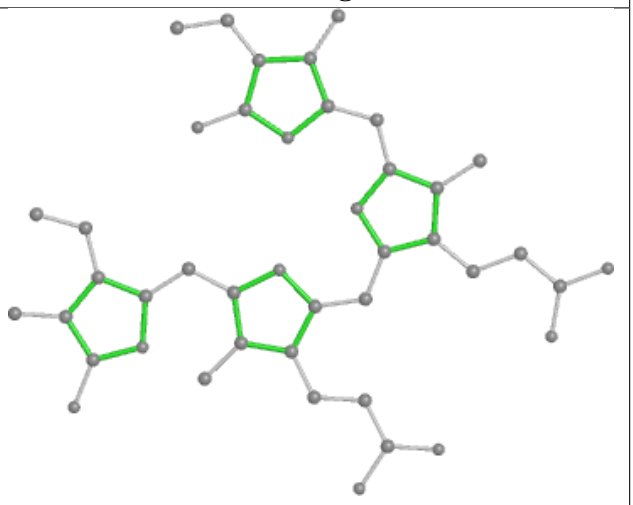
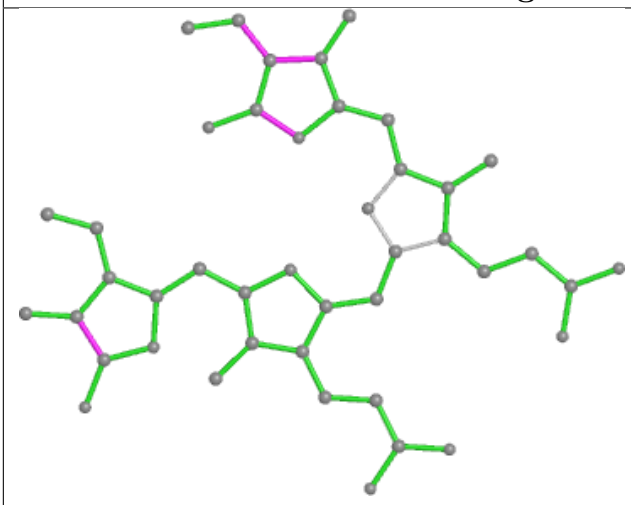


Rings

Ligand PEB F4 202



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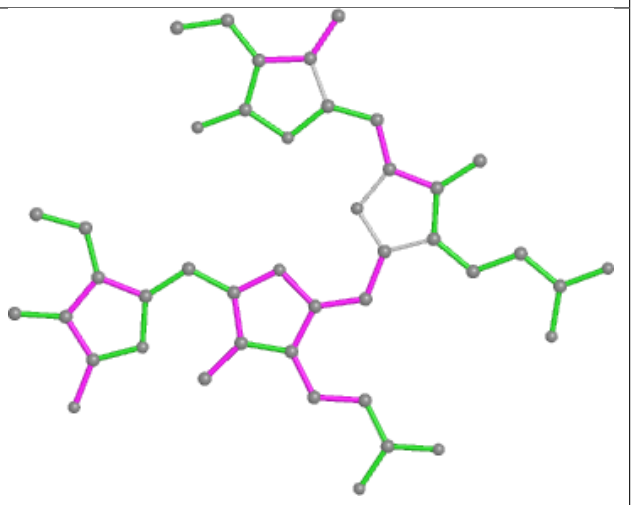

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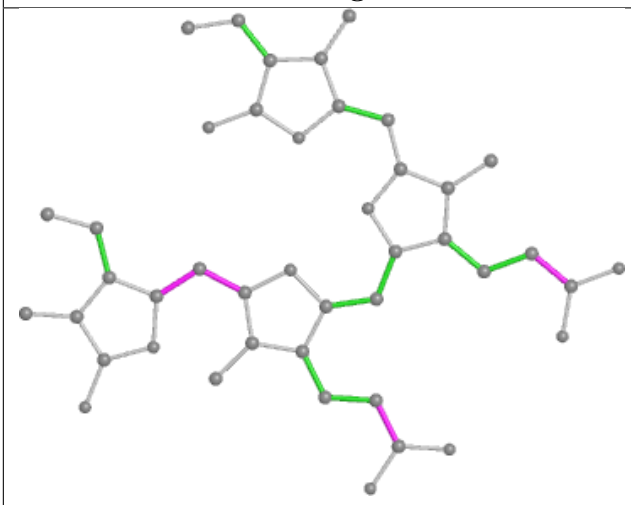

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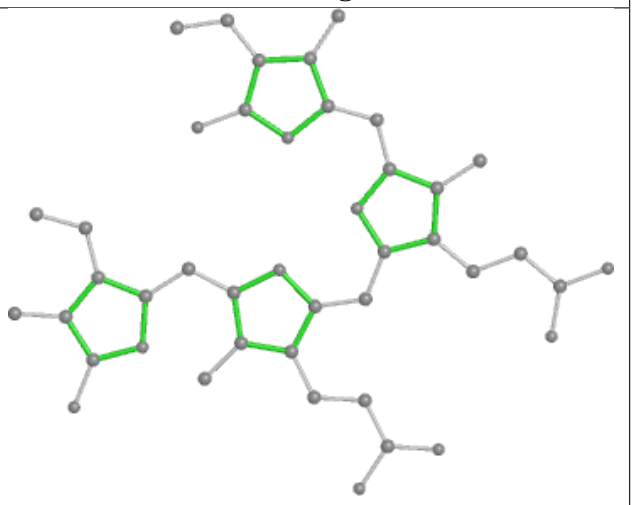
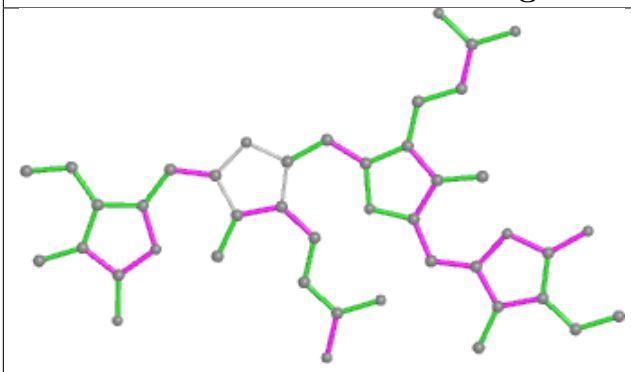


Rings

Ligand CYC t1 201



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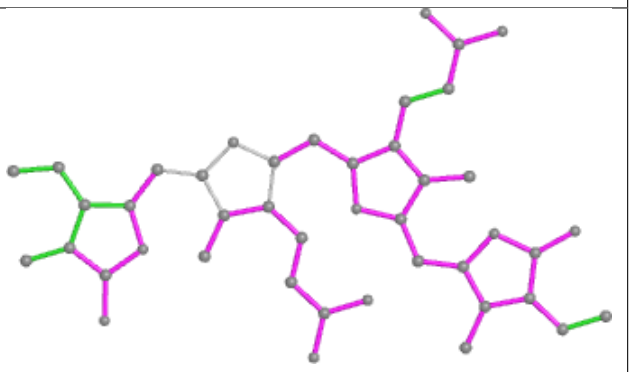

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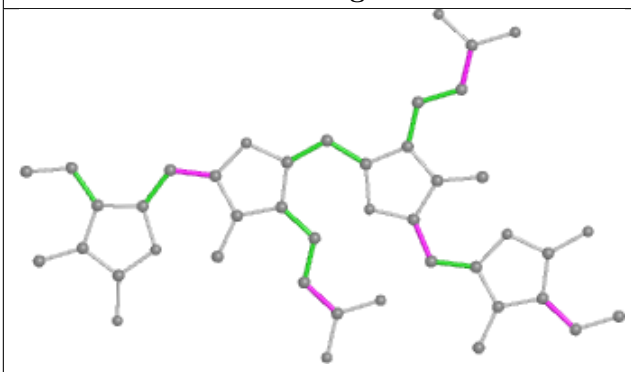

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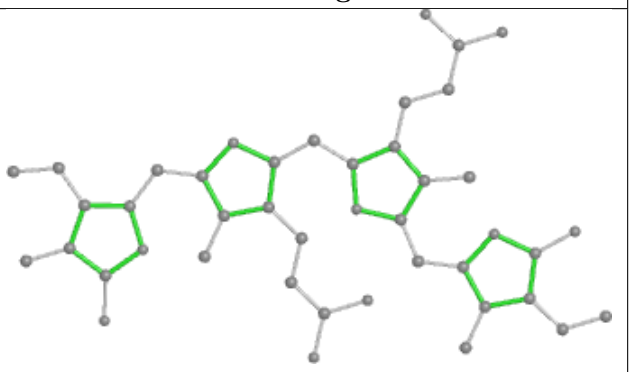
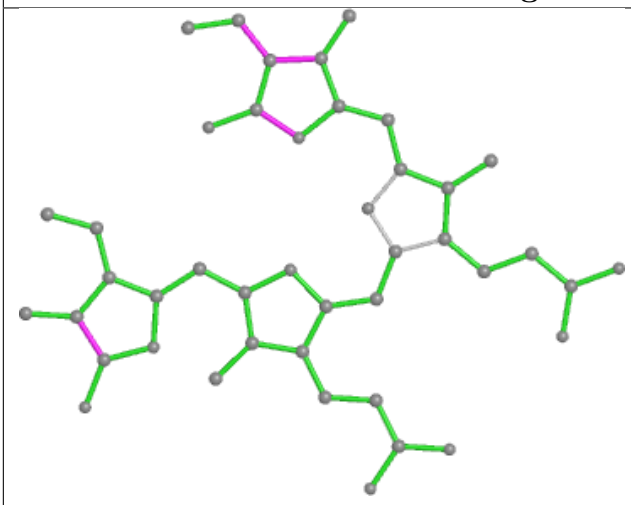


Rings

Ligand PEB c4 202



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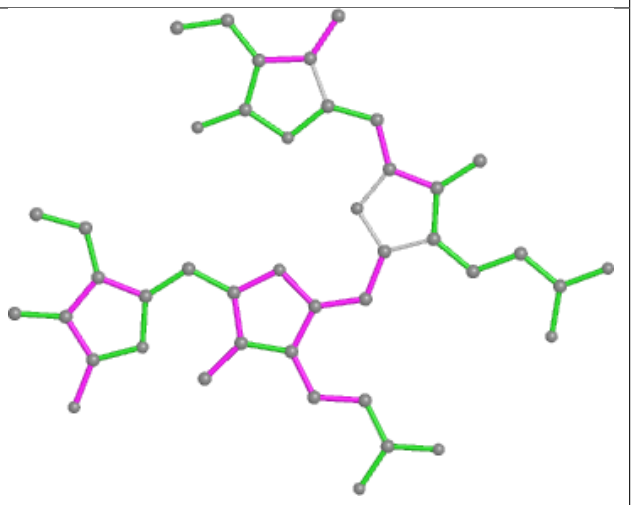
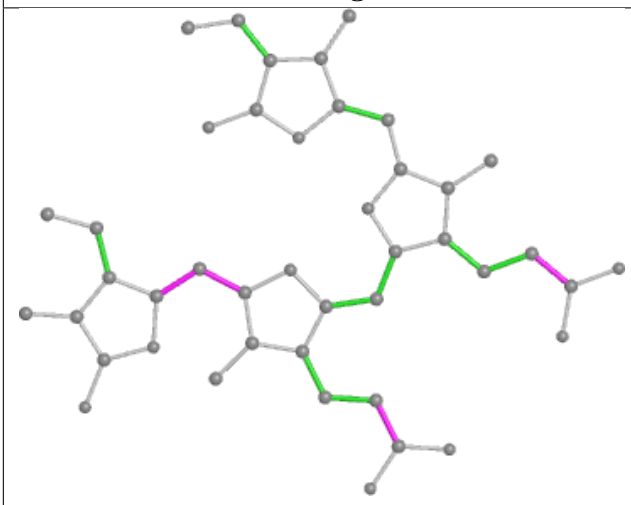
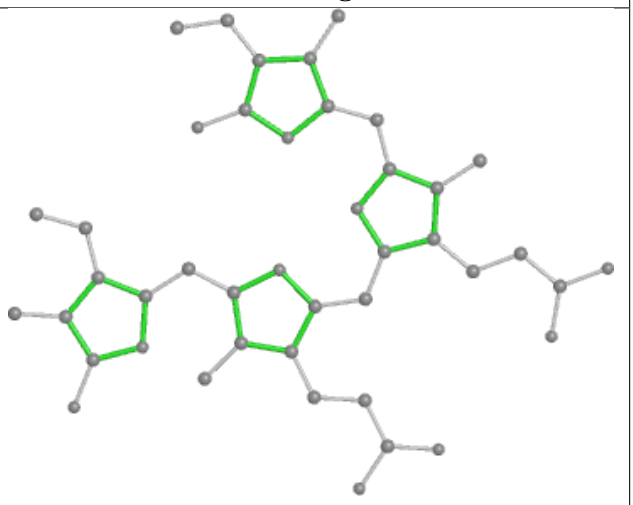


Bond angles

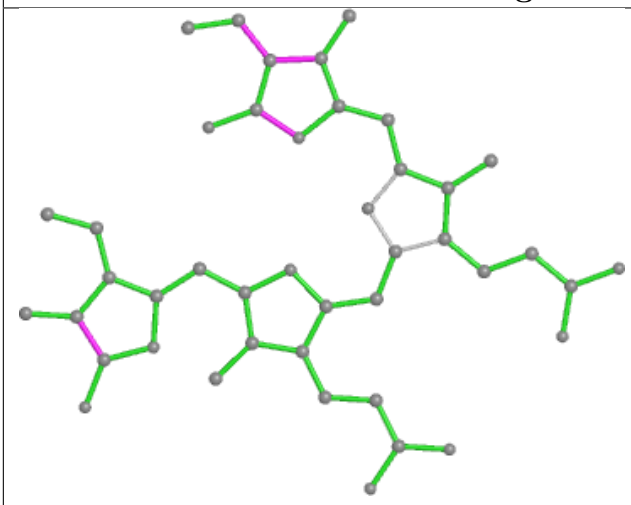


Torsions



Rings

Ligand PEB R5 201



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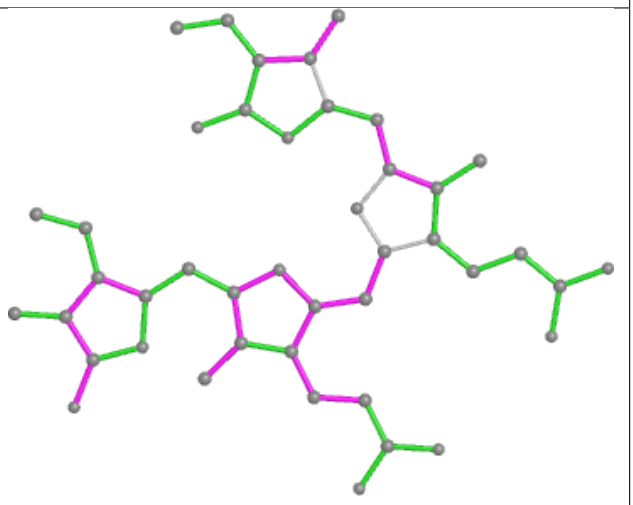

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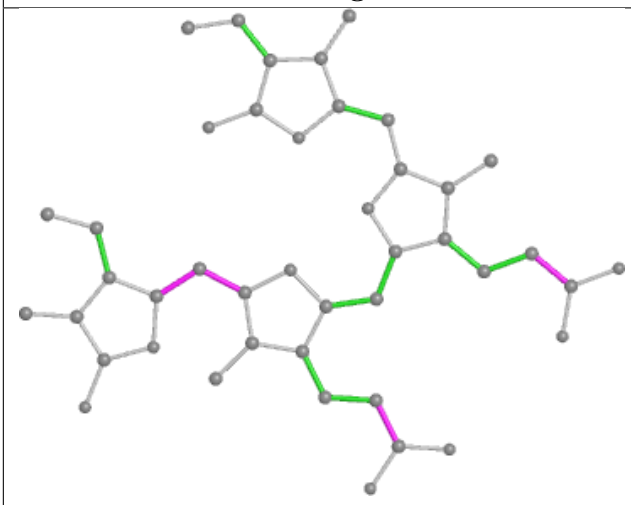

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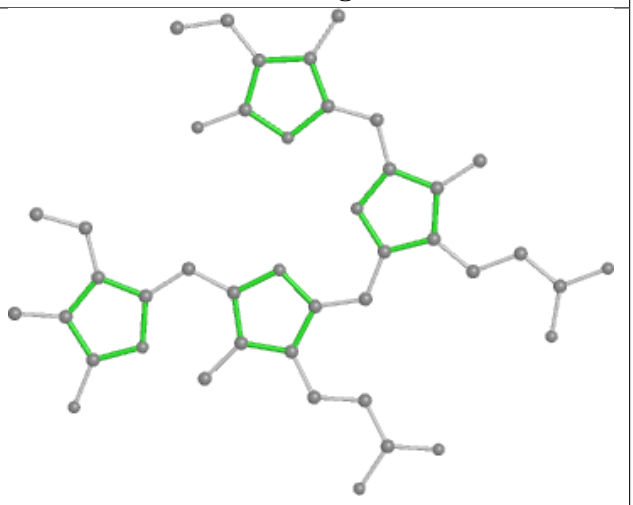
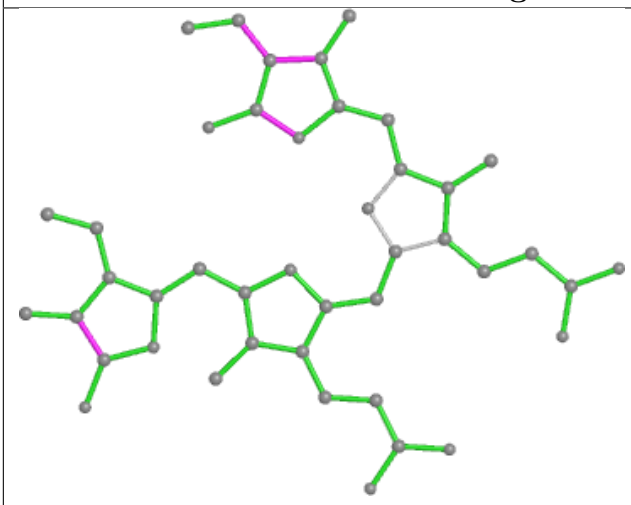


Rings

Ligand PEB iH 1001



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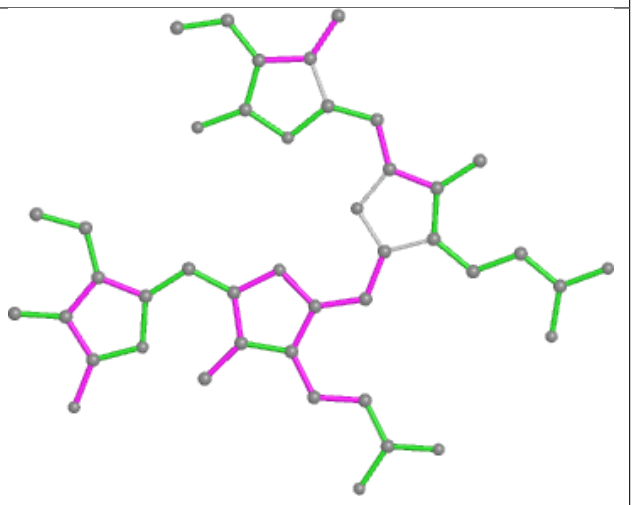

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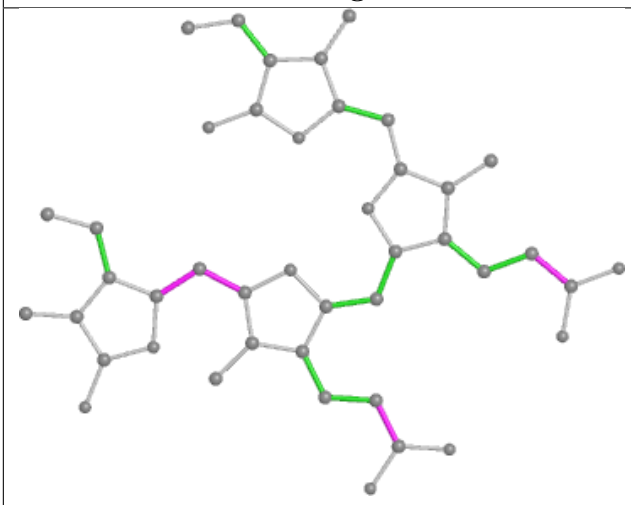

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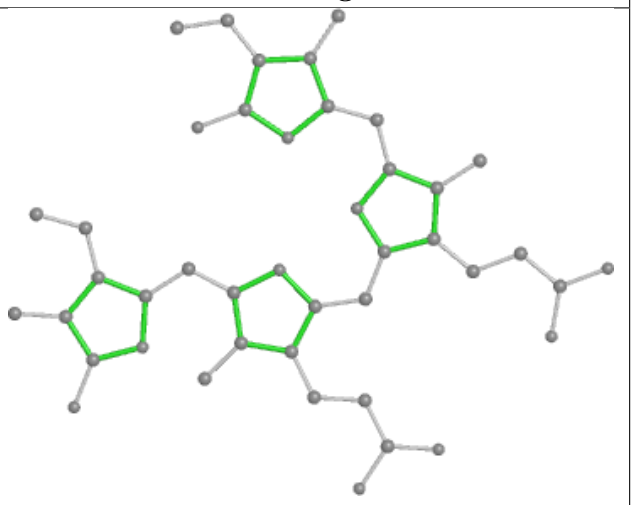
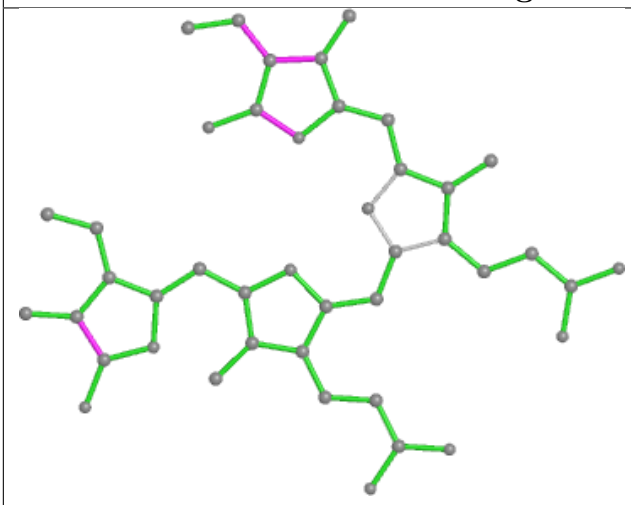


Rings

Ligand PEB w2 203



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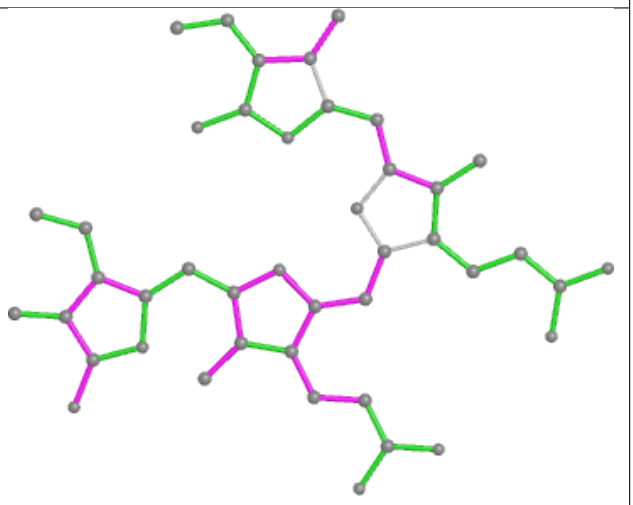

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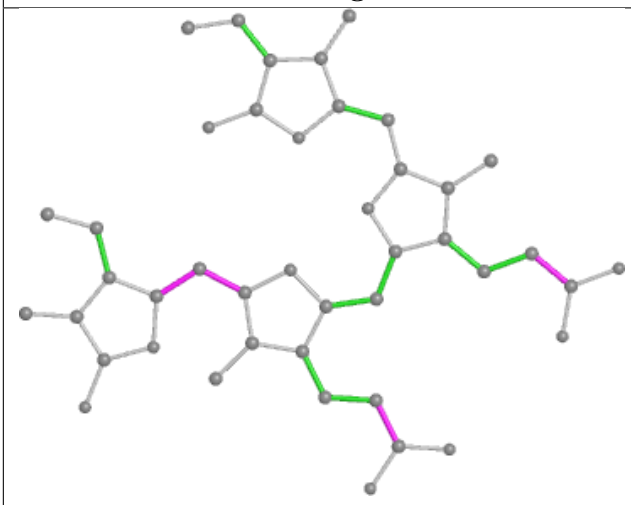

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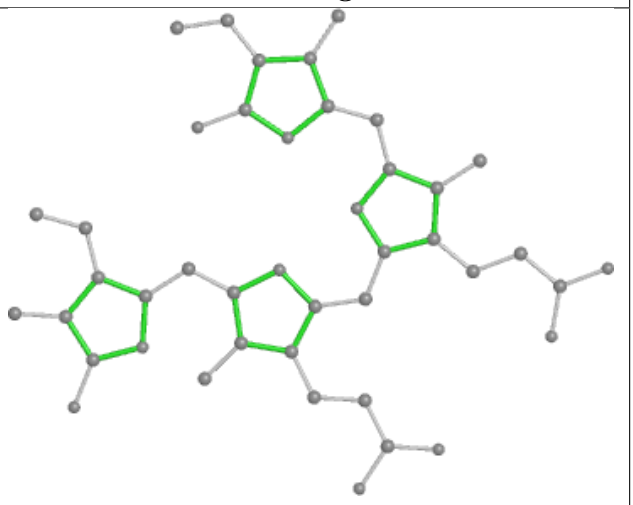
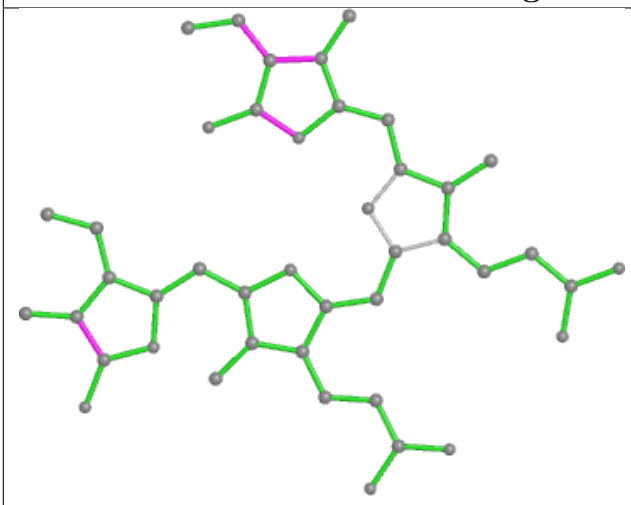


Rings

Ligand PEB fk 201



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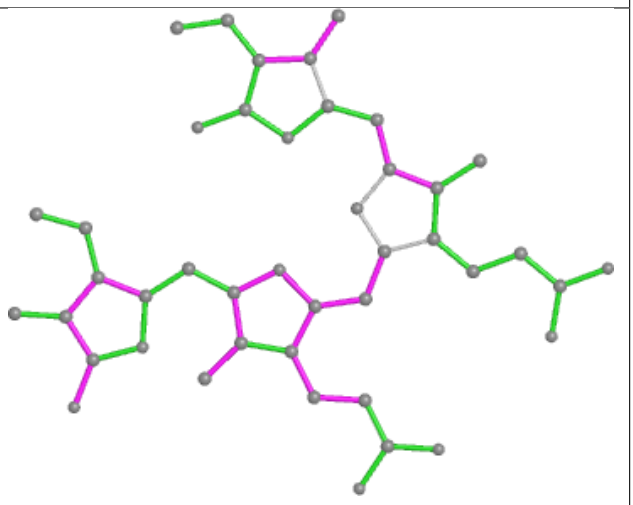

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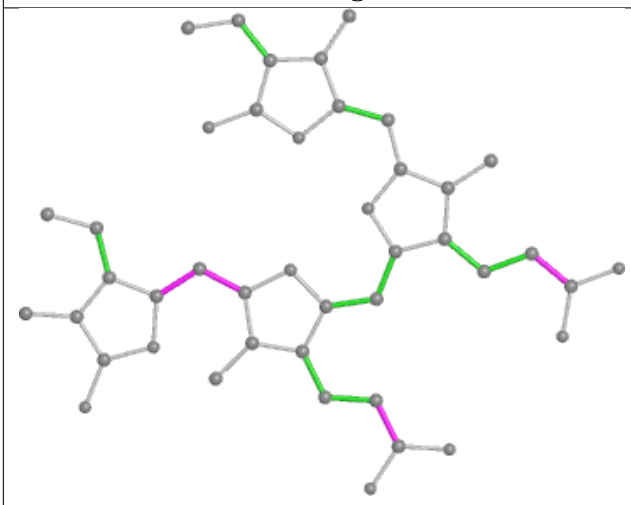

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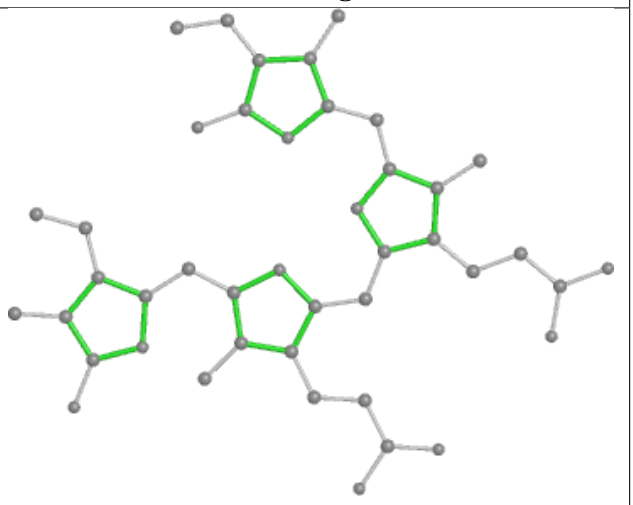
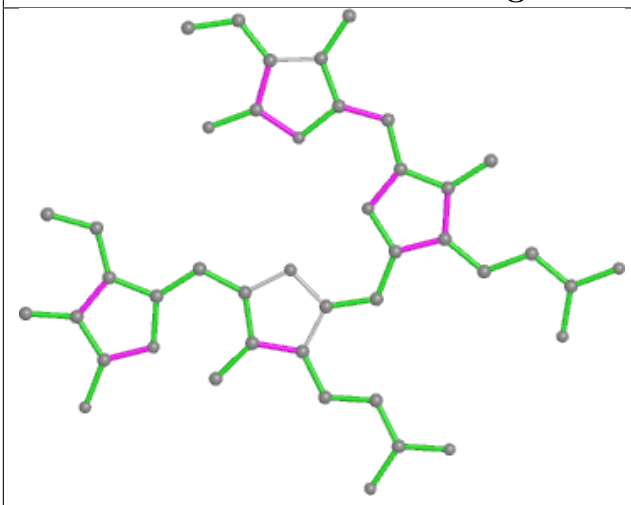


Rings

Ligand PUB jK 1003



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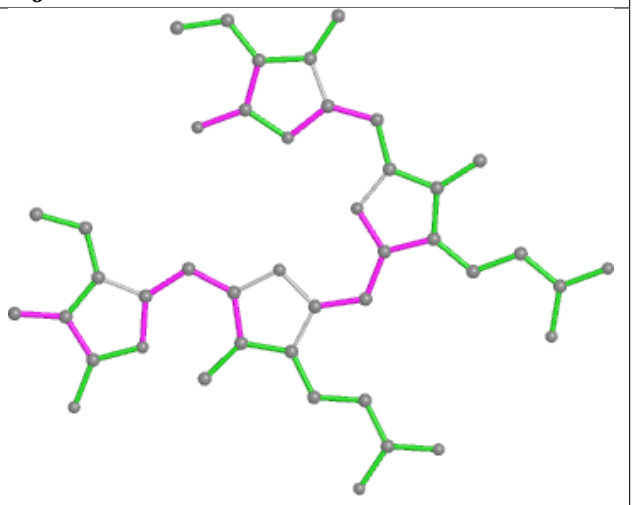

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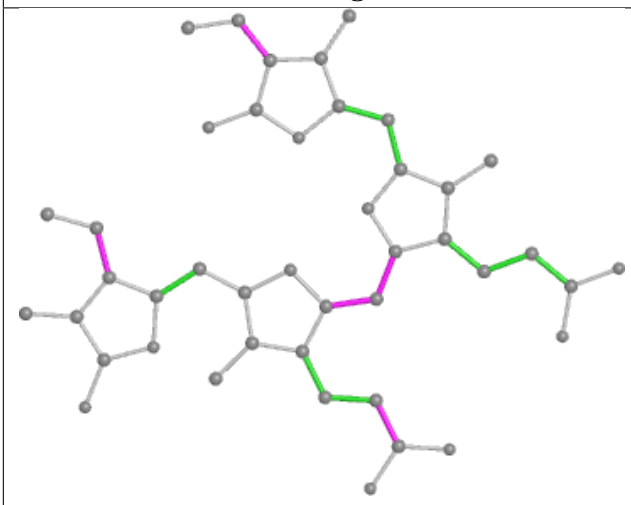

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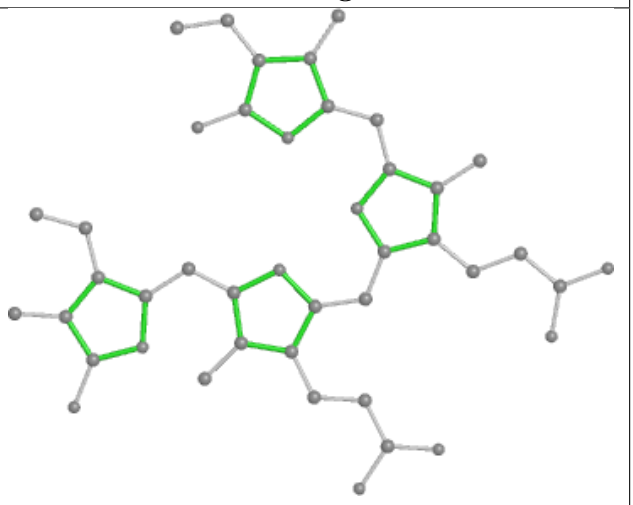

Rings

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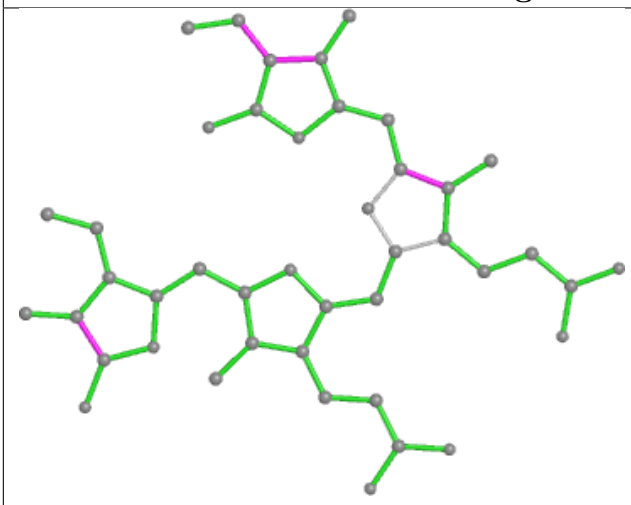

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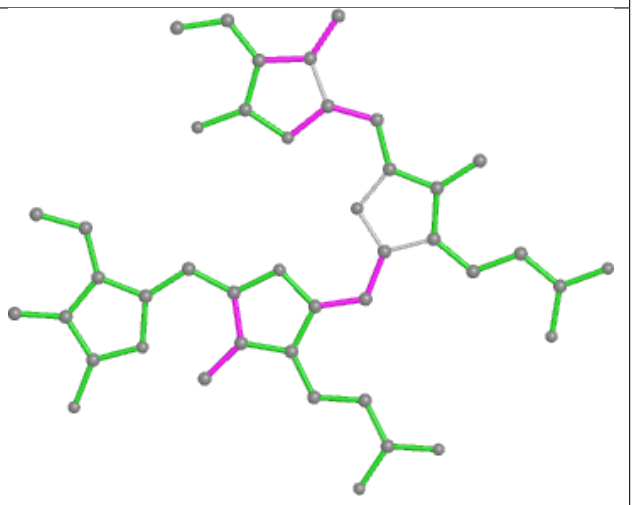

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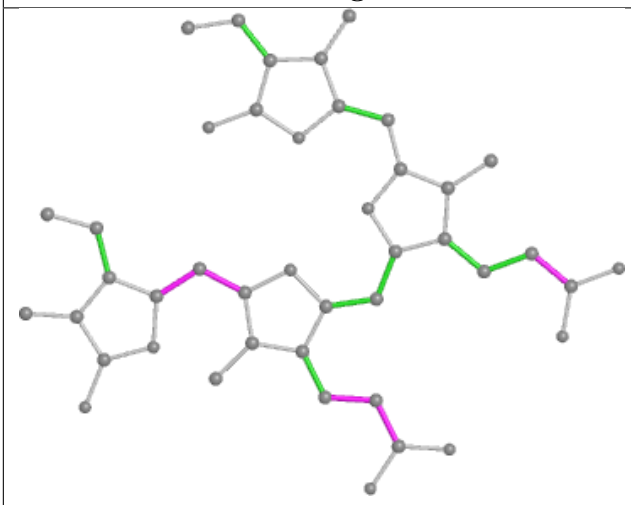

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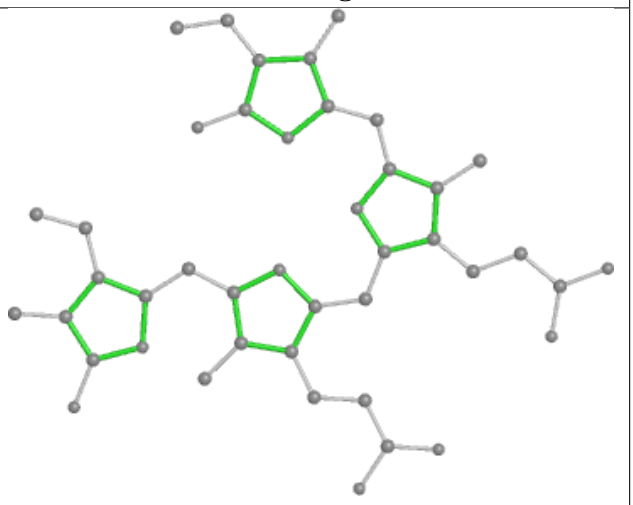

Rings

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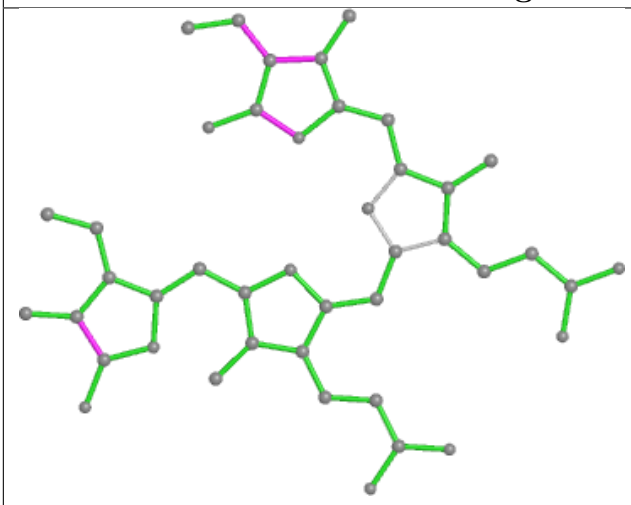

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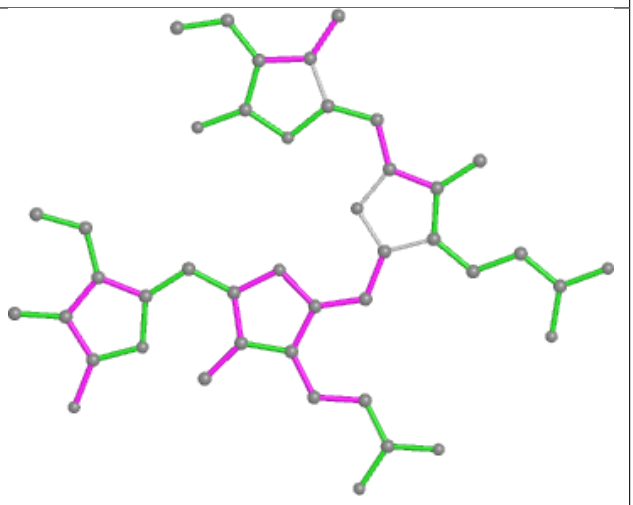

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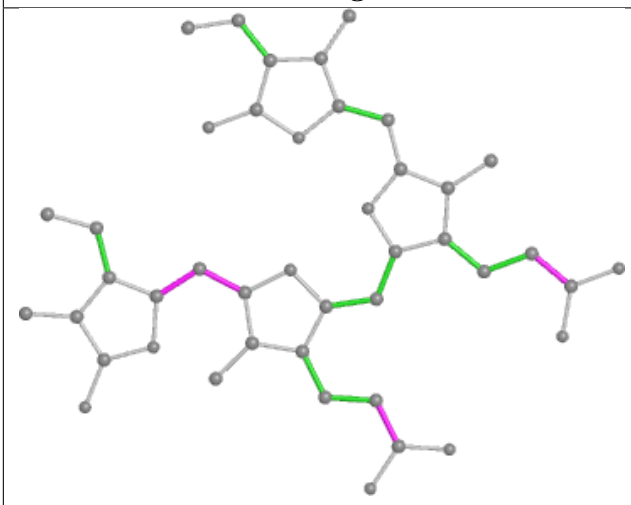

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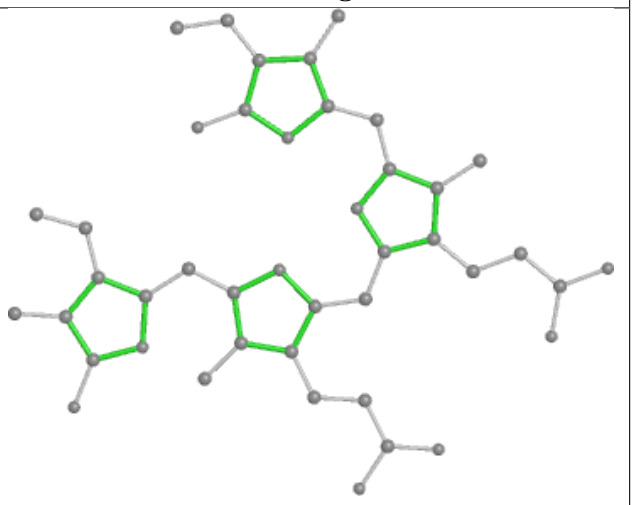
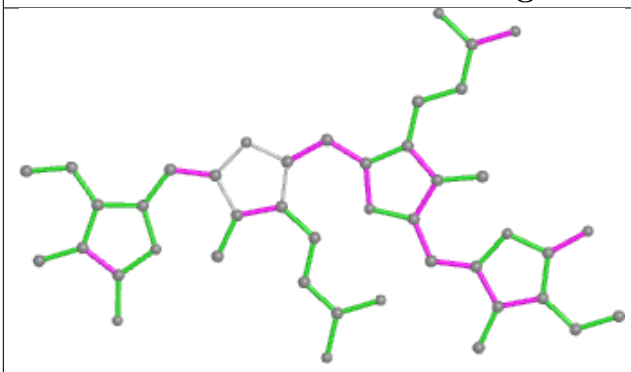


Rings

Ligand CYC y1 201



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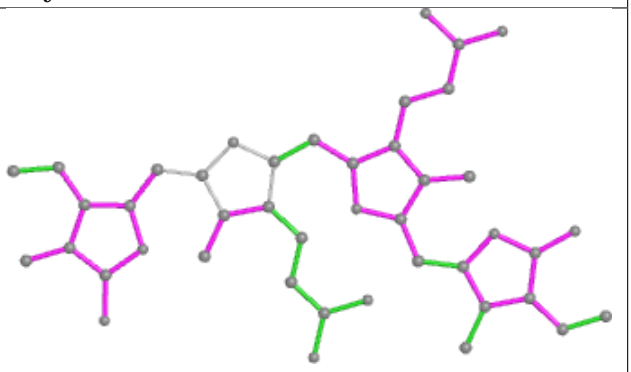

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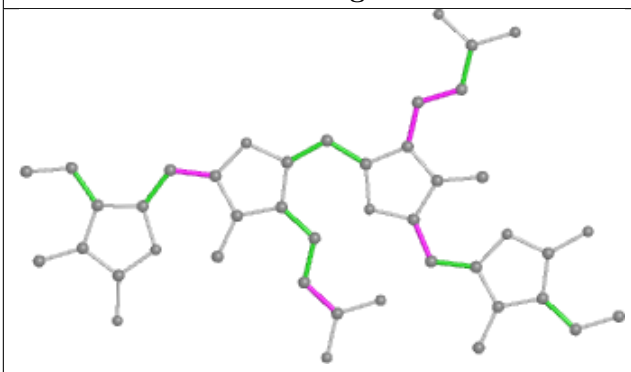

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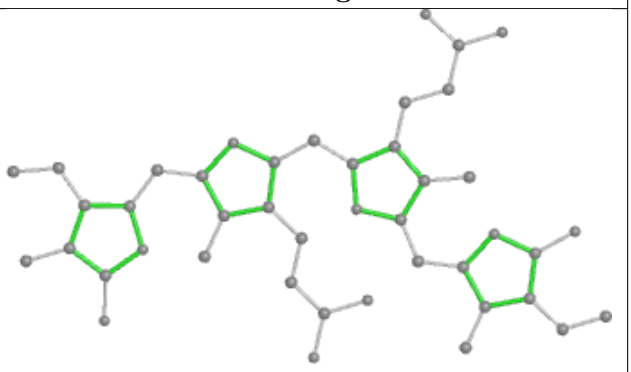
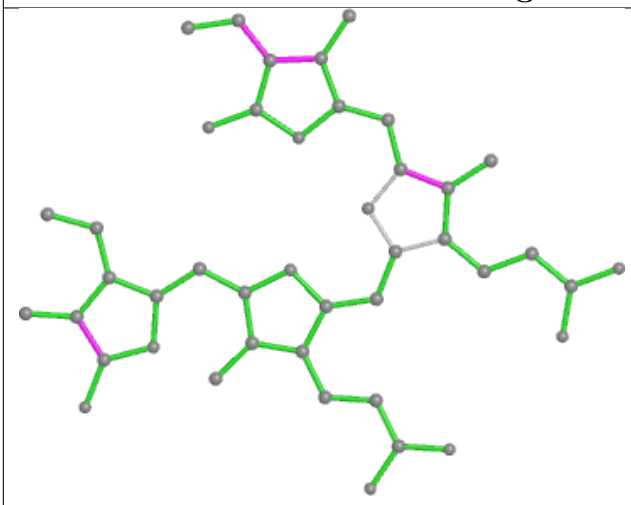


Rings

Ligand PEB bE 202



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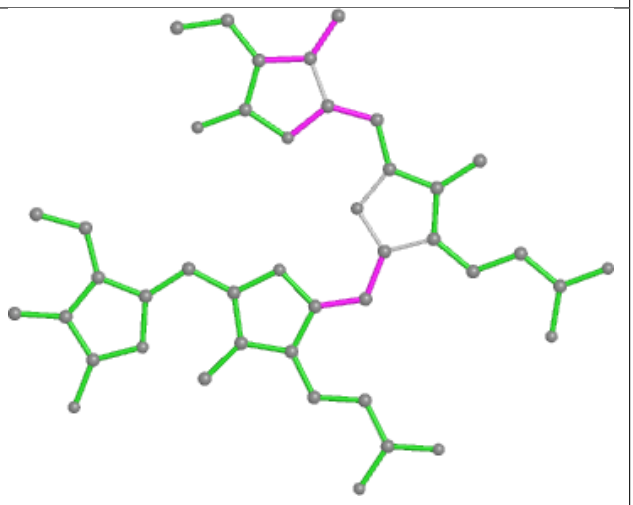

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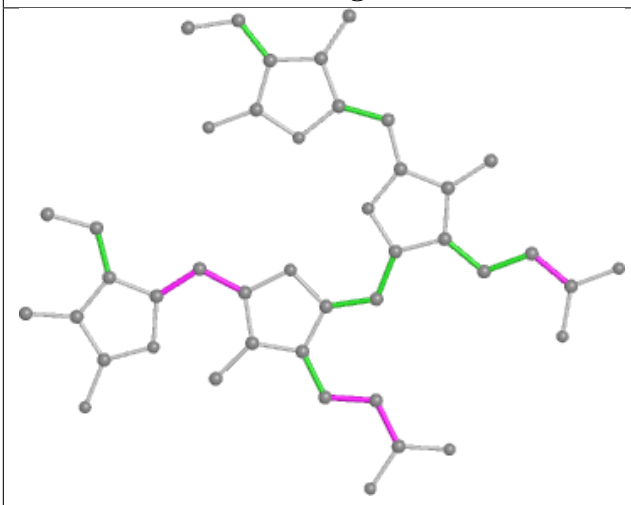

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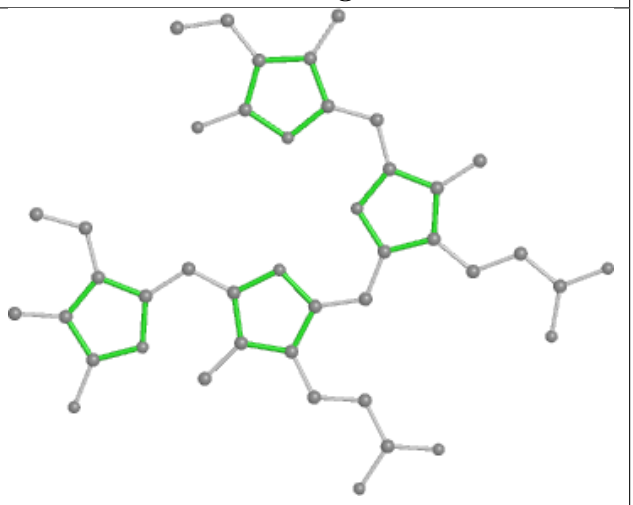
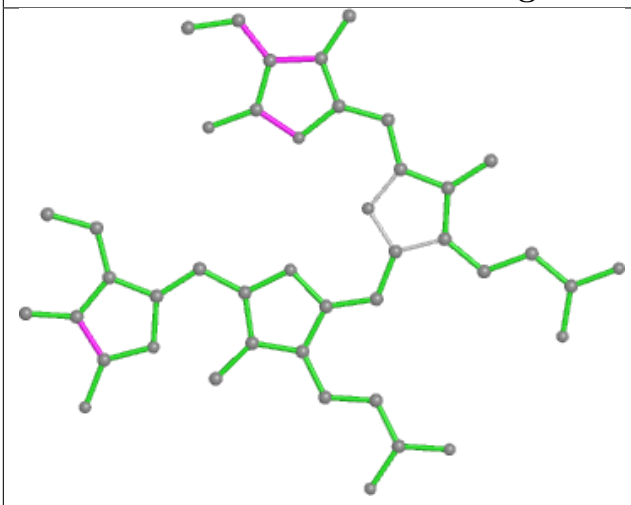


Rings

Ligand PEB aL 202



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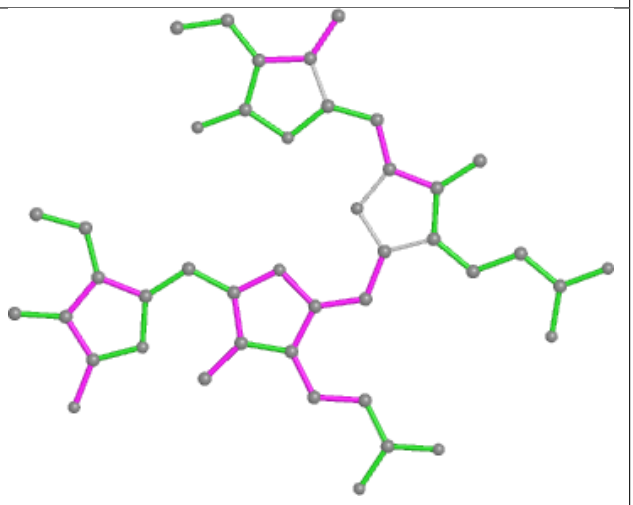

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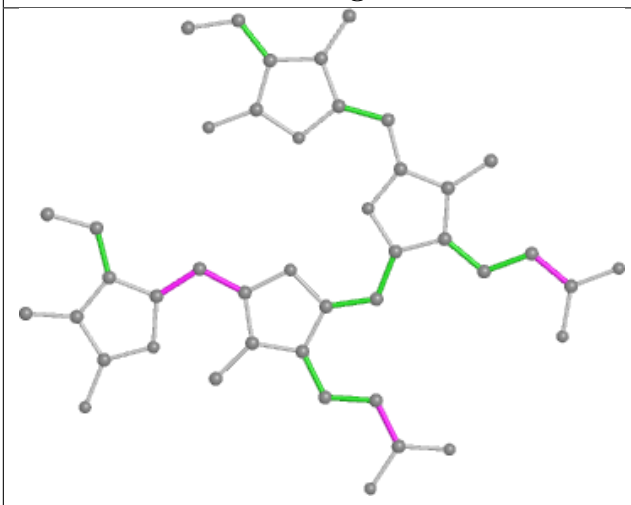

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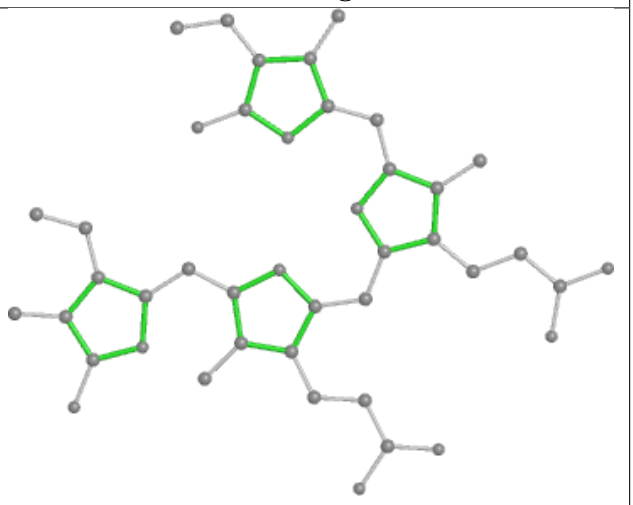
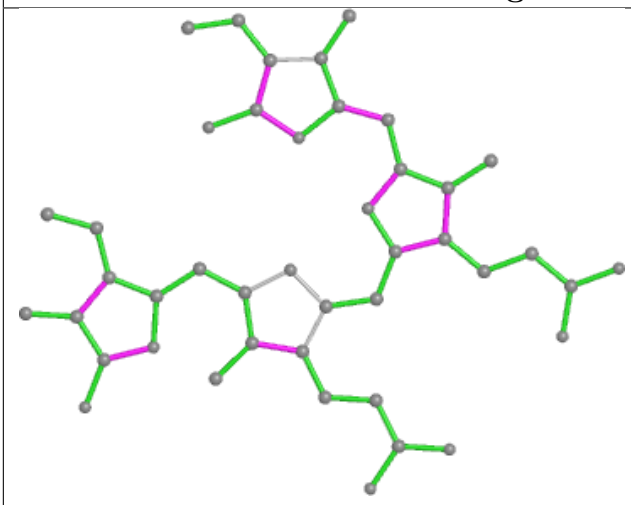


Rings

Ligand PUB Z9 1005



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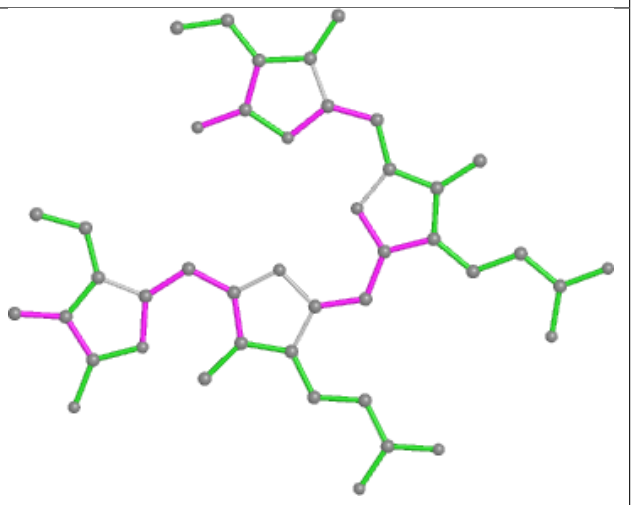

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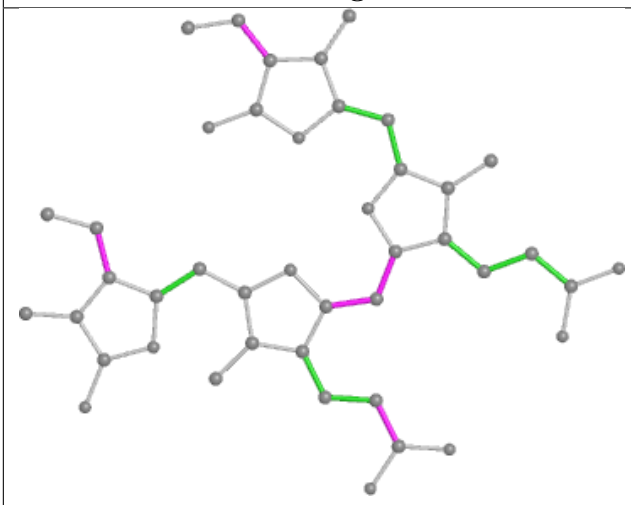

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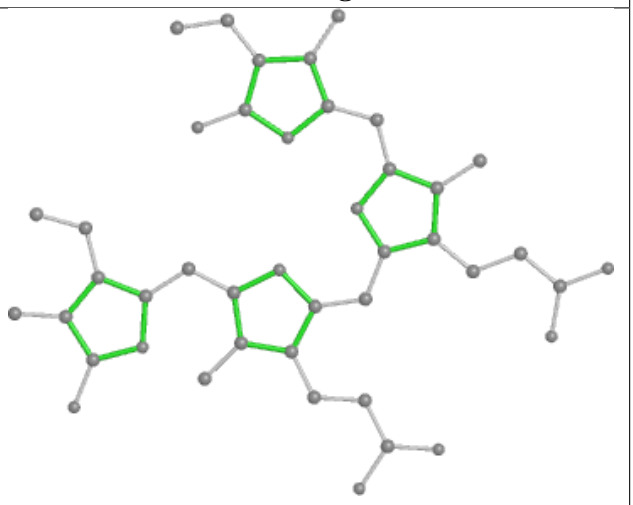
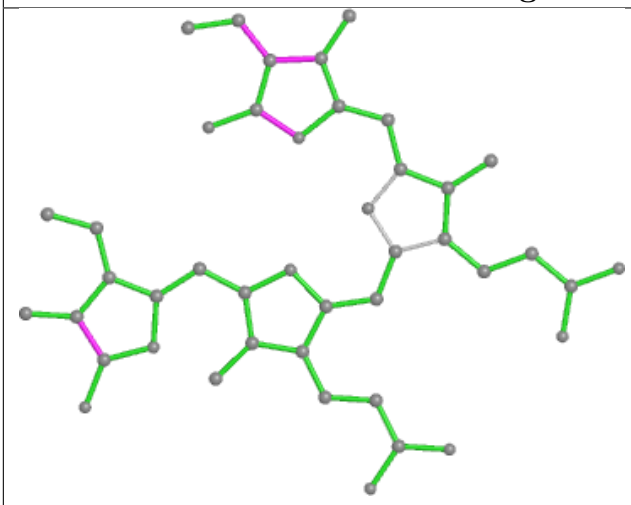


Rings

Ligand PEB y6 202



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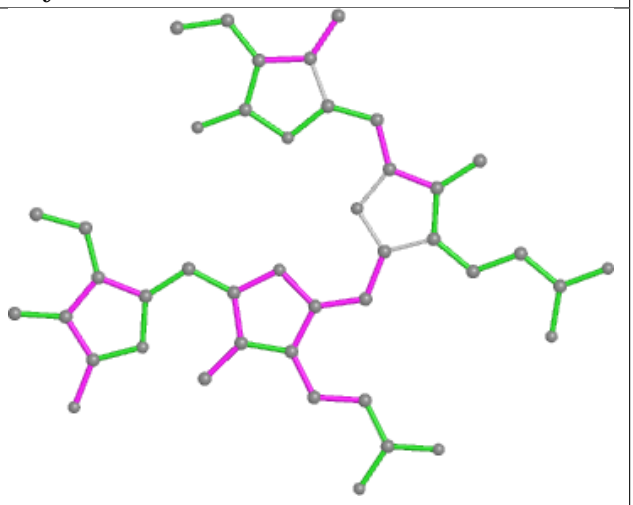
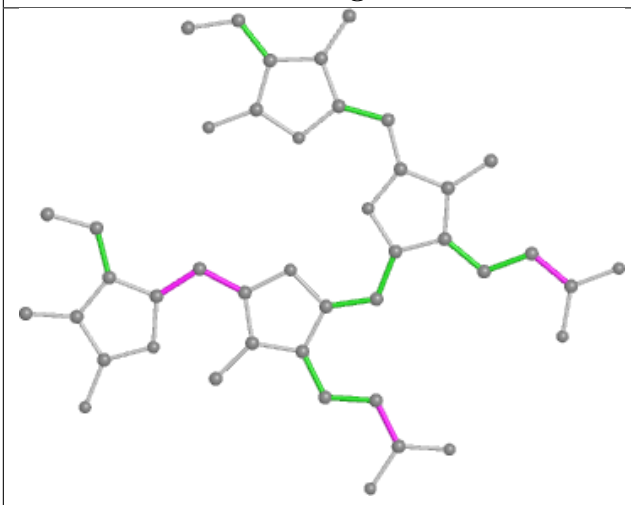


Bond angles



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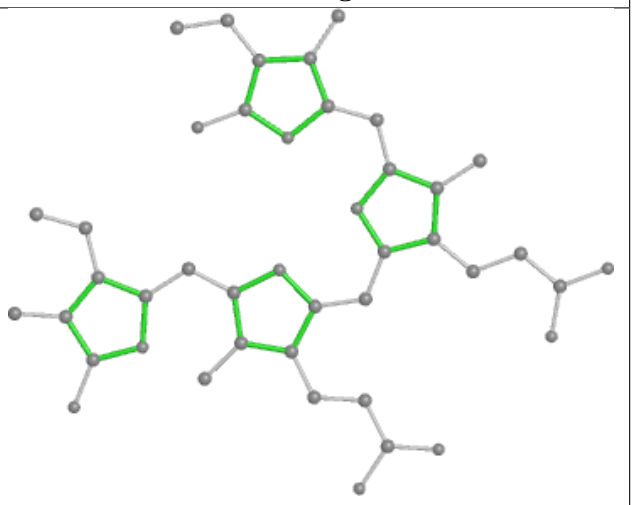
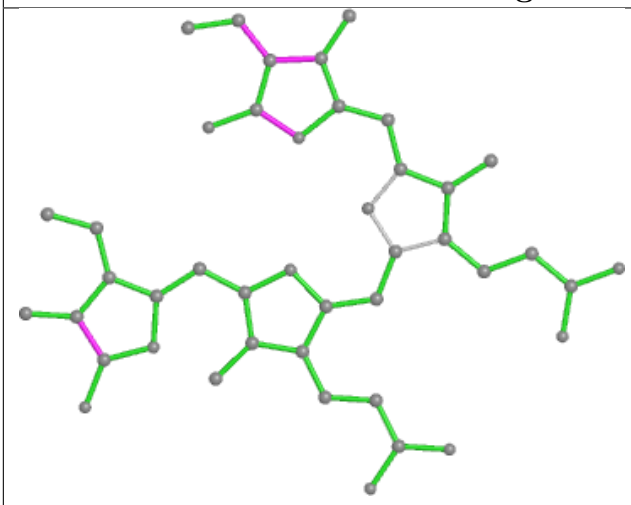


Rings

Ligand PEB aQ 202



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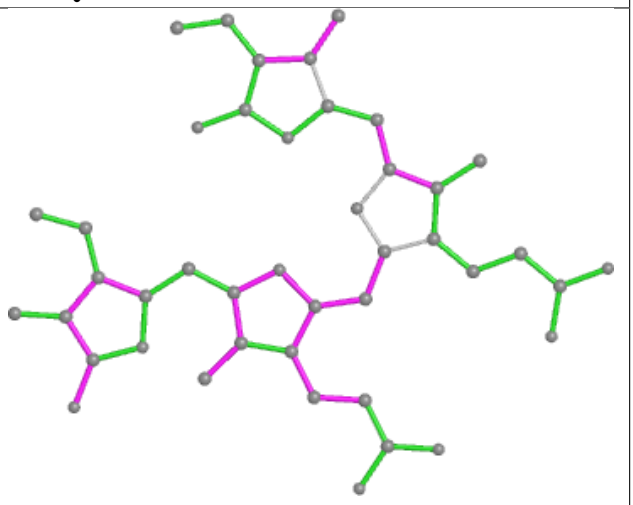
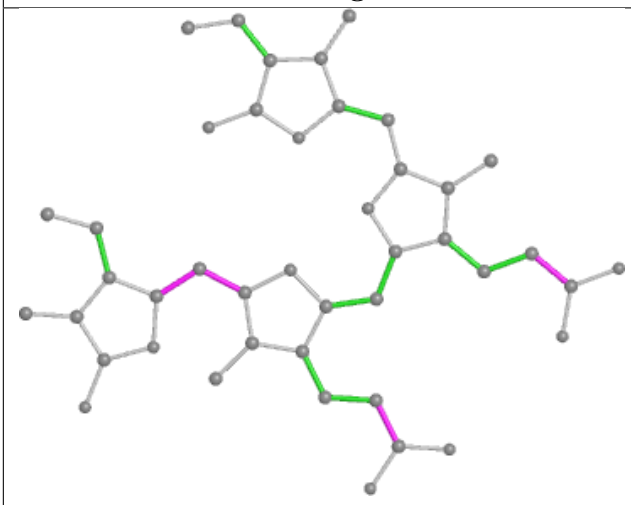
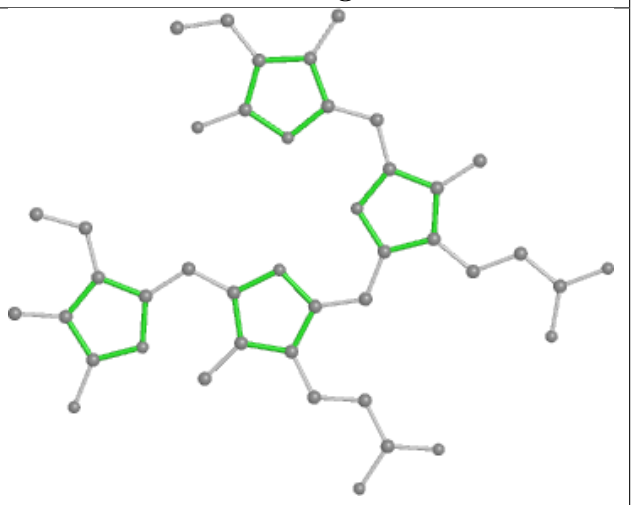


Bond angles

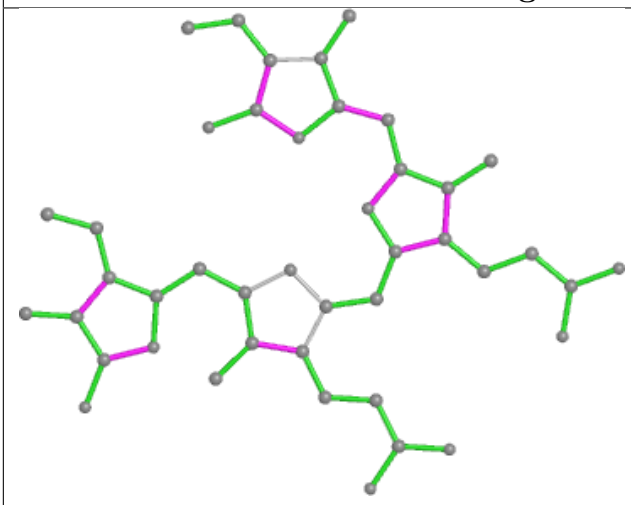


Torsions



Rings

Ligand PUB eg 203



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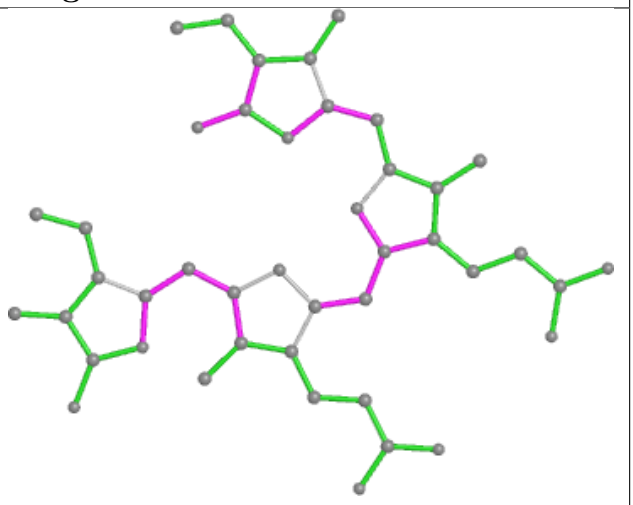
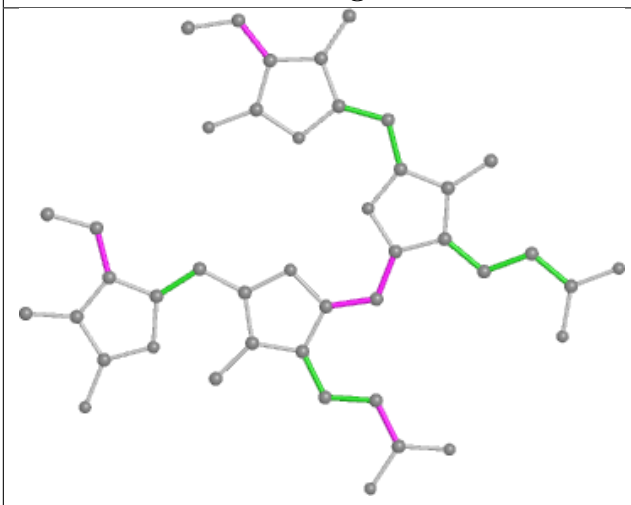


Bond angles



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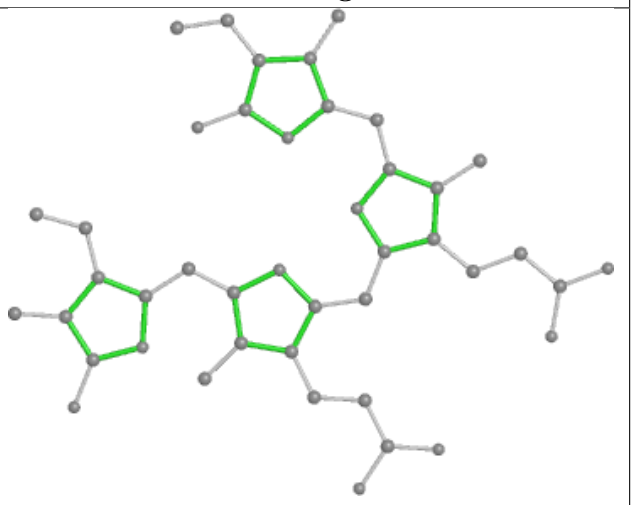
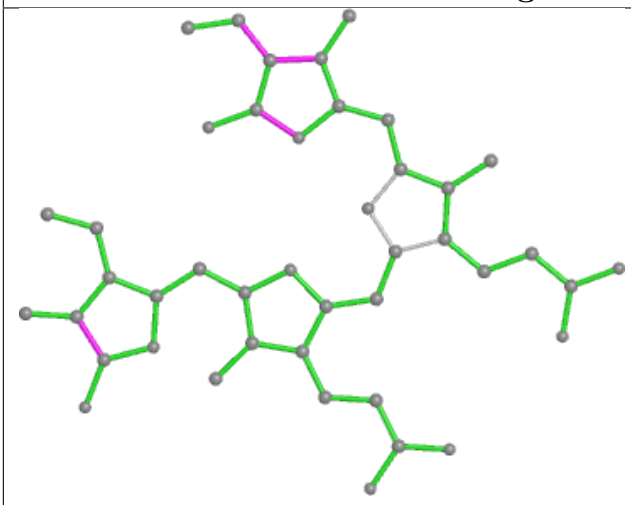


Rings

Ligand PEB eP 203



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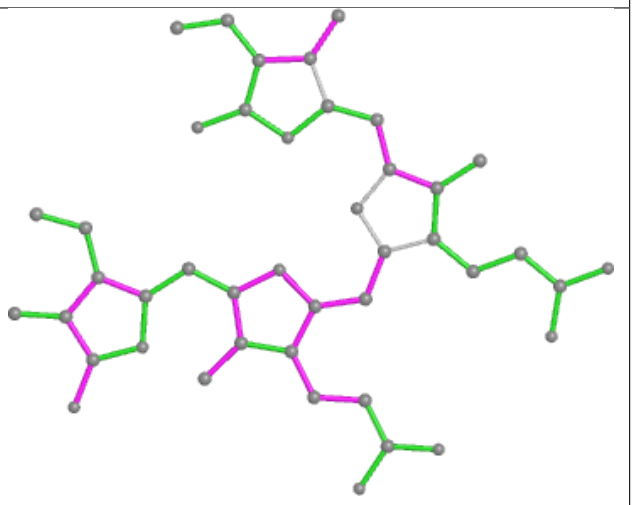

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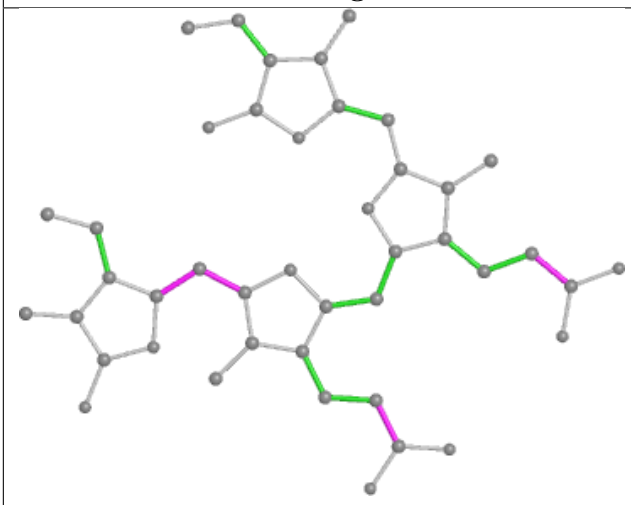

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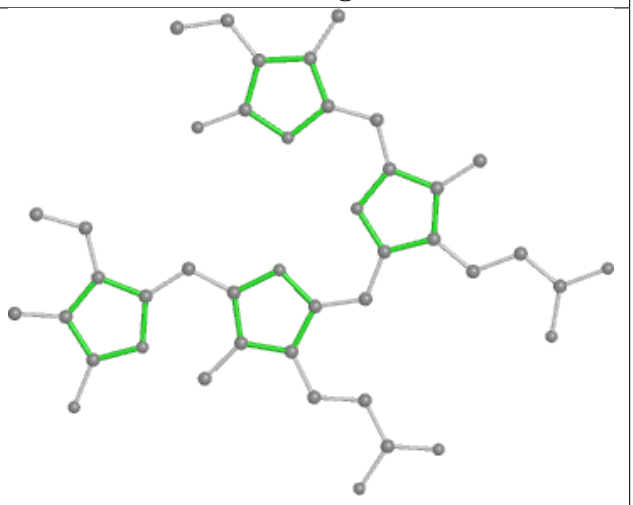
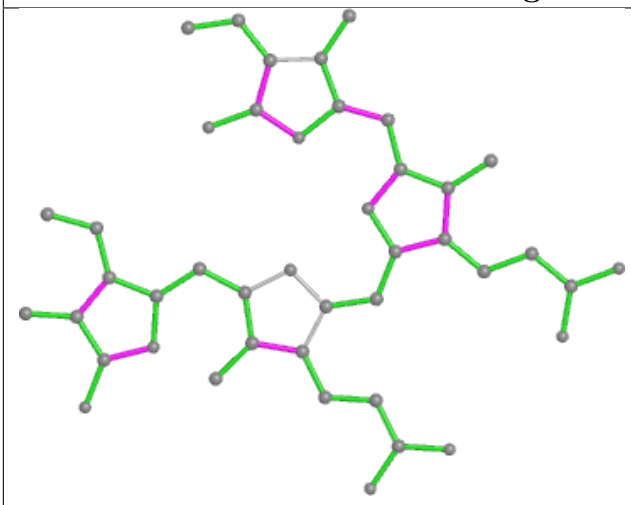


Rings

Ligand PUB fs 203



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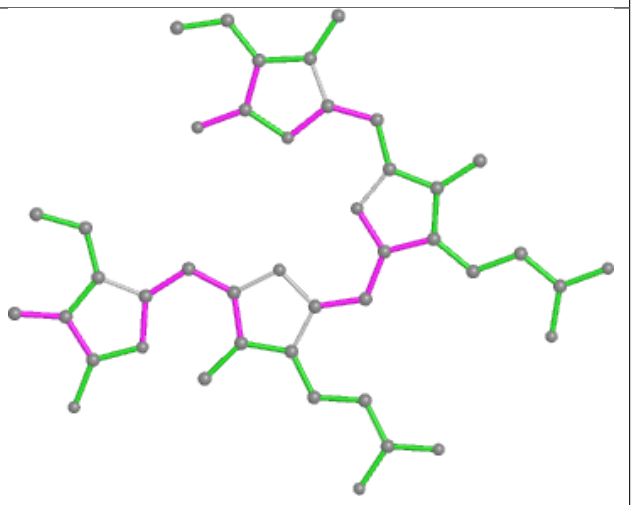

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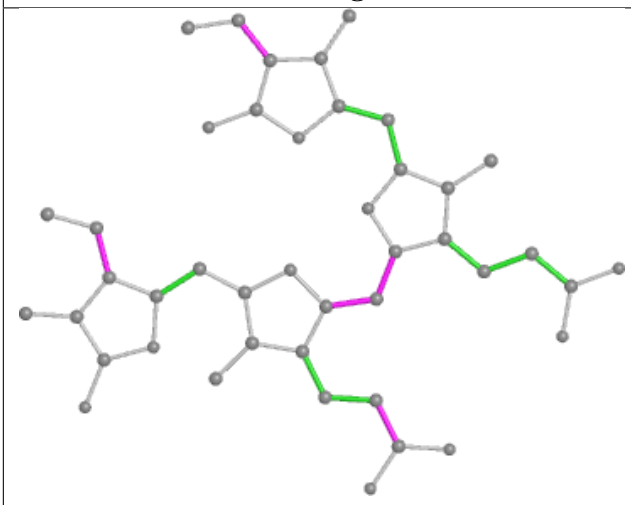

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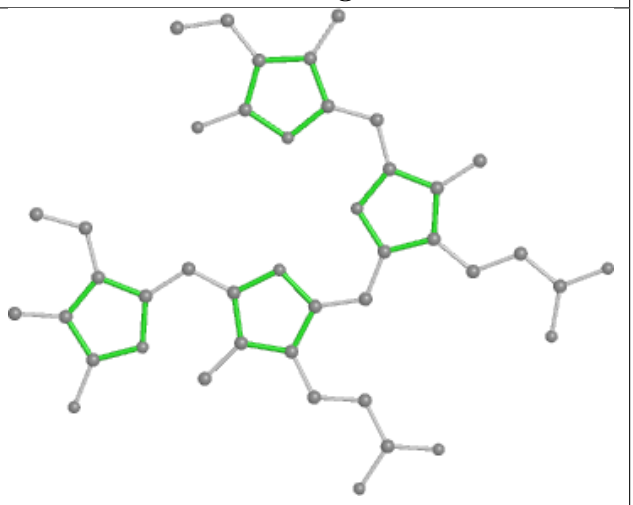
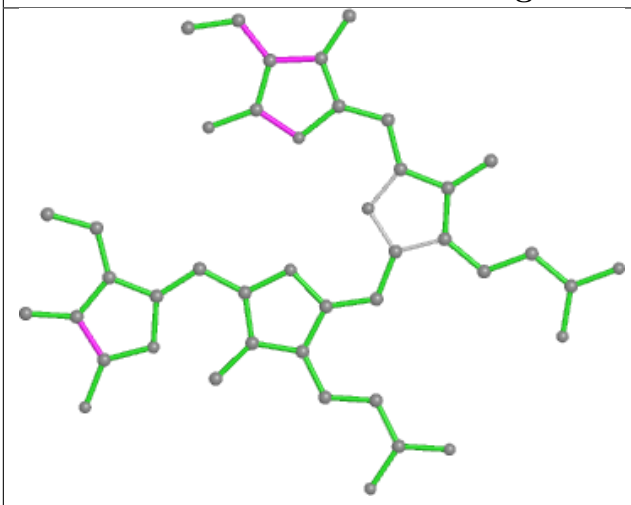


Rings

Ligand PEB Q6 201



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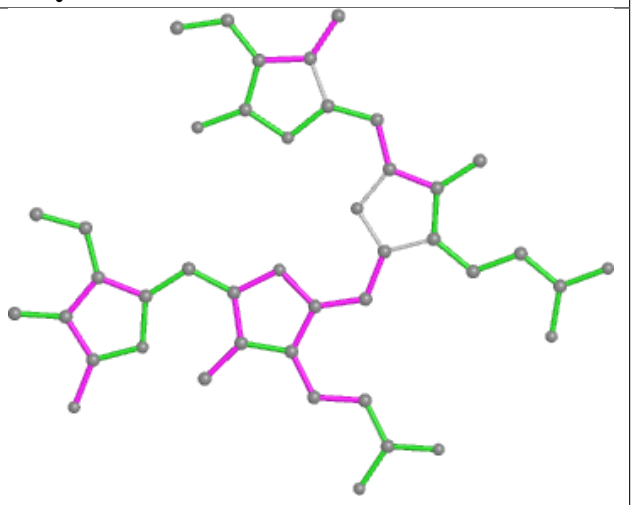

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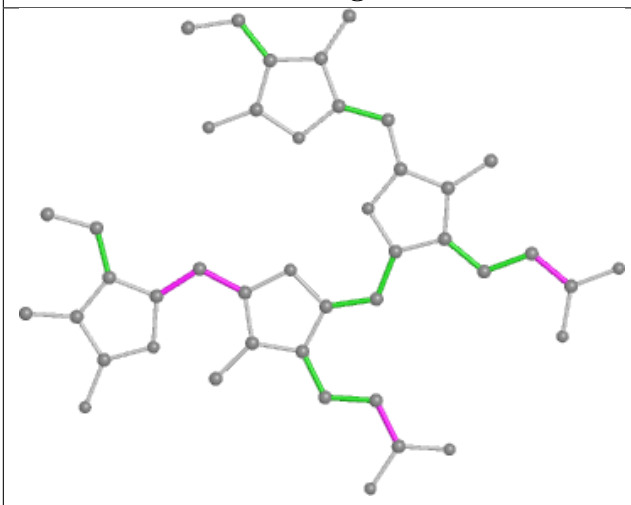

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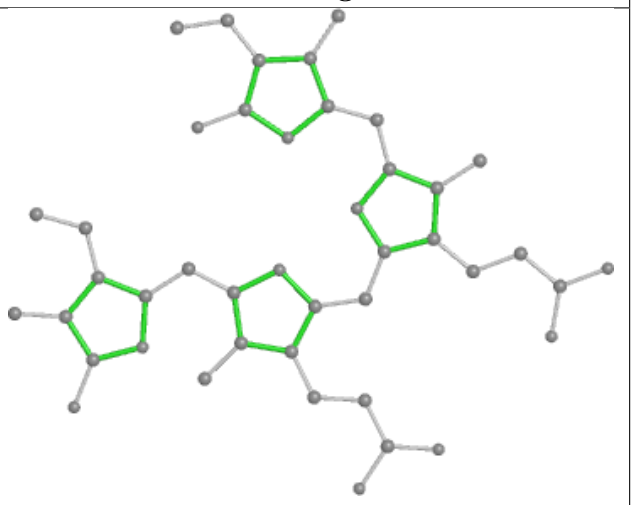
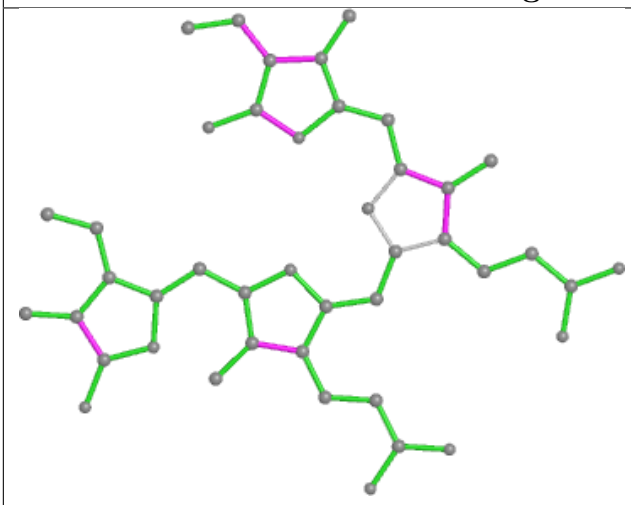


Rings

Ligand PEB fq 202



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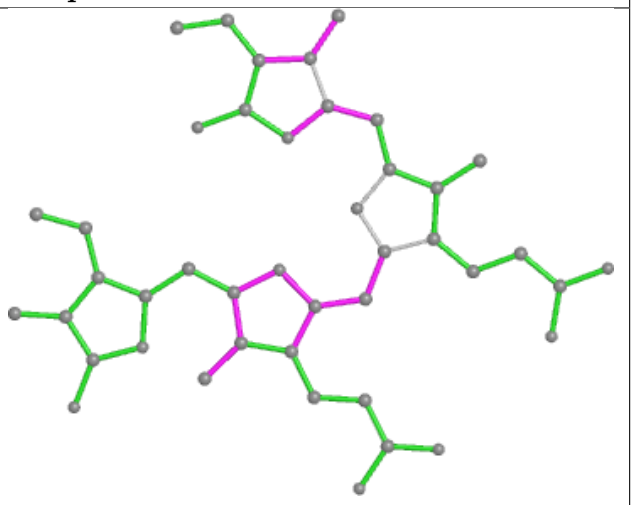

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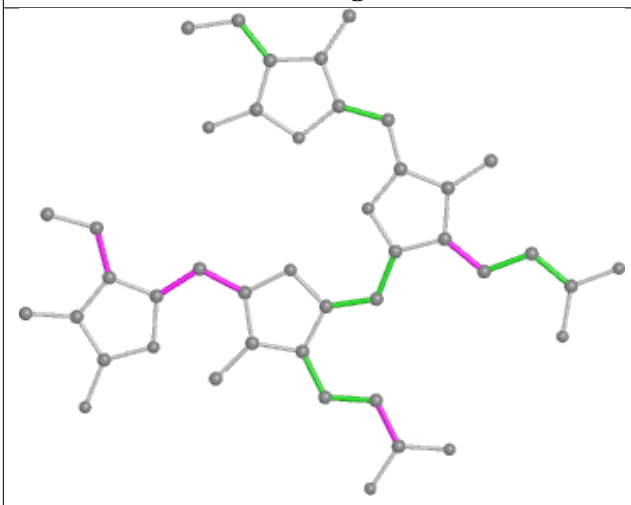

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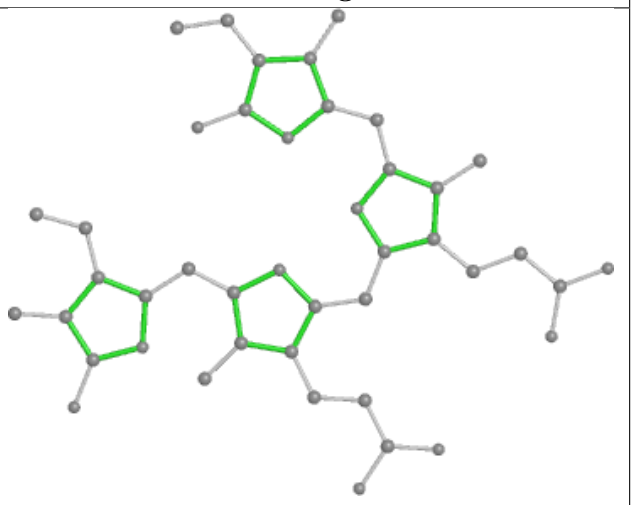
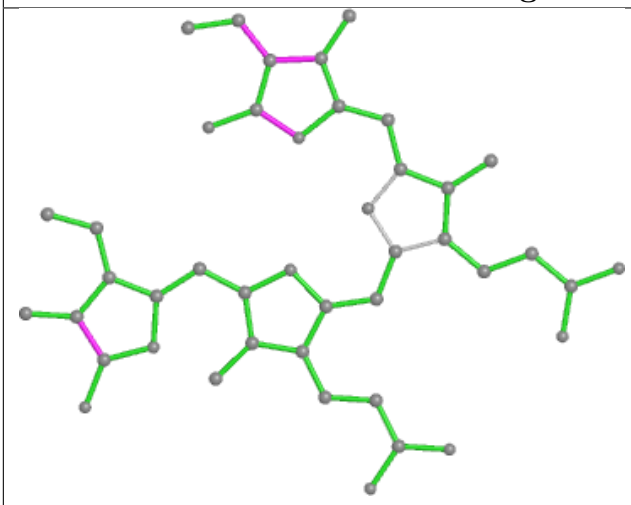


Rings

Ligand PEB cp 201



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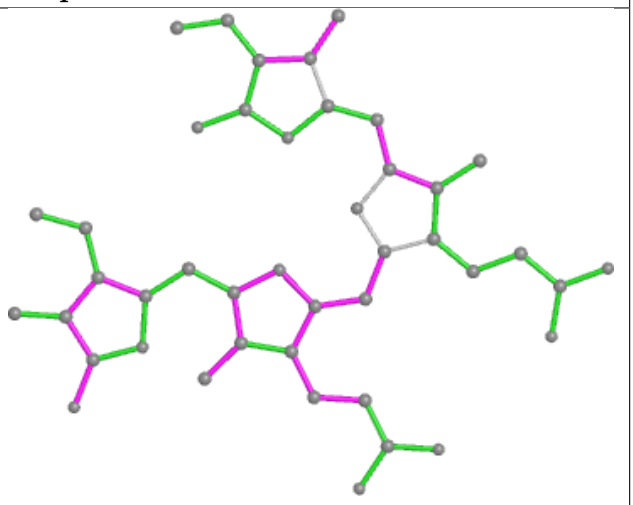

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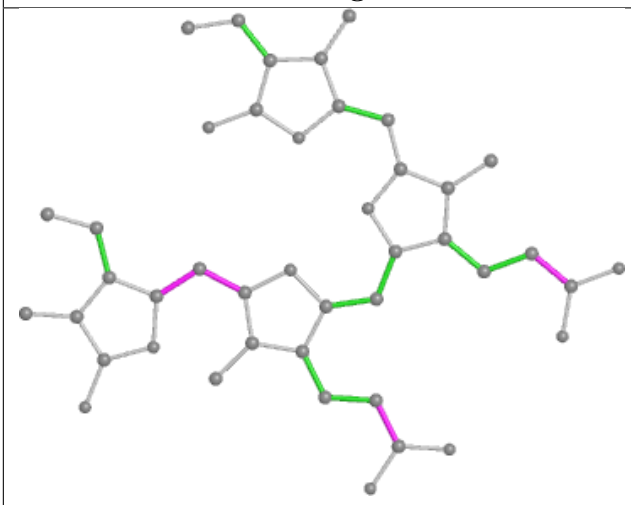

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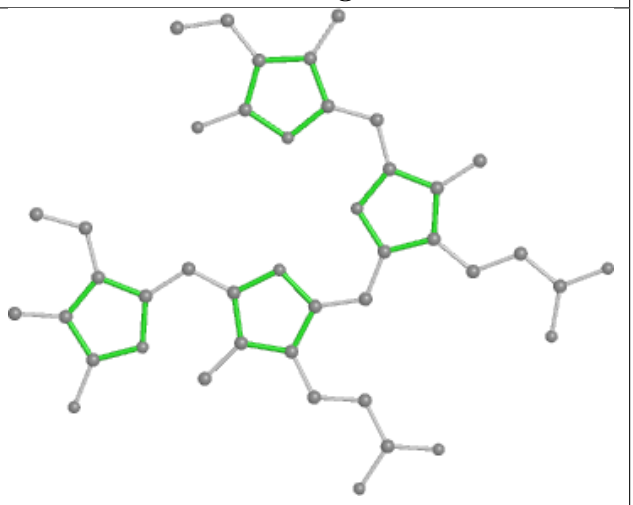
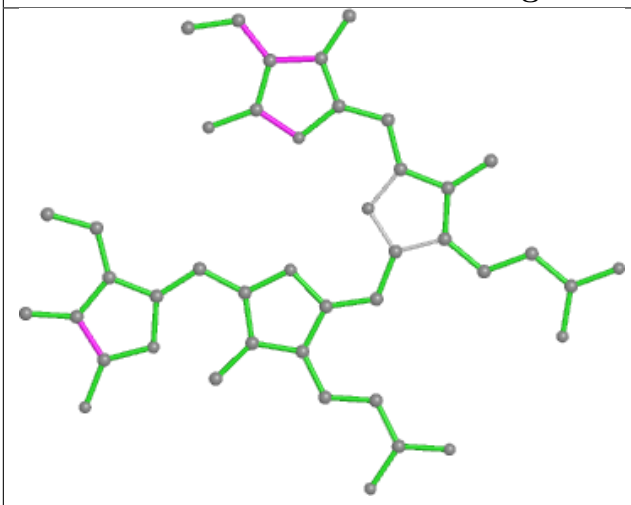


Rings

Ligand PEB t5 201



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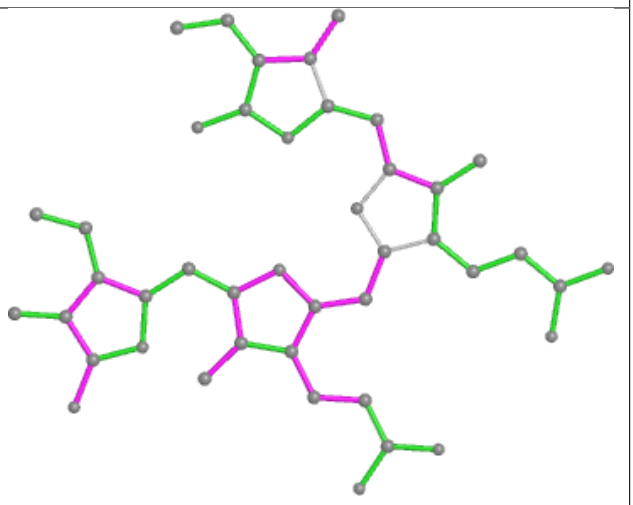

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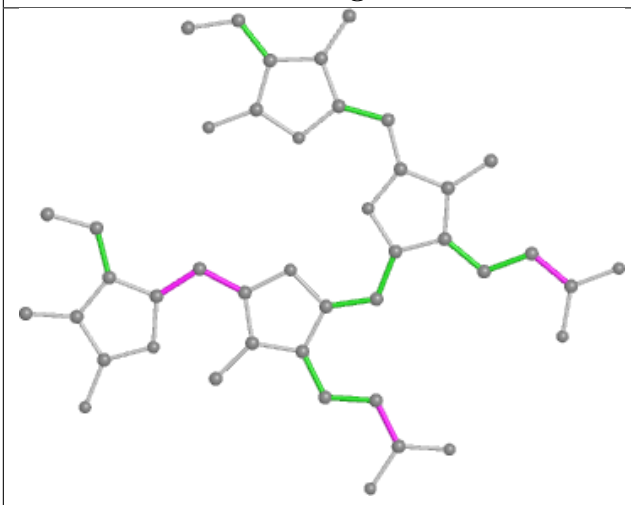

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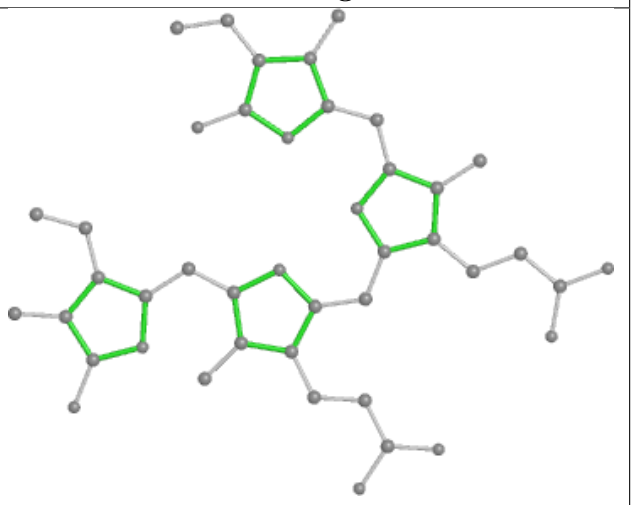

Rings

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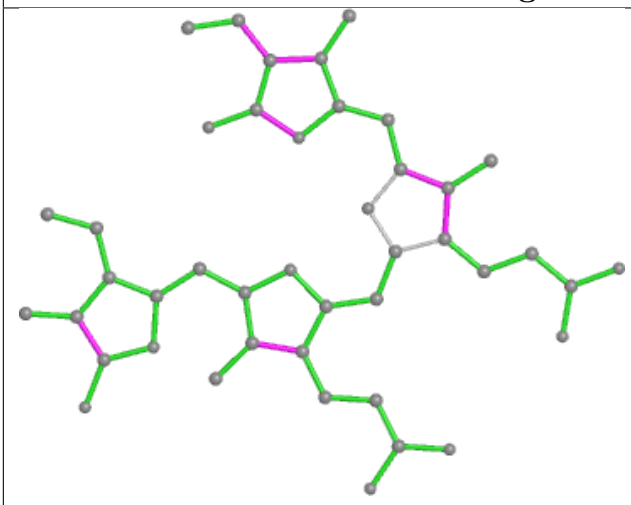

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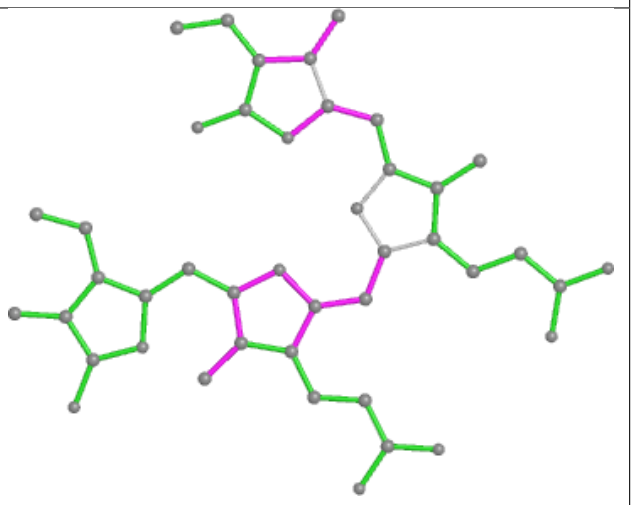

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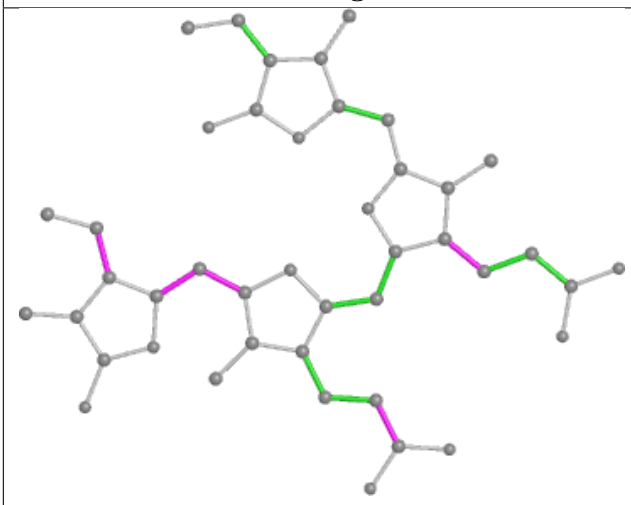

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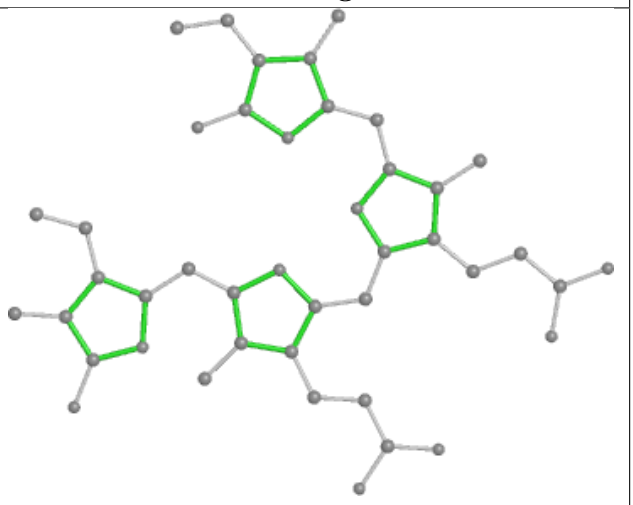

Rings

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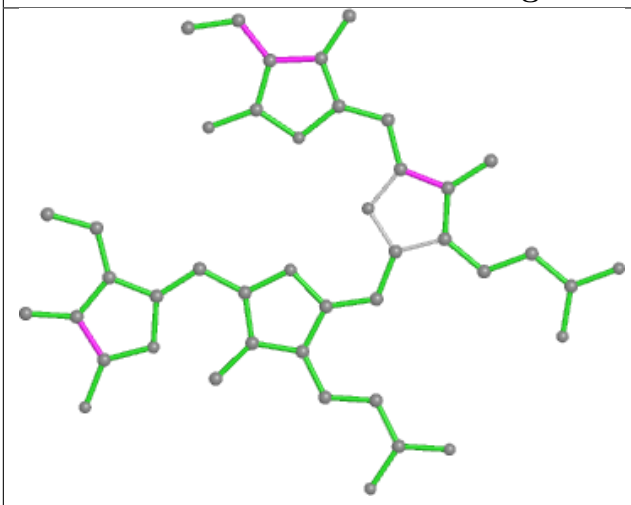

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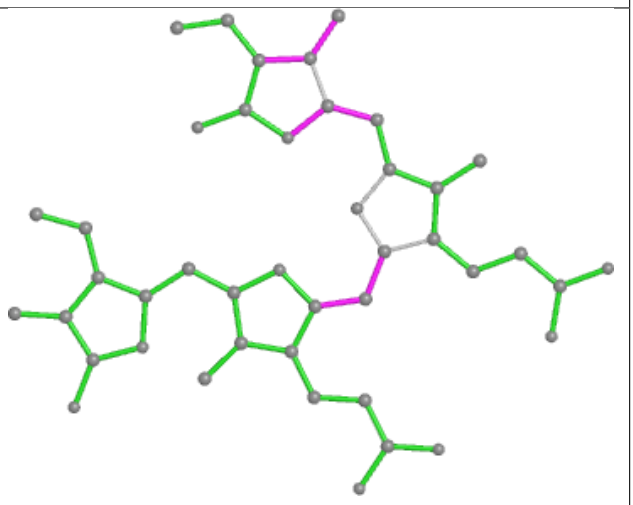

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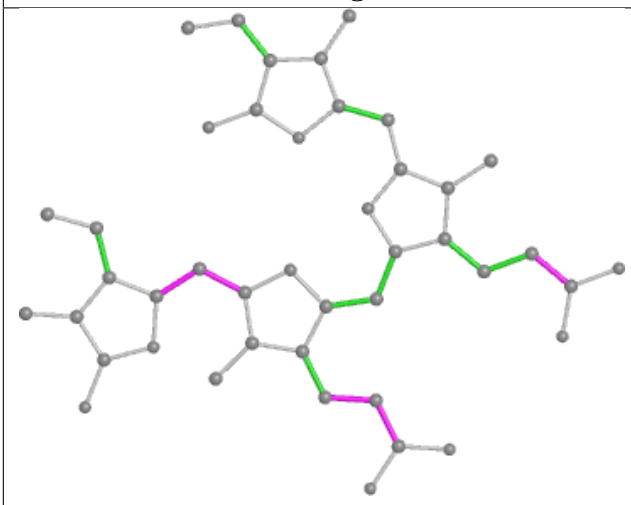

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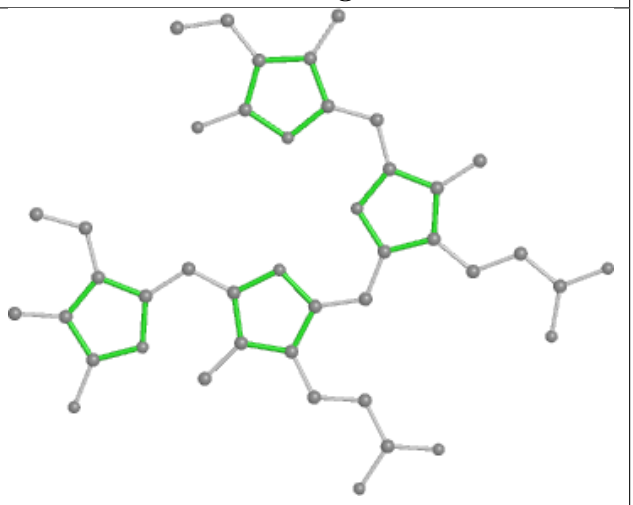
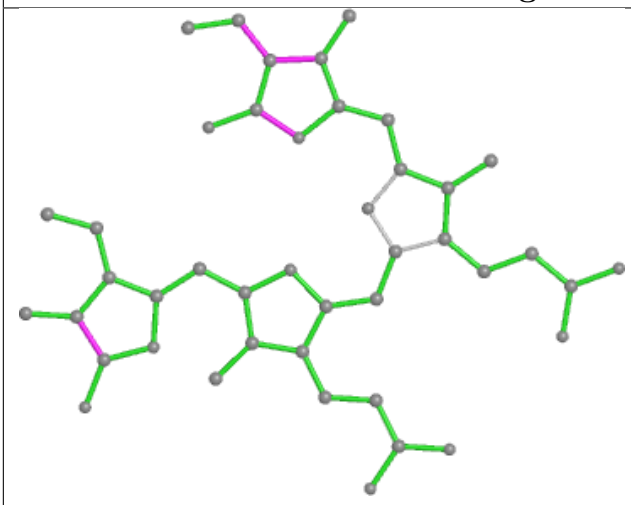


Rings

Ligand PEB ah 201



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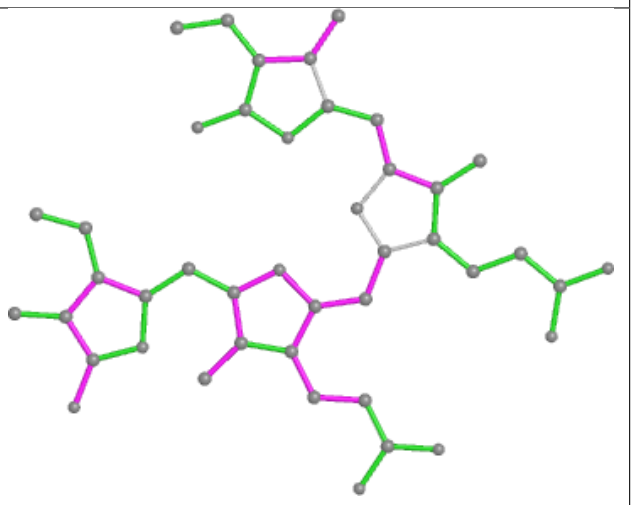

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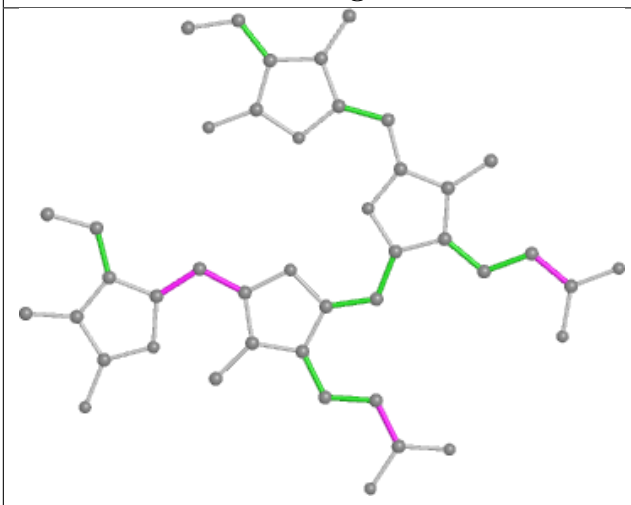

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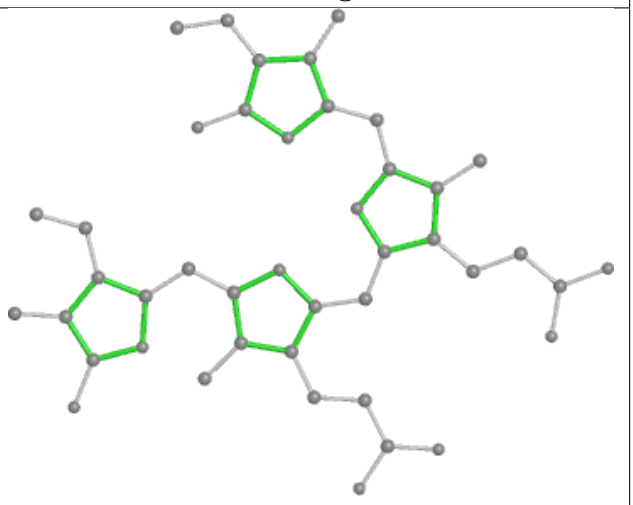
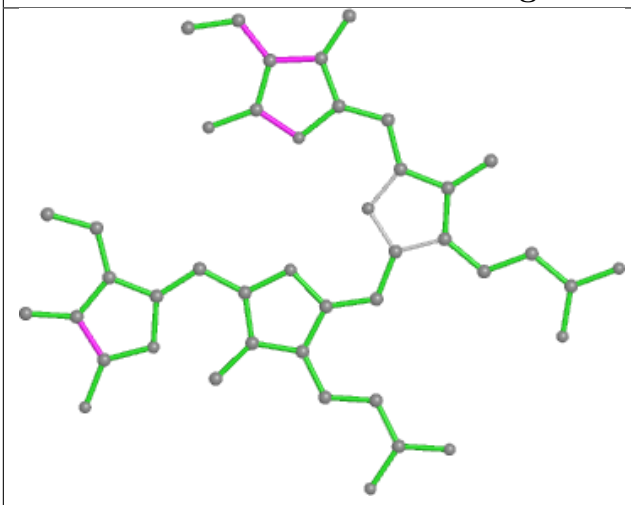


Rings

Ligand PEB q4 201



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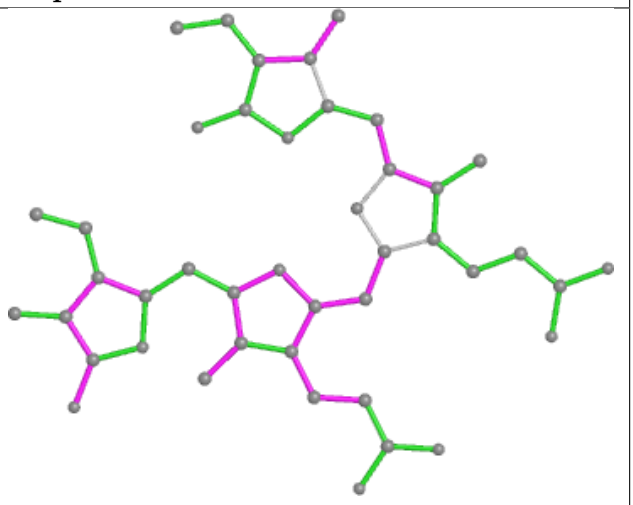

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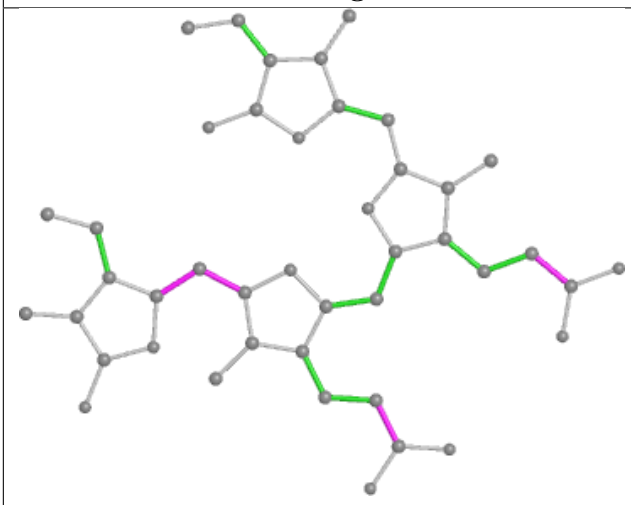

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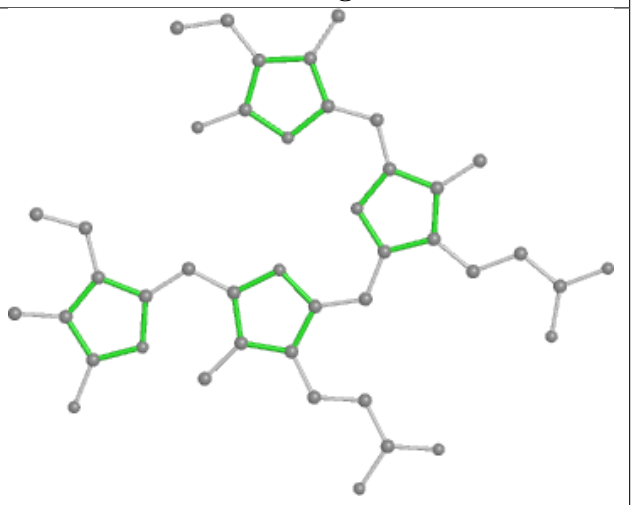
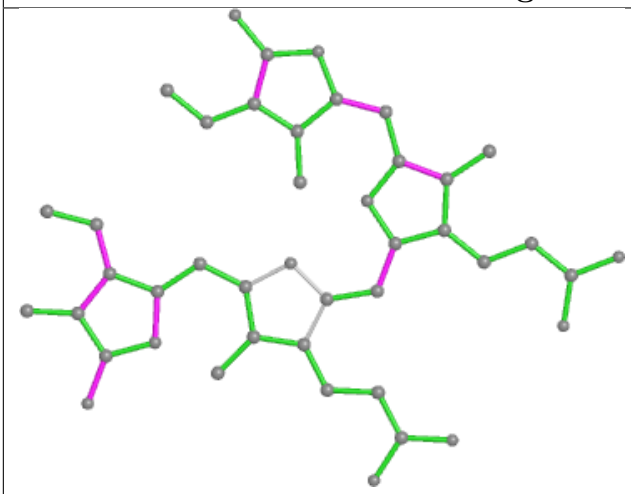


Rings

Ligand PVN 44 303



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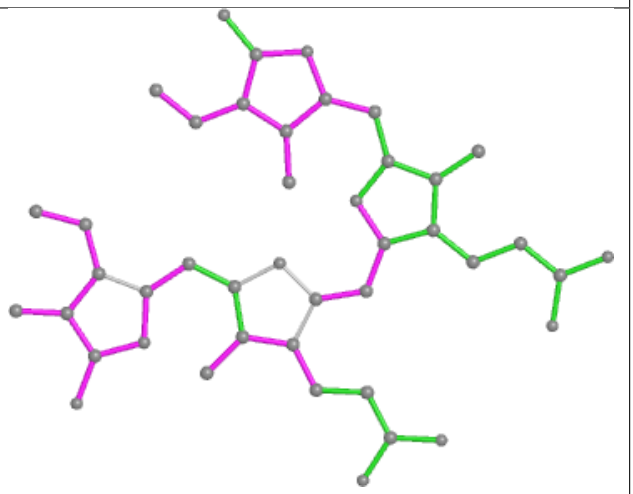

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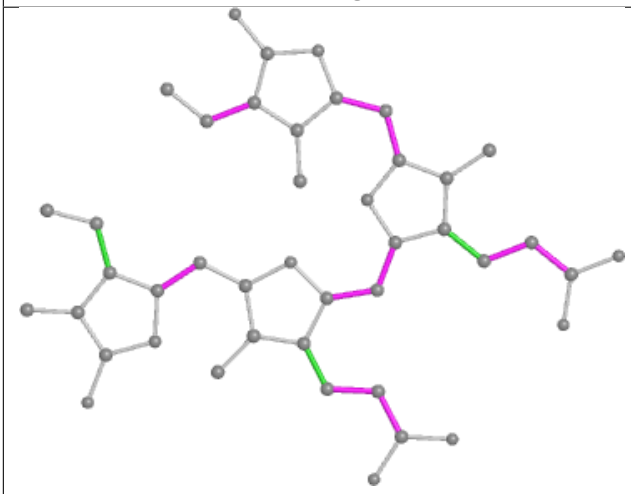

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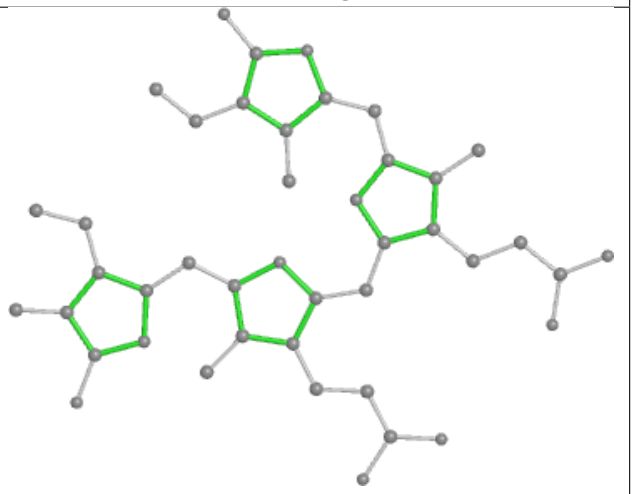
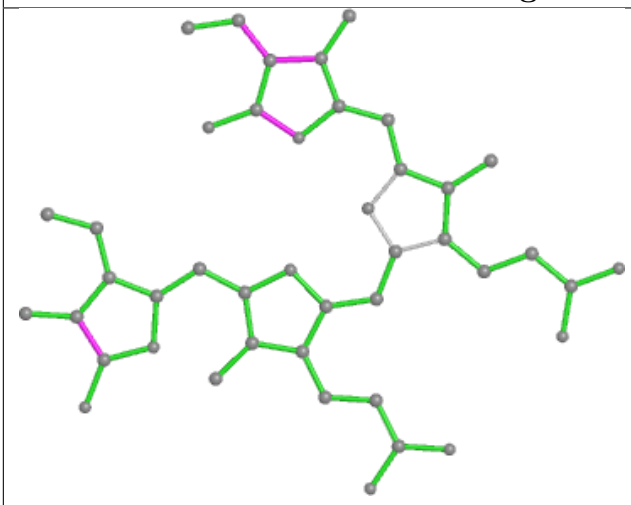


Rings

Ligand PEB aJ 201



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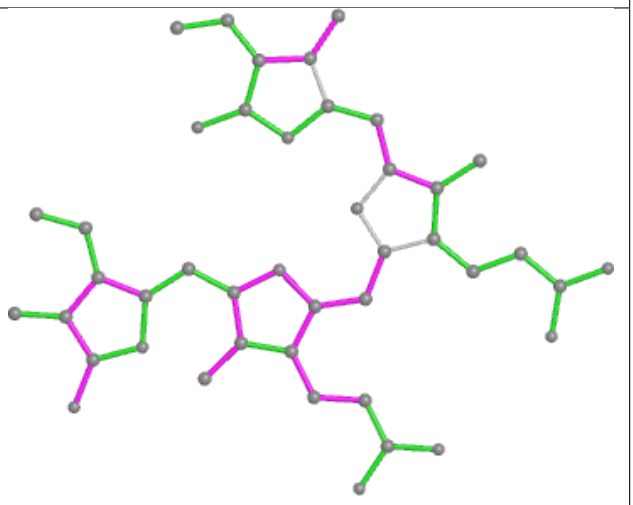

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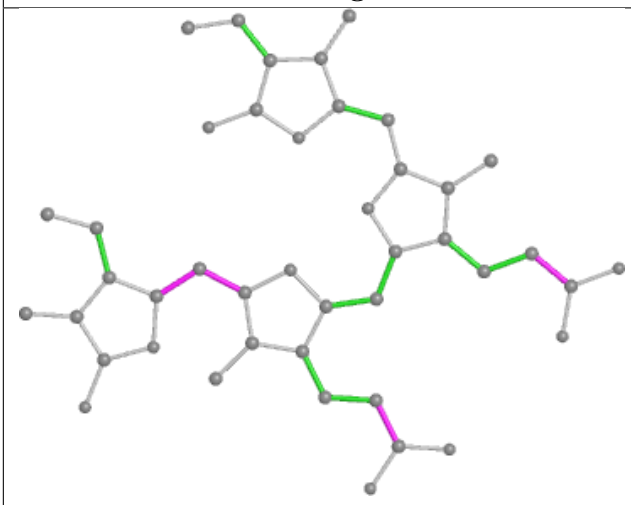

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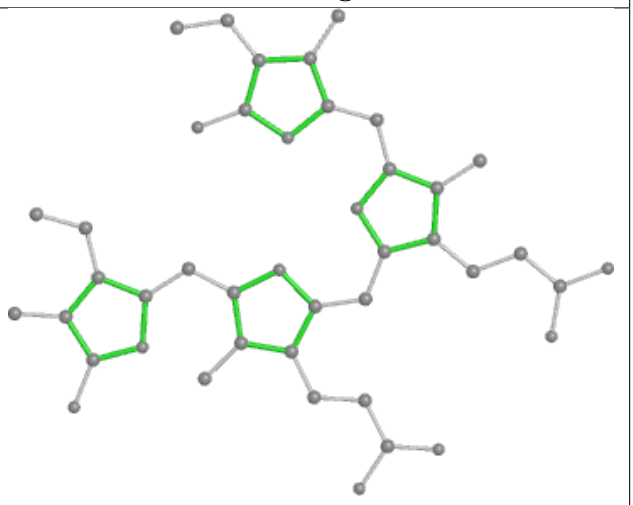
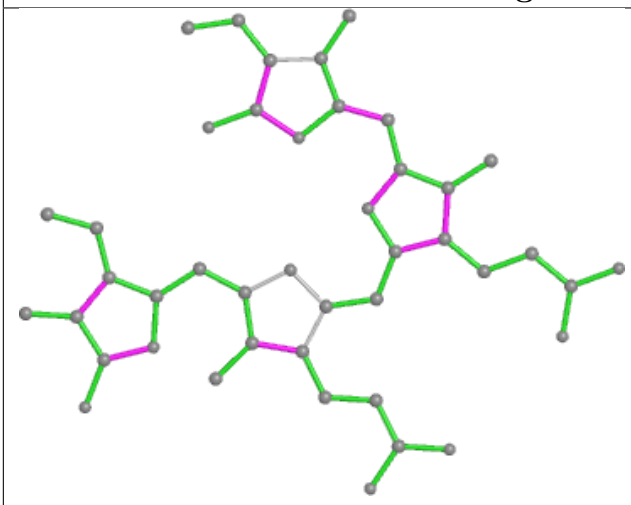
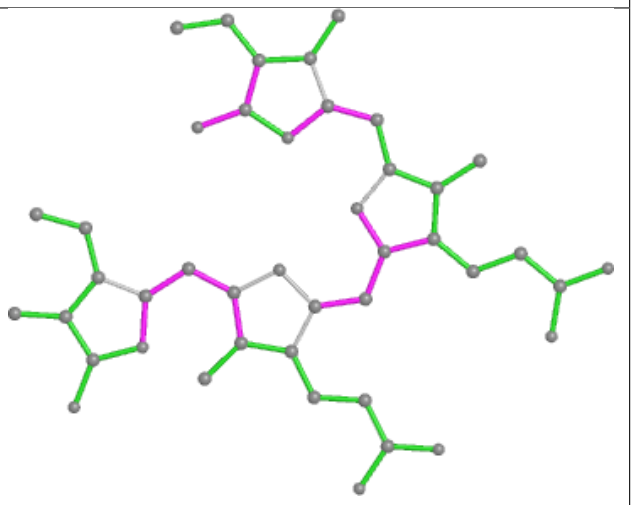


Rings

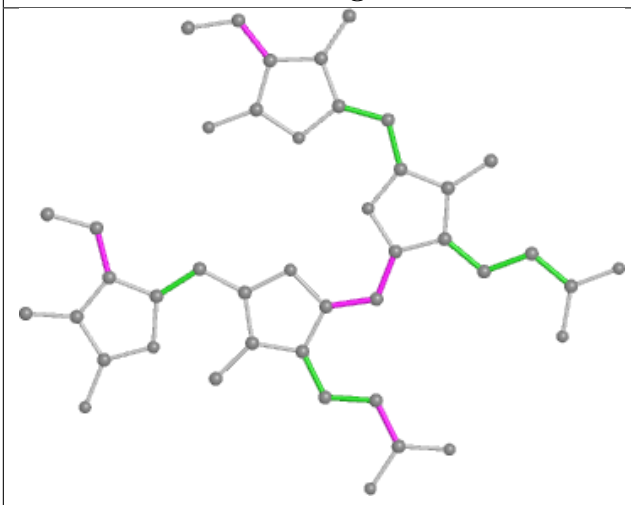
Ligand PUB Z4 203



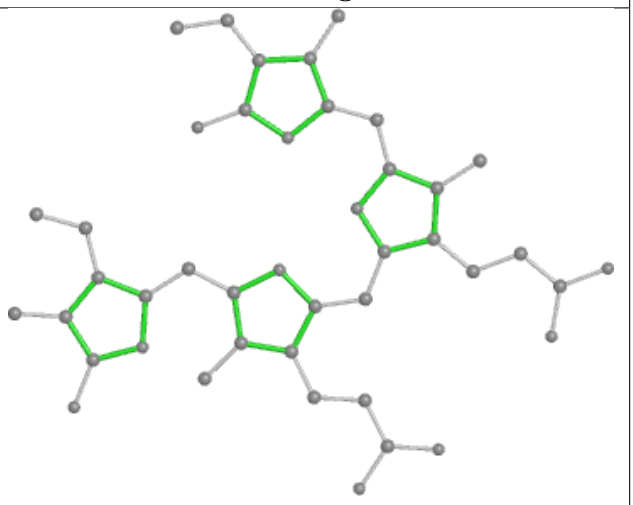
Bond lengths



Bond angles

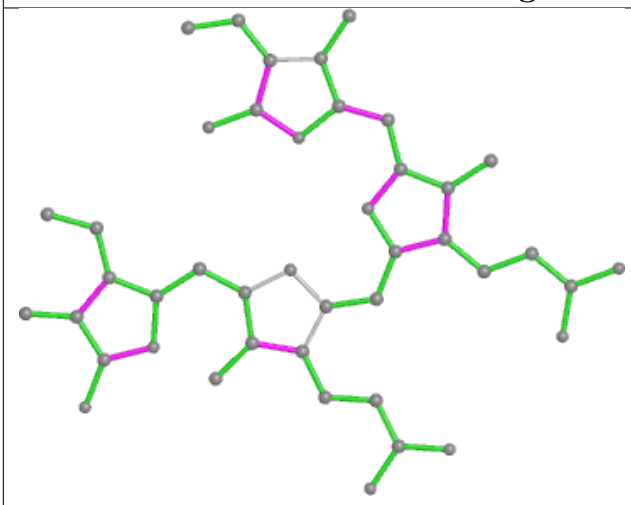


Torsions



Rings

Ligand PUB c9 305



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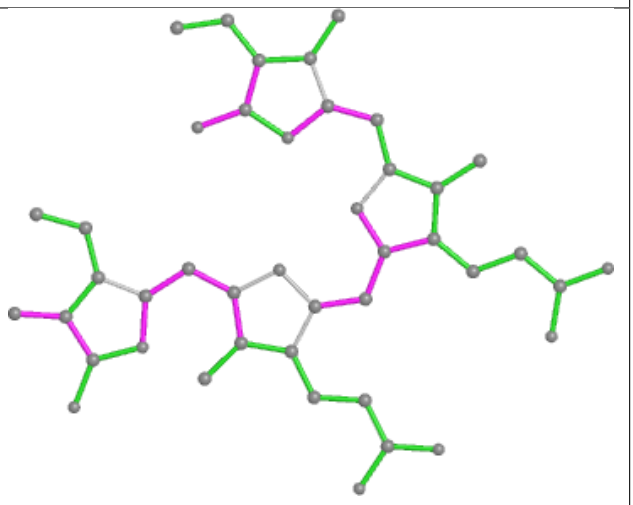

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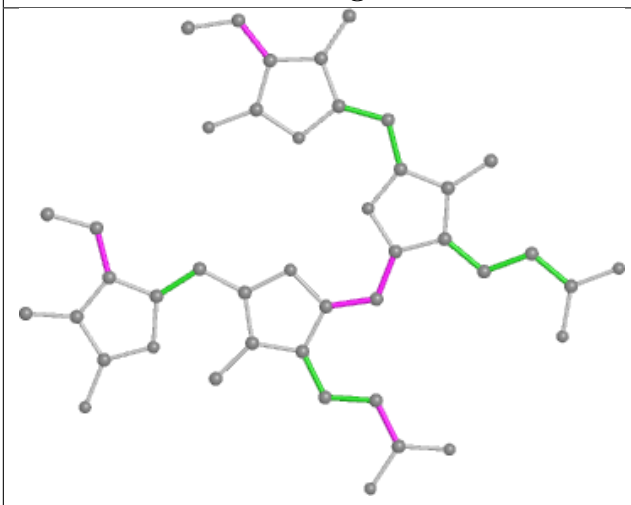

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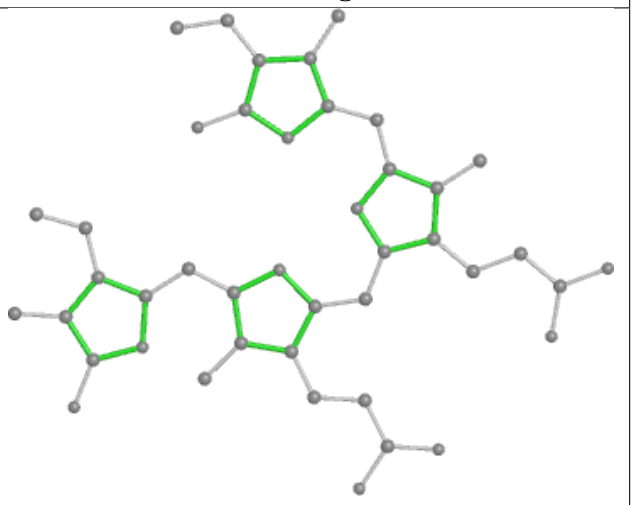
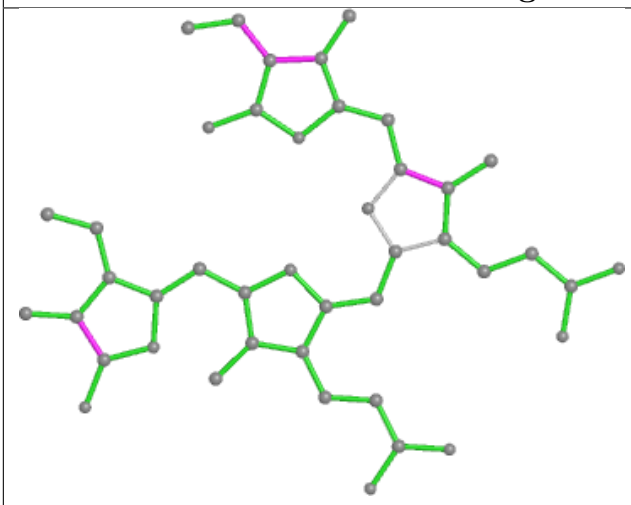


Rings

Ligand PEB u8 202



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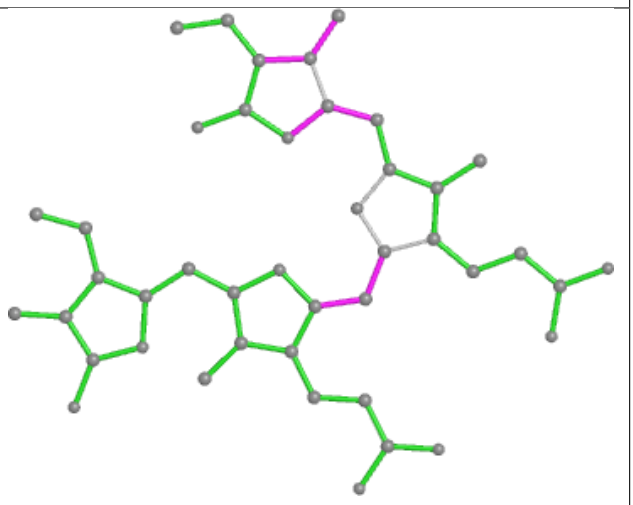

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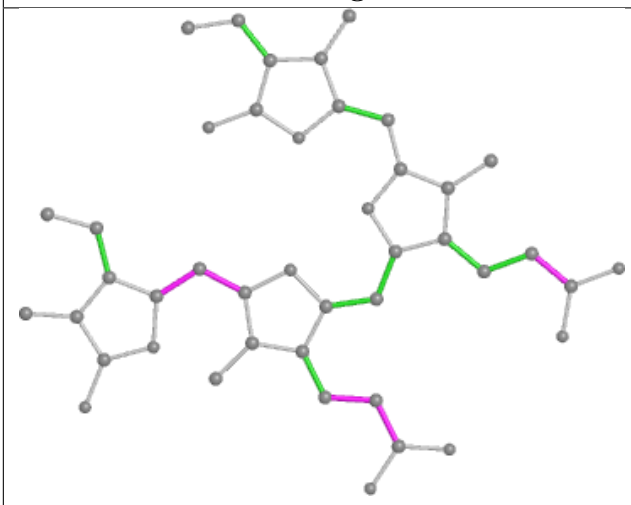

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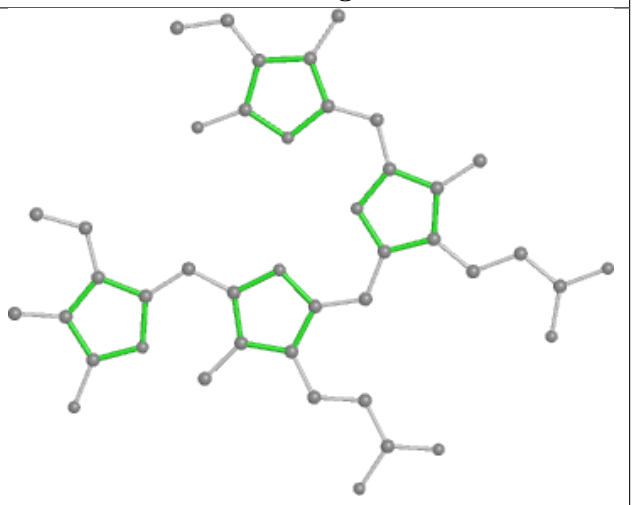
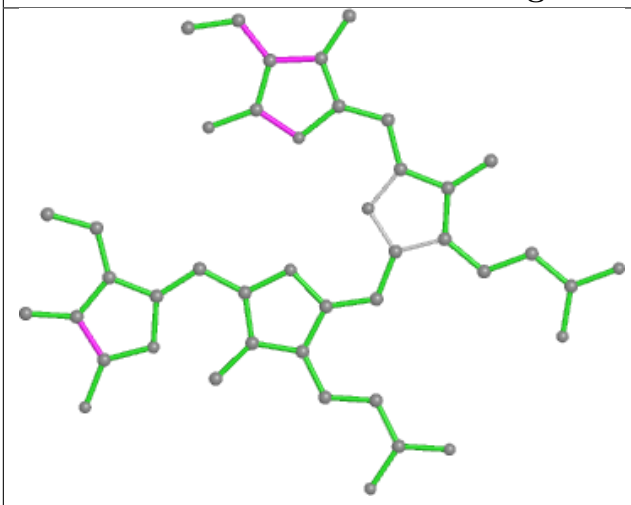


Rings

Ligand PEB ff 204



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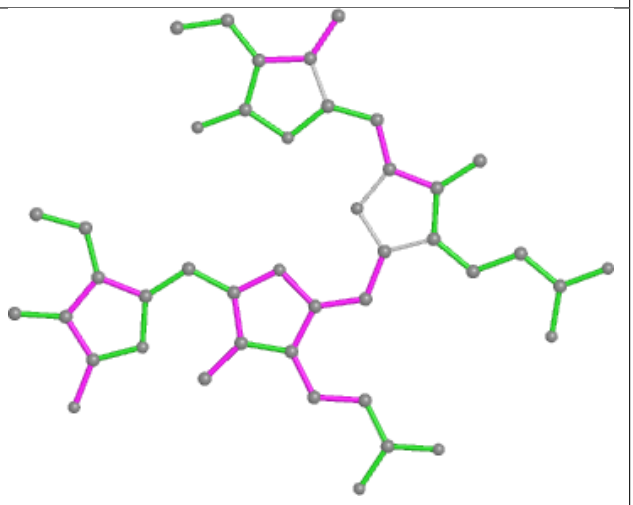

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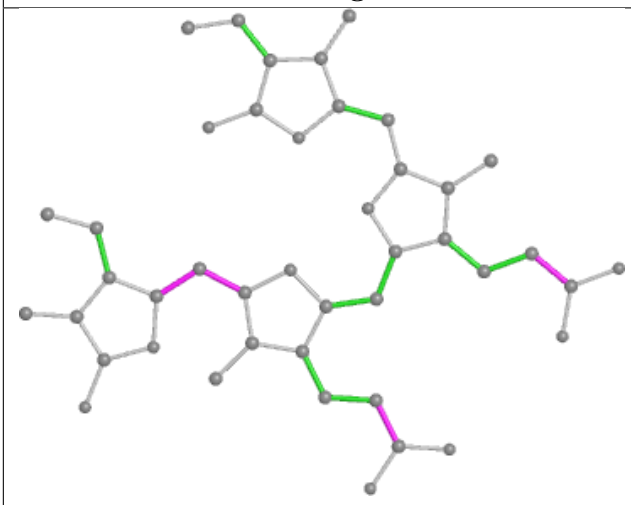

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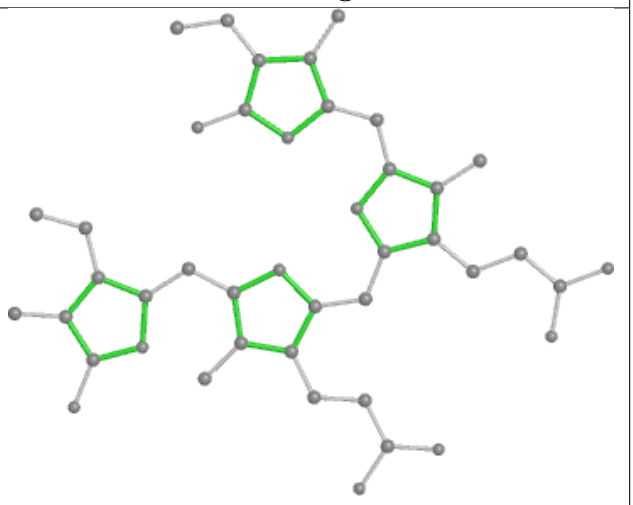
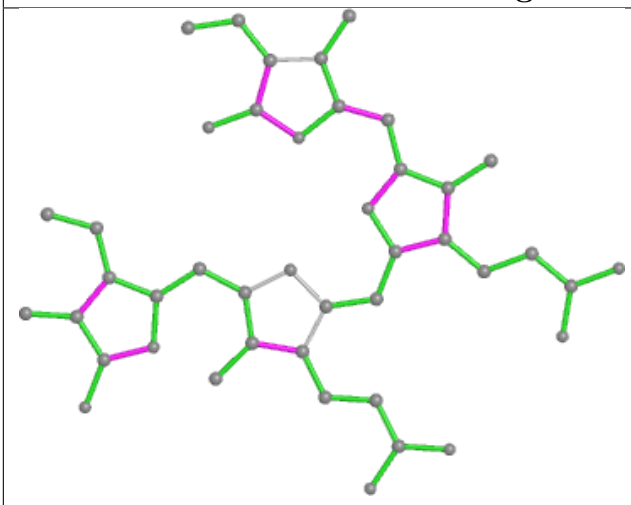


Rings

Ligand PUB Z6 203



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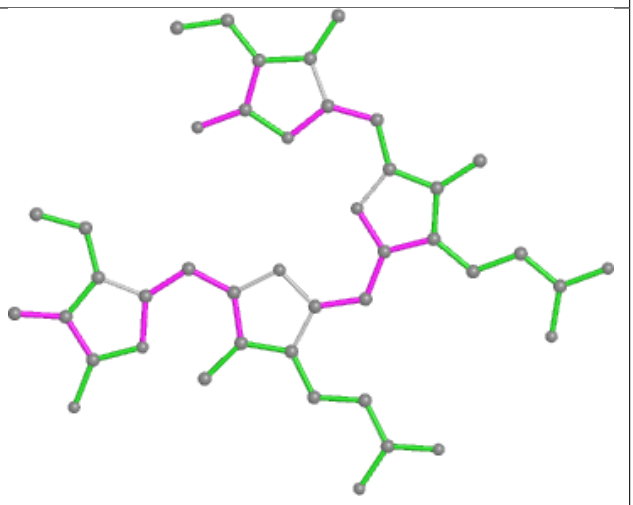

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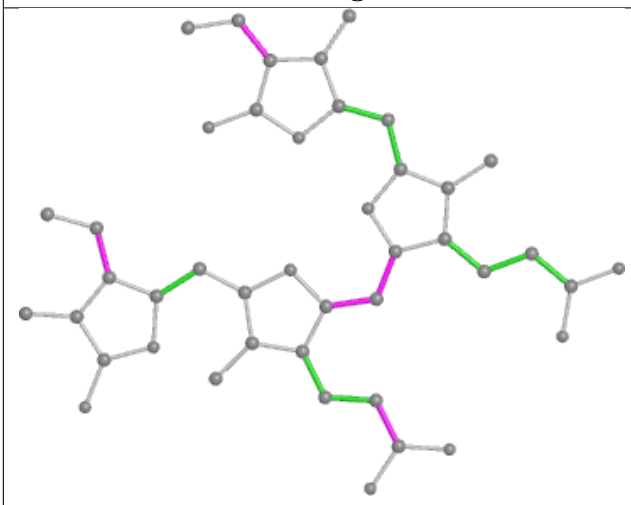

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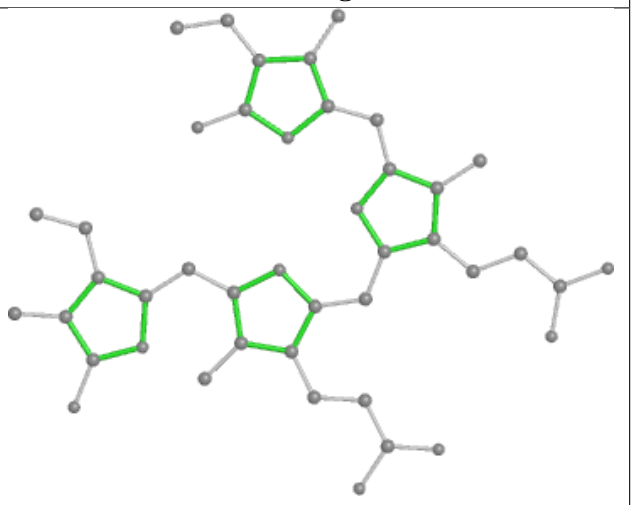

Rings

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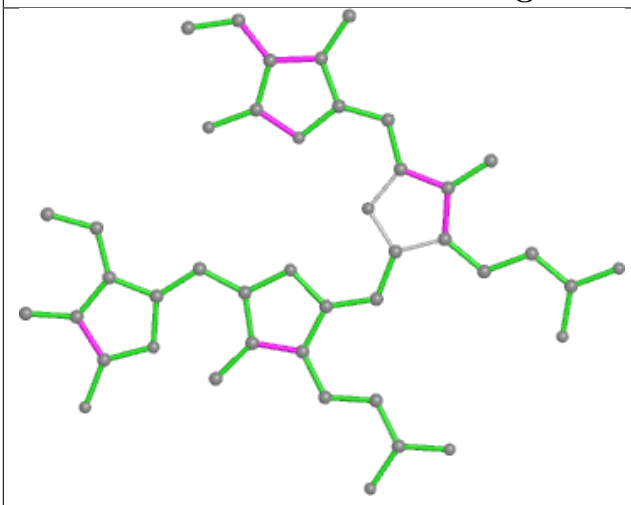

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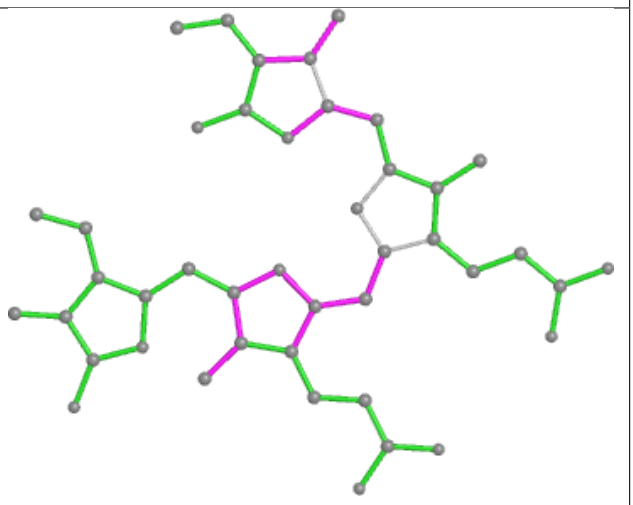

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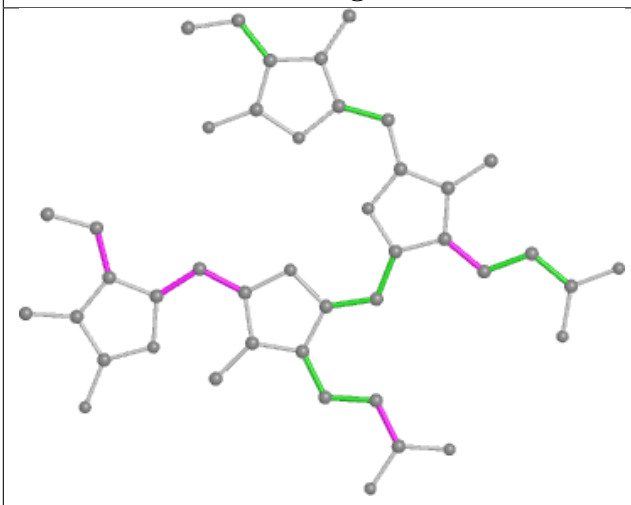

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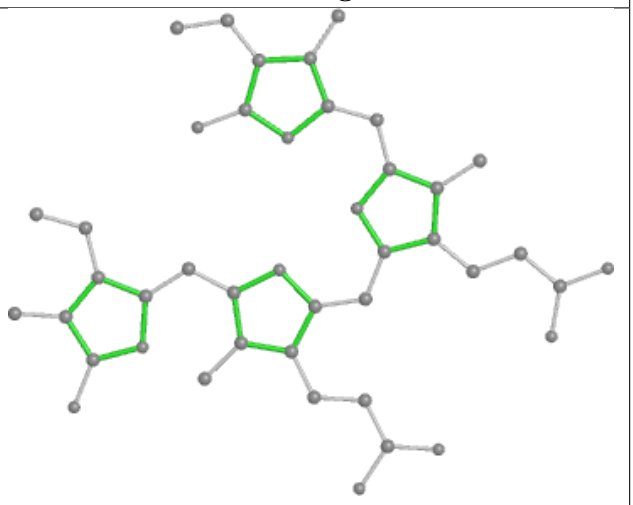
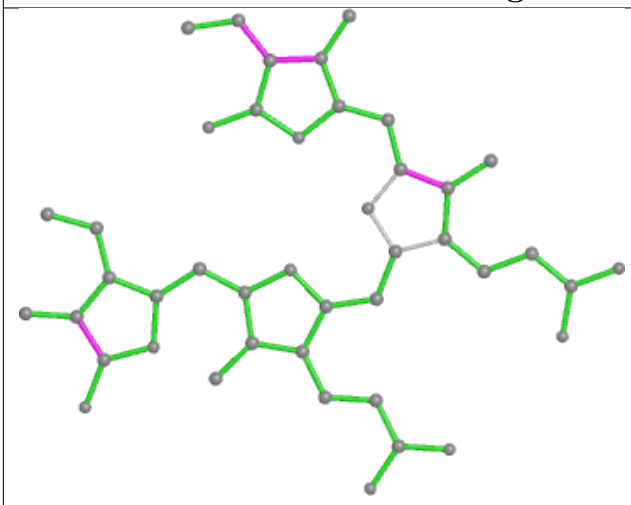


Rings

Ligand PEB C3 1002



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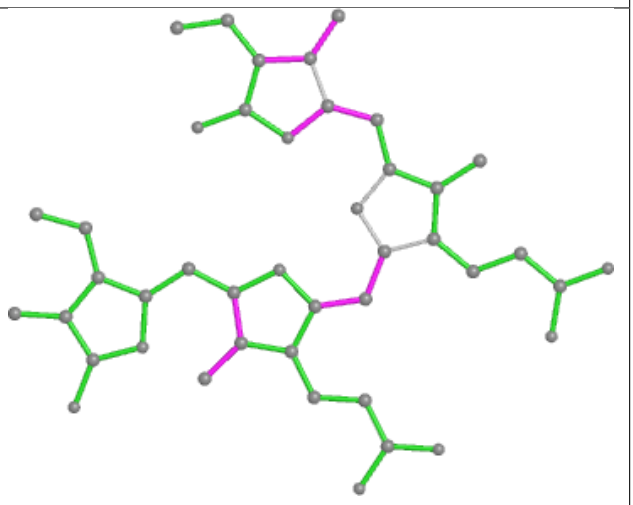

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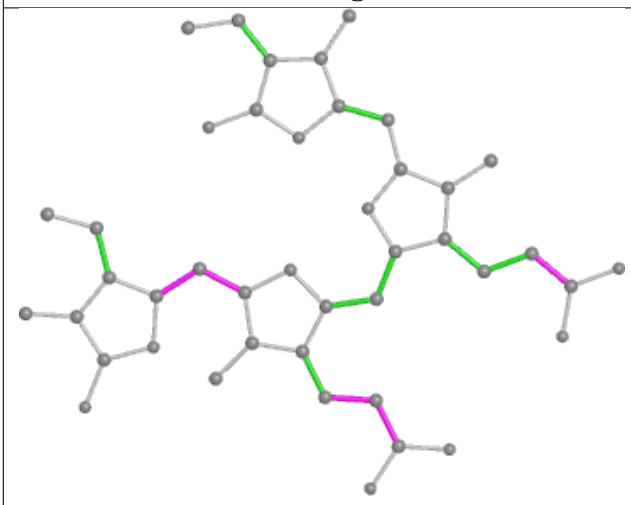

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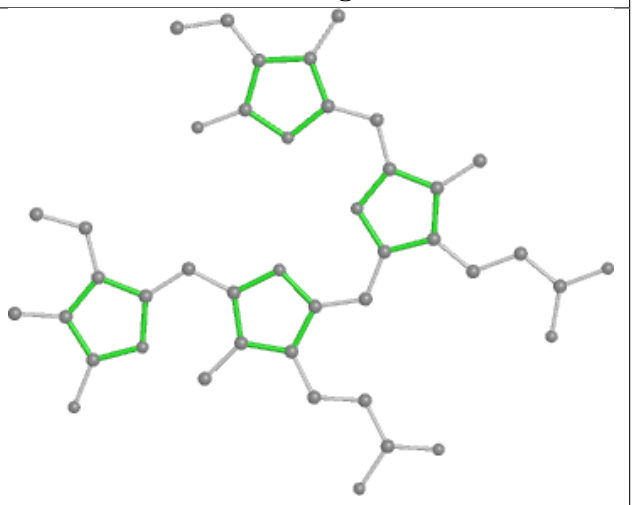
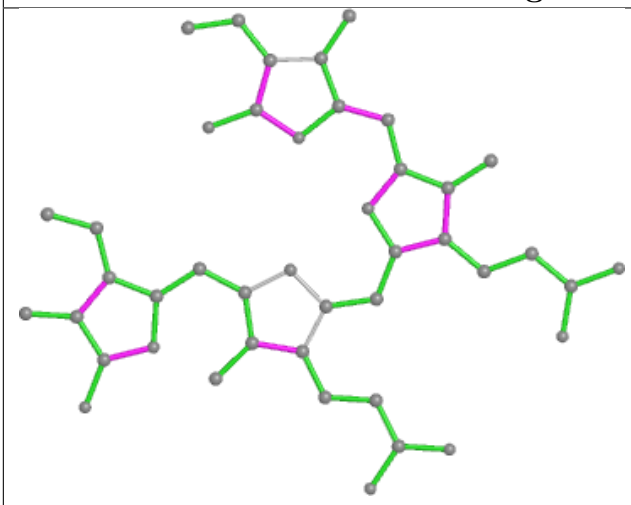


Rings

Ligand PUB fi 203



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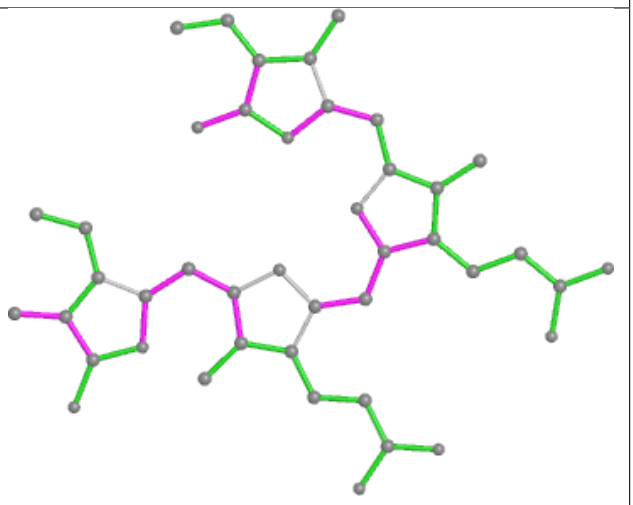

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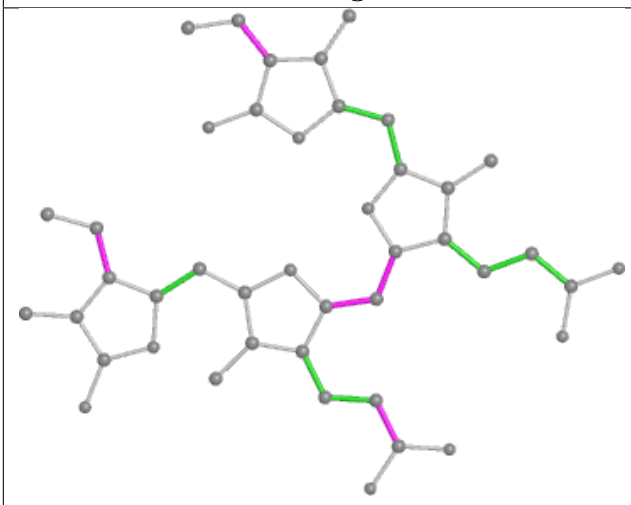

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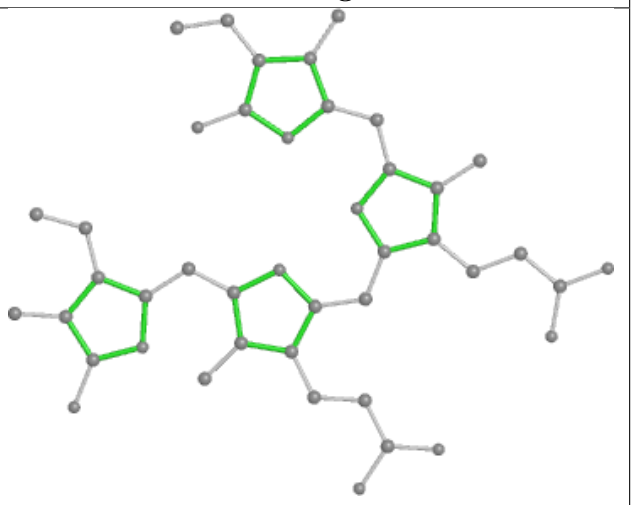
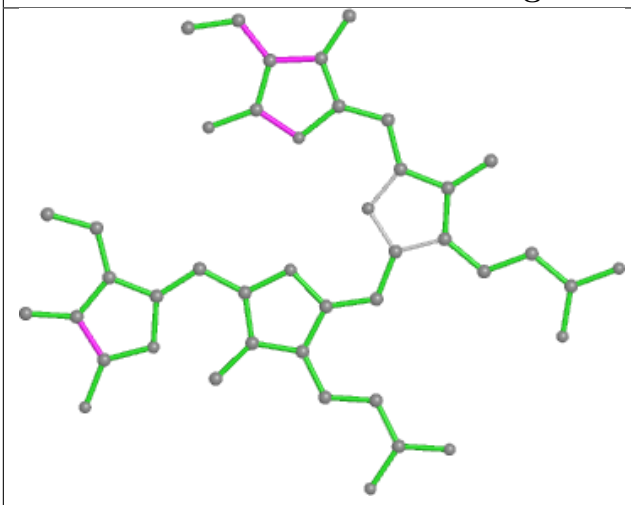


Rings

Ligand PEB i7 201



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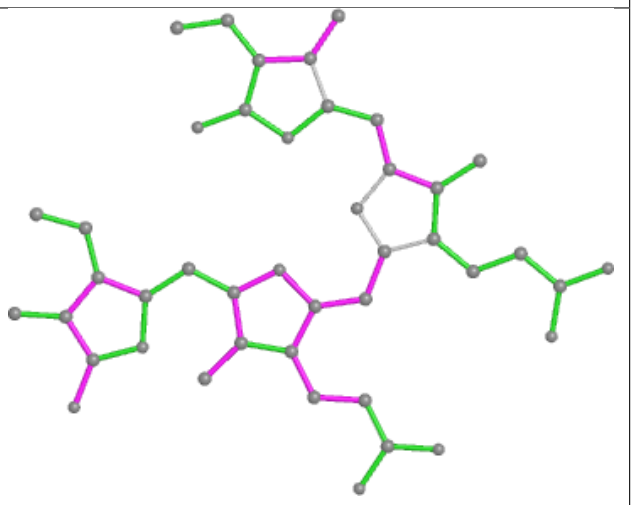

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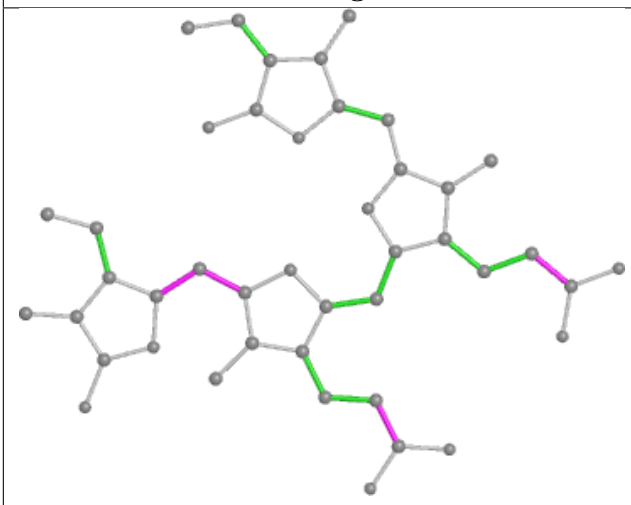

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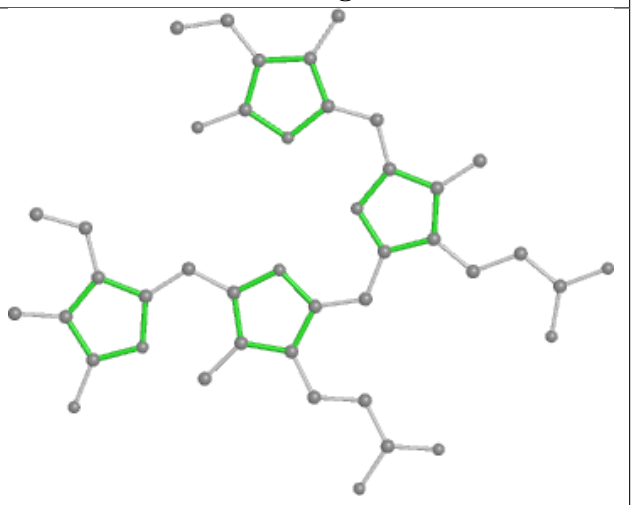
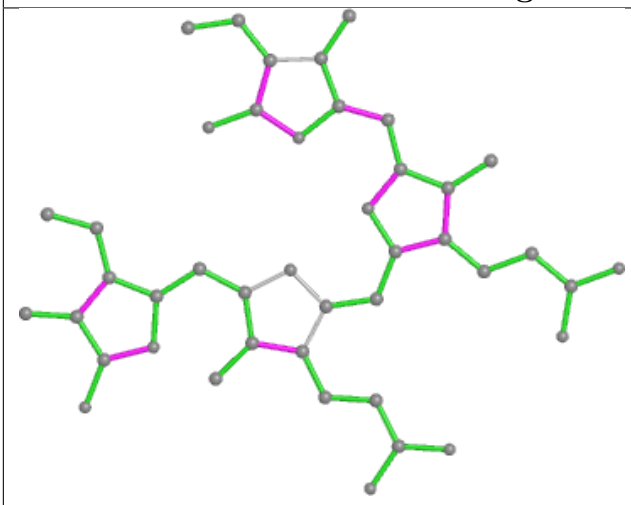


Rings

Ligand PUB L2 203



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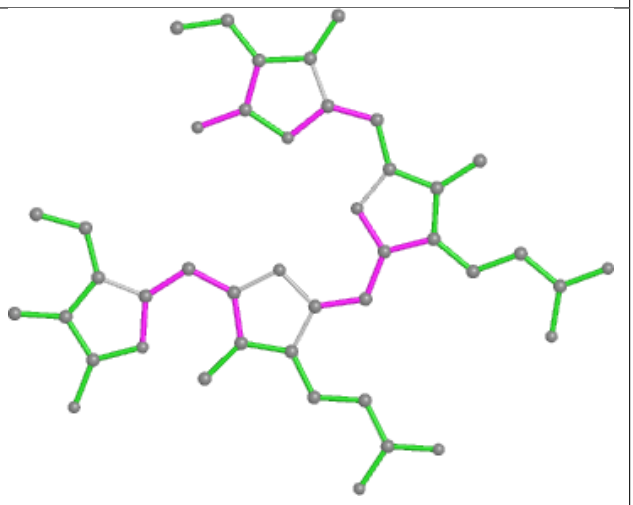

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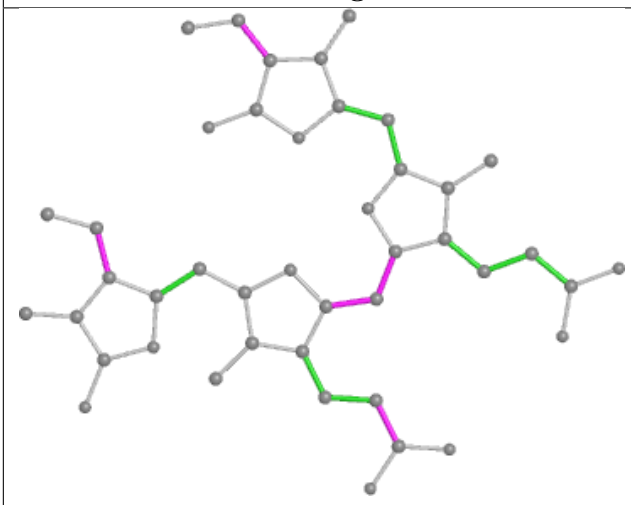

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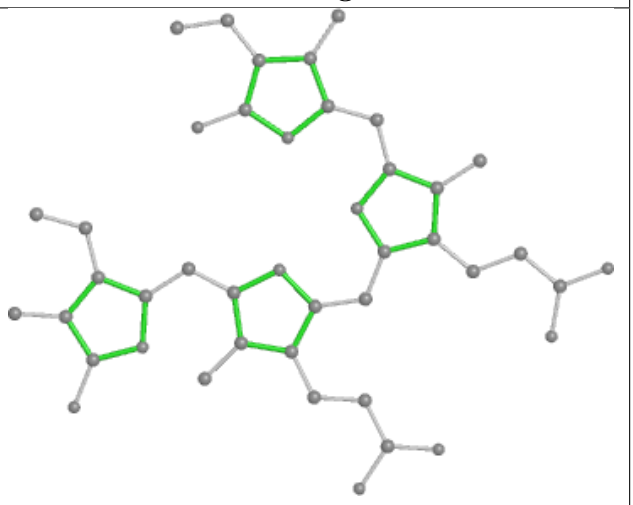
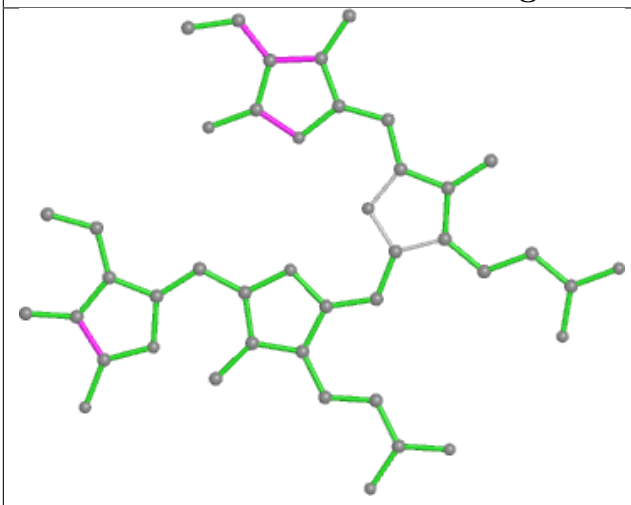


Rings

Ligand PEB v2 201



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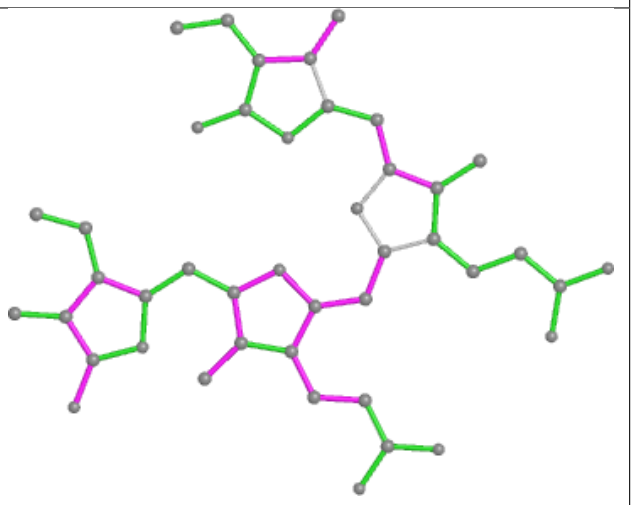

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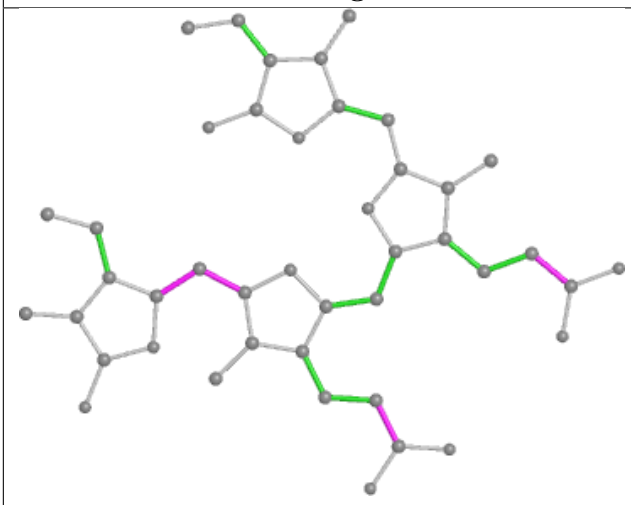

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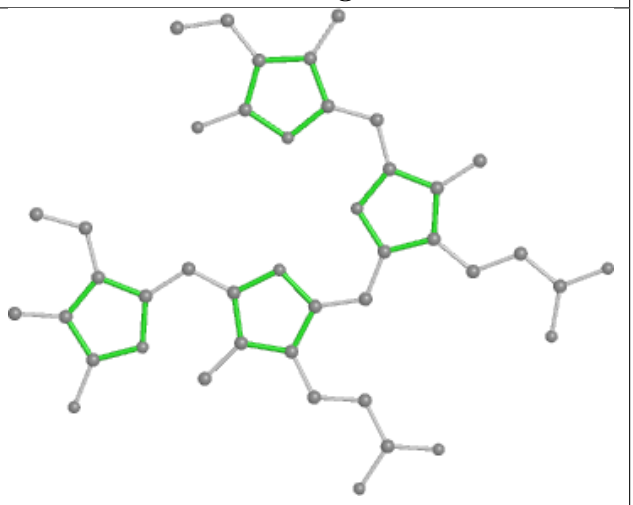
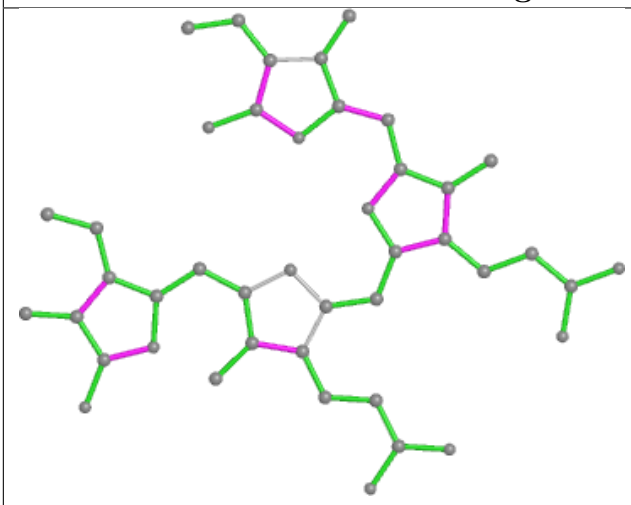


Rings

Ligand PUB T2 203



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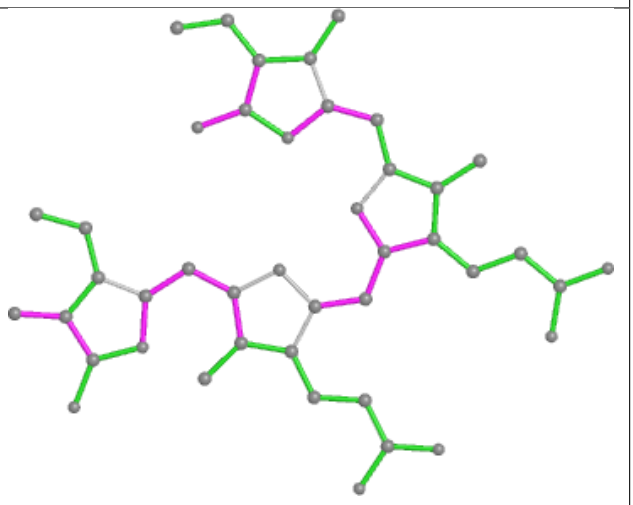

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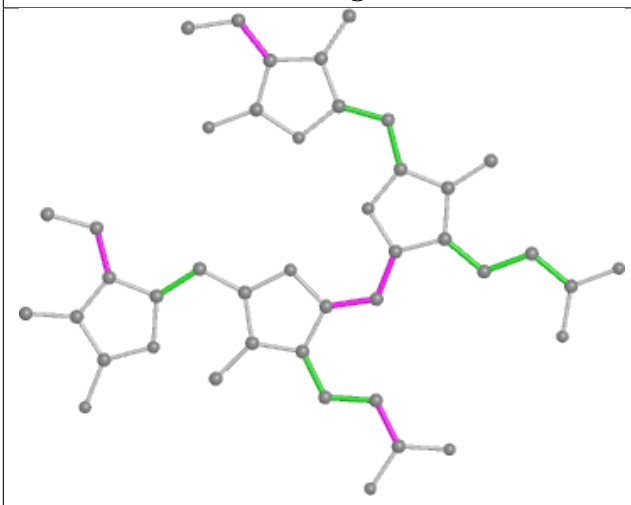

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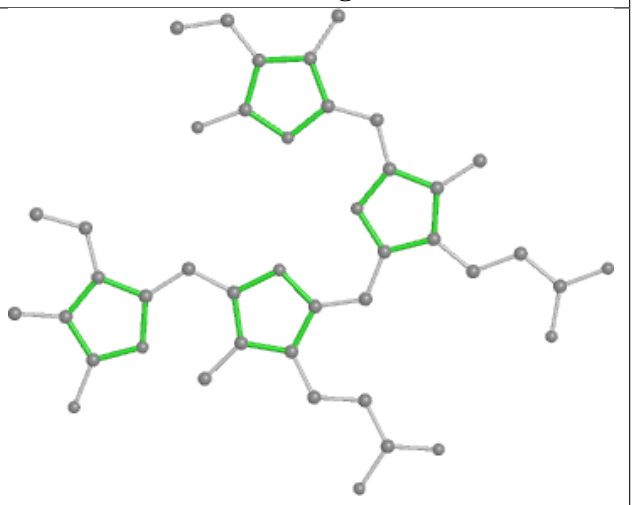
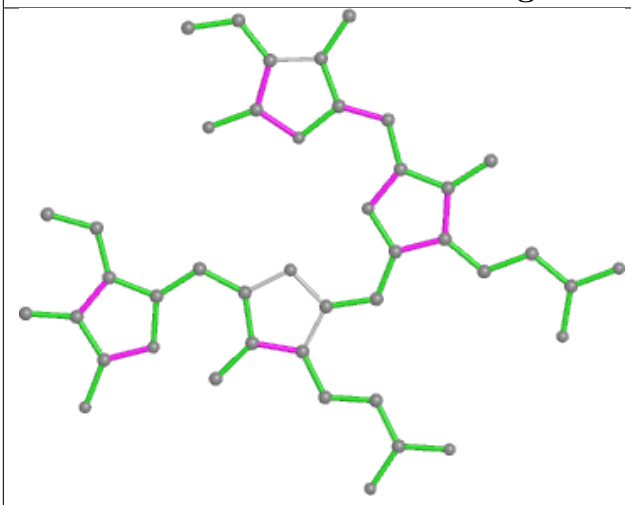


Rings

Ligand PUB v7 203



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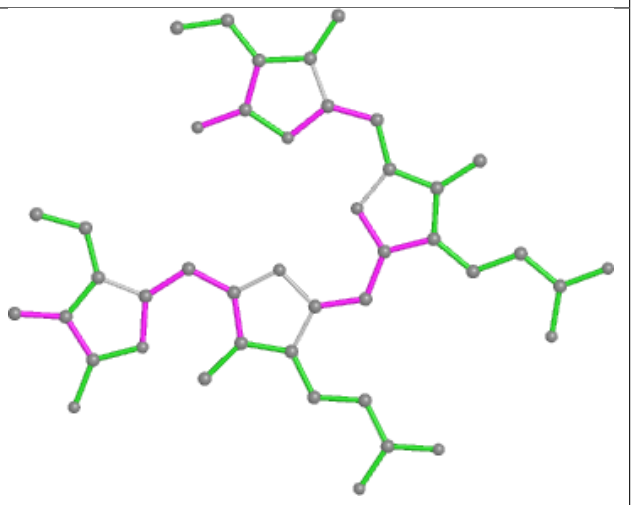
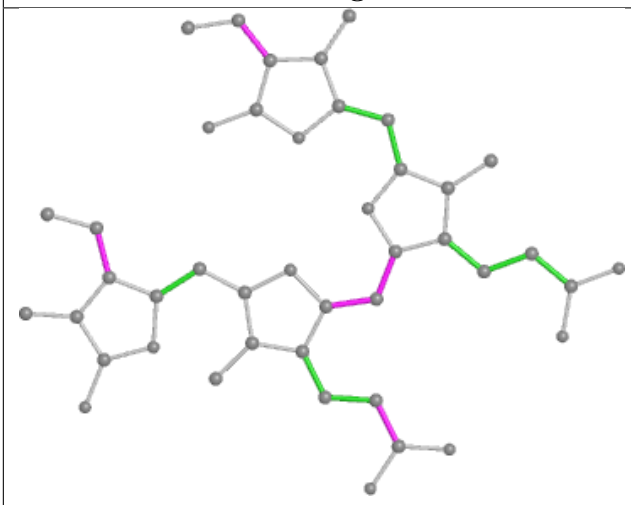


Bond angles



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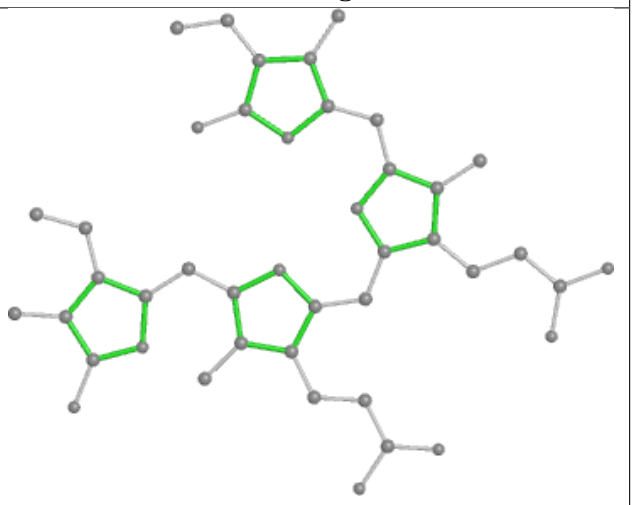
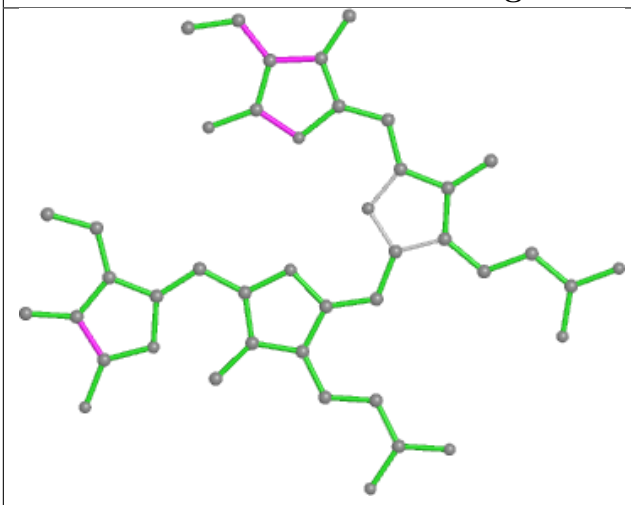


Rings

Ligand PEB m4 1001



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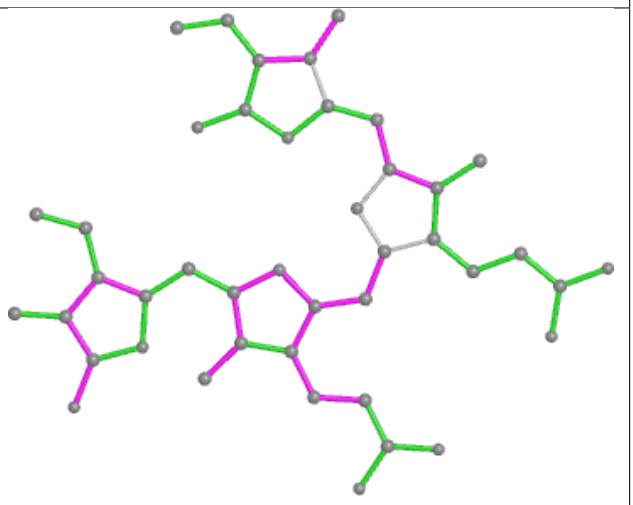
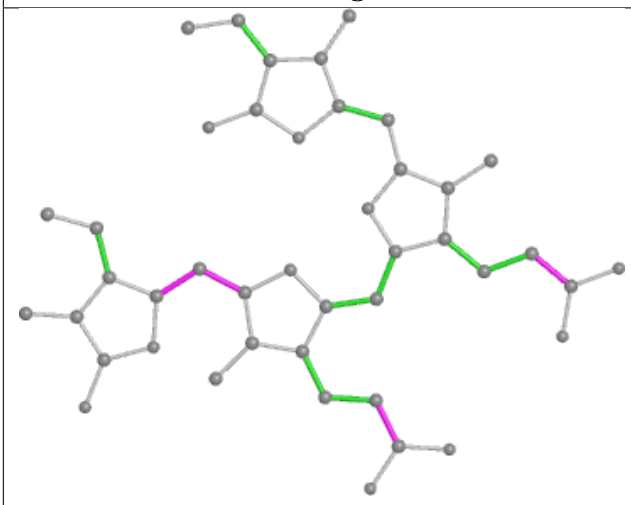
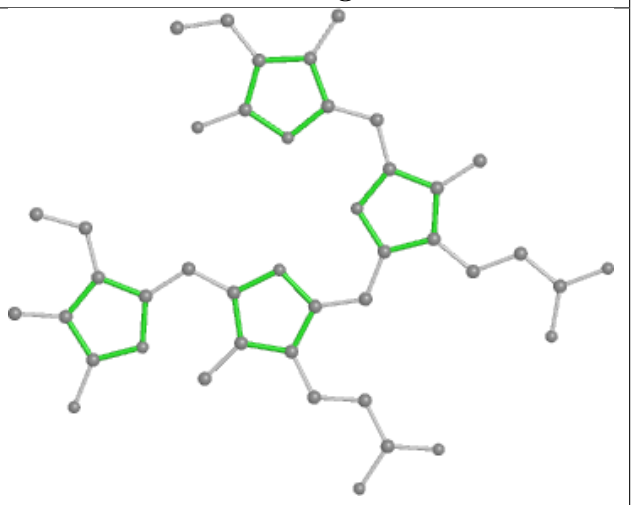


Bond angles

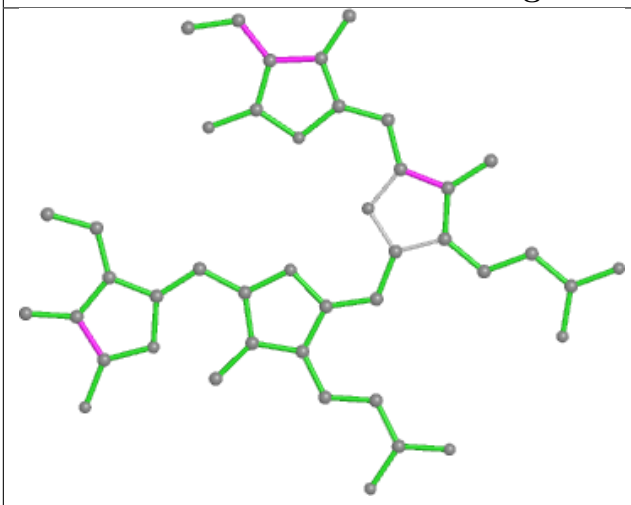


Torsions



Rings

Ligand PEB fg 202



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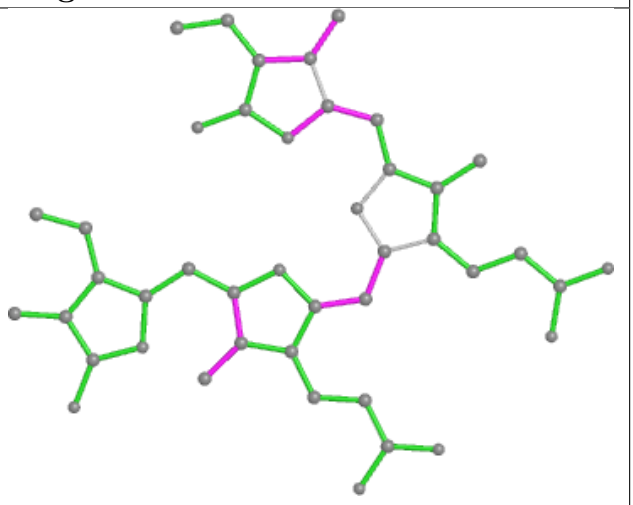

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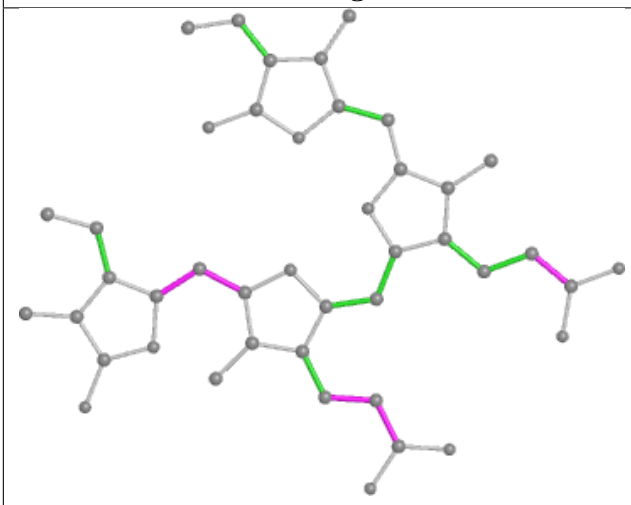

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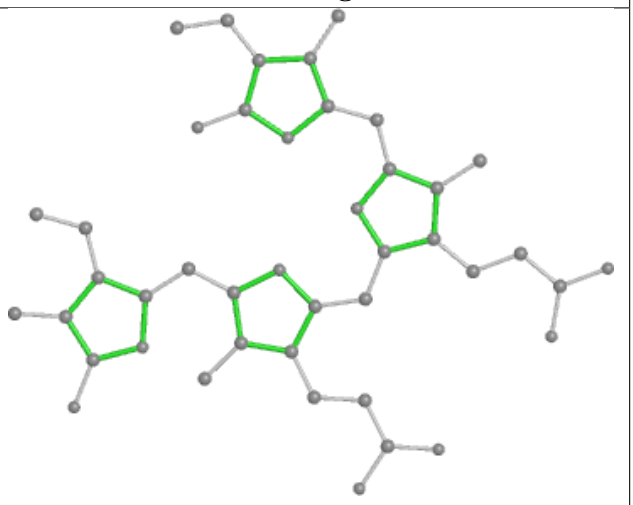
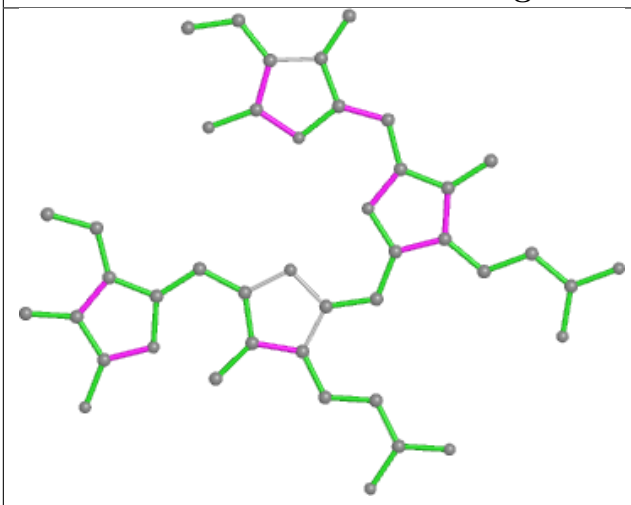


Rings

Ligand PUB B5 203



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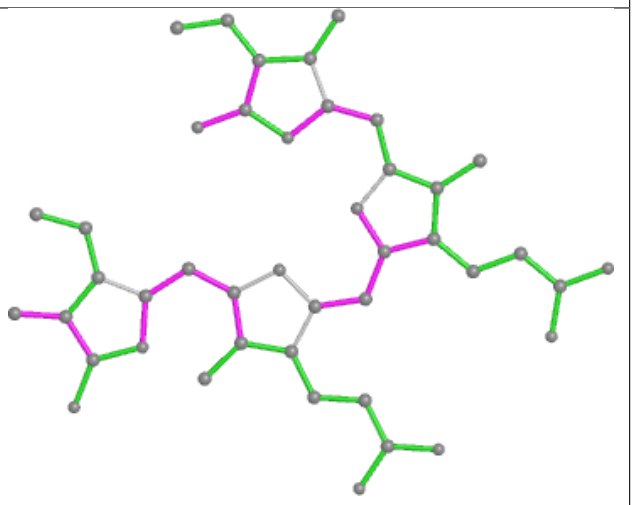

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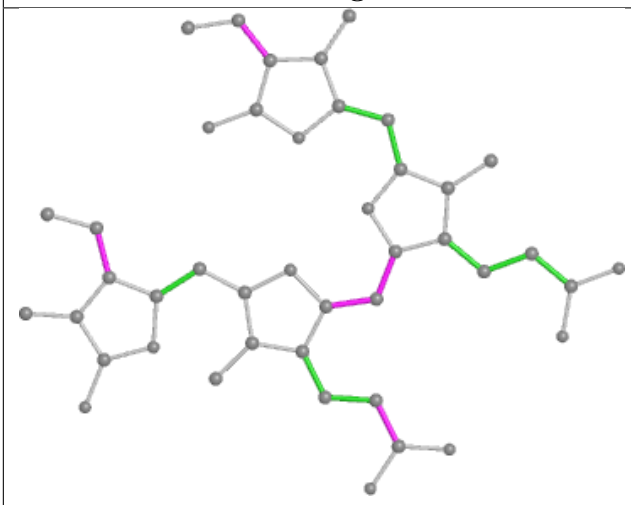

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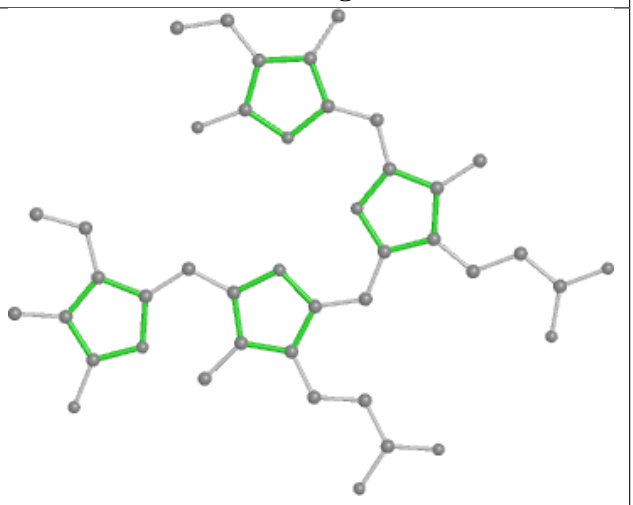
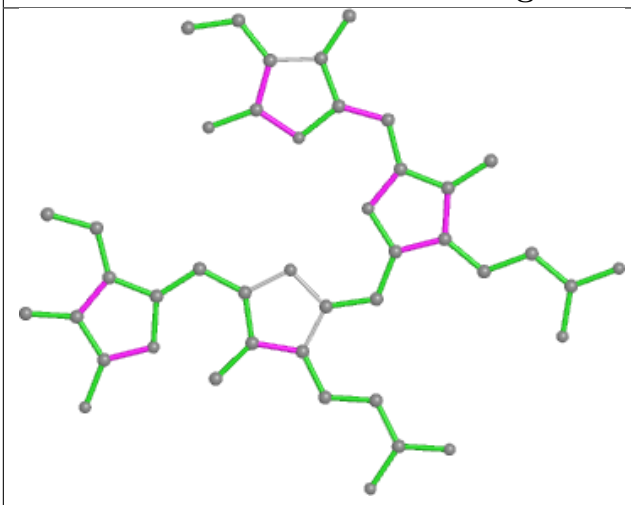


Rings

Ligand PUB p2 203



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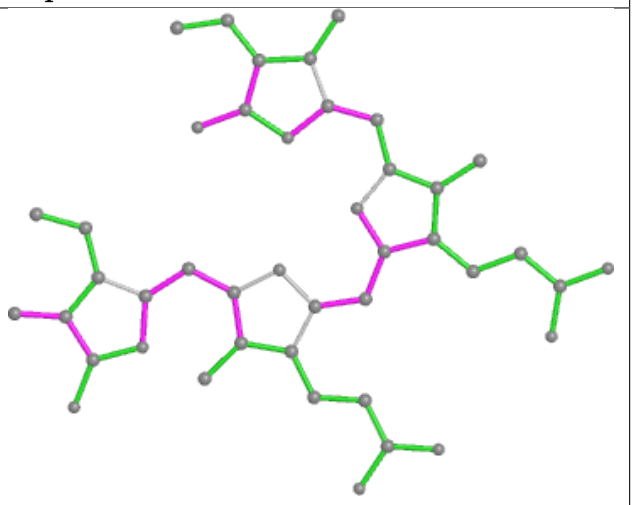

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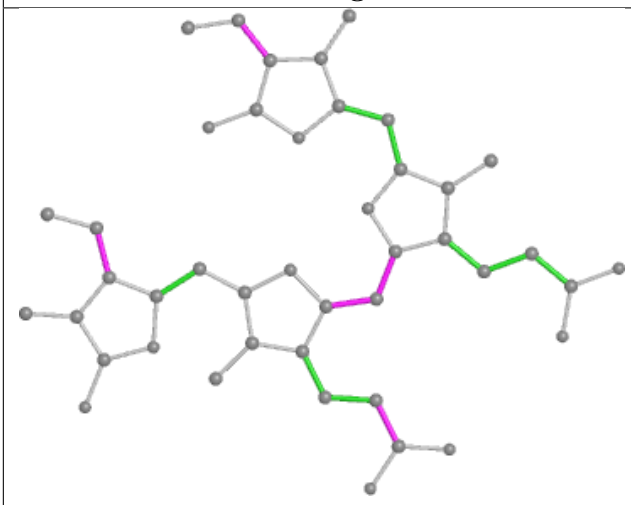

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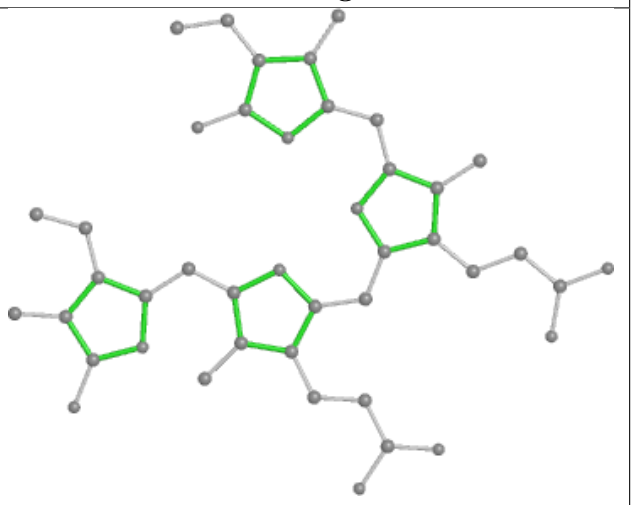
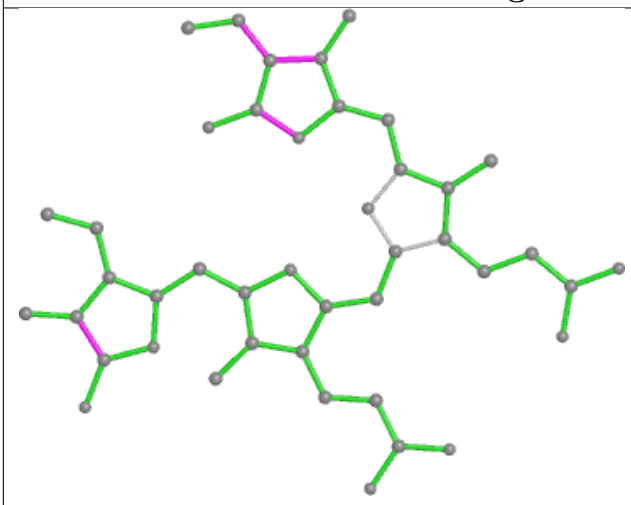


Rings

Ligand PEB E2 1001



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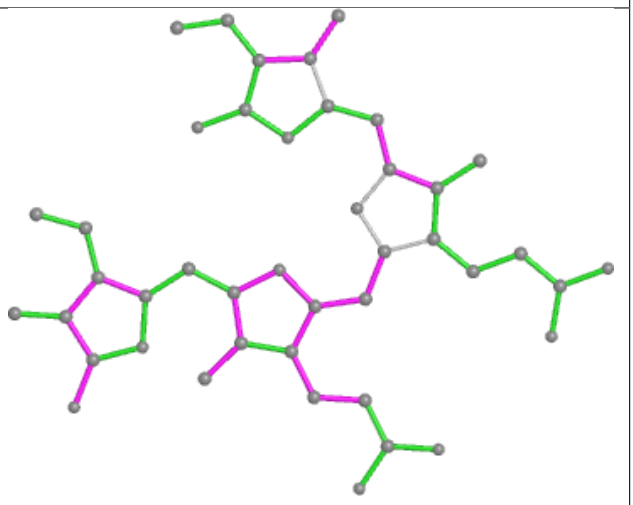

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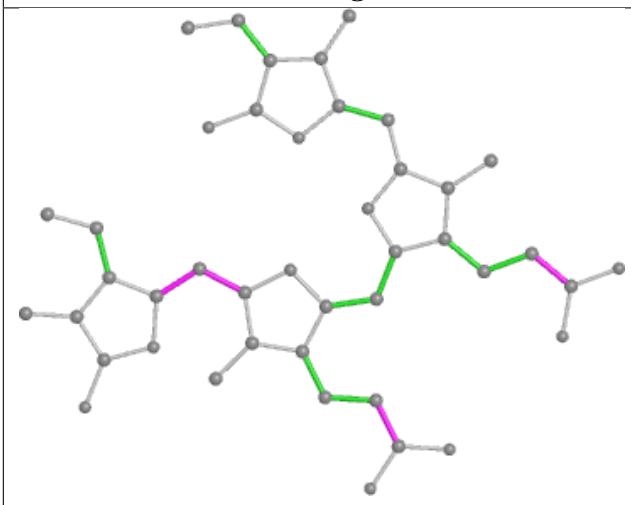

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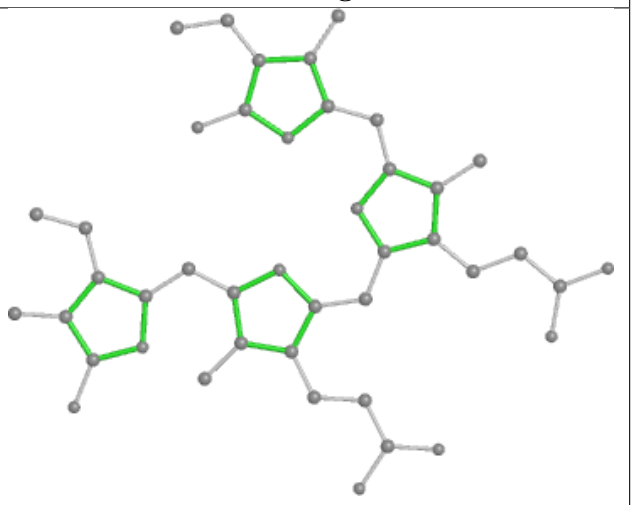
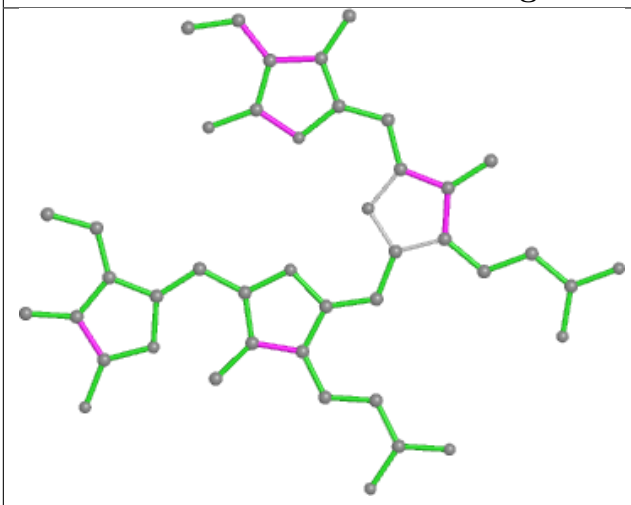


Rings

Ligand PEB en 202



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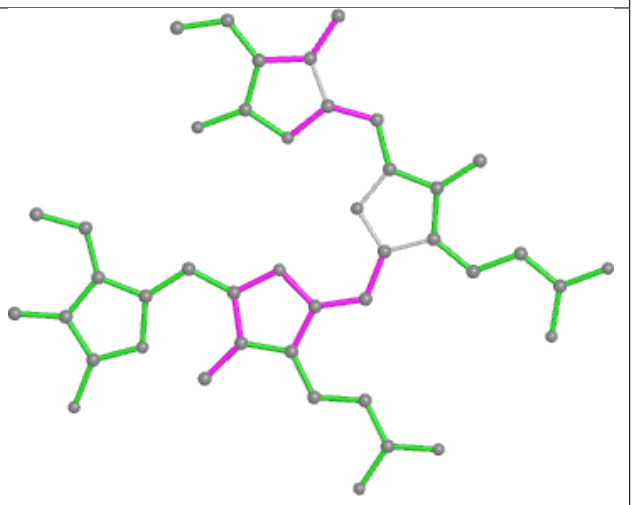

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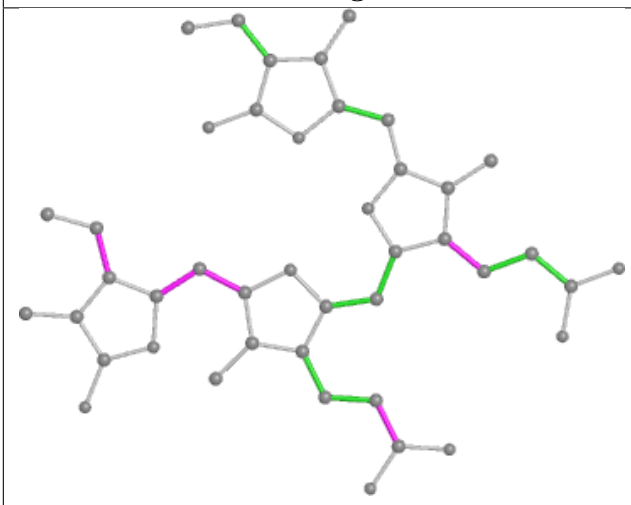

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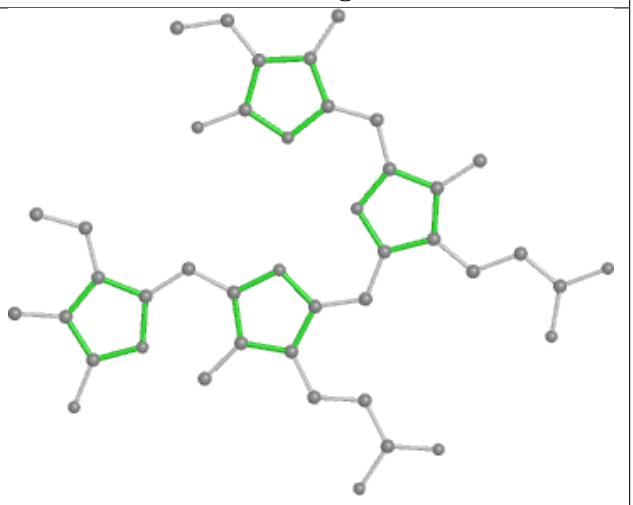

Rings

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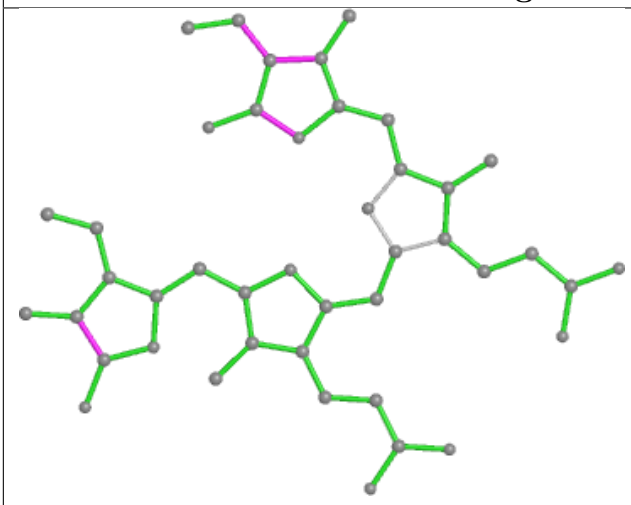

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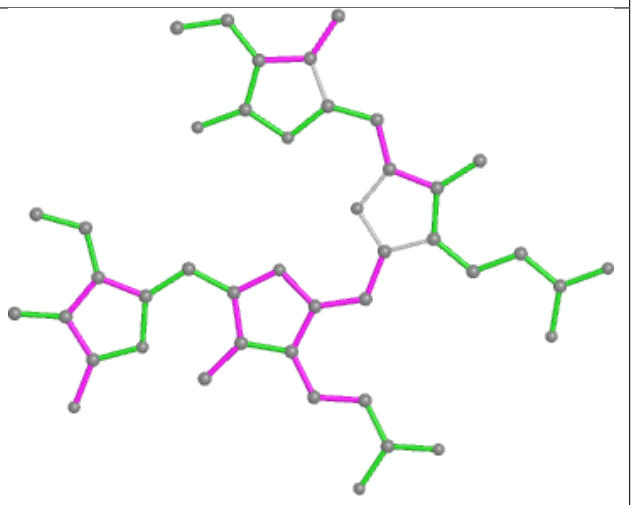

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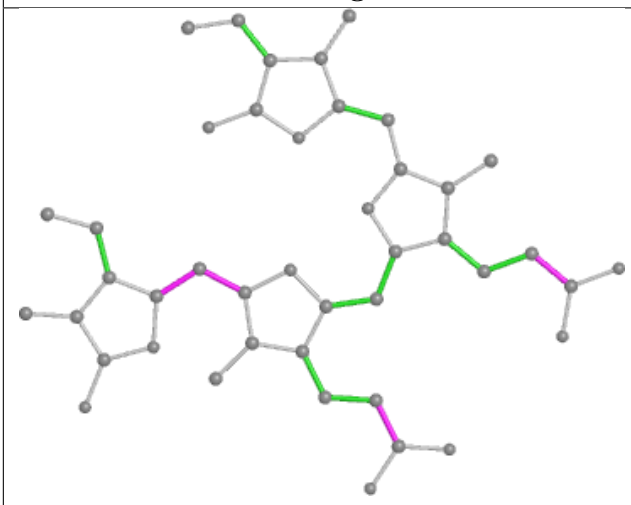

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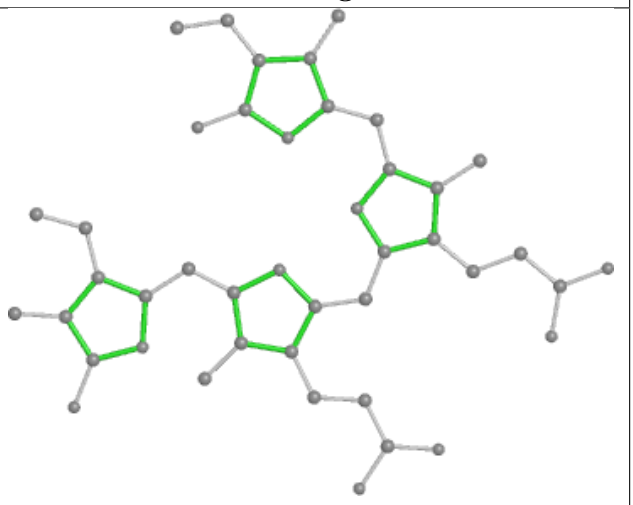

Rings

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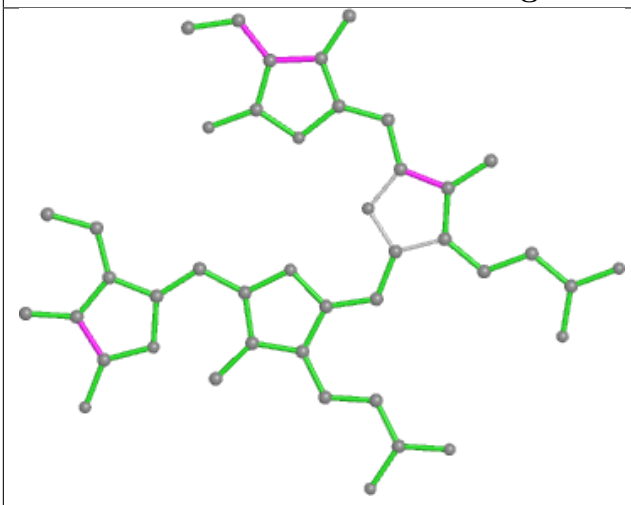

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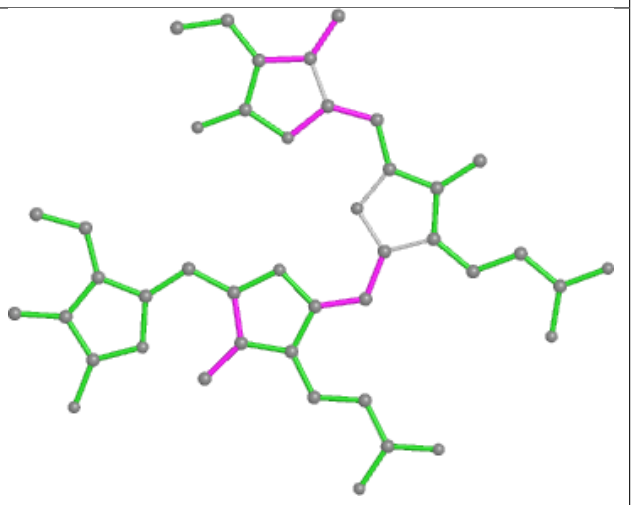

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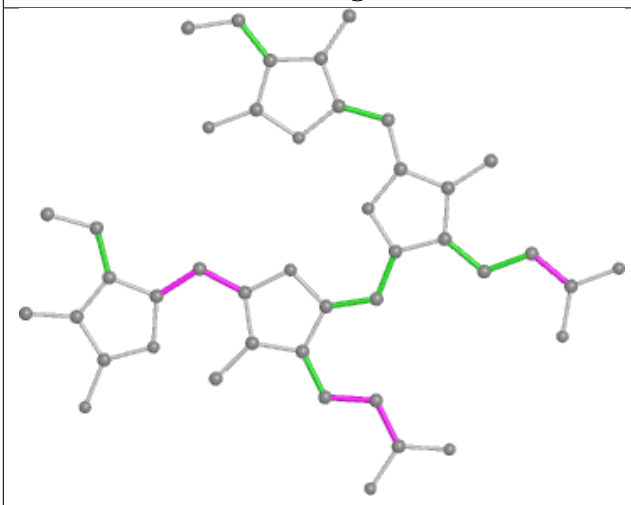

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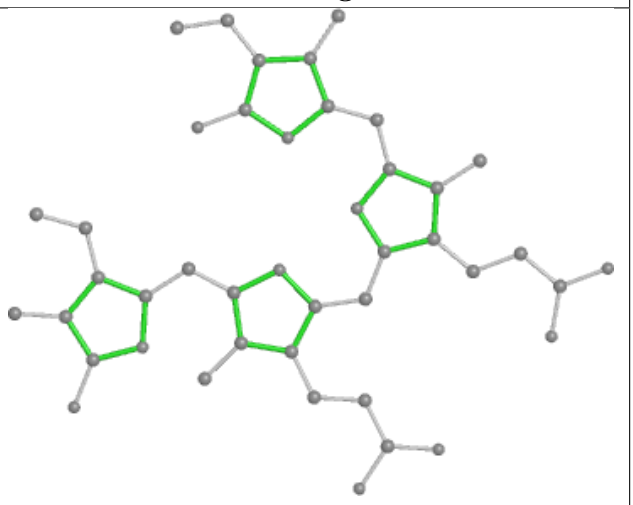
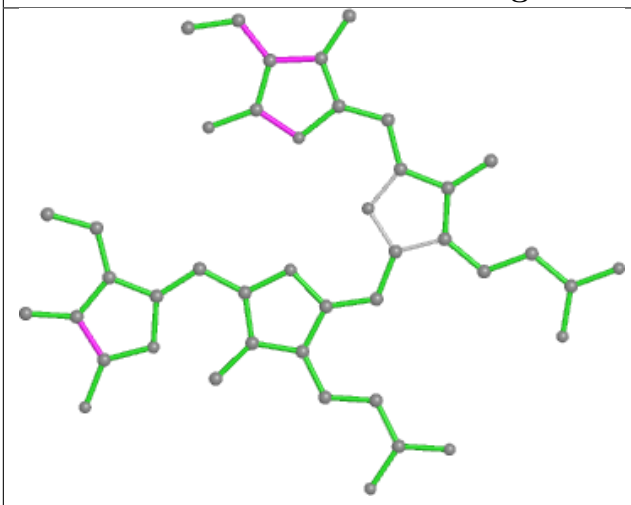


Rings

Ligand PEB ey 1002



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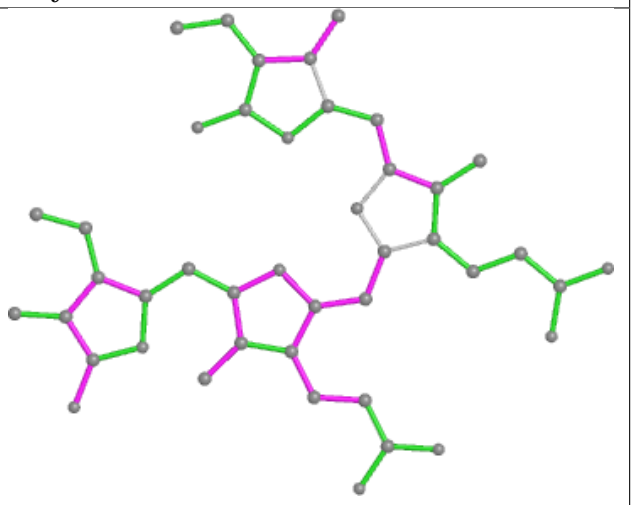
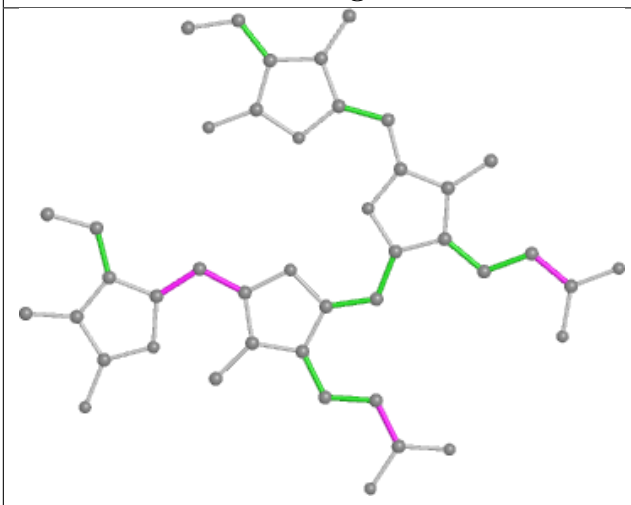


Bond angles



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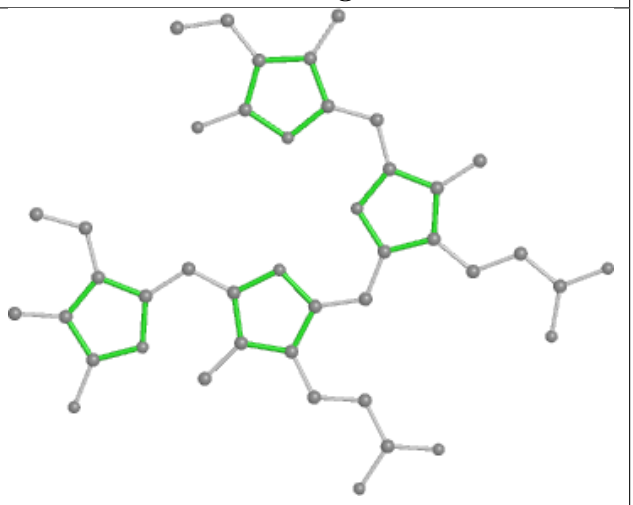
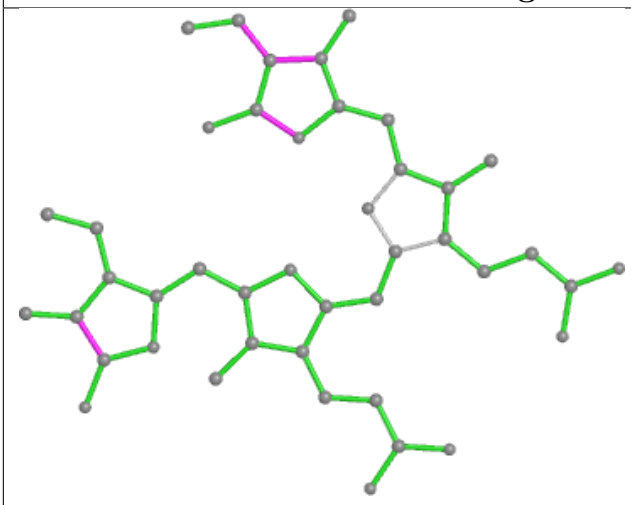


Rings

Ligand PEB L9 201



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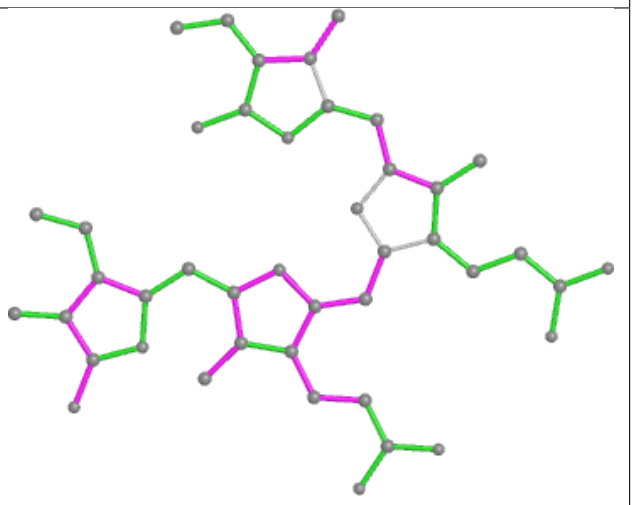

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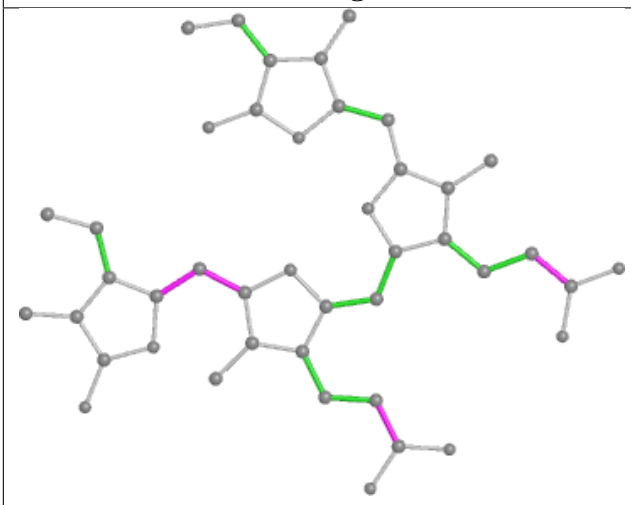

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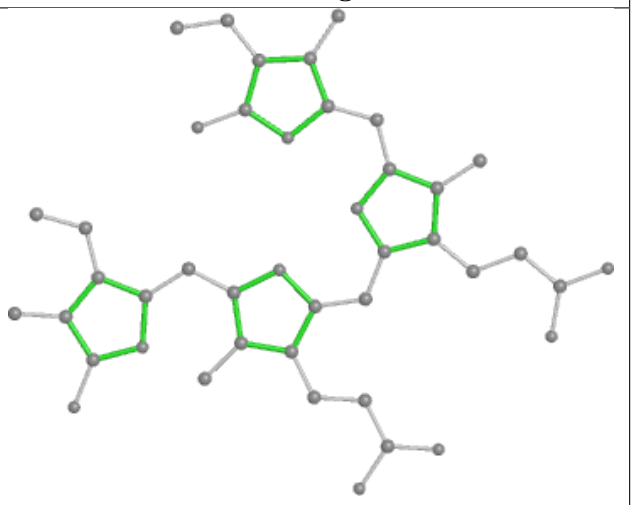
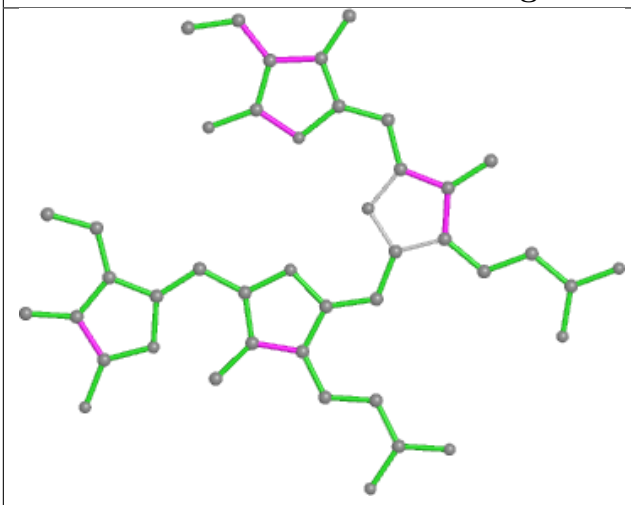


Rings

Ligand PEB ev 202



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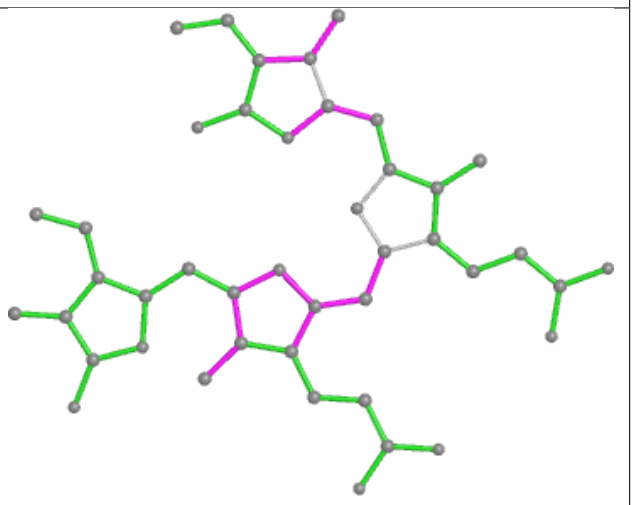

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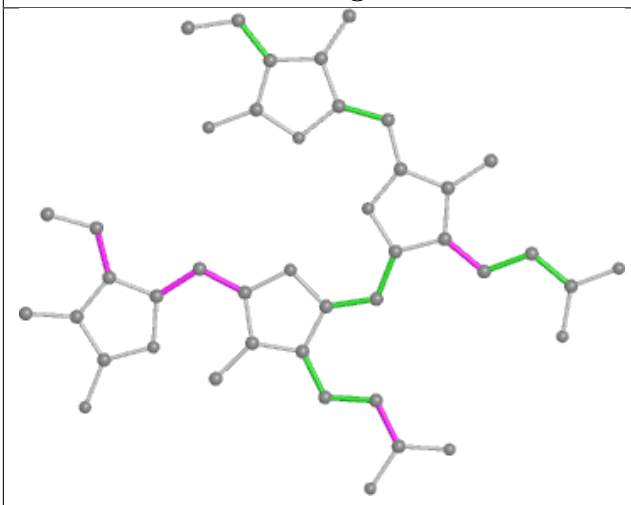

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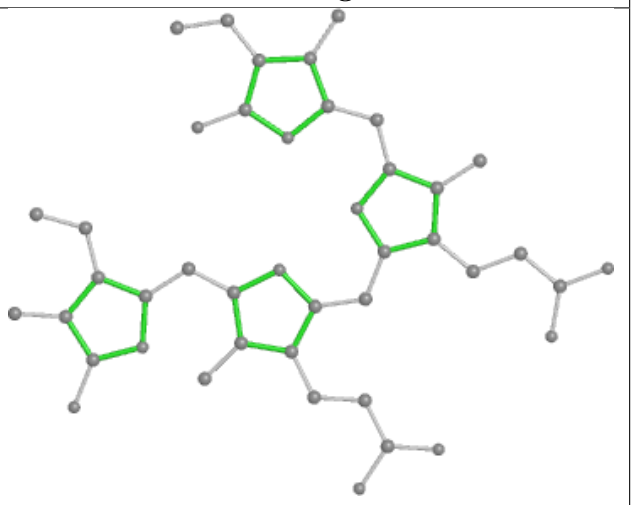
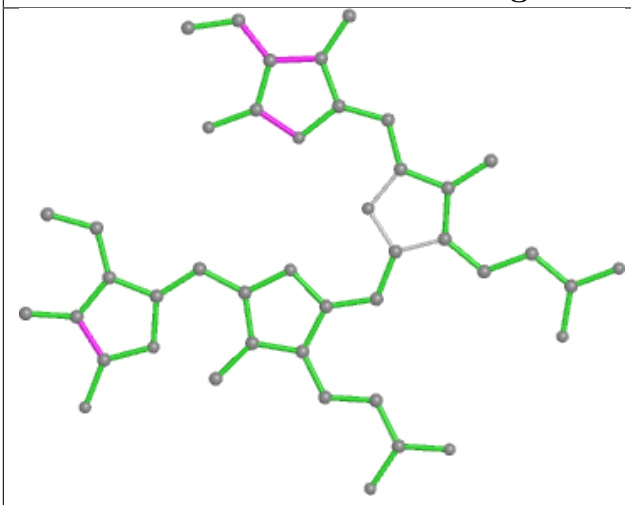


Rings

Ligand PEB y4 1001



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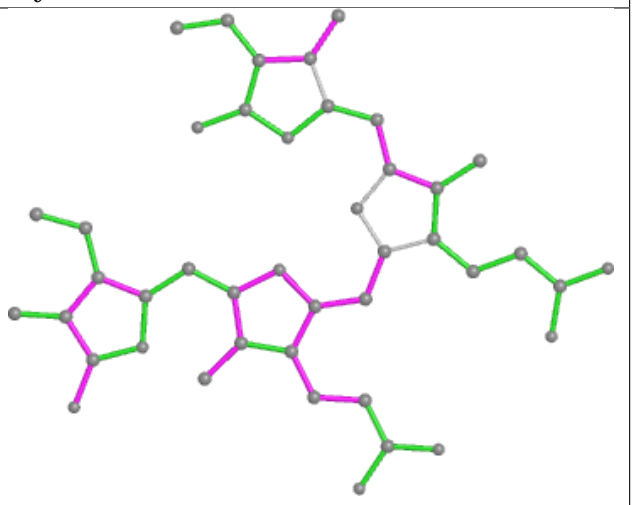

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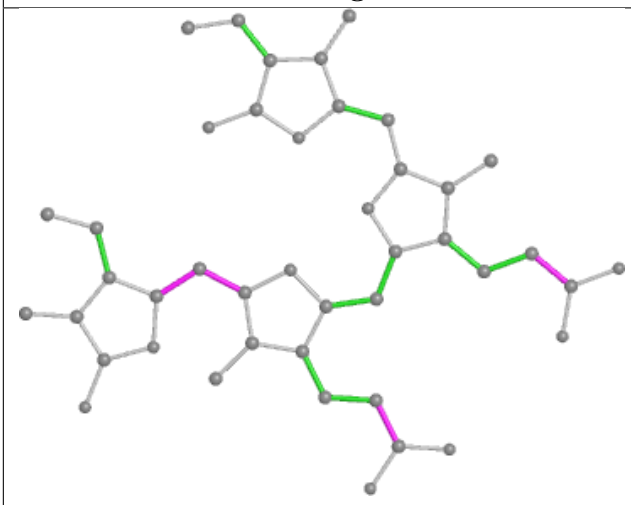

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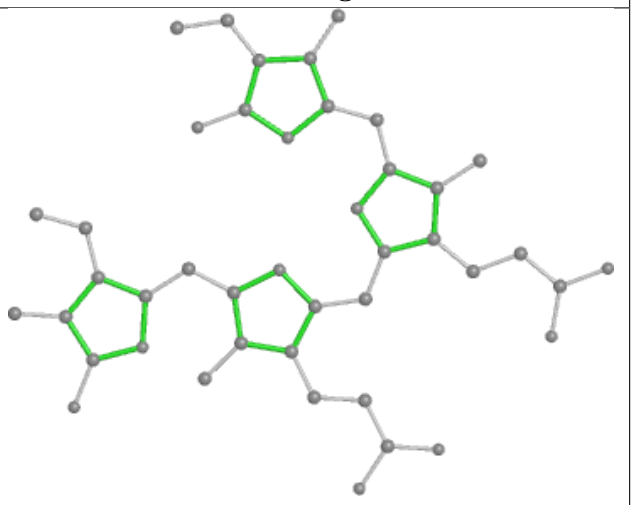

Rings

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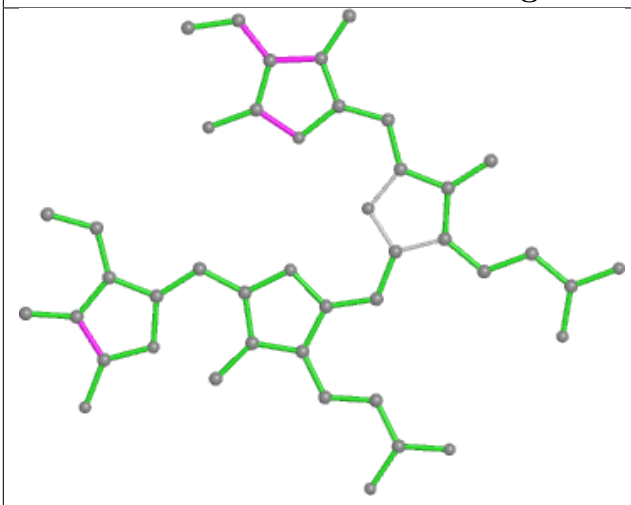

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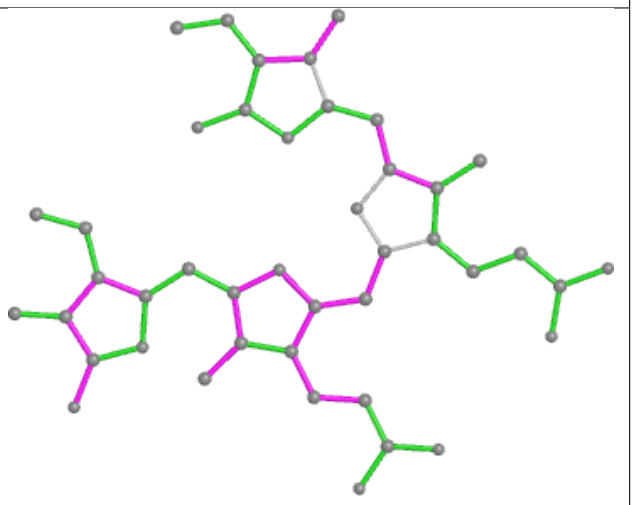

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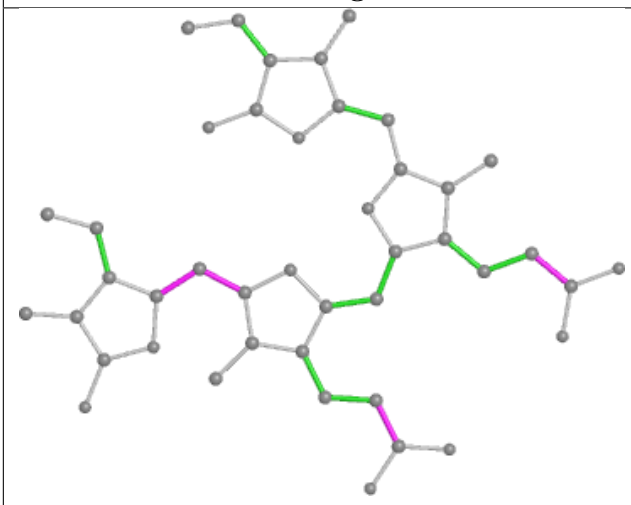

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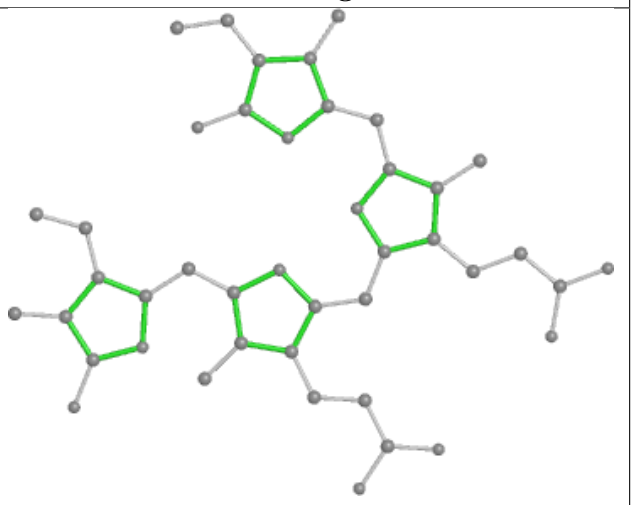
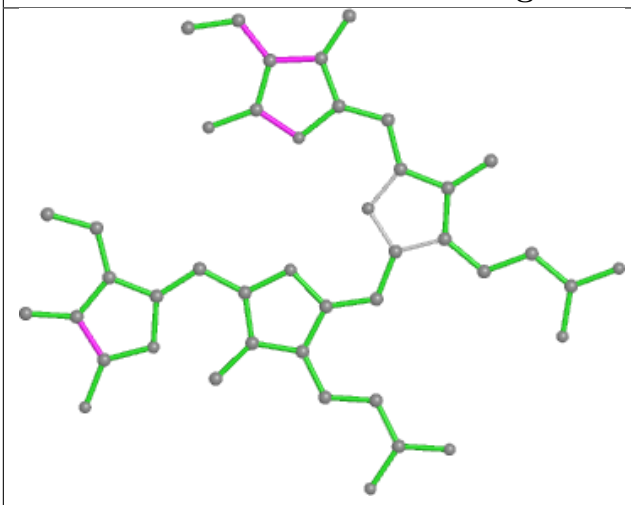


Rings

Ligand PEB aB 201



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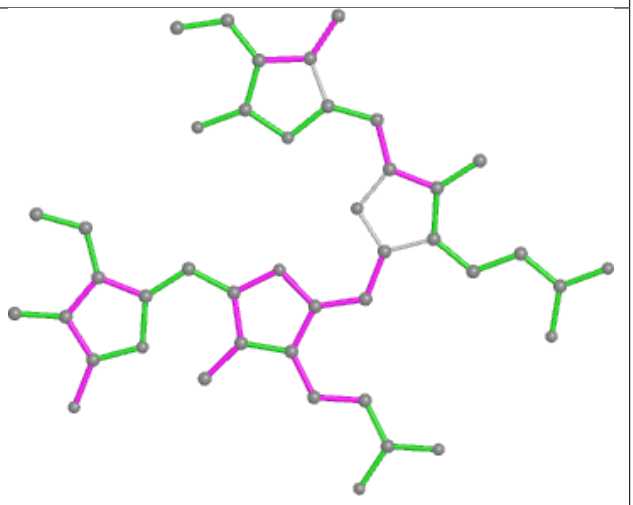

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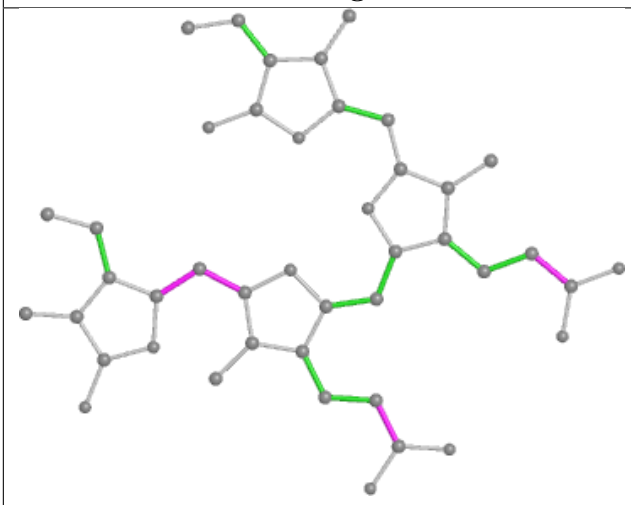
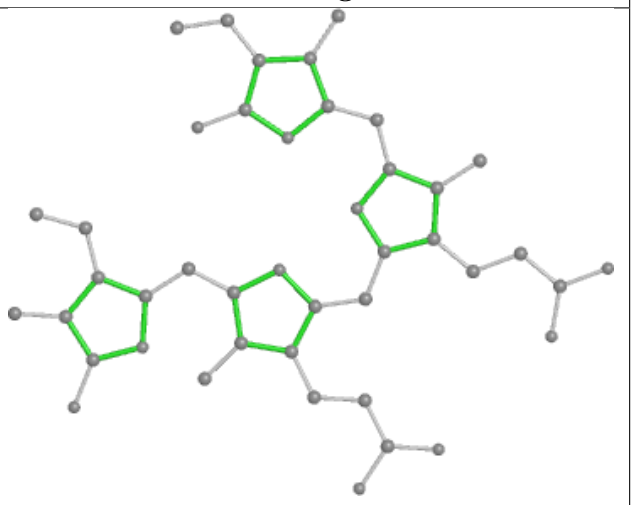
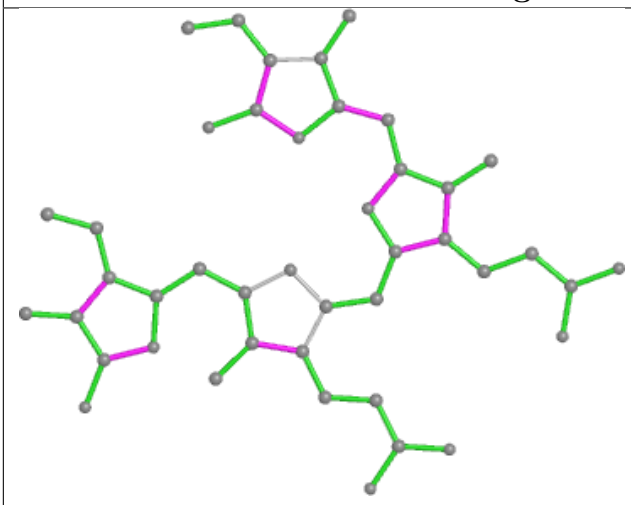


Torsions



Rings

Ligand PUB bP 203



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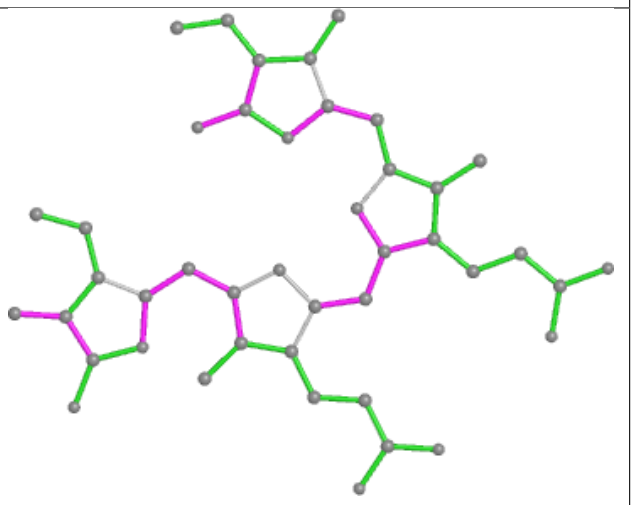
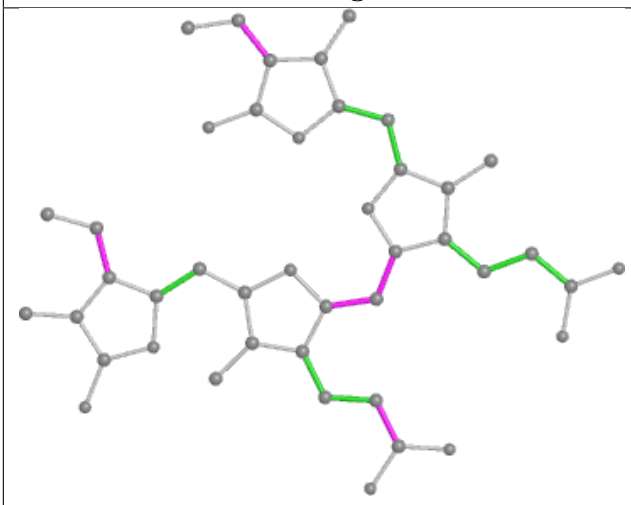


Bond angles



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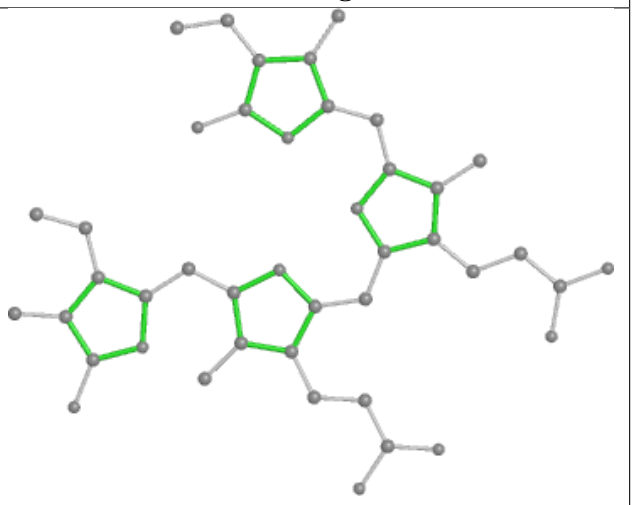
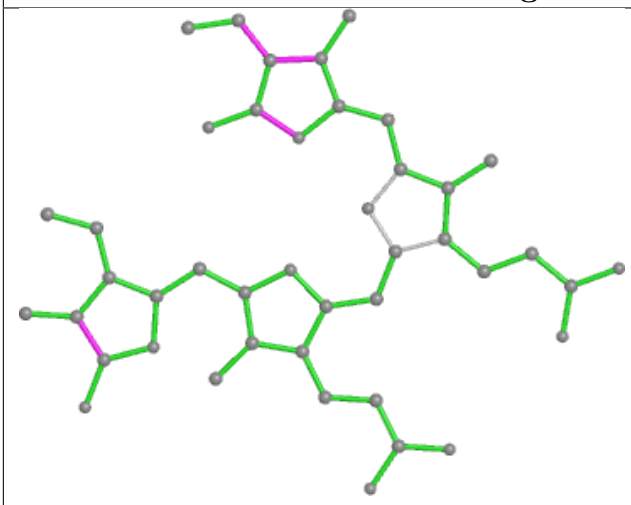


Rings

Ligand PEB eJ 201



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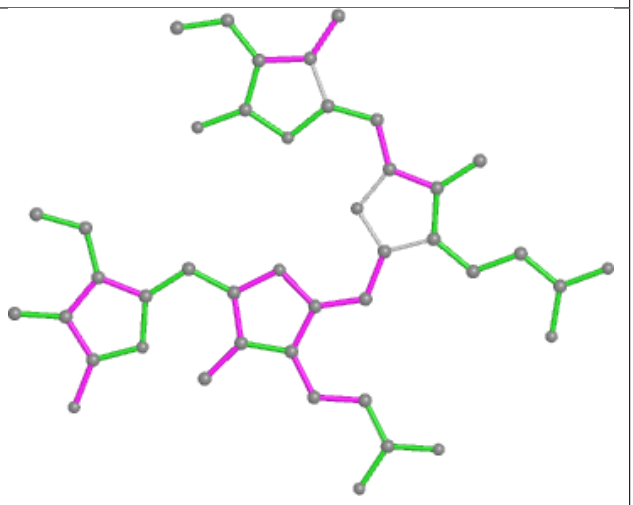

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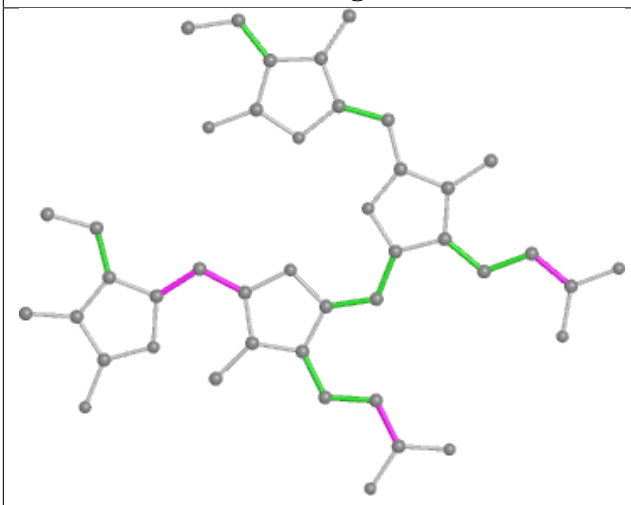

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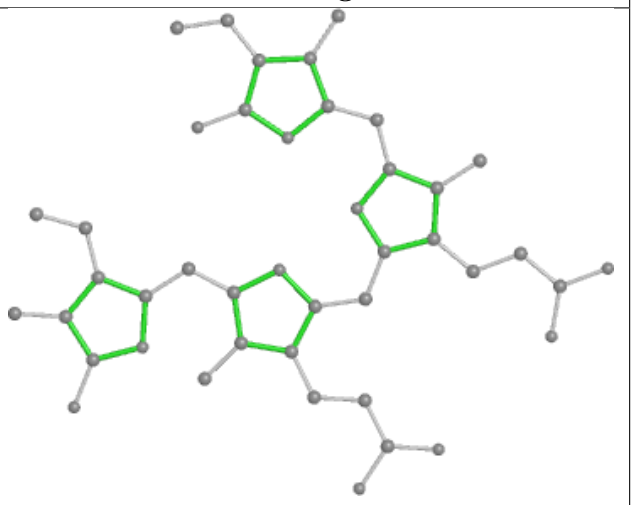
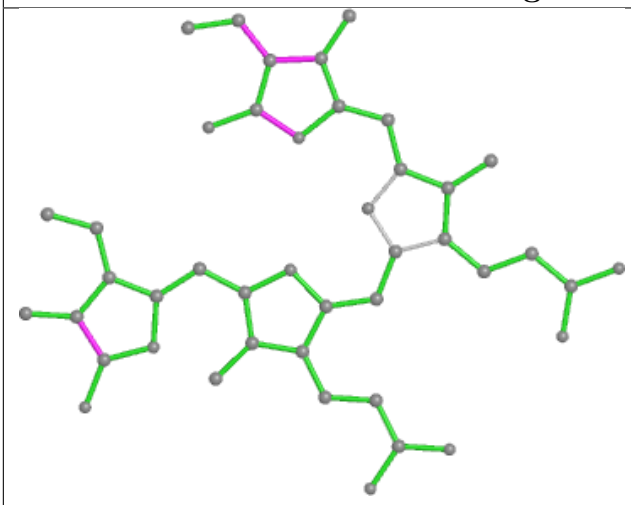


Rings

Ligand PEB j8 201



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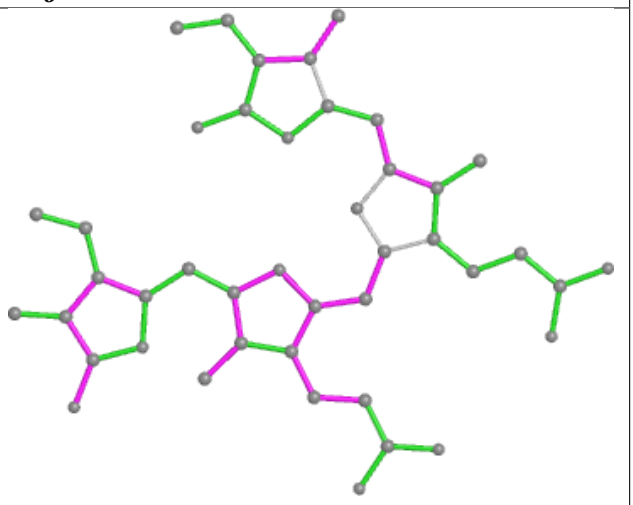

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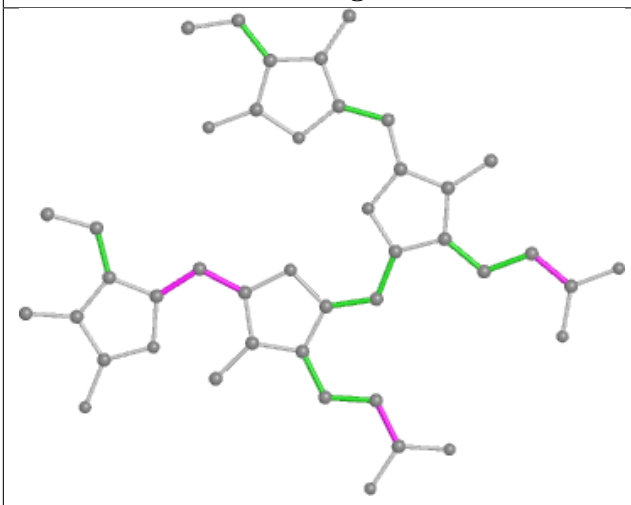

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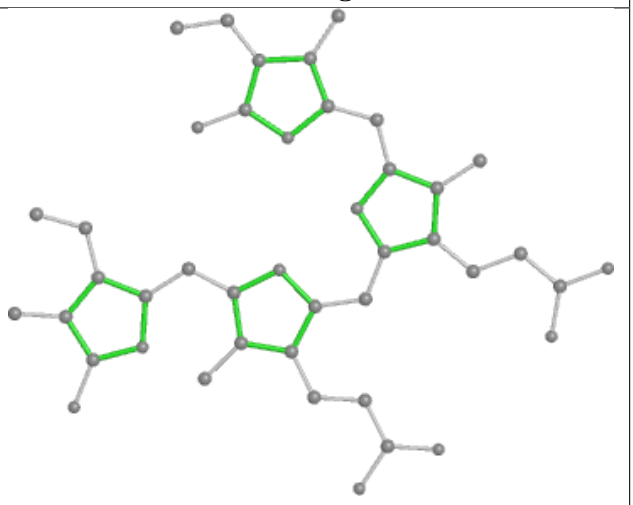
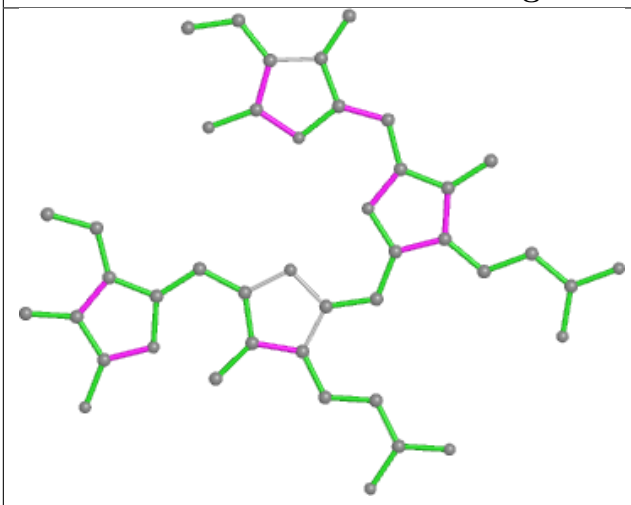


Rings

Ligand PUB el 203



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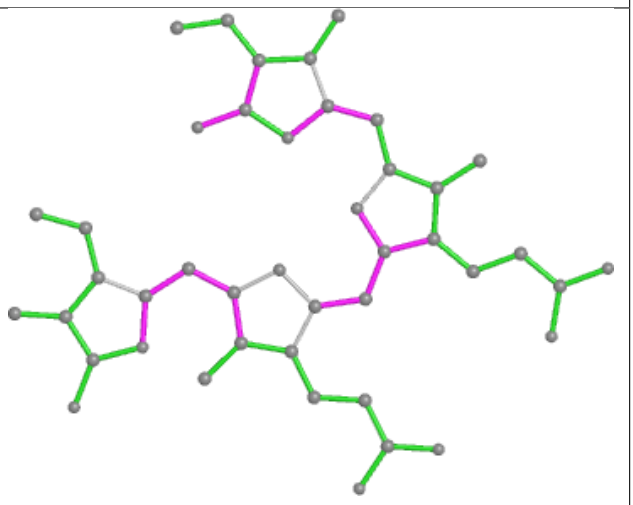

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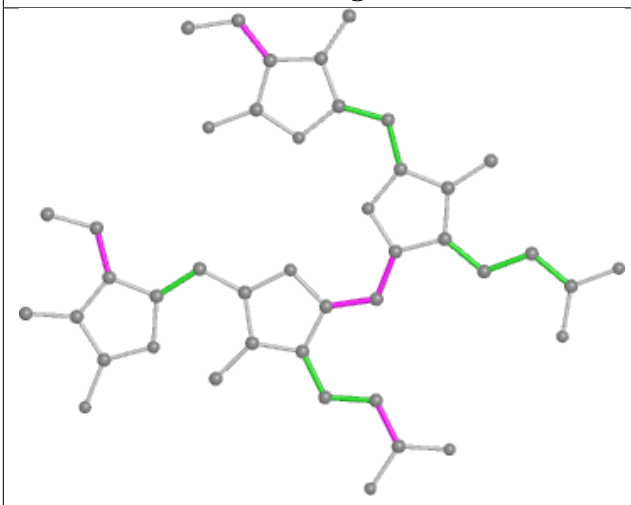

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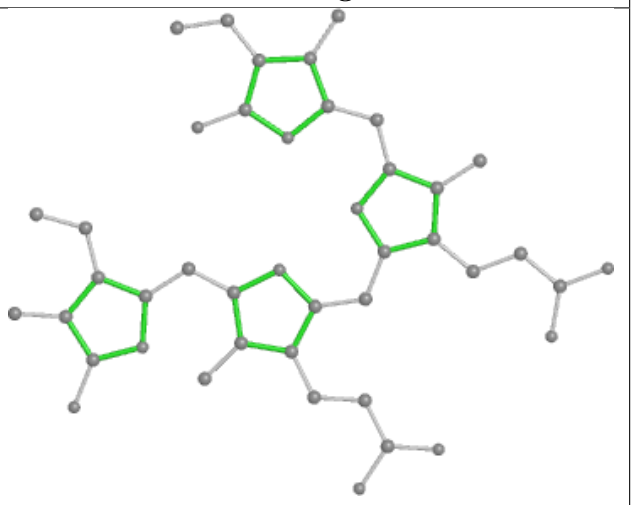
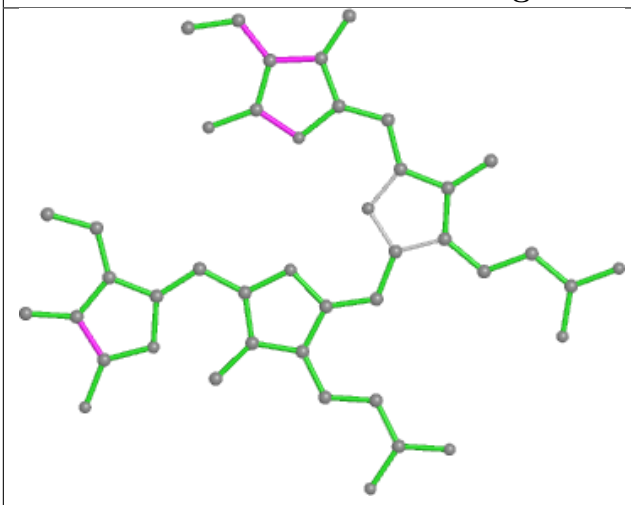


Rings

Ligand PEB ez 1003



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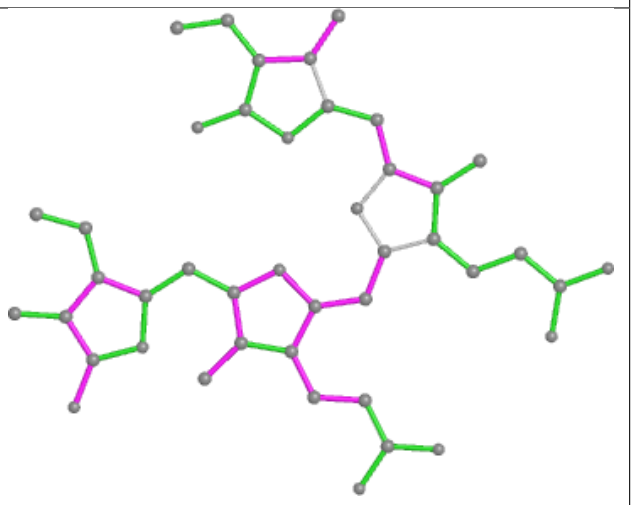

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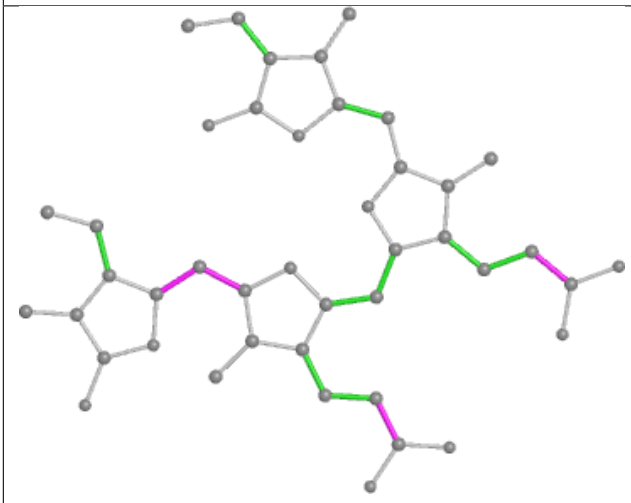

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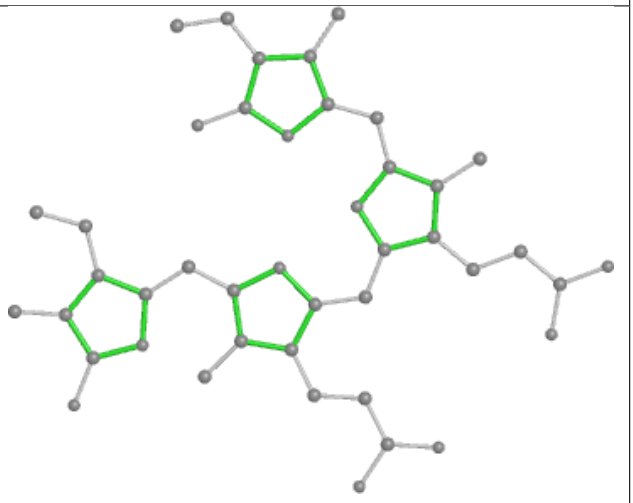

Rings

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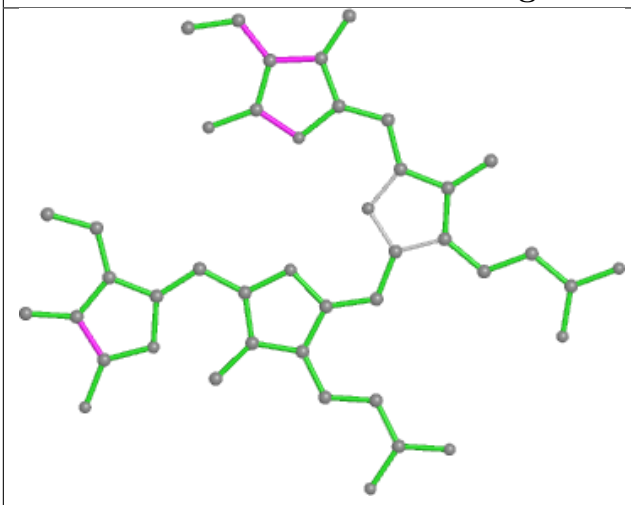

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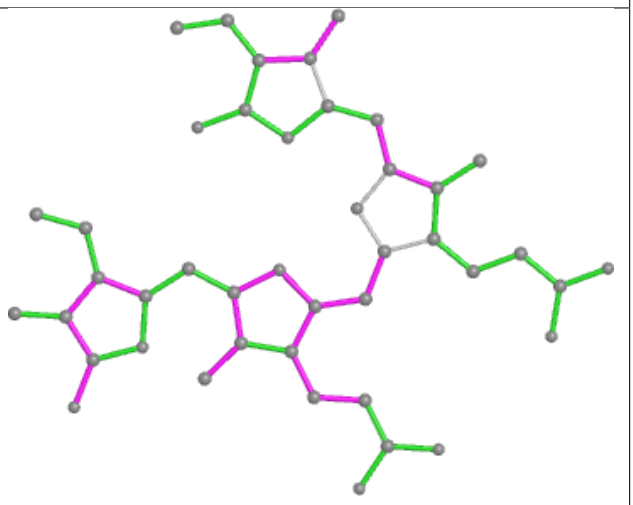

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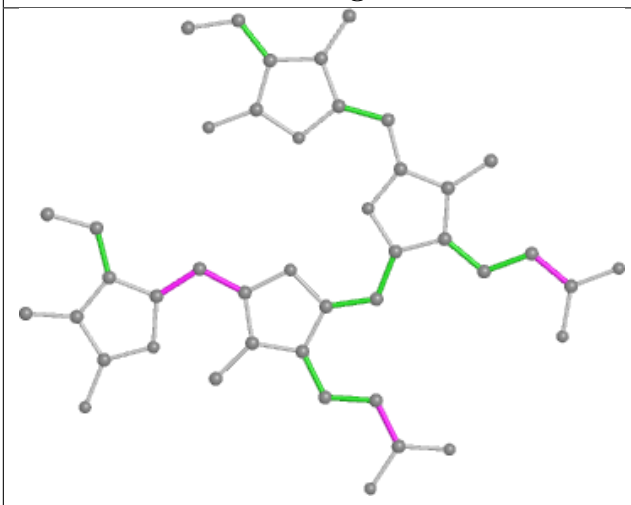

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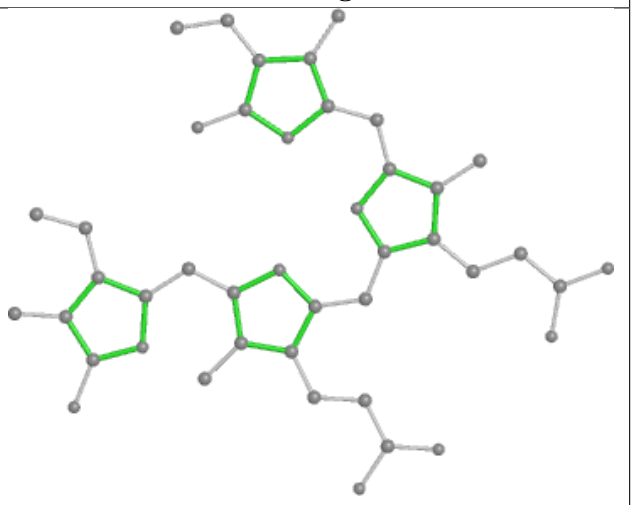
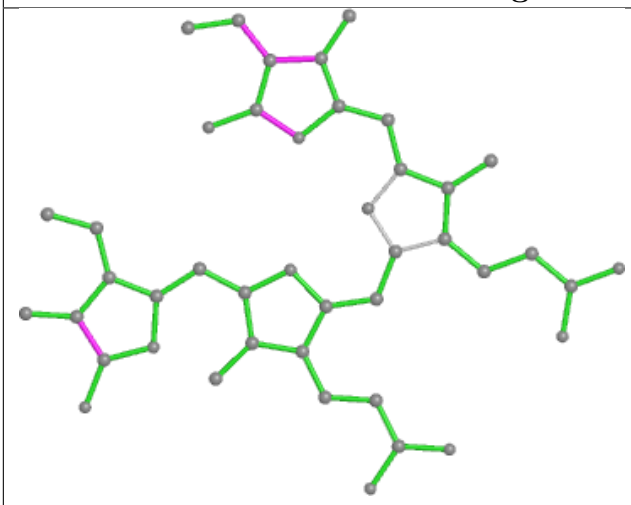


Rings

Ligand PEB cW 202



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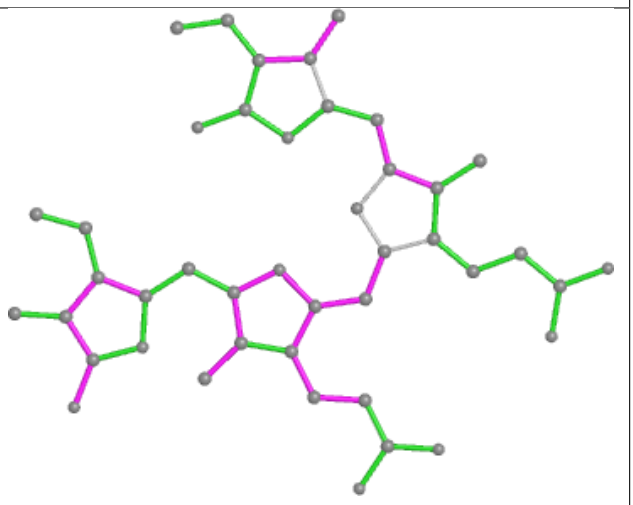

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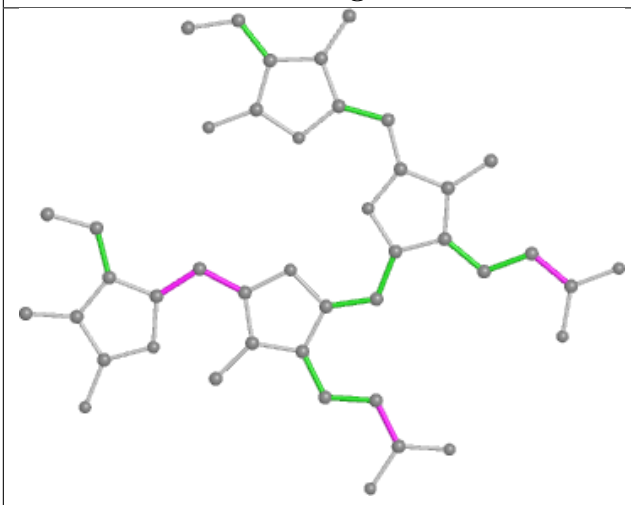

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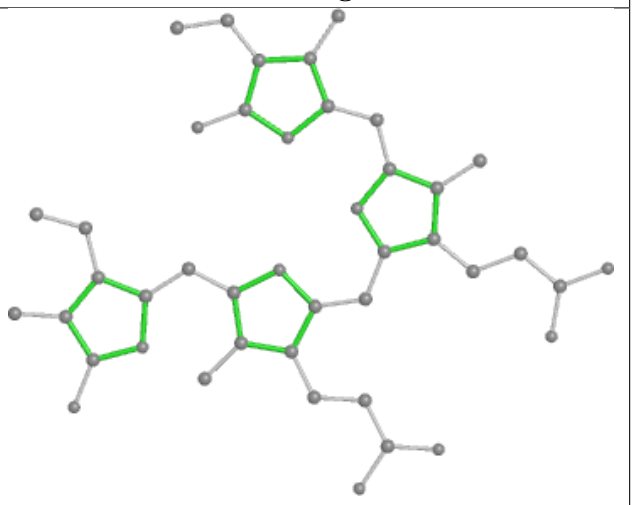
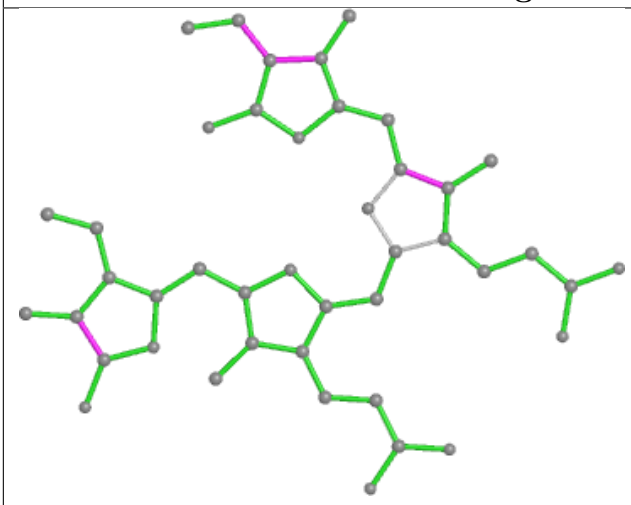


Rings

Ligand PEB U7 202



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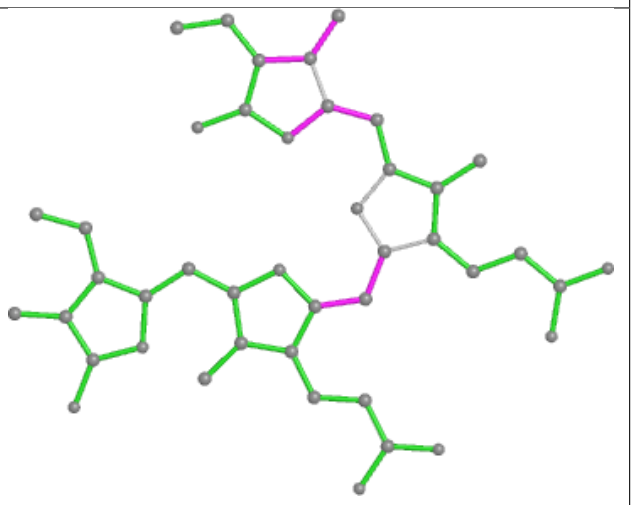

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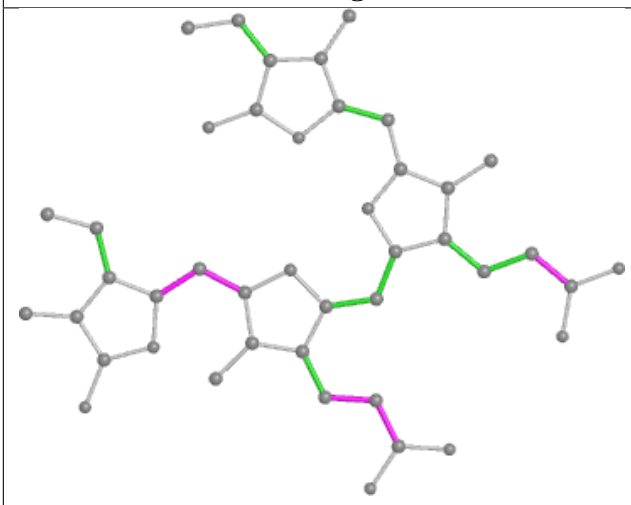

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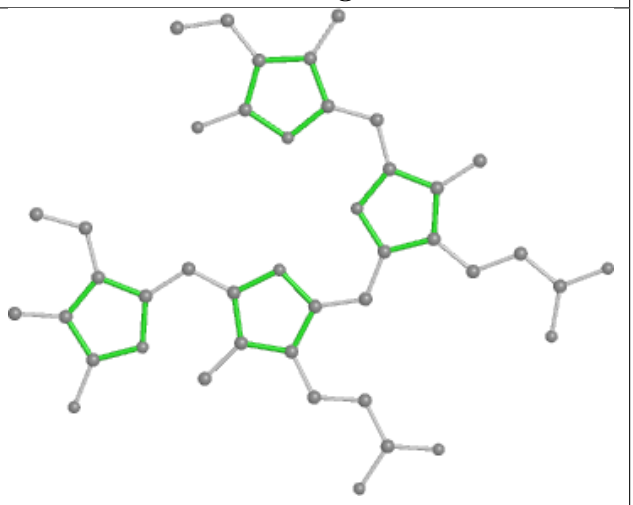

Rings

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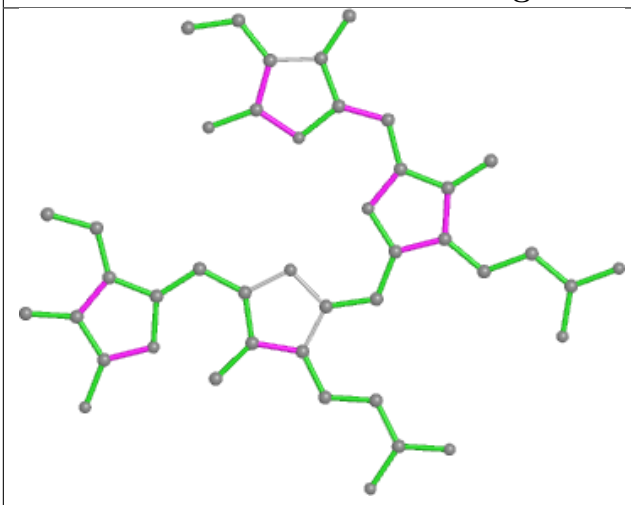

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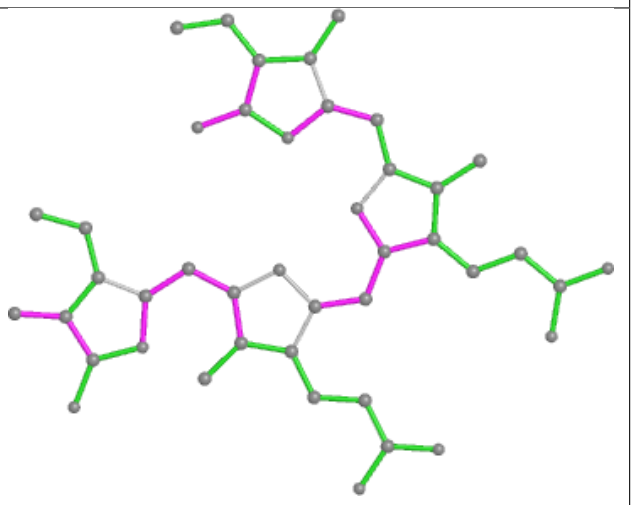

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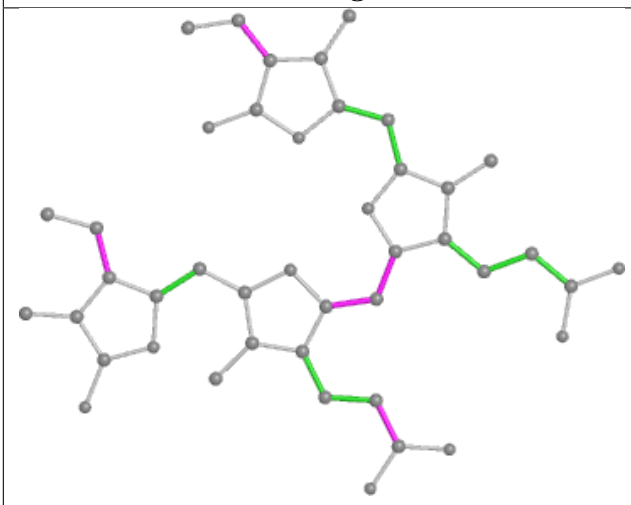

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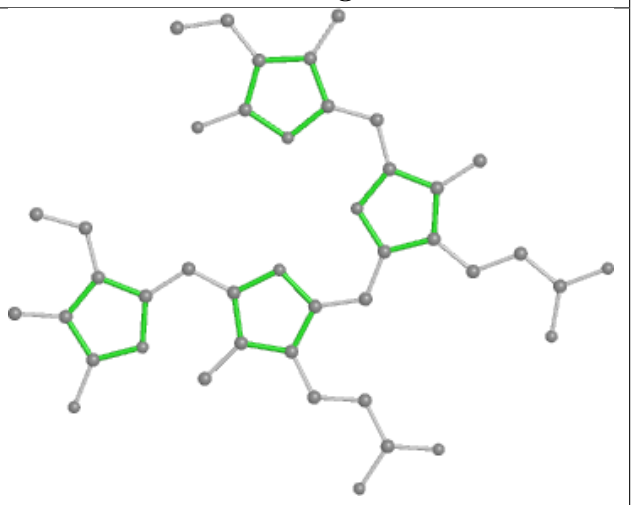
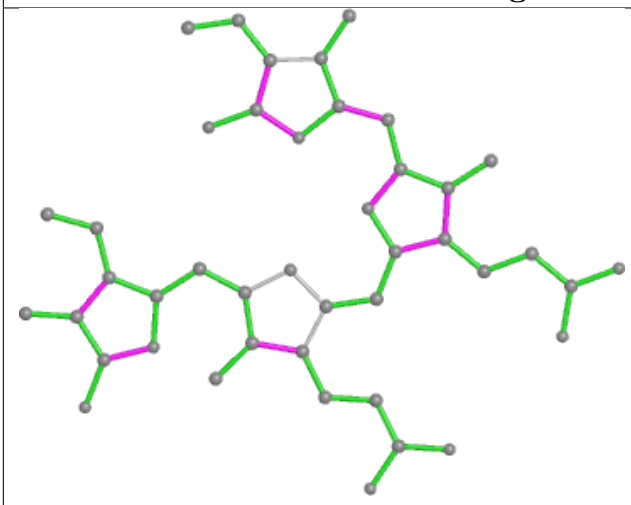


Rings

Ligand PUB ey 1006



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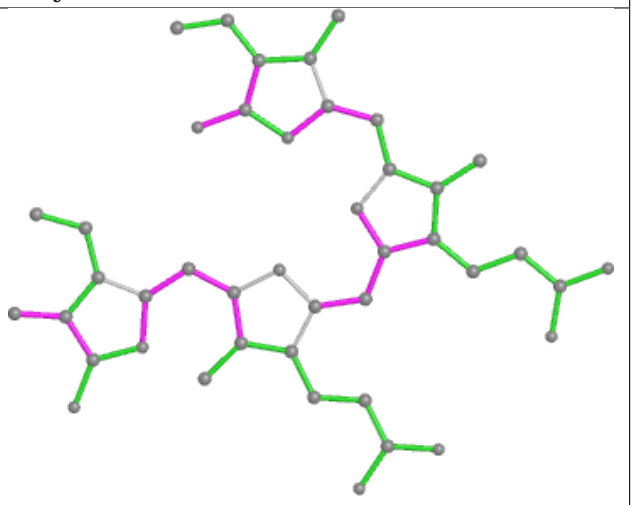

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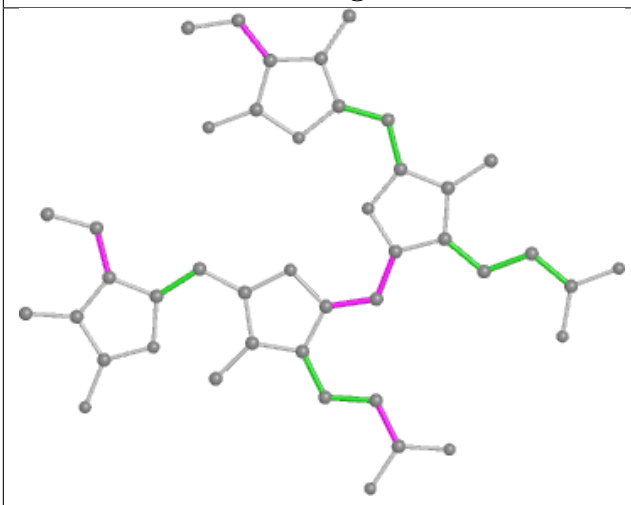

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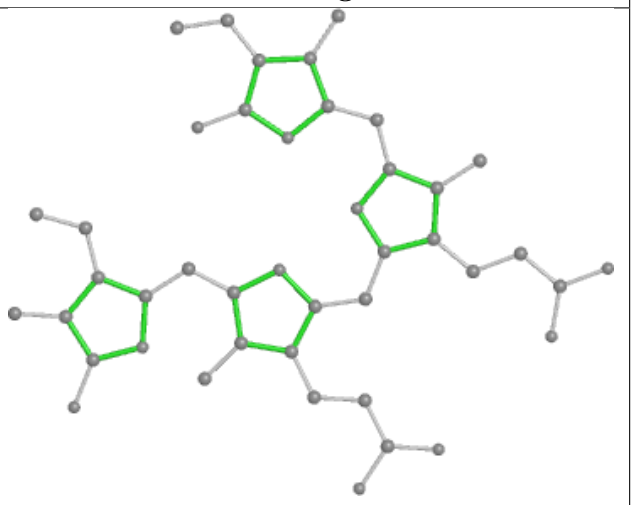
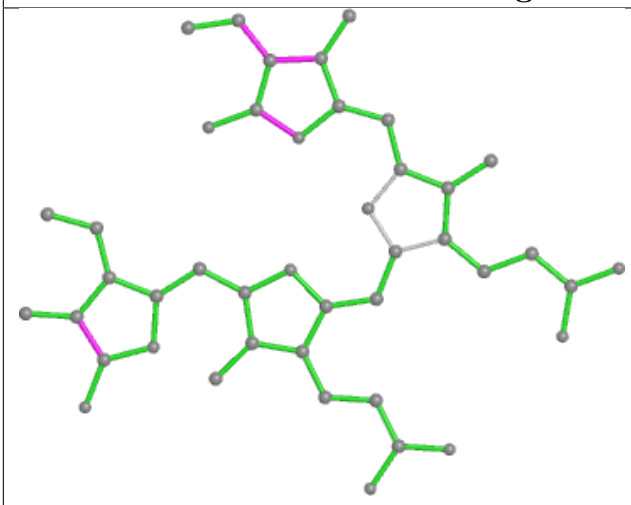


Rings

Ligand PEB A5 201



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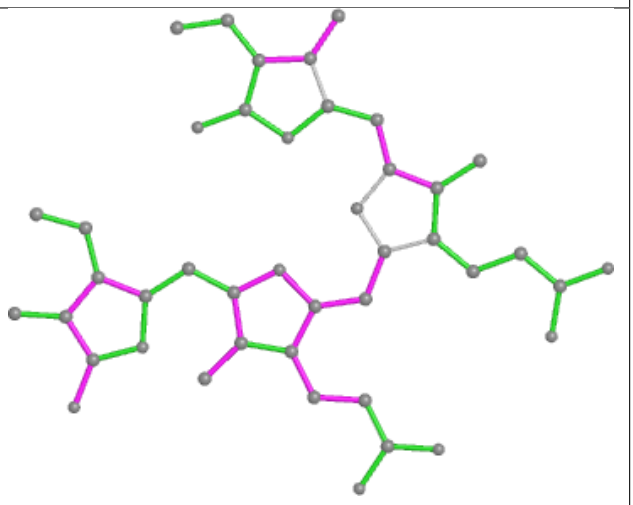

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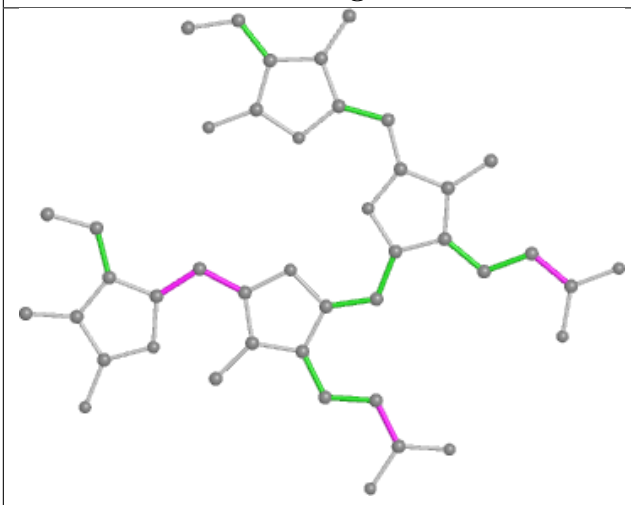

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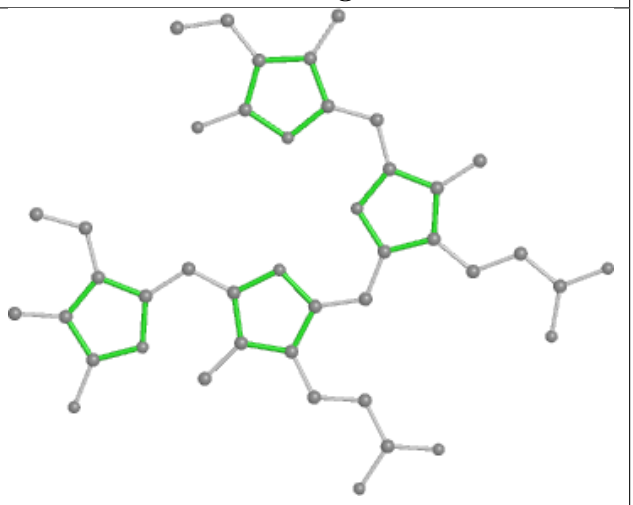
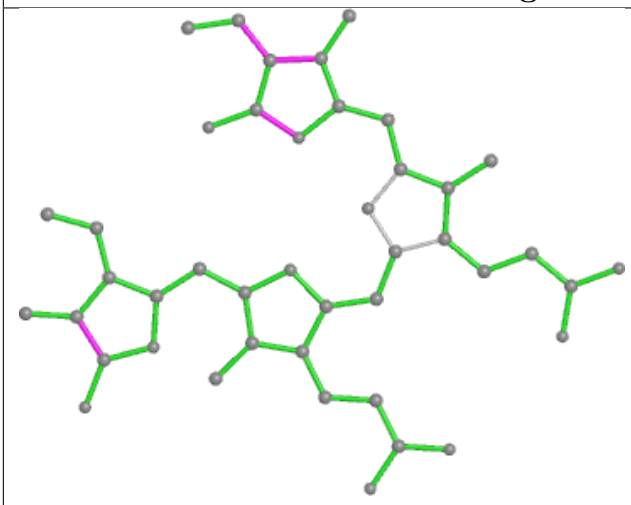


Rings

Ligand PEB aq 201



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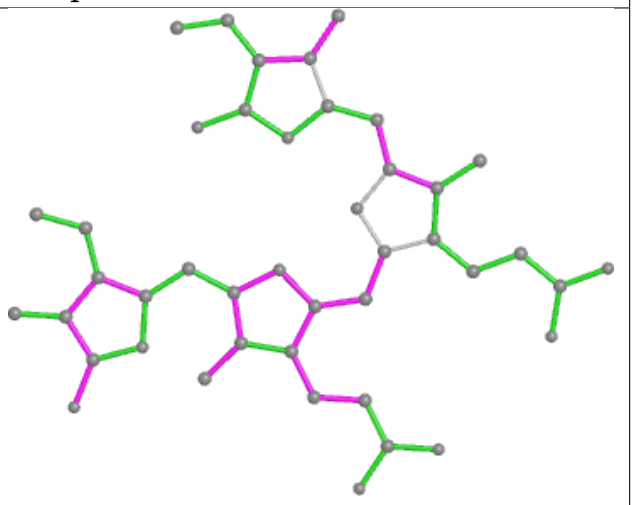

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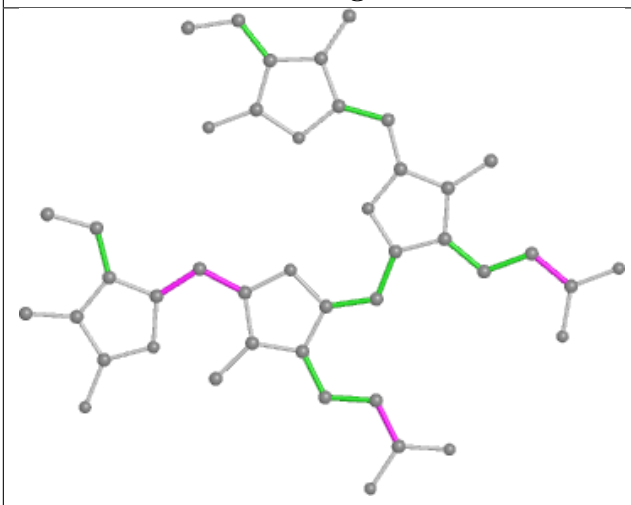

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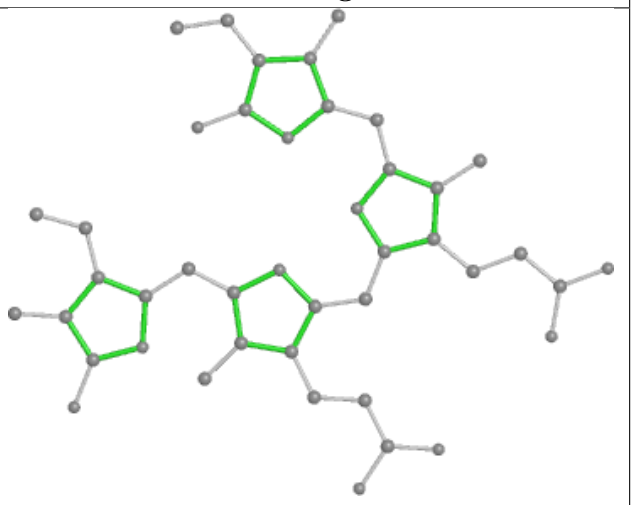
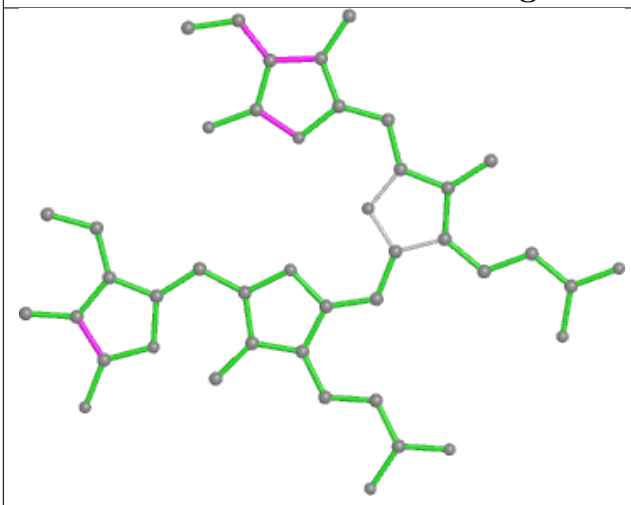


Rings

Ligand PEB q9 201



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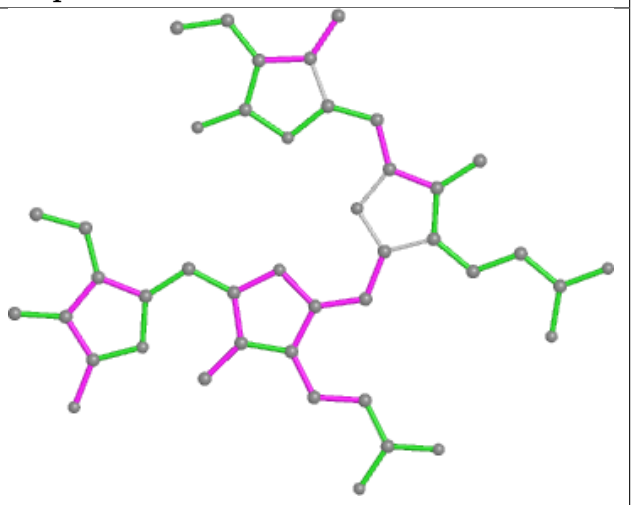
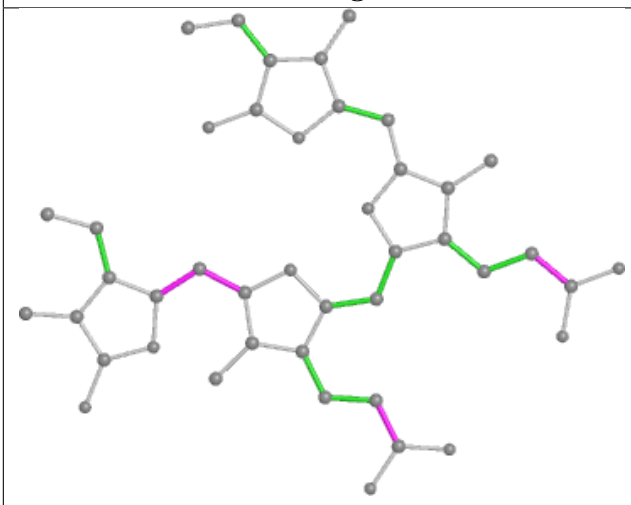


Bond angles



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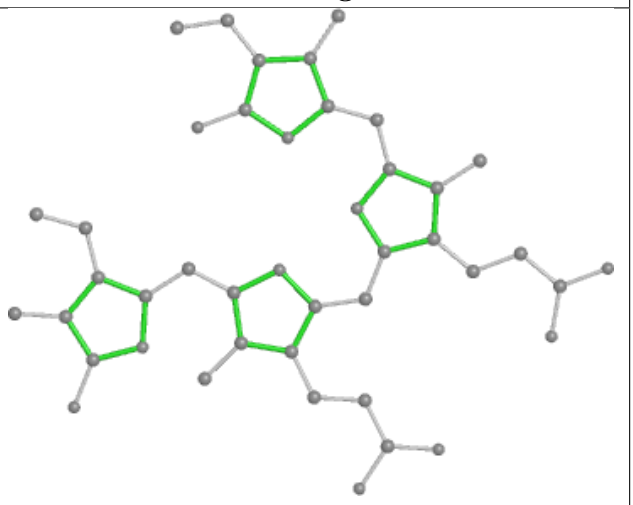
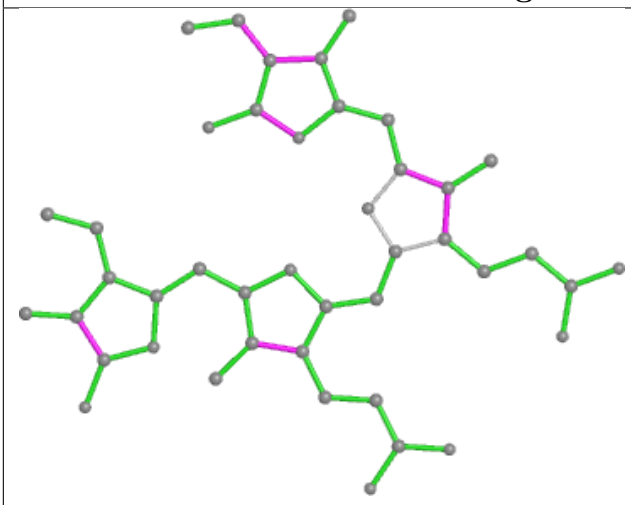
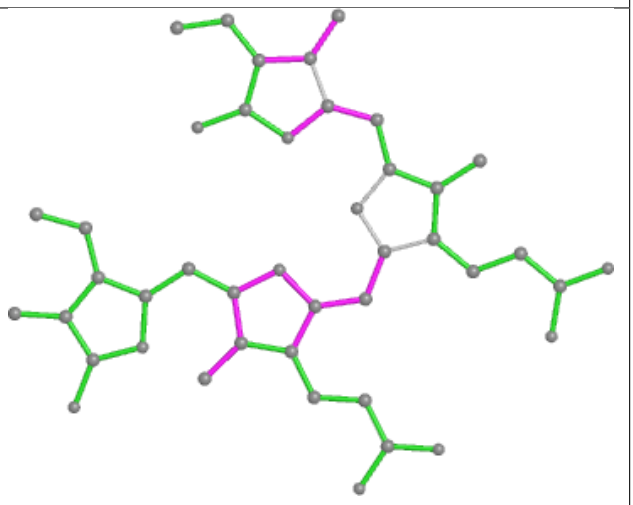


Rings

Ligand PEB R6 202



Bond lengths



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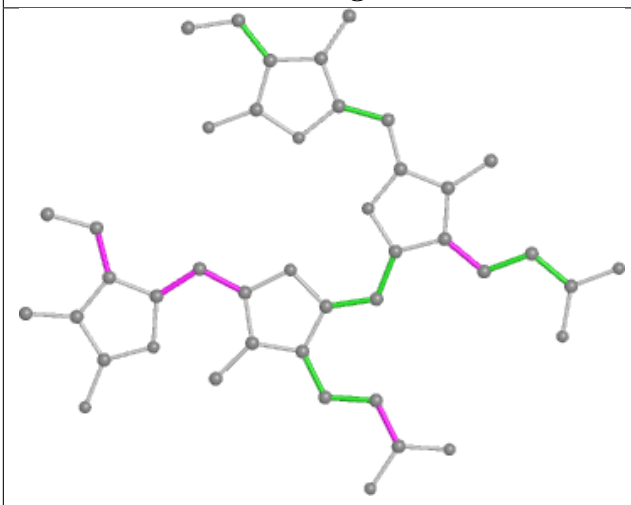
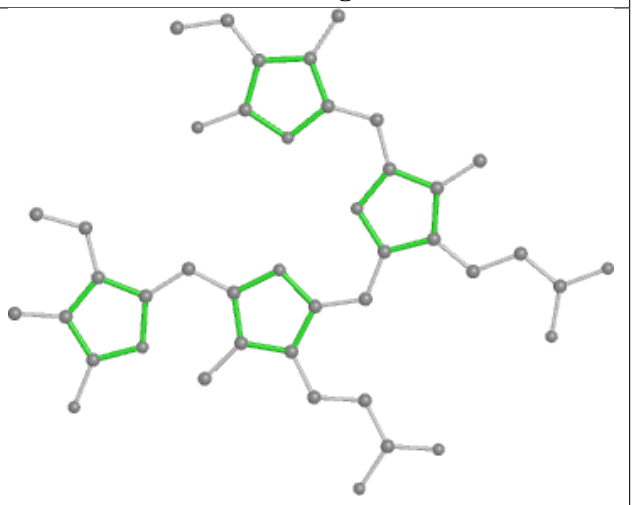
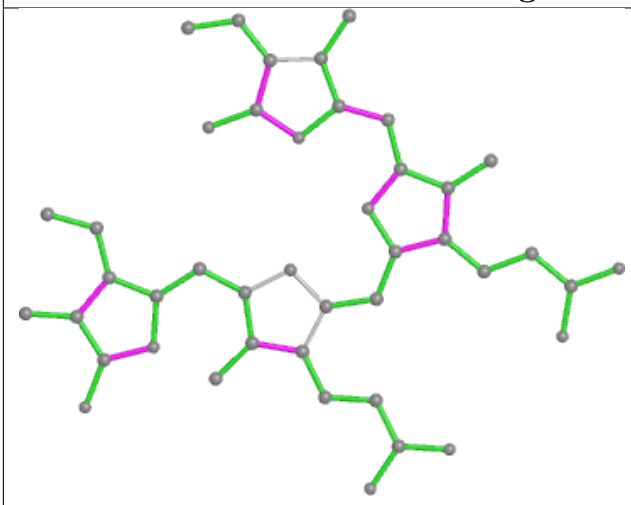


Torsions



Rings

Ligand PUB z7 203



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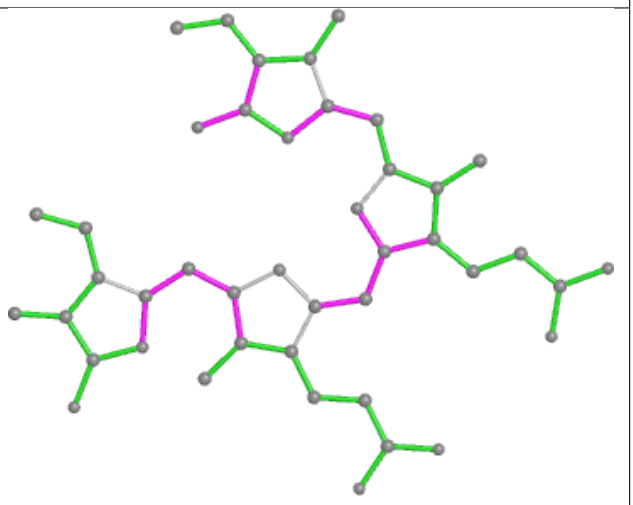

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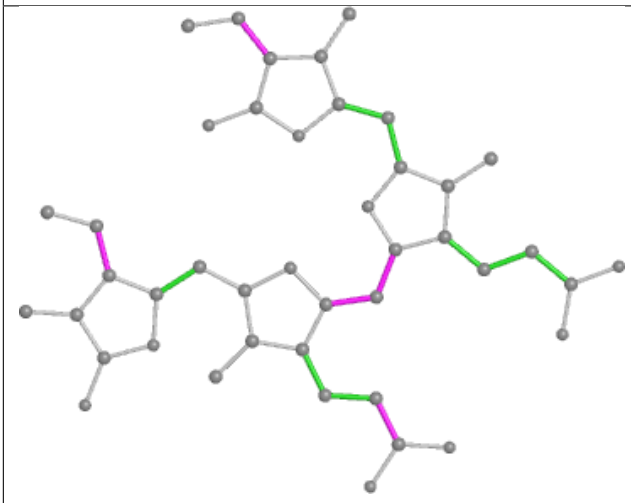

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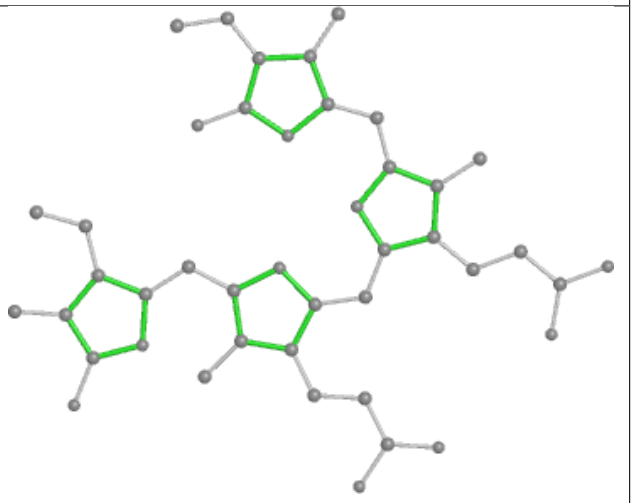
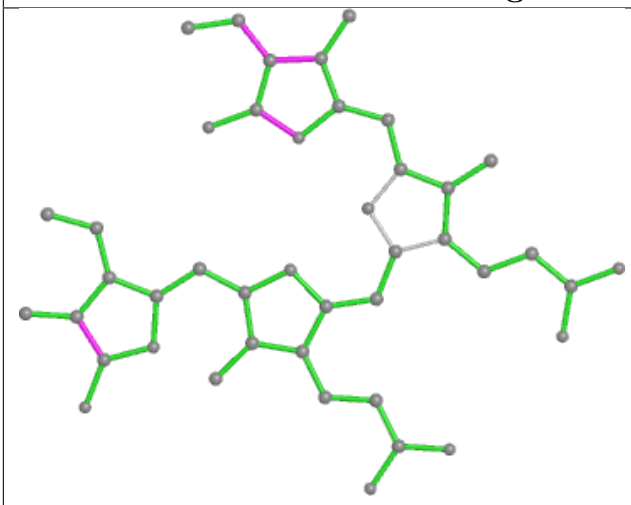


Rings

Ligand PEB V8 1001



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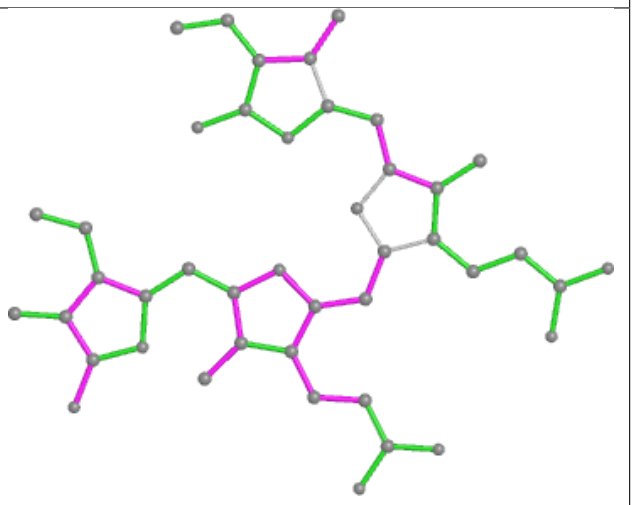

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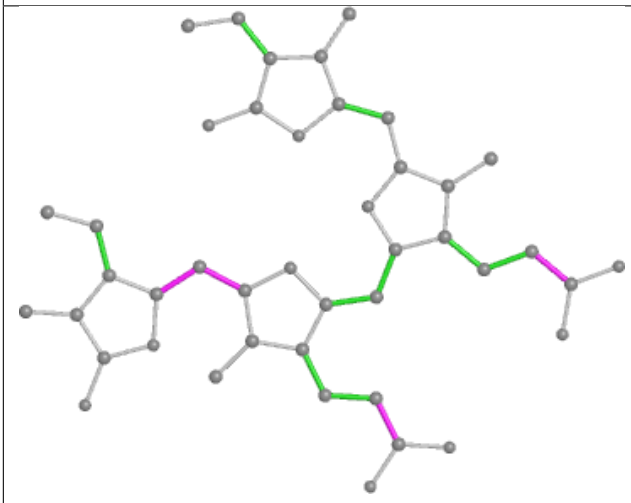

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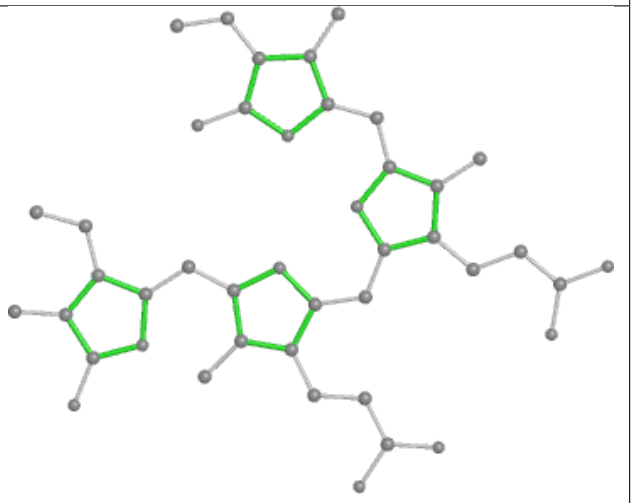
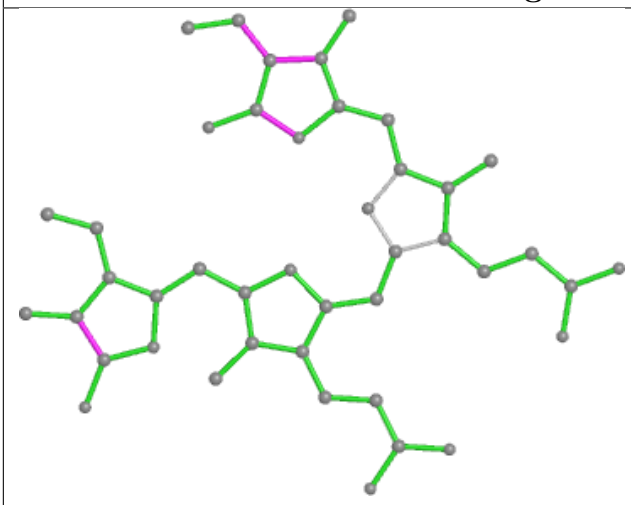


Rings

Ligand PEB le 201



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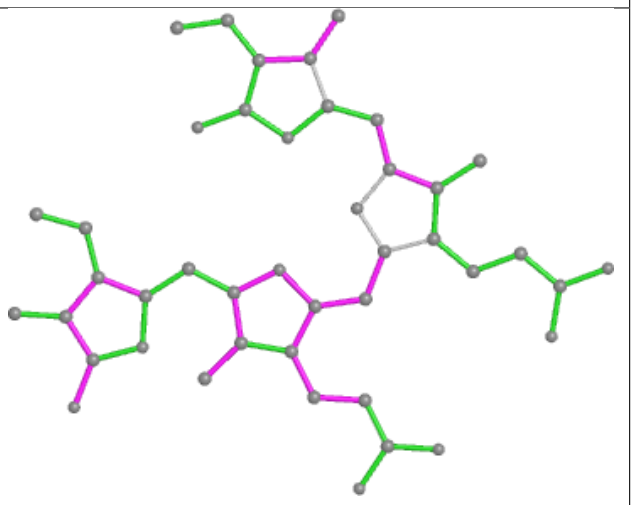

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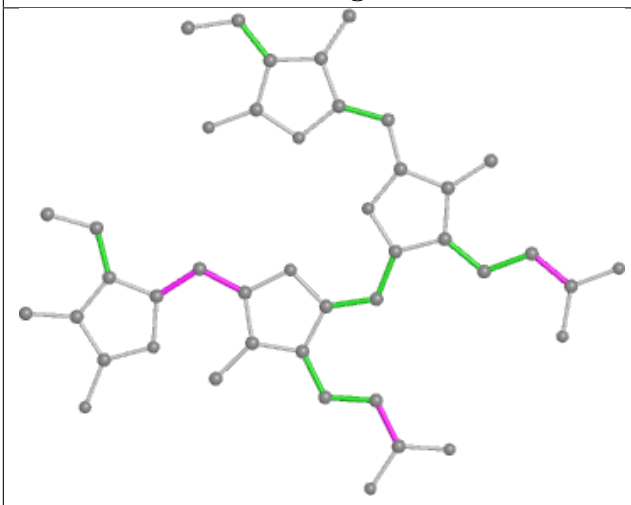

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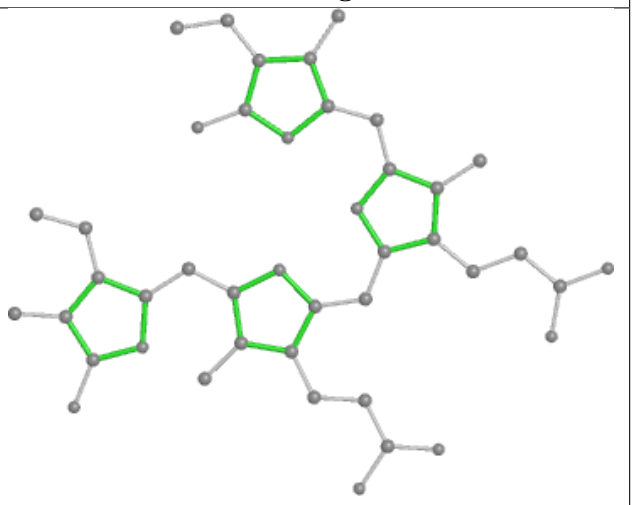

Rings

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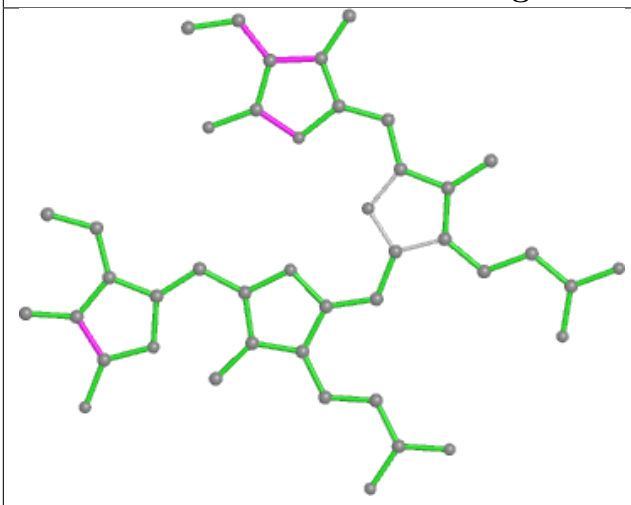

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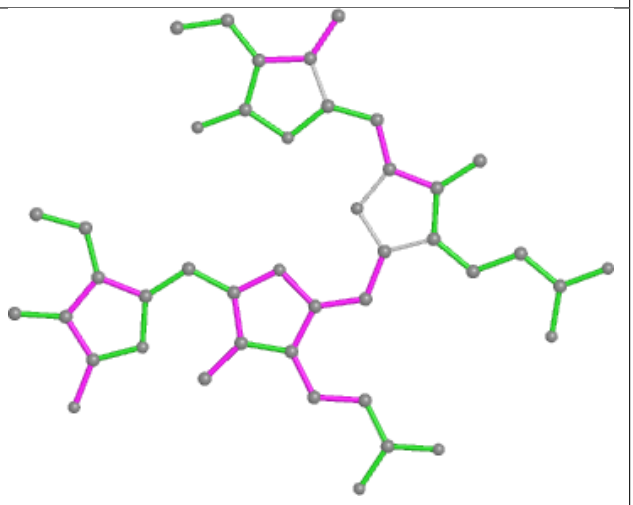

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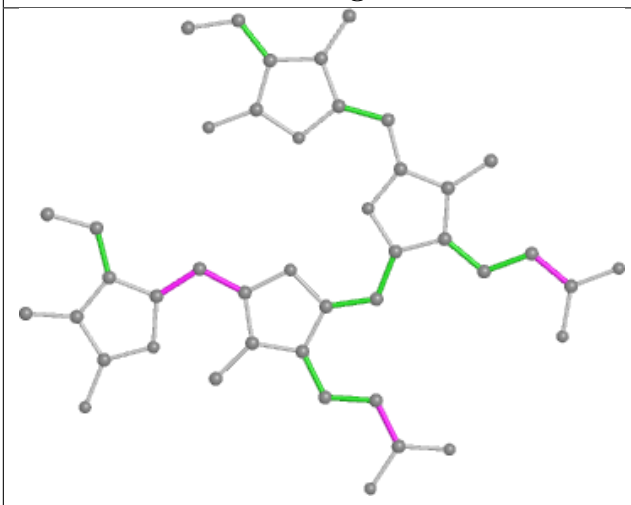

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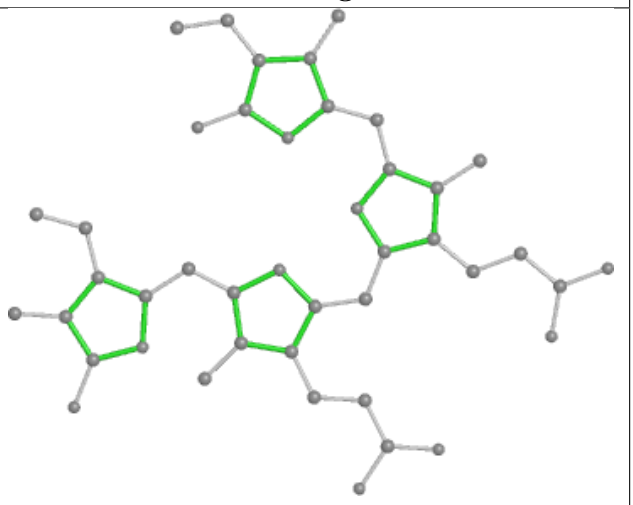

Rings

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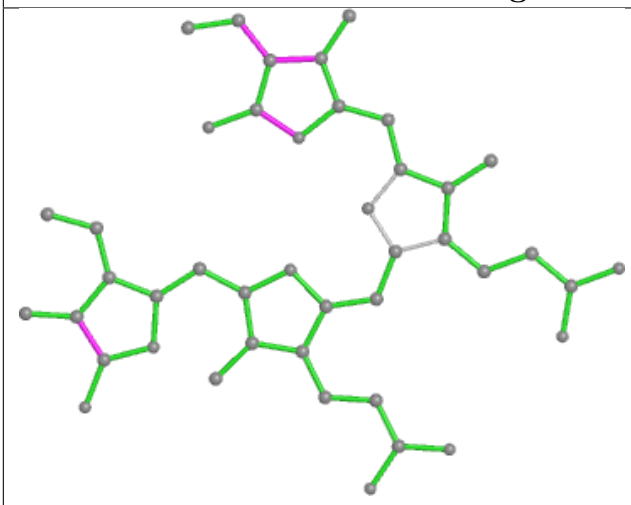

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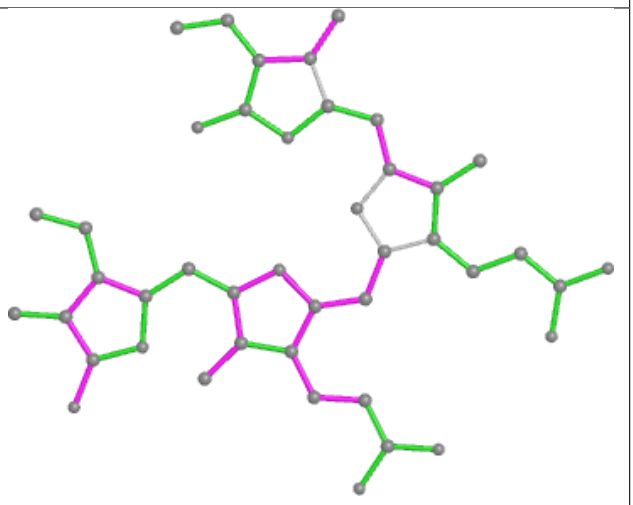

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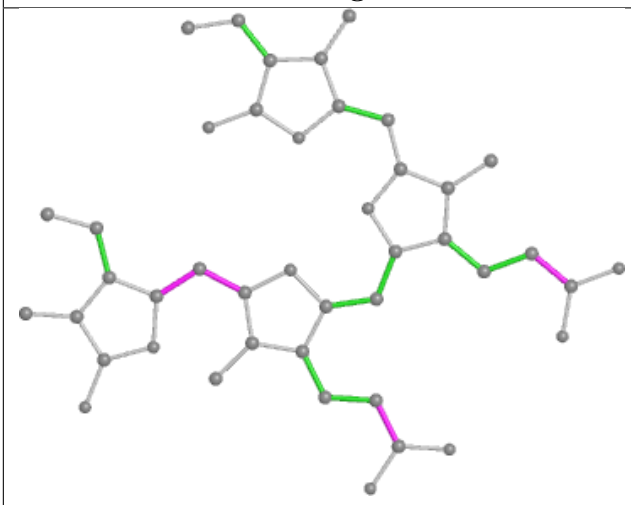

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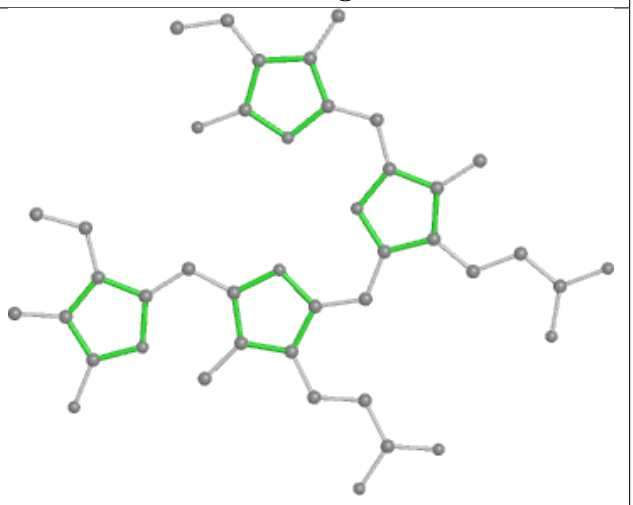

Rings

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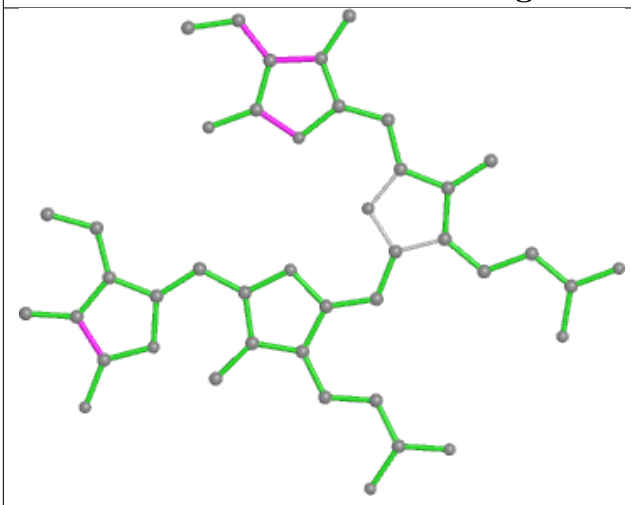

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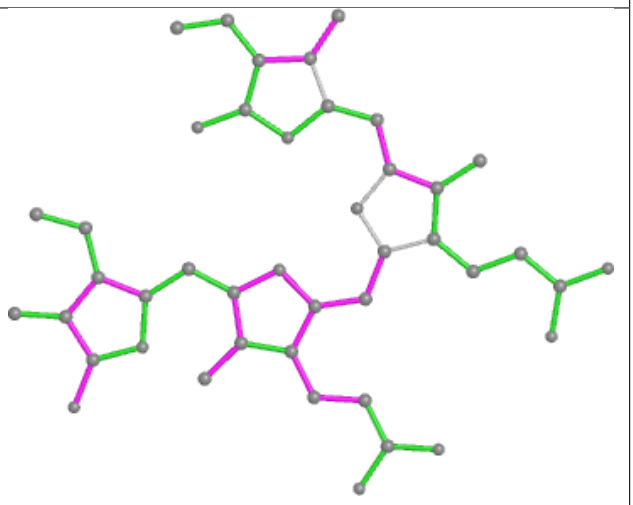

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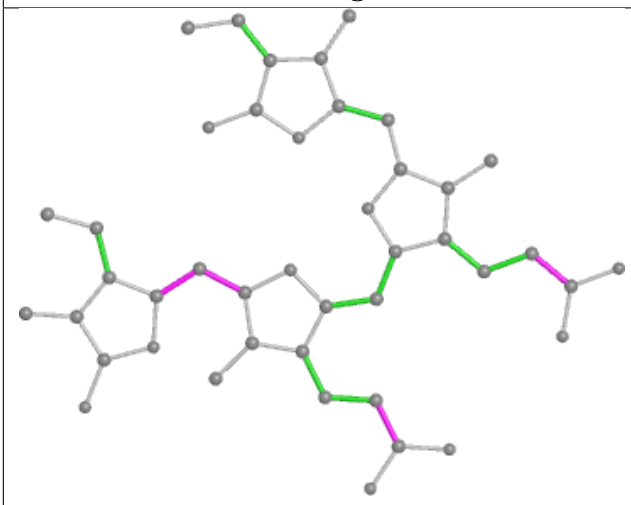

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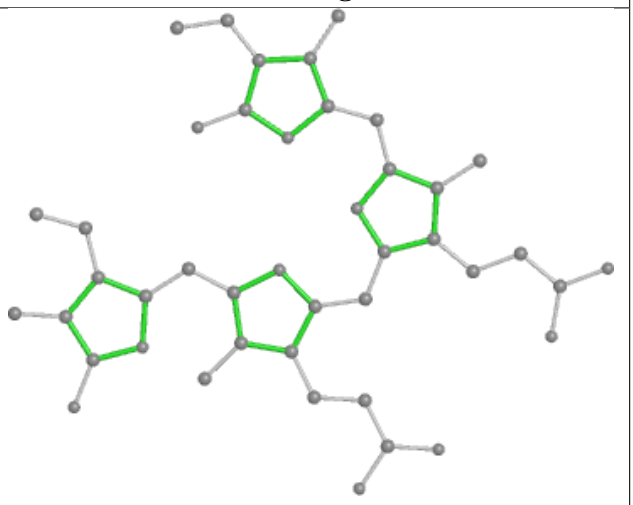

Rings

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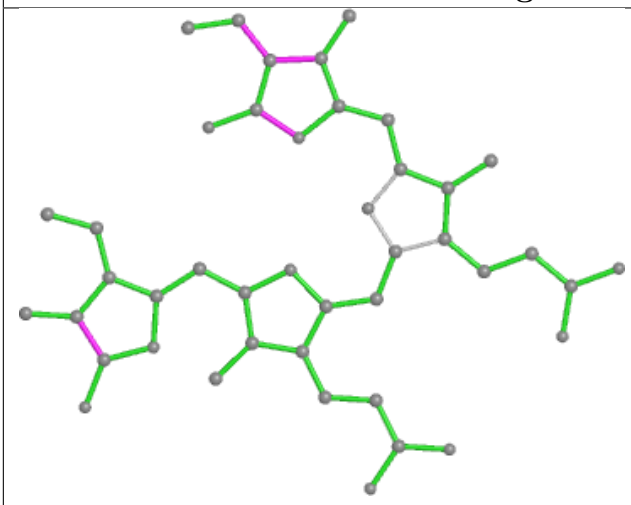

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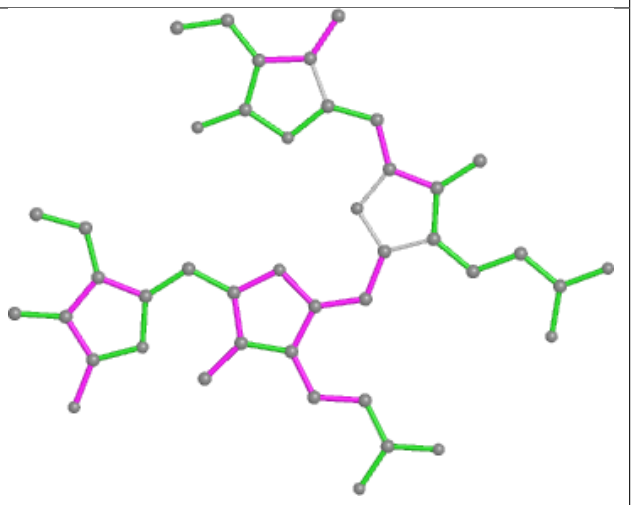

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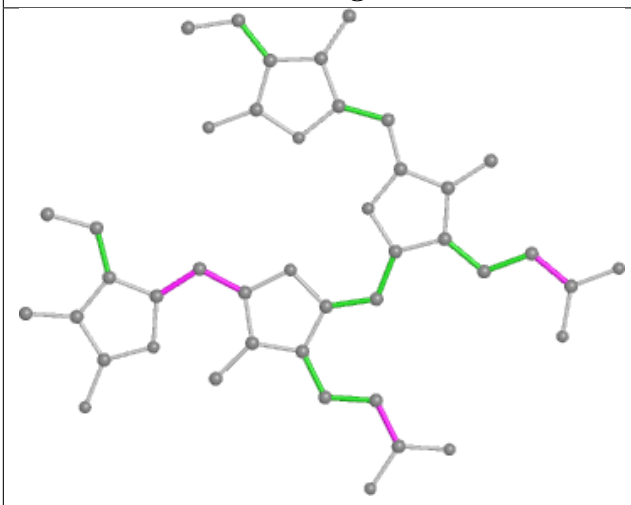

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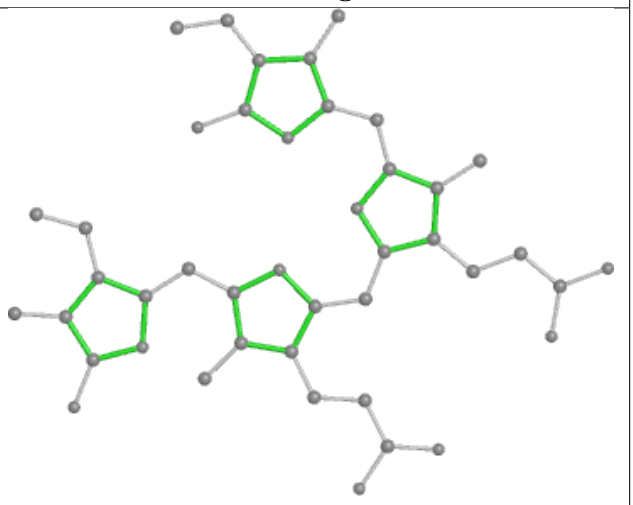

Rings

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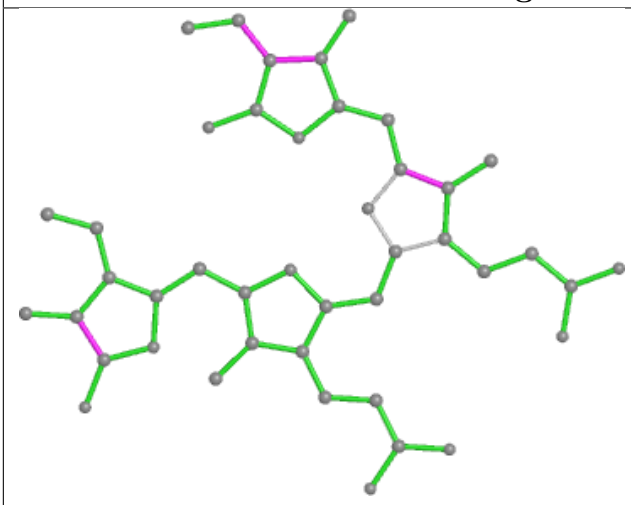

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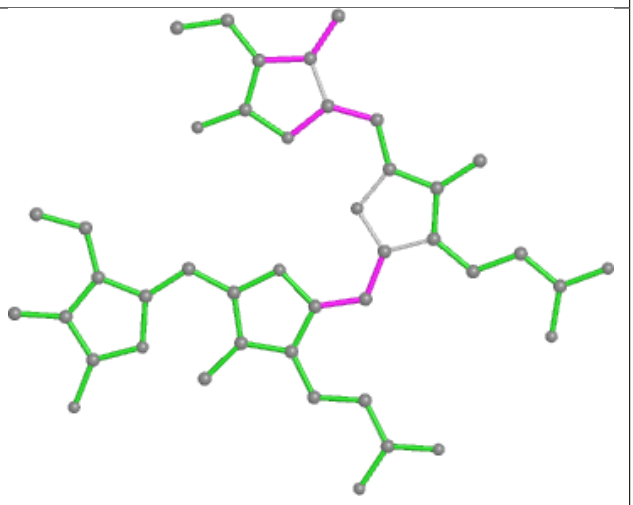

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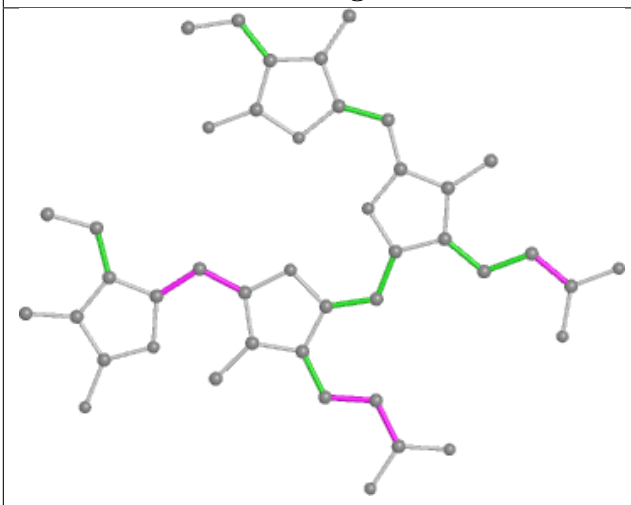

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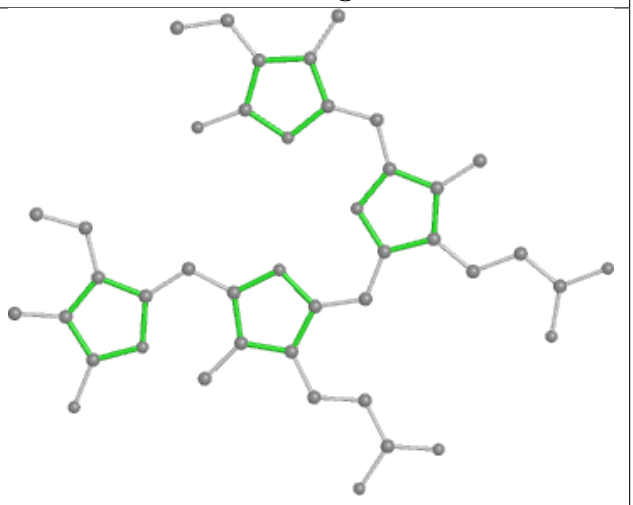

Rings

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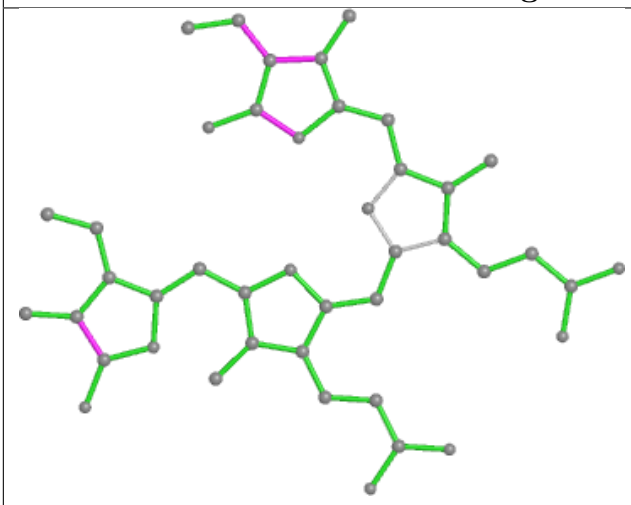

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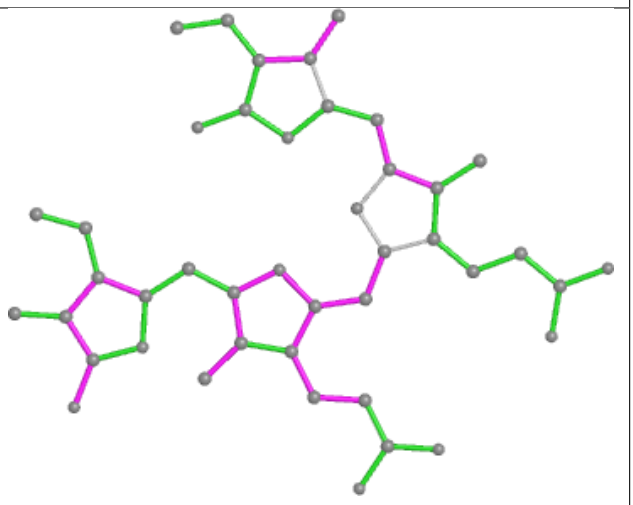

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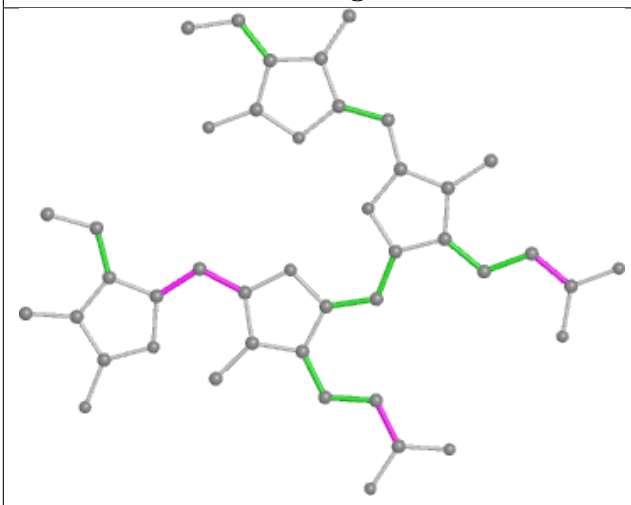

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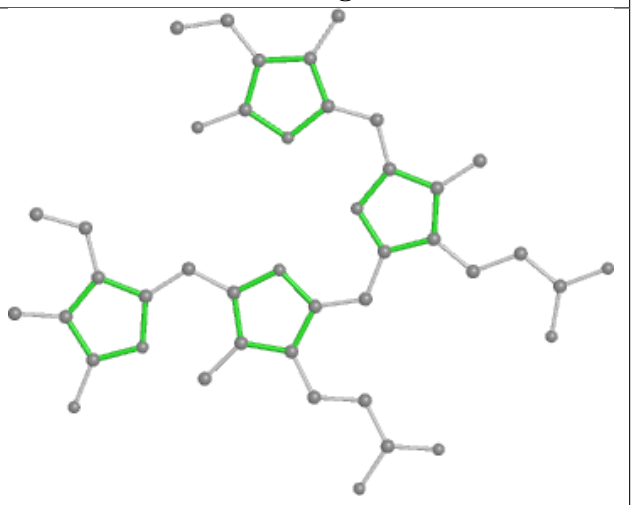
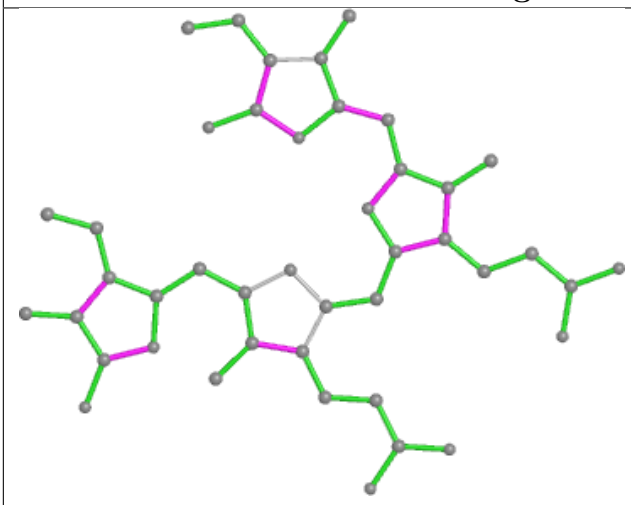


Rings

Ligand PUB A8 203



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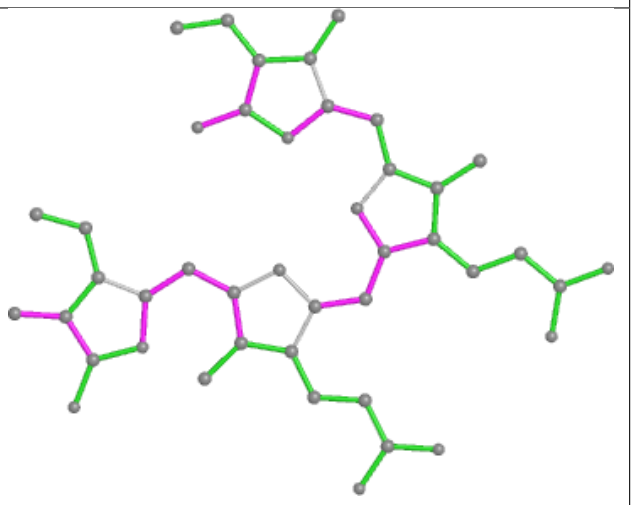

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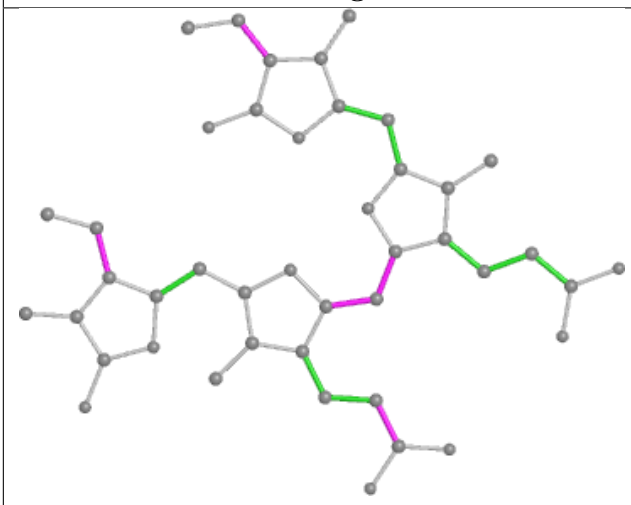

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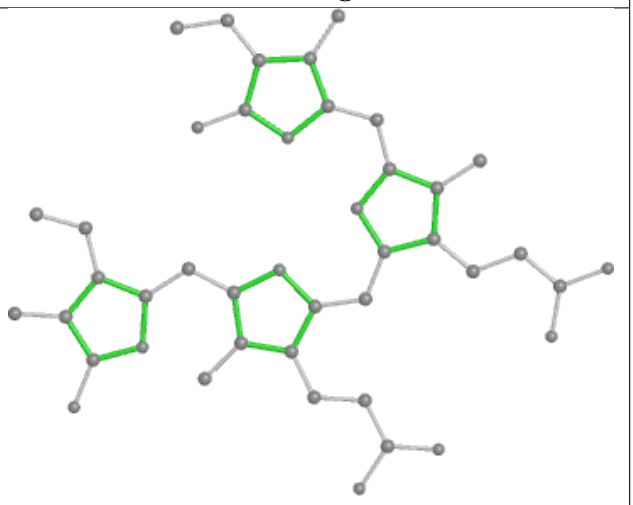

Rings

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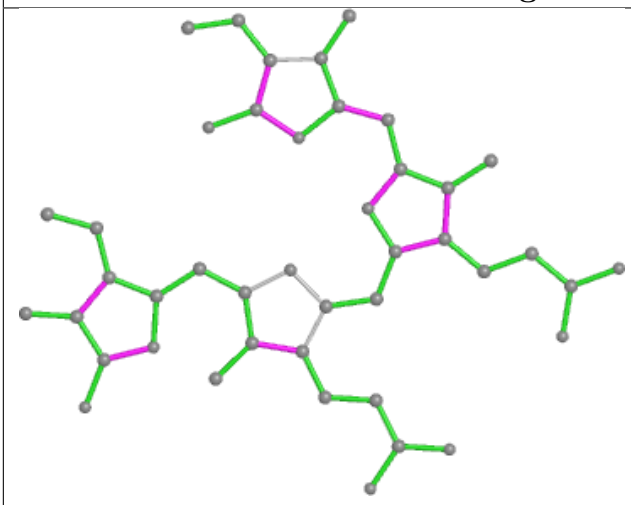

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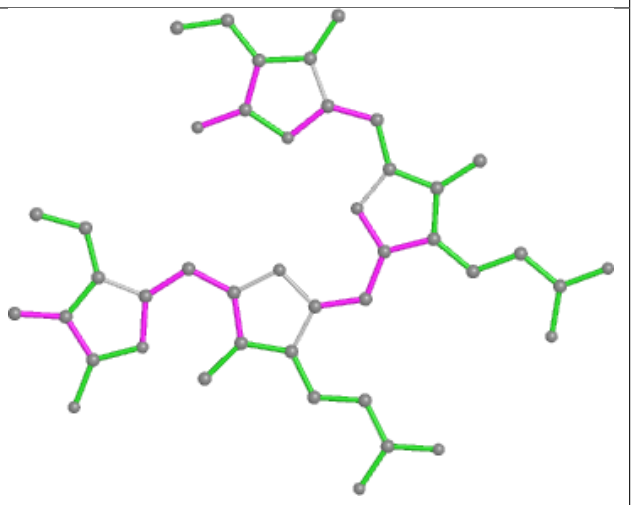

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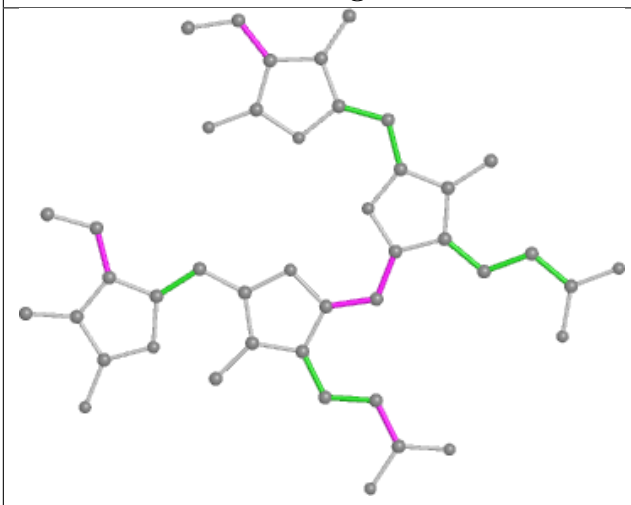

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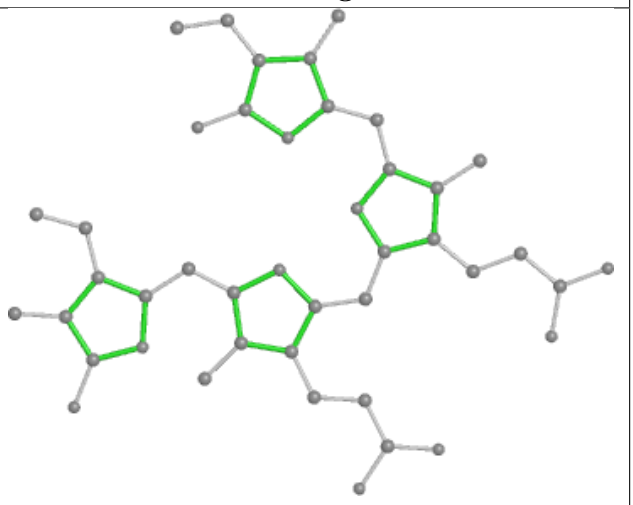
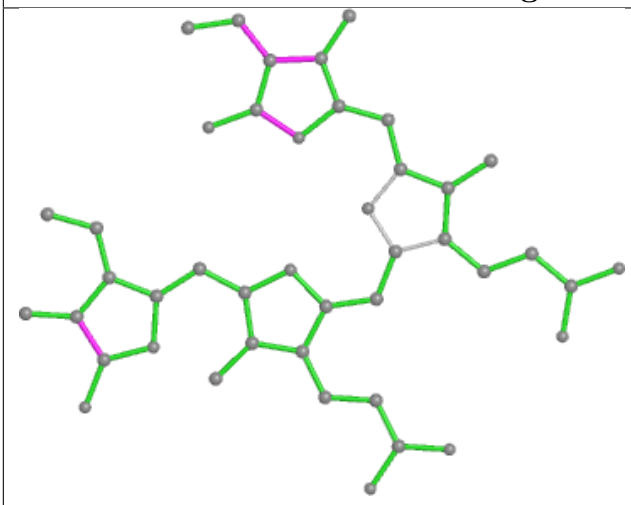


Rings

Ligand PEB gz 301



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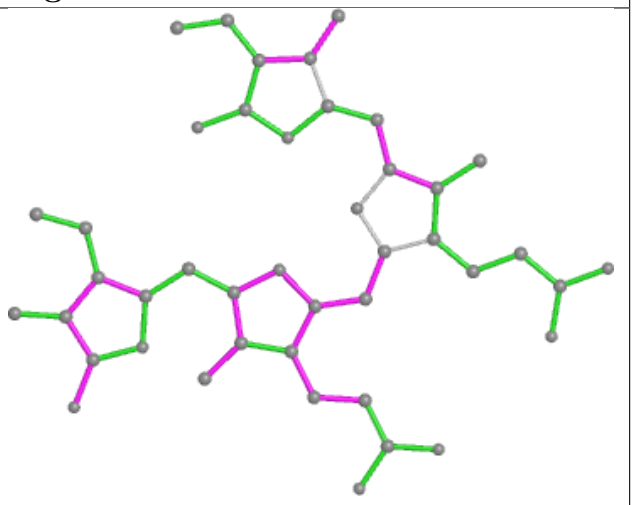

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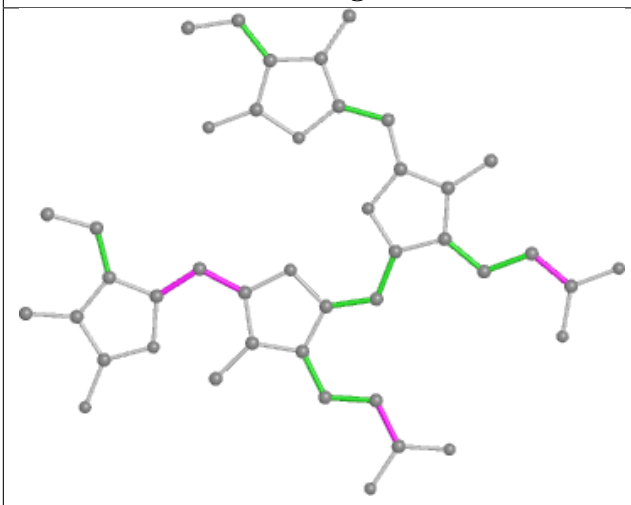

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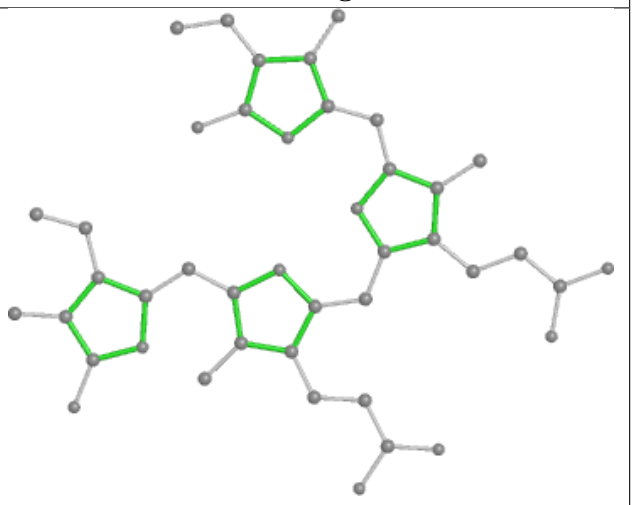

Rings

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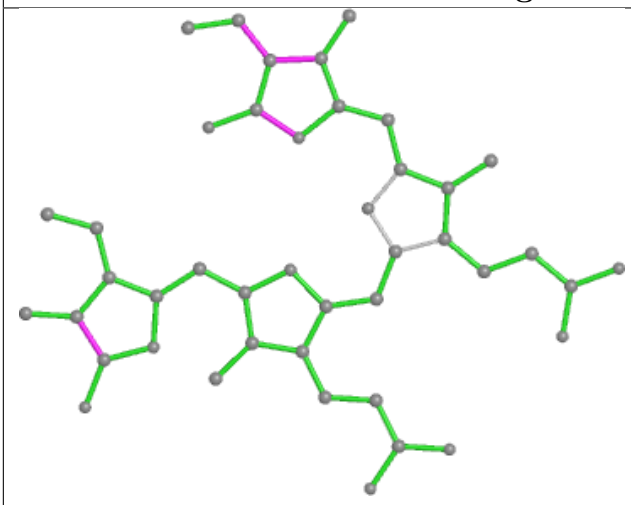

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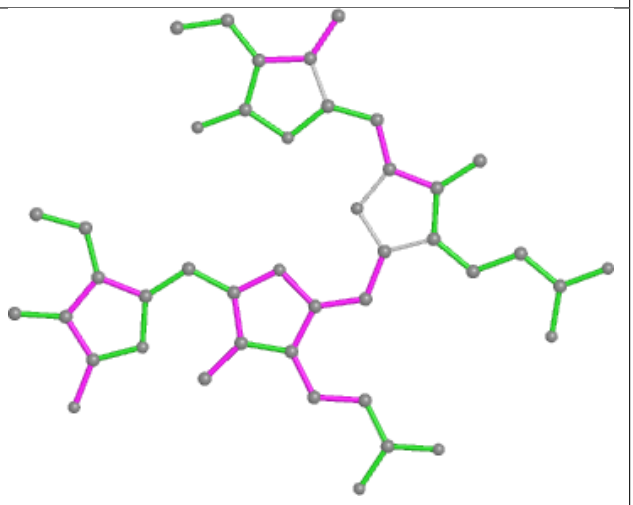
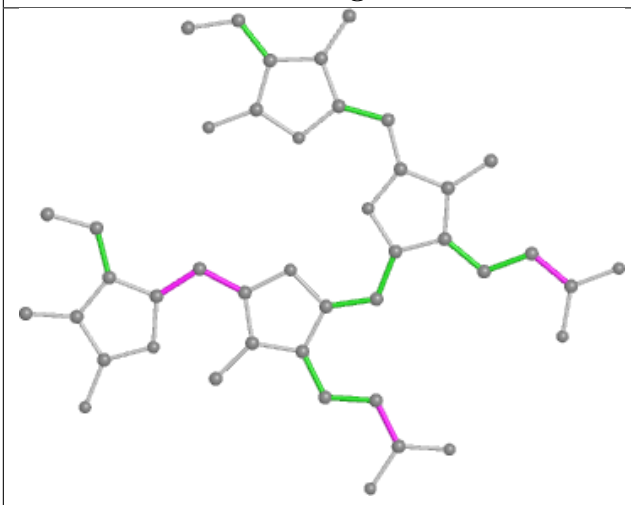
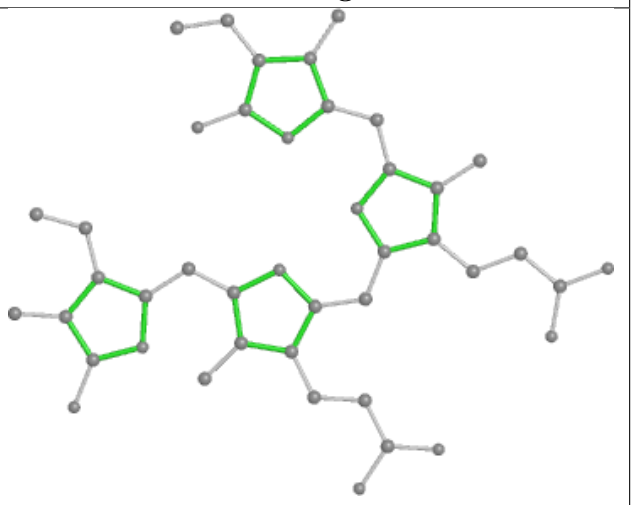


Bond angles

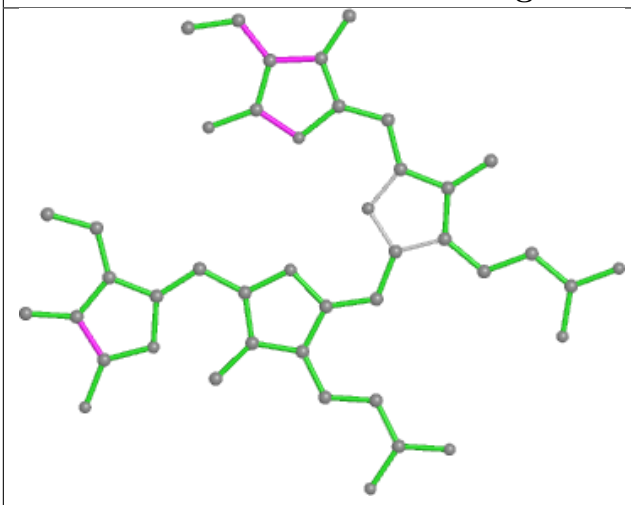


Torsions



Rings

Ligand PEB eH 202



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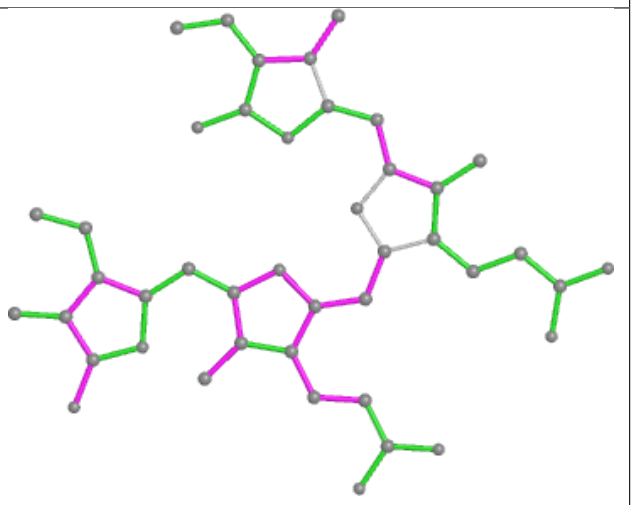

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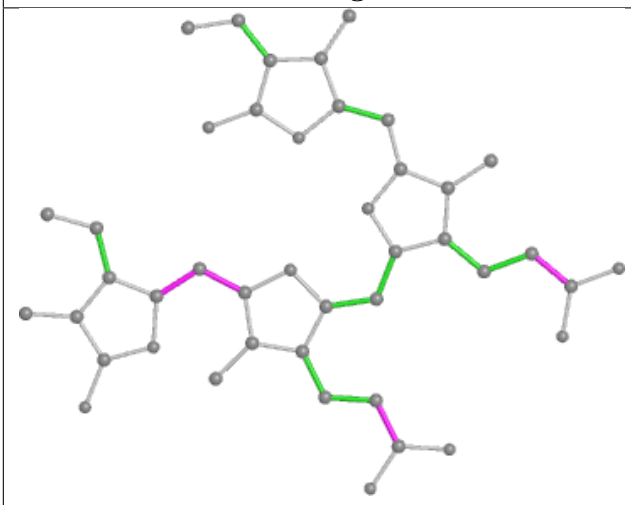

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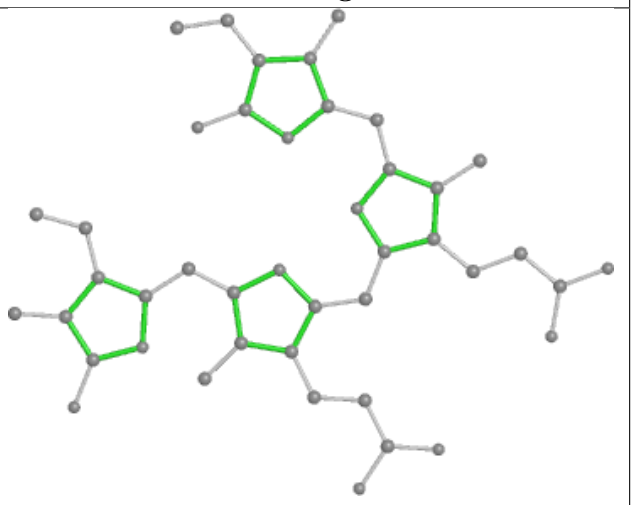
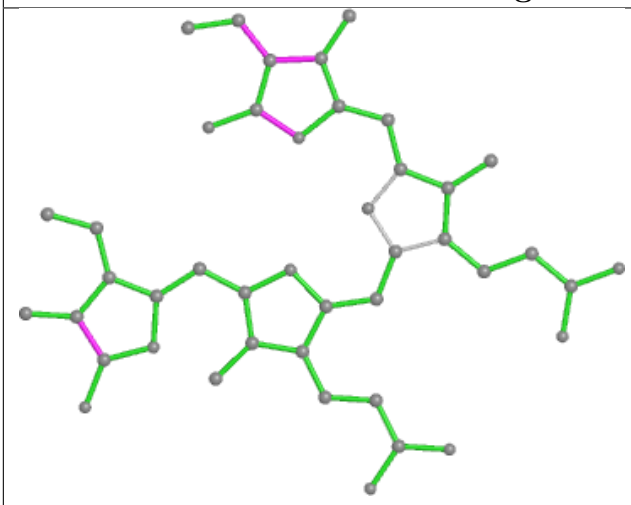


Rings

Ligand PEB G7 201



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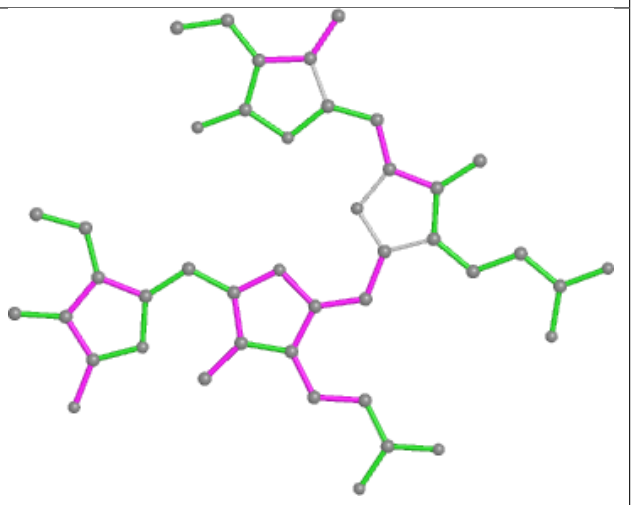

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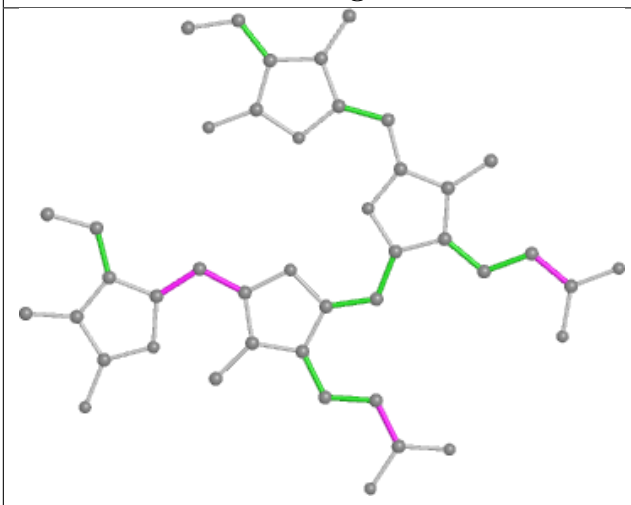

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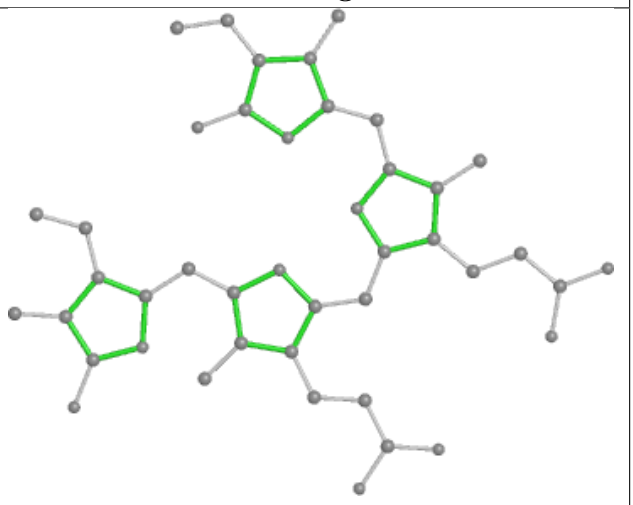
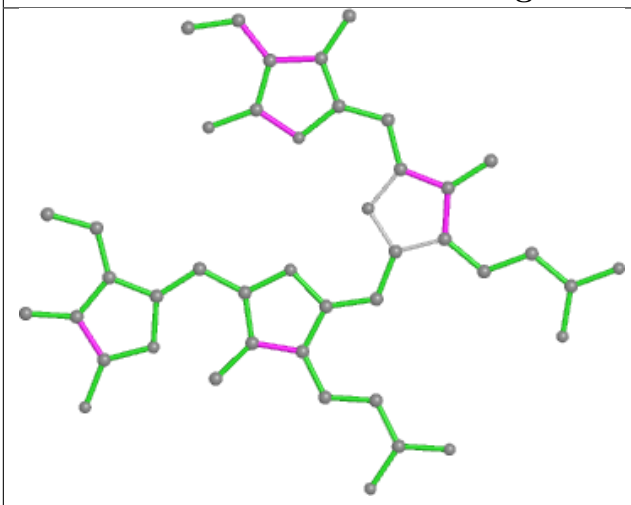


Rings

Ligand PEB V3 202



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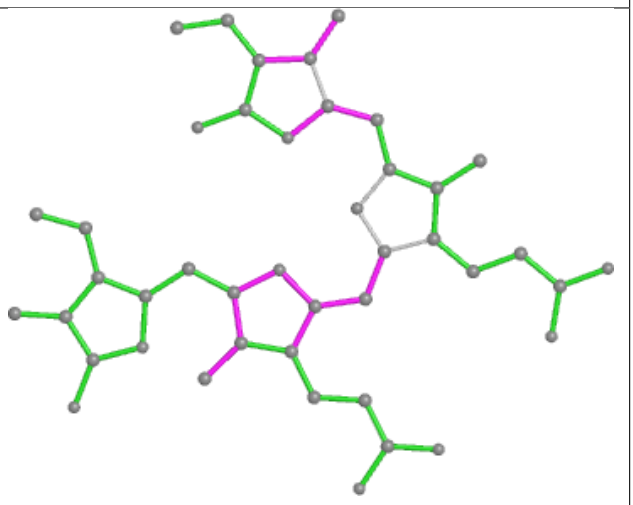

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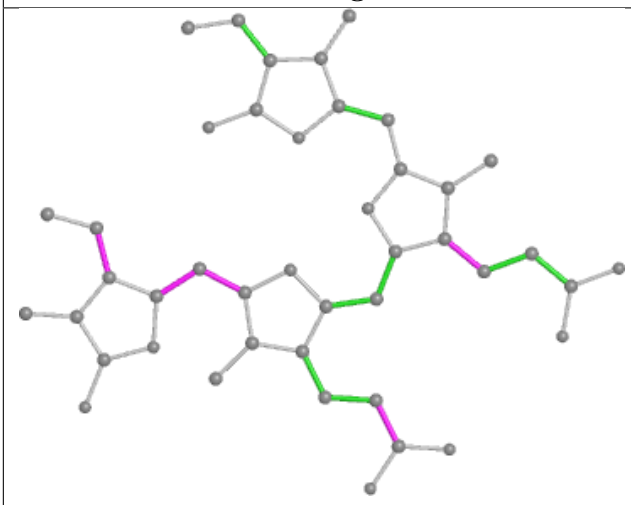

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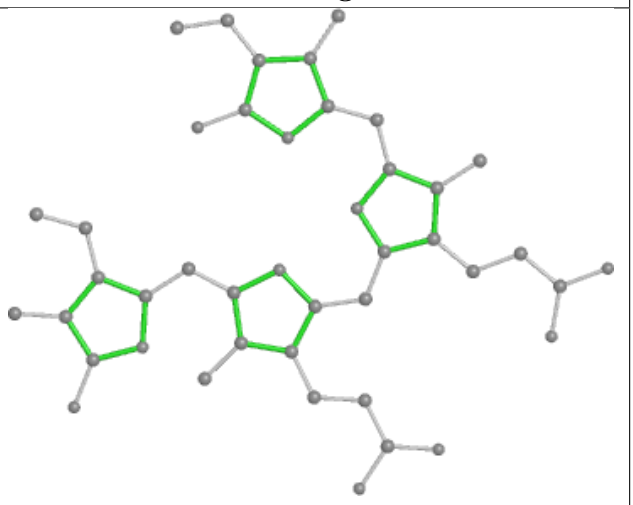
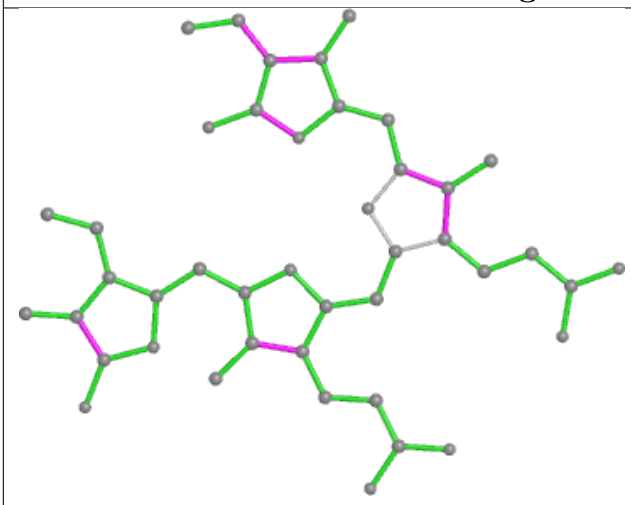


Rings

Ligand PEB ad 202



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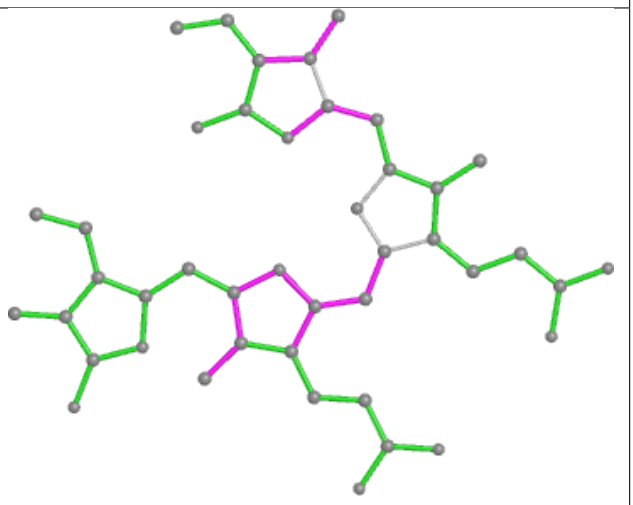

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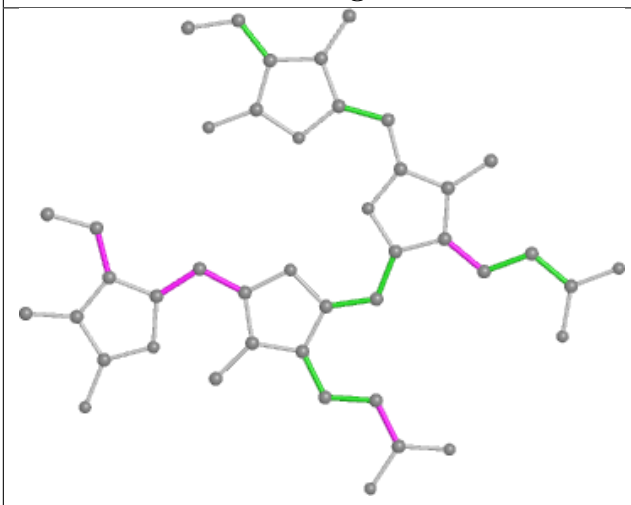

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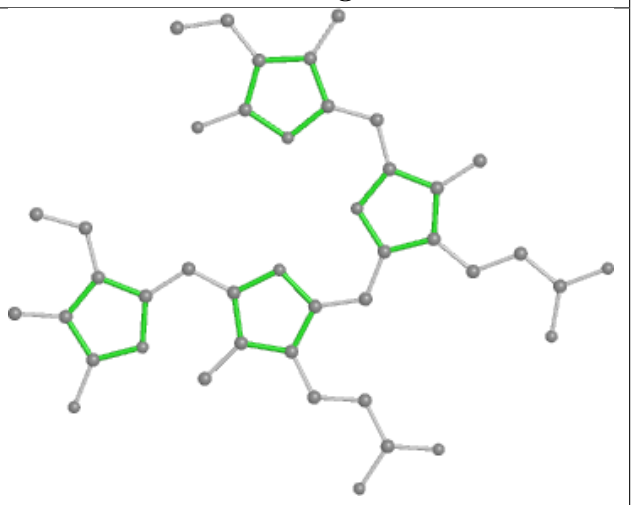

Rings

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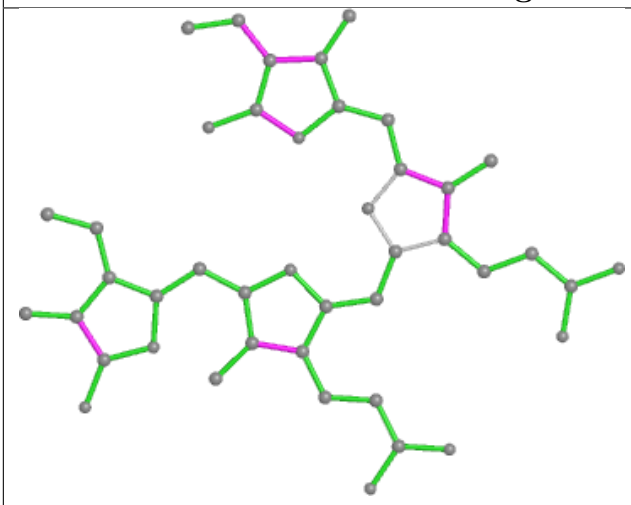

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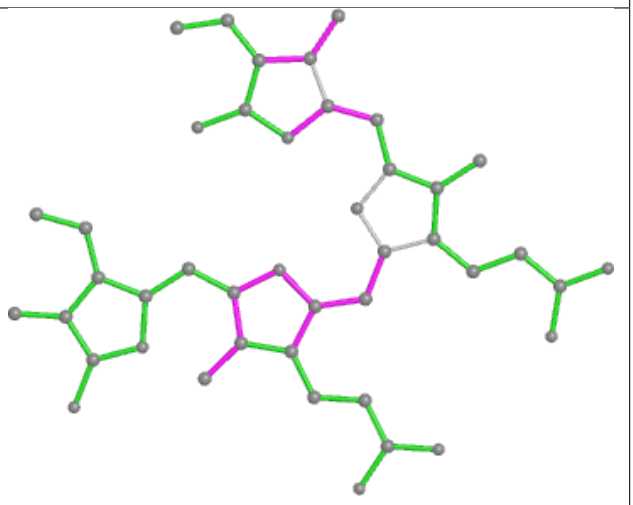

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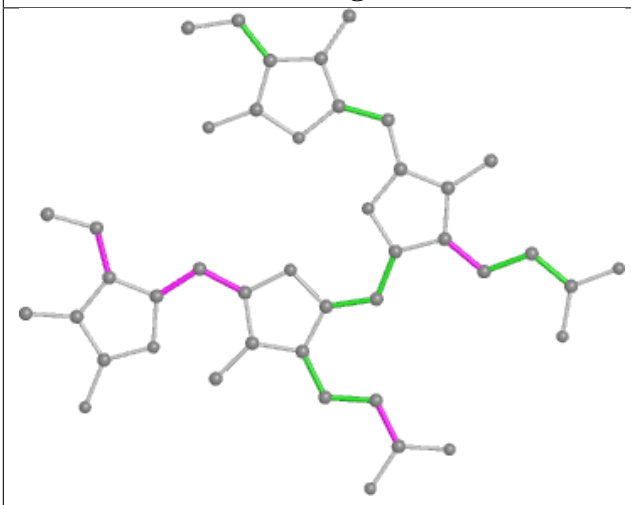

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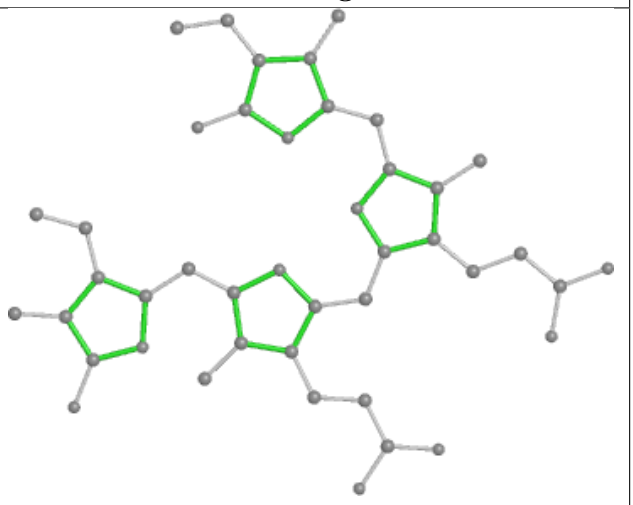

Rings

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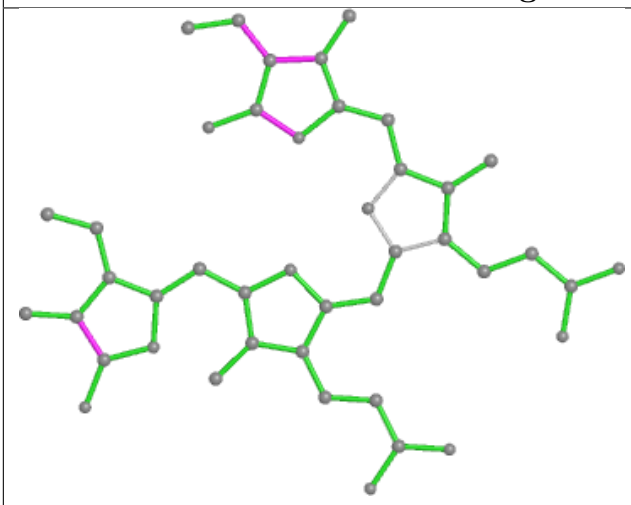

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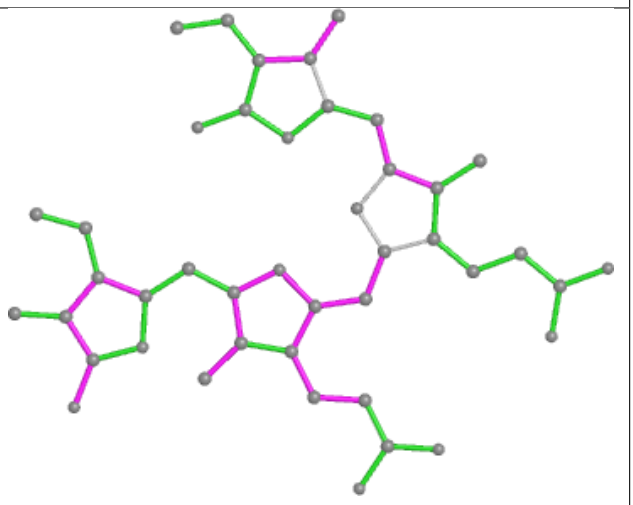

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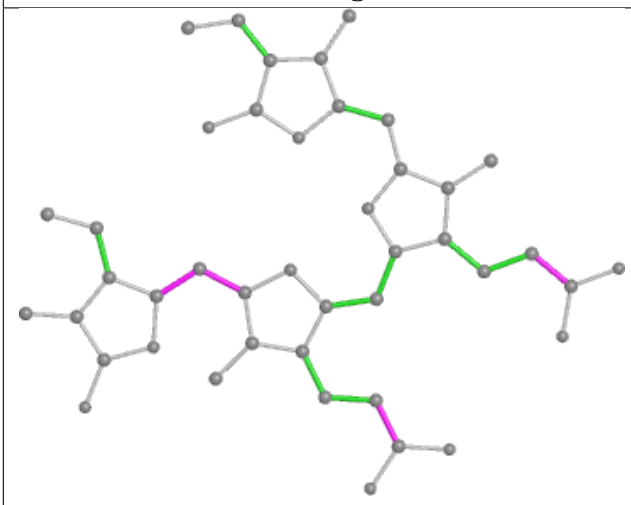

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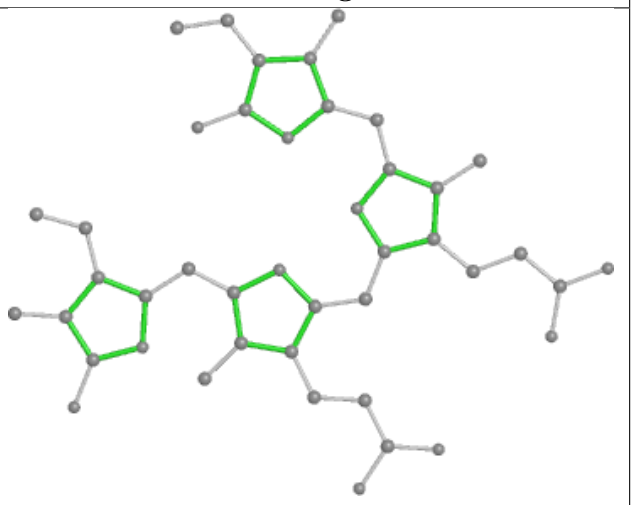
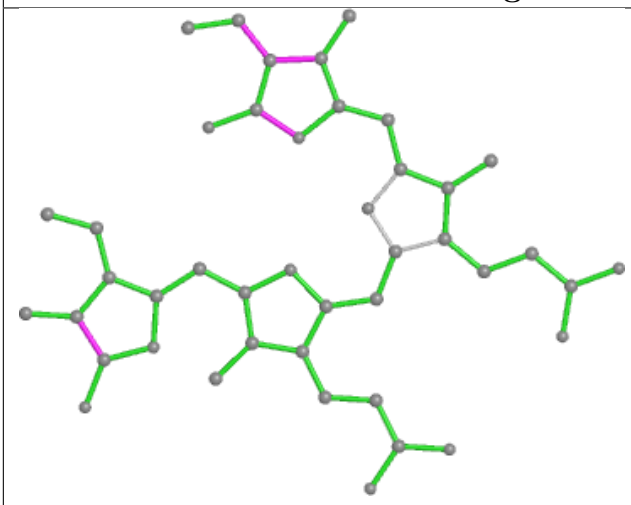


Rings

Ligand PEB eM 1002



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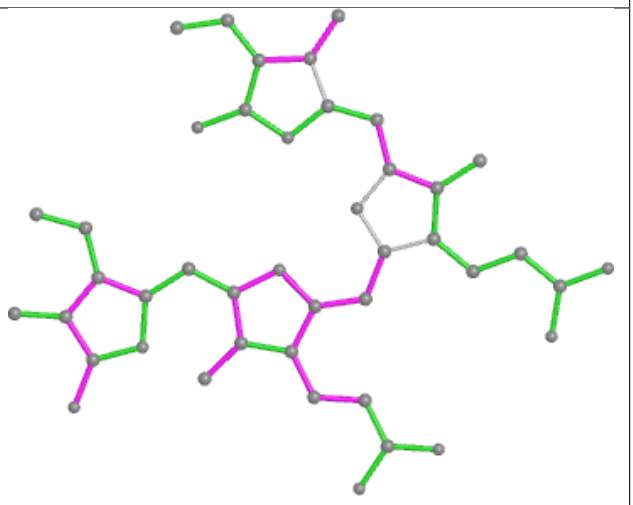

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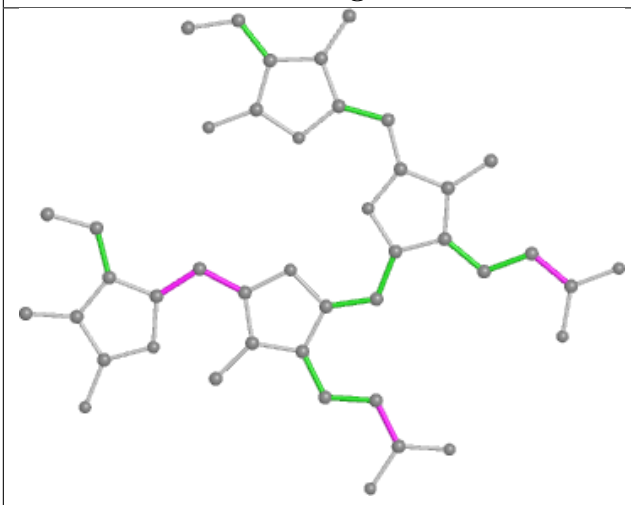

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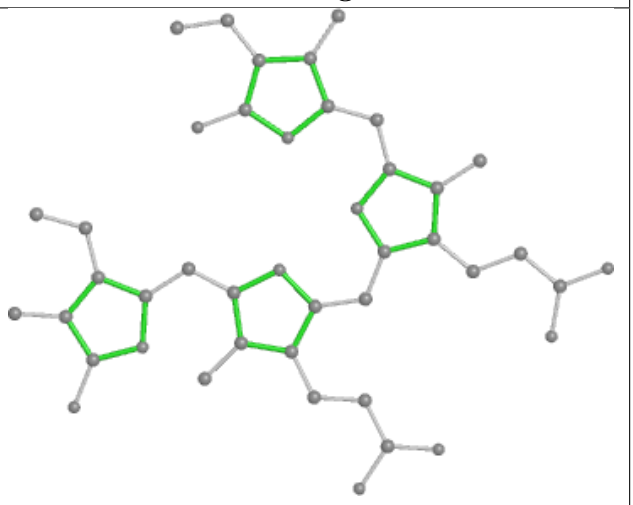
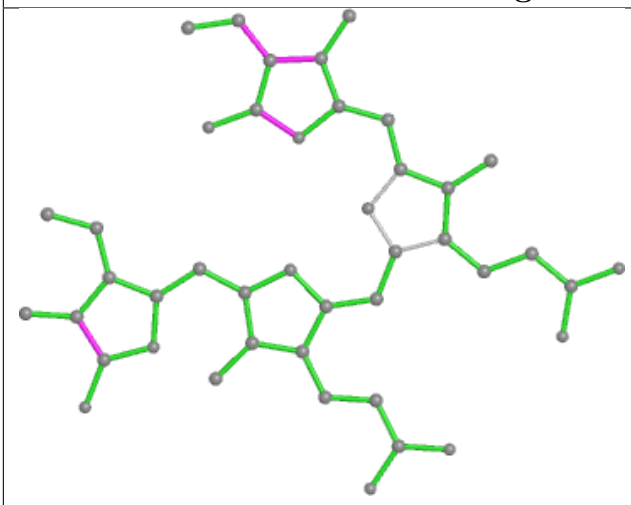


Rings

Ligand PEB N2 202



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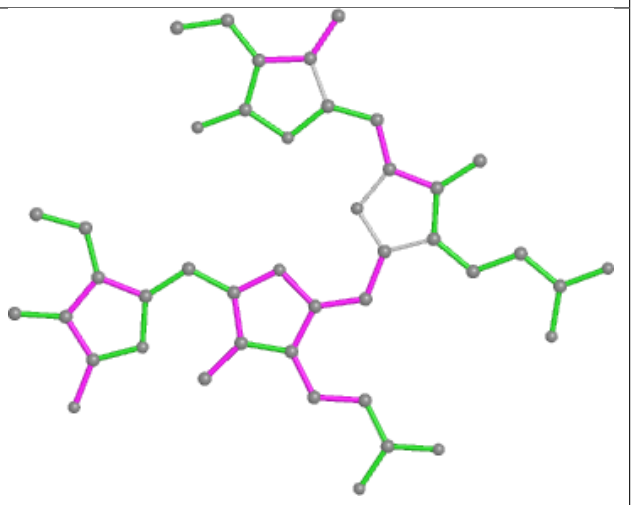

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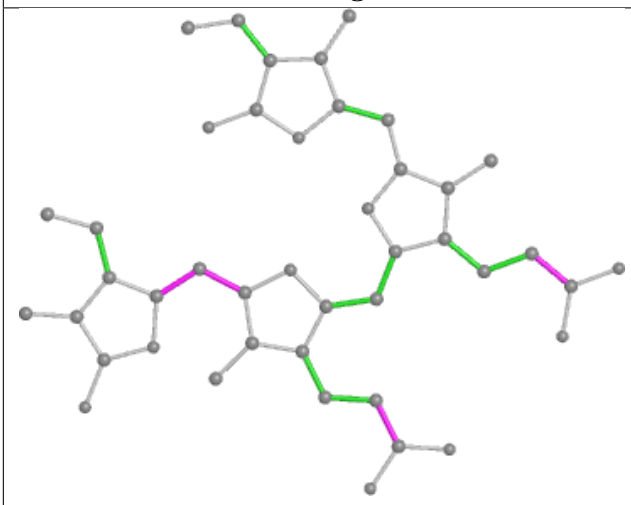

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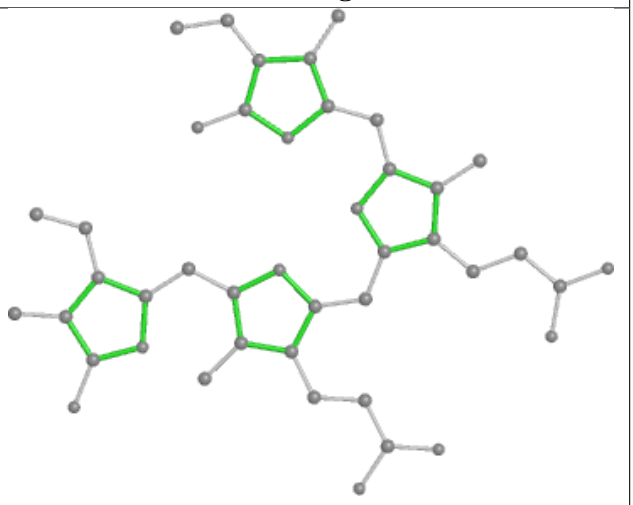
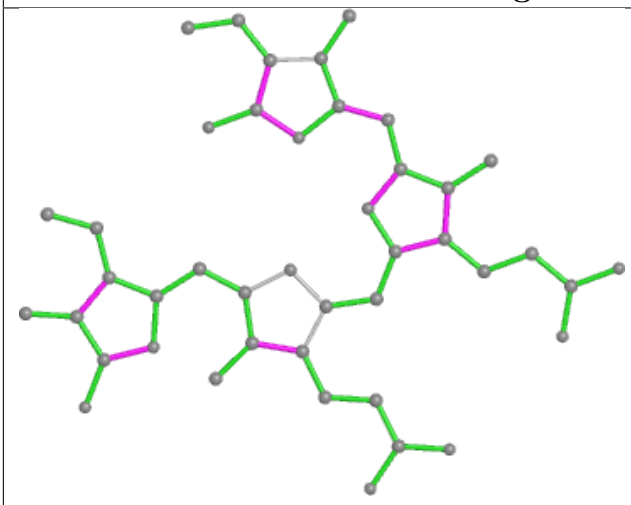


Rings

Ligand PUB Q8 203



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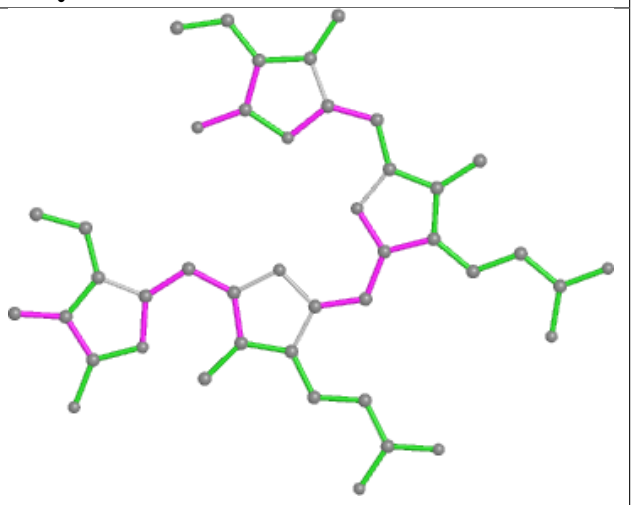

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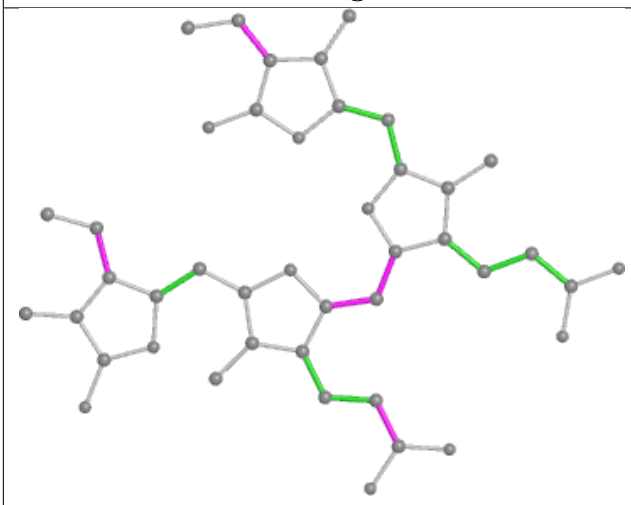

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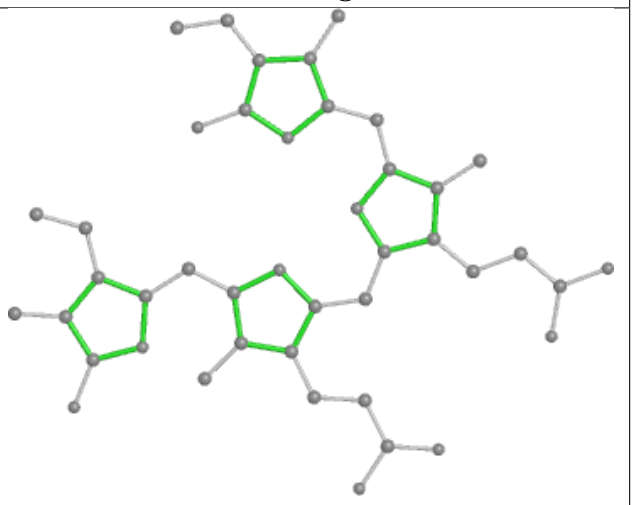
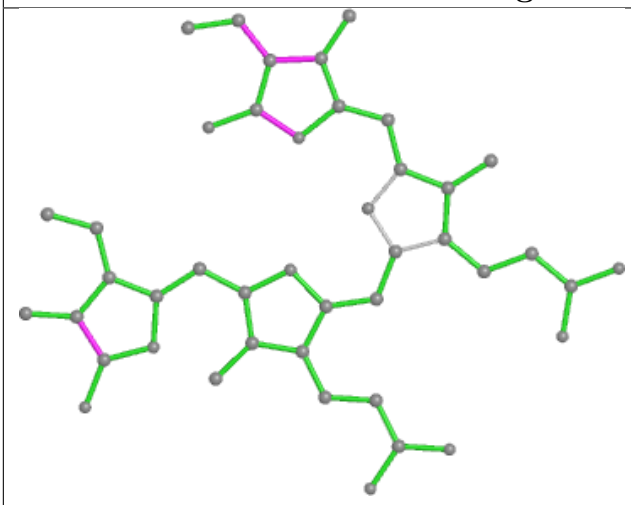


Rings

Ligand PEB B2 502



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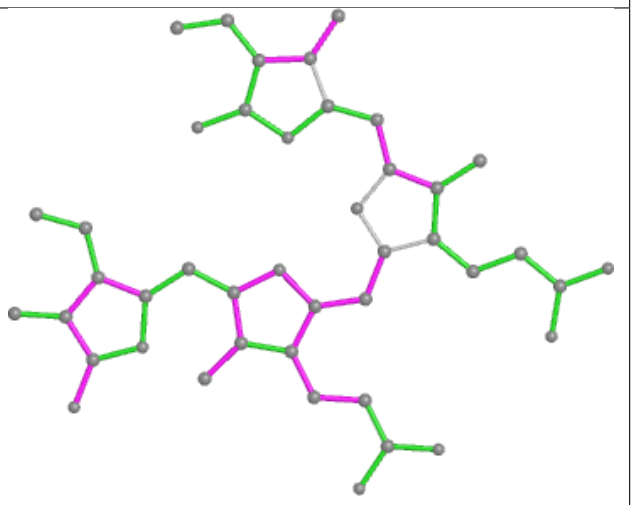

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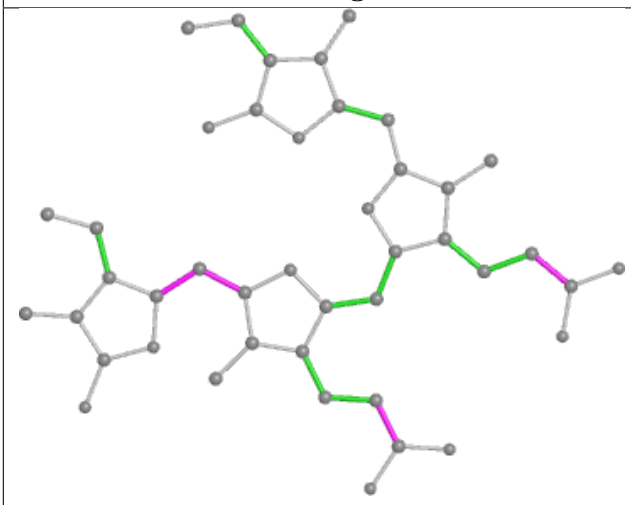

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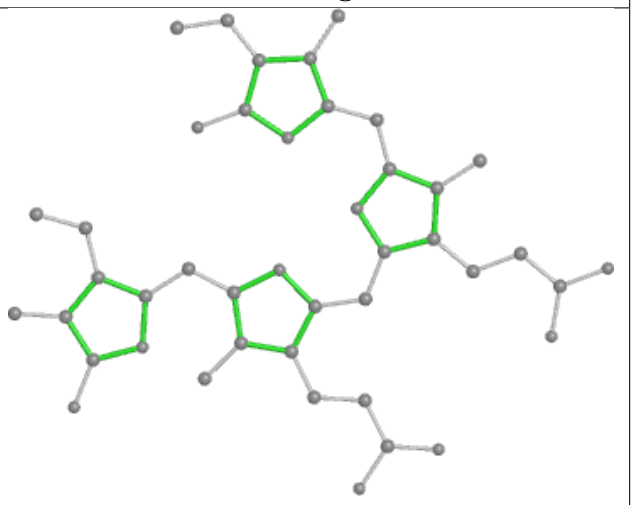
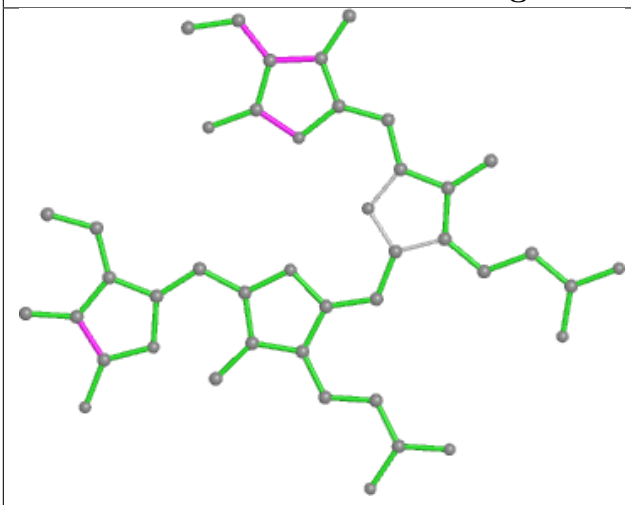


Rings

Ligand PEB b5 1001



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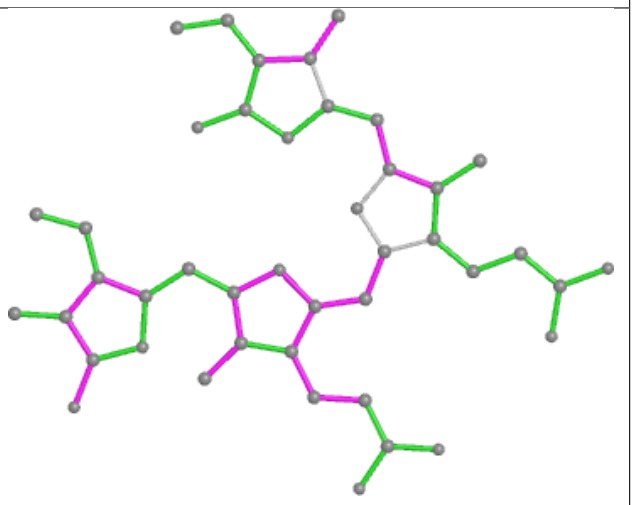

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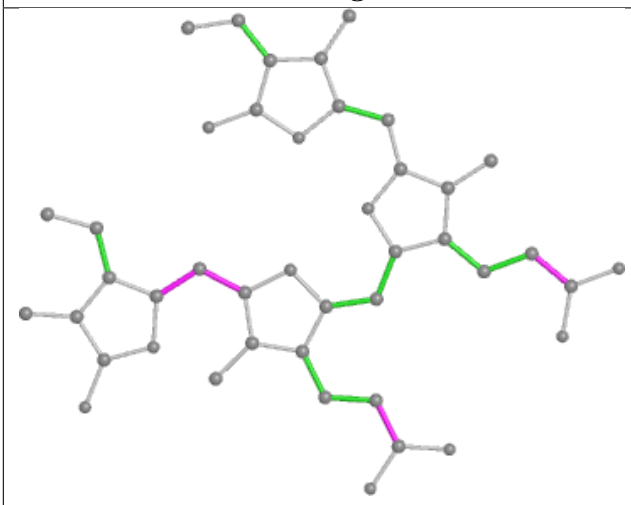

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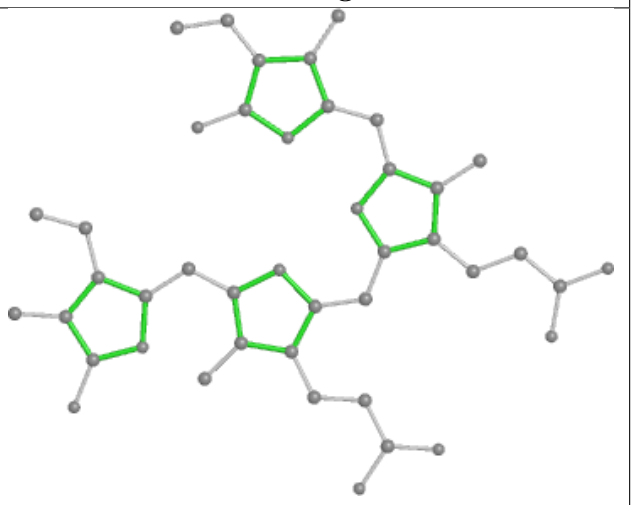
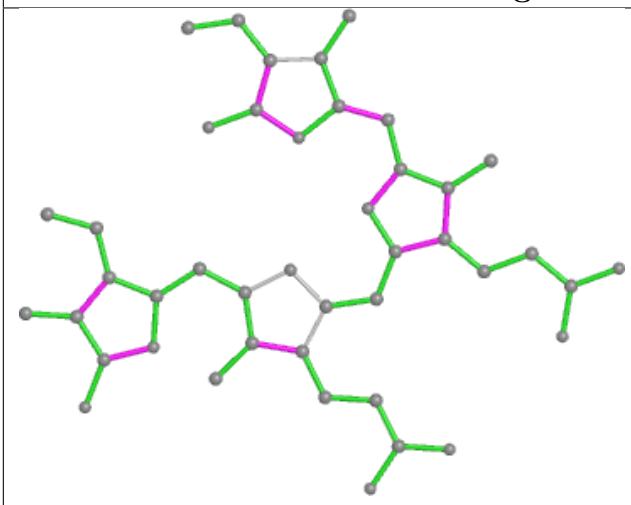


Rings

Ligand PUB w8 203



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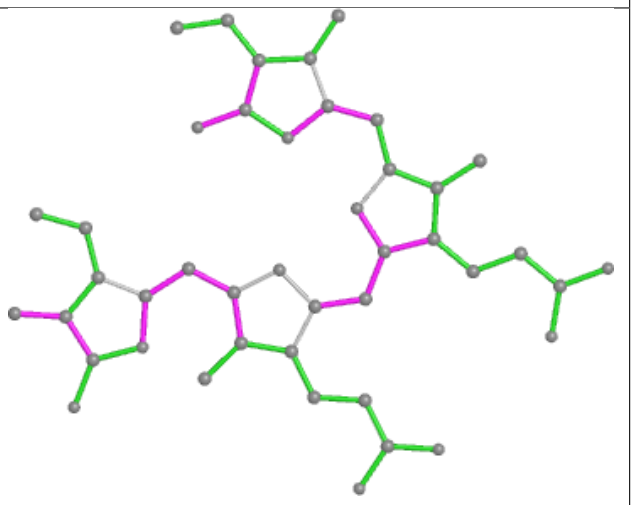
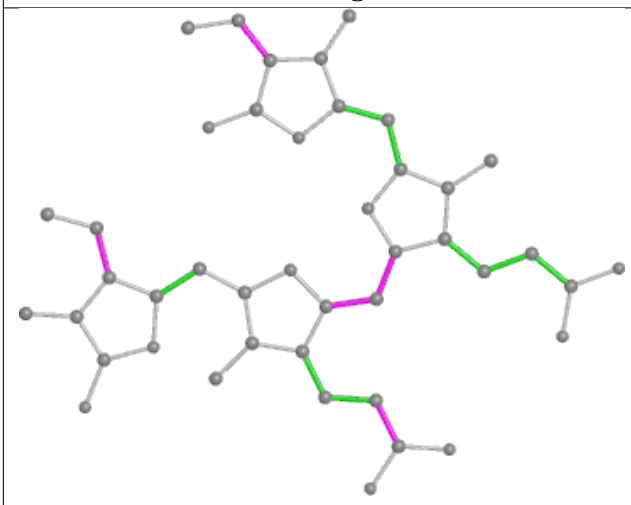


Bond angles



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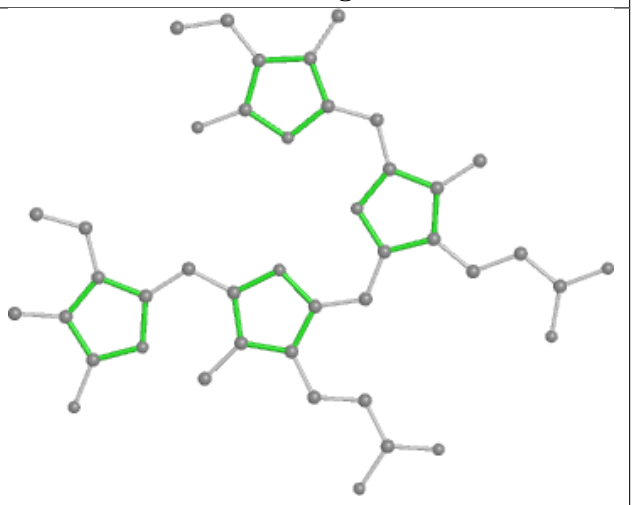
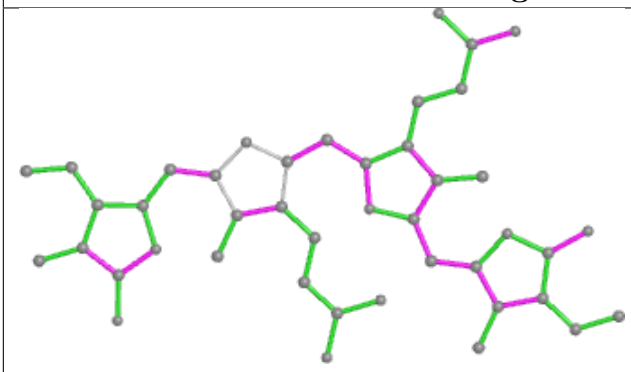


Rings

Ligand CYC m1 201



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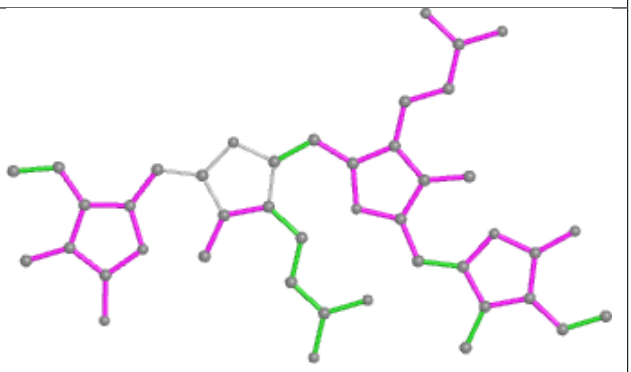
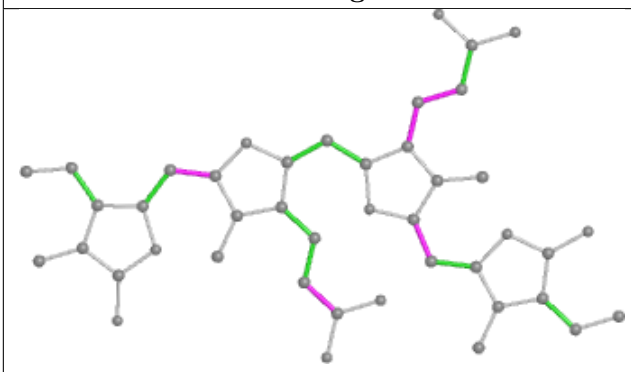
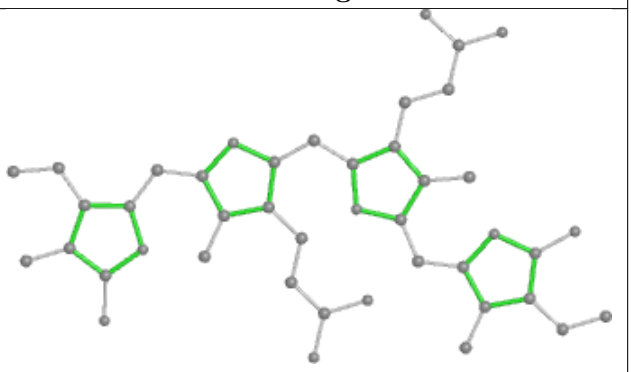


Bond angles

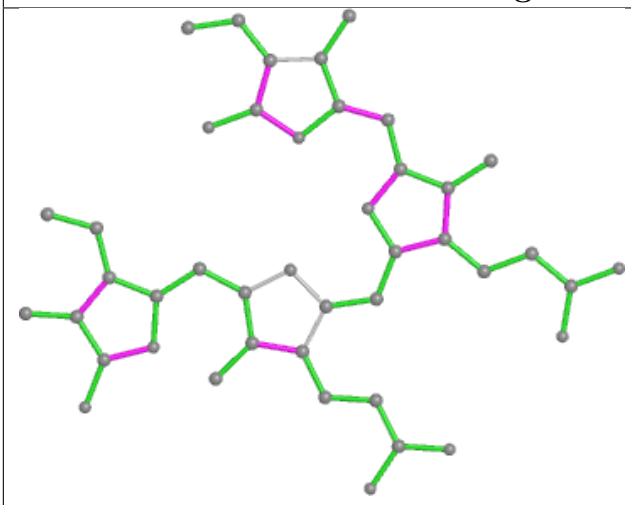


Torsions



Rings

Ligand PUB T8 304



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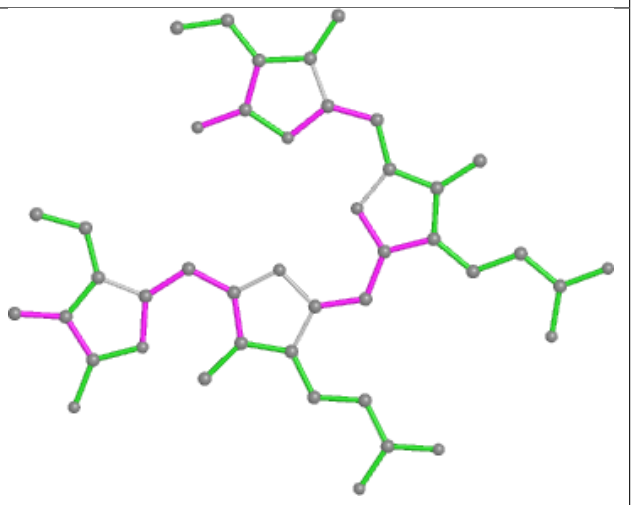

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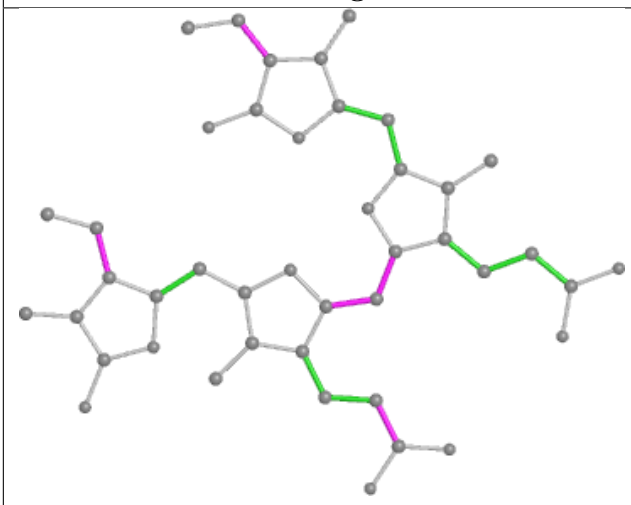

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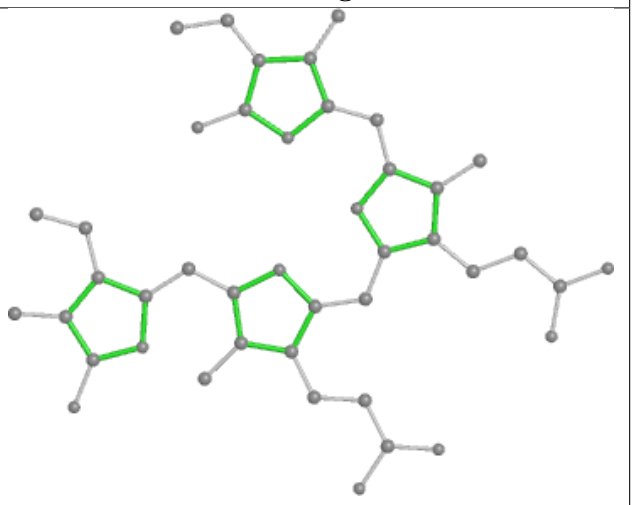
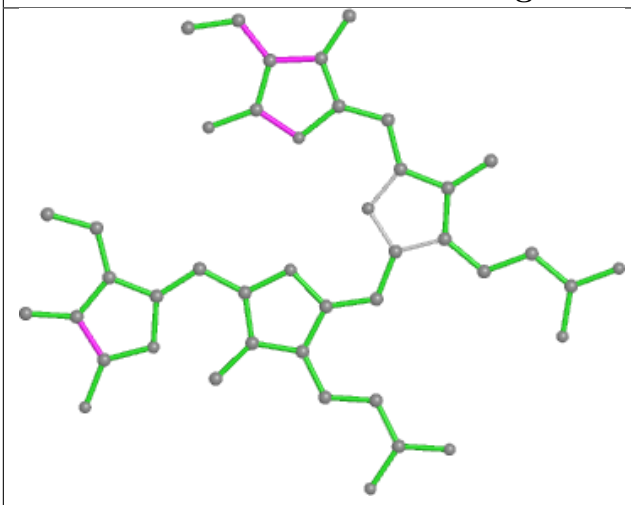


Rings

Ligand PEB Y8 202



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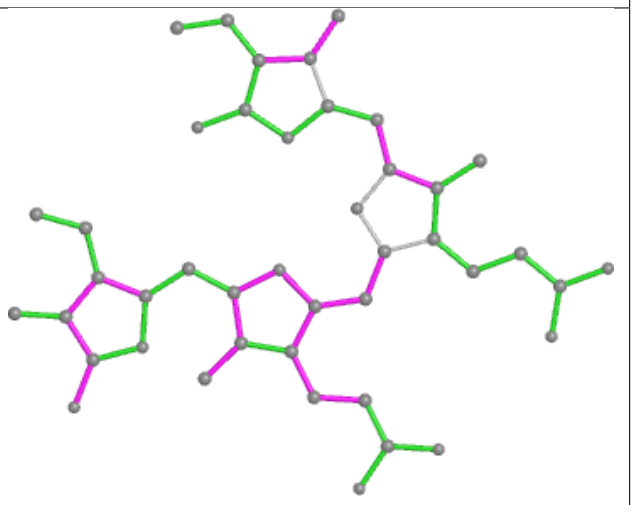

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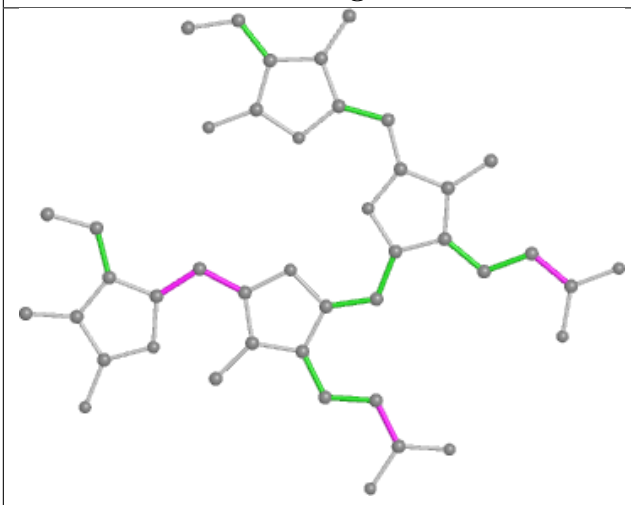

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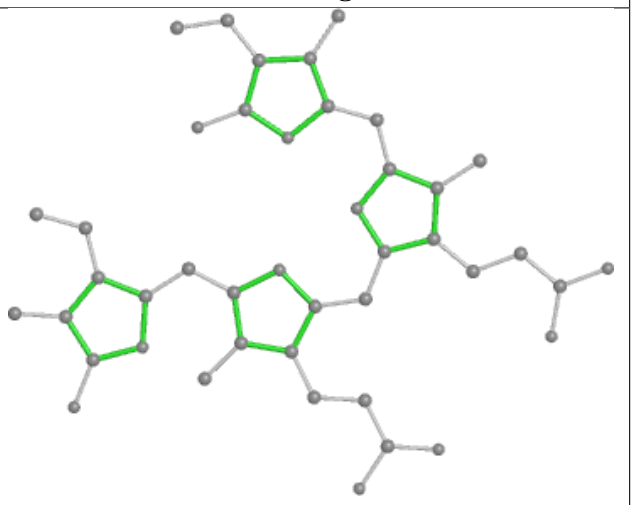
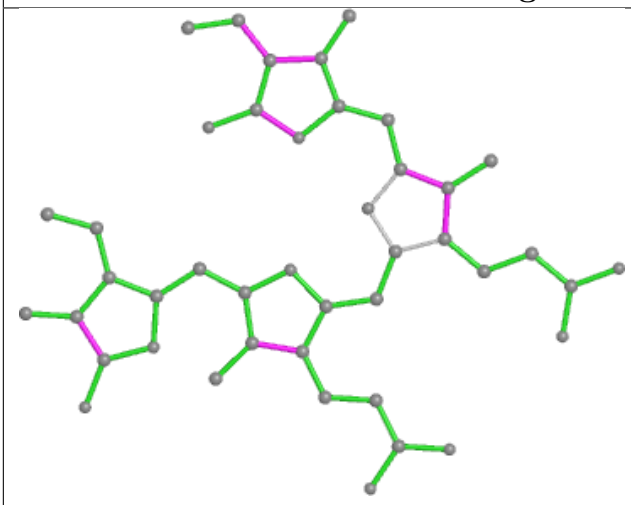


Rings

Ligand PEB cL 202



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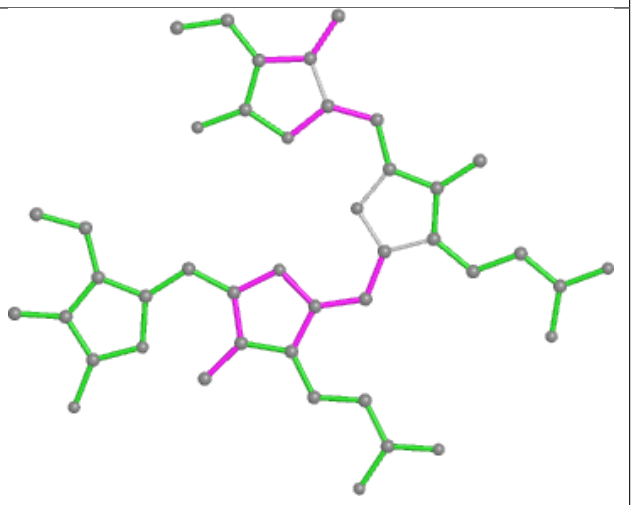

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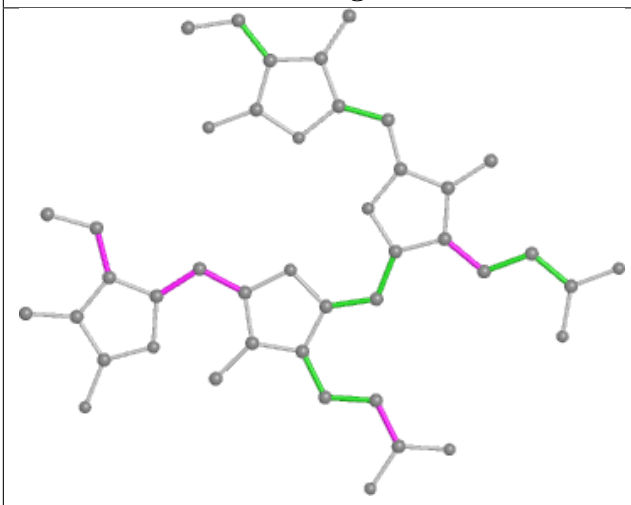

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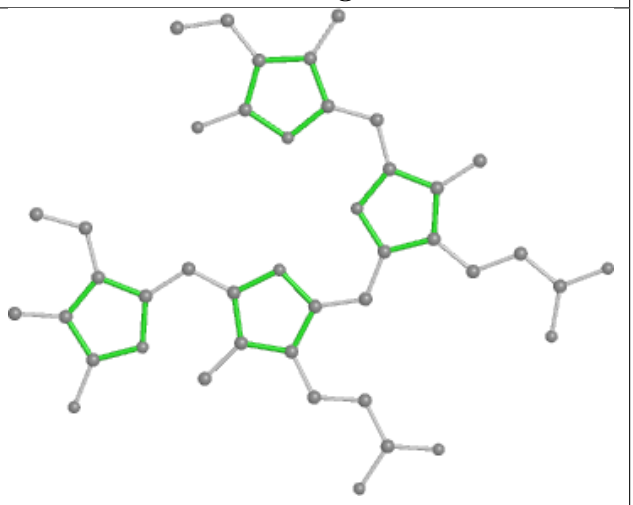
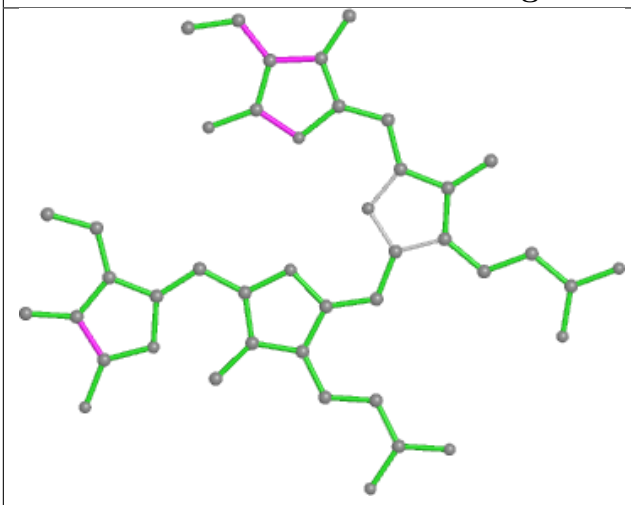


Rings

Ligand PEB r7 201



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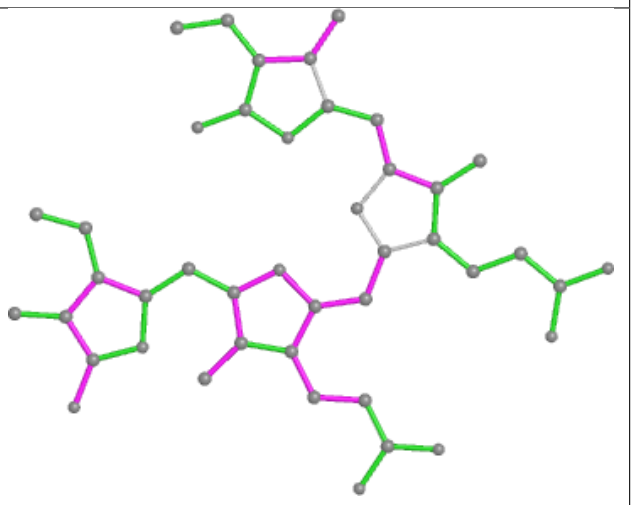

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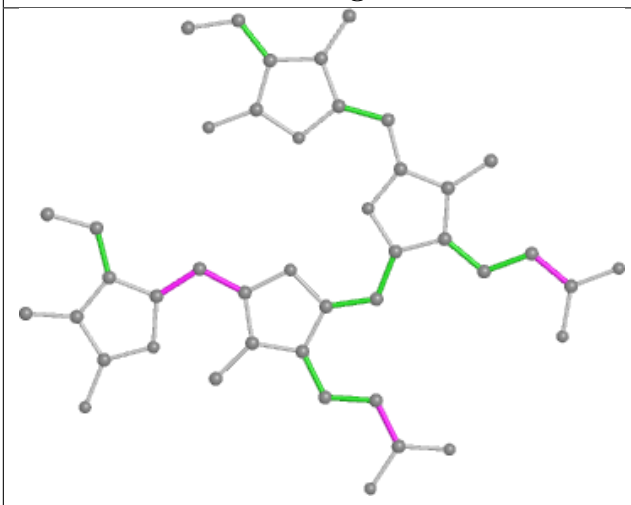

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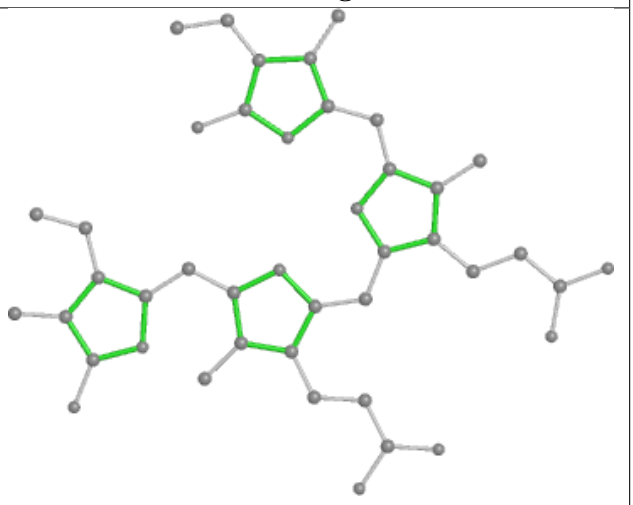

Rings

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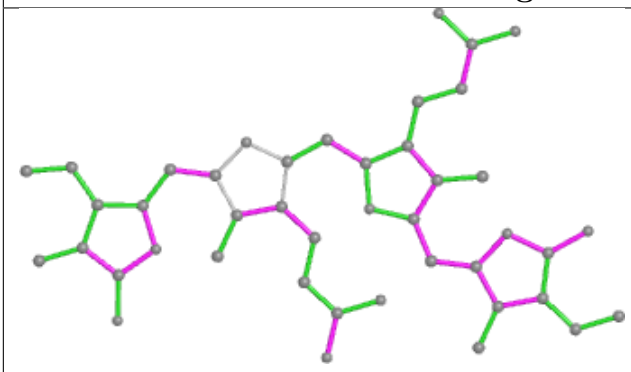

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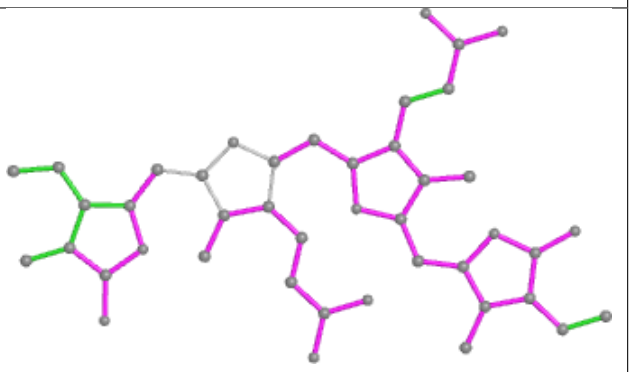

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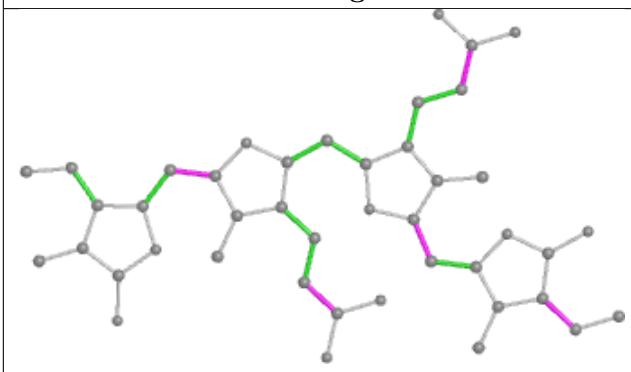

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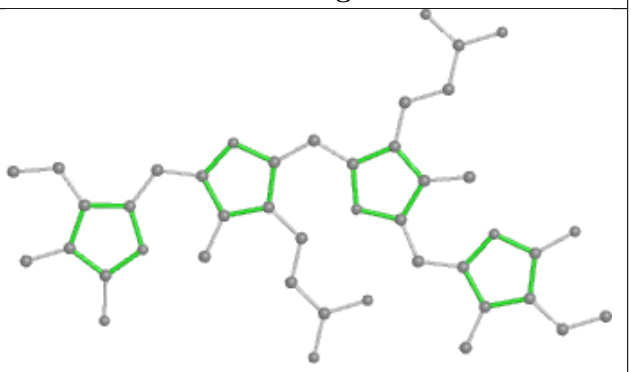

Rings

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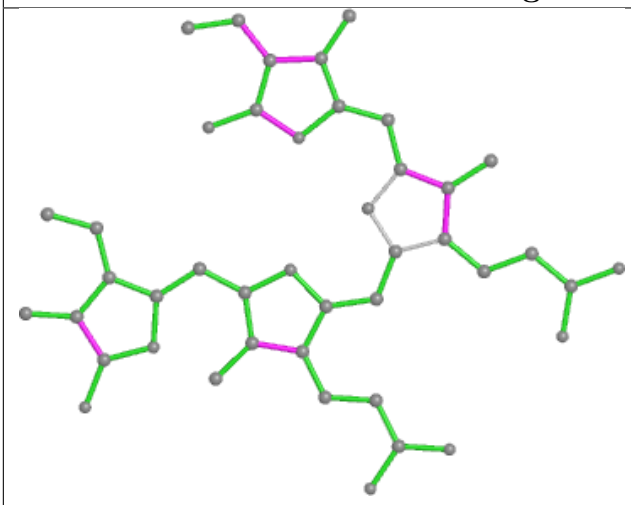

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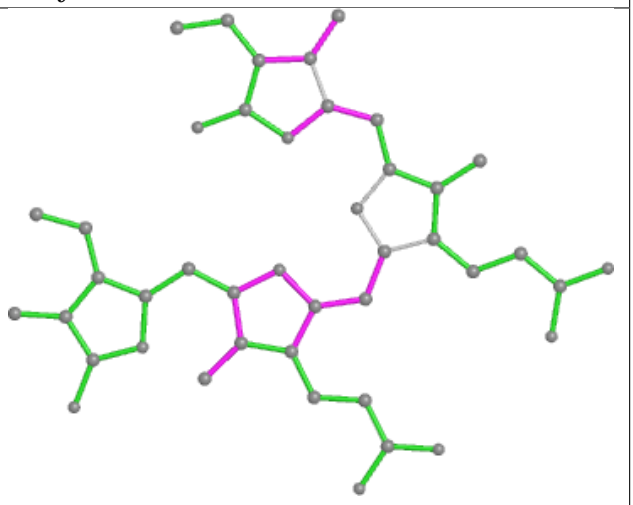

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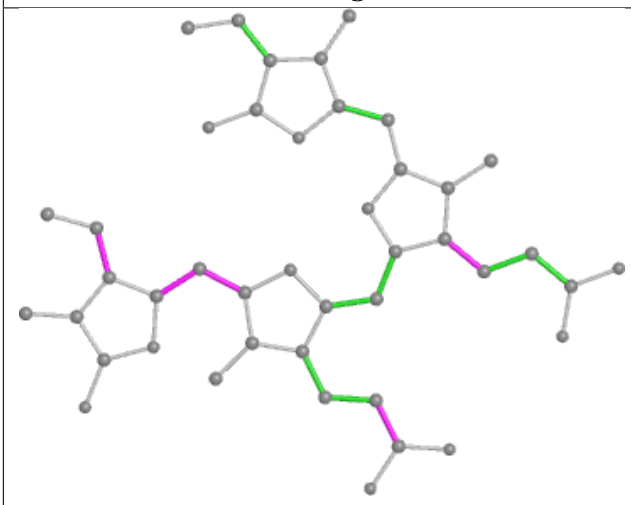

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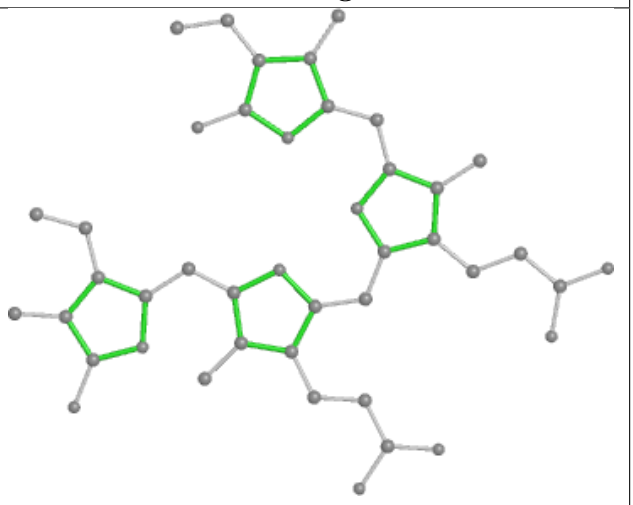
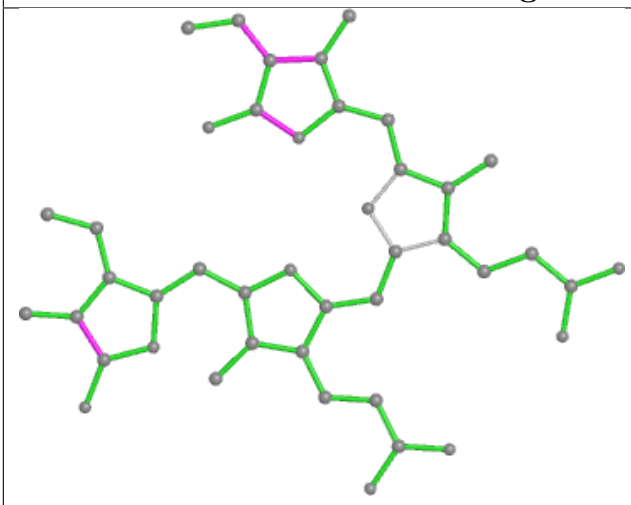


Rings

Ligand PEB g7 201



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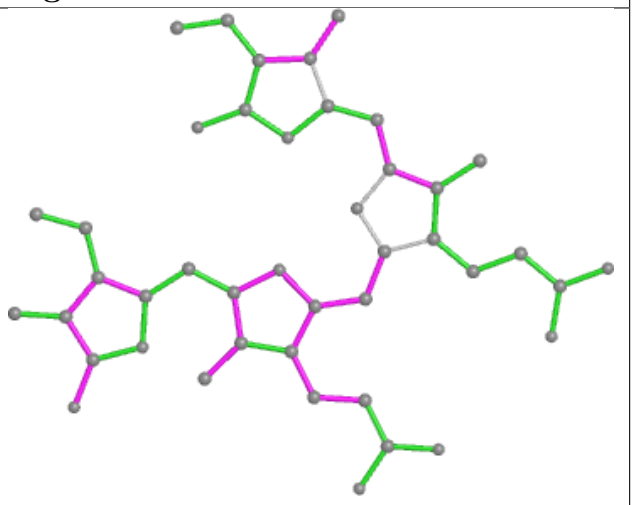

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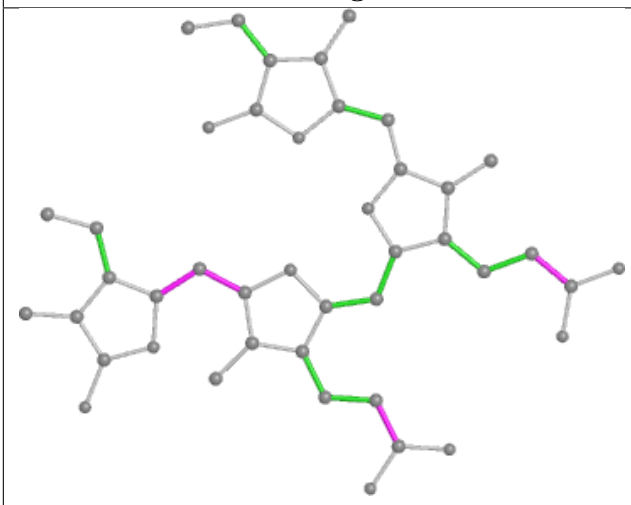

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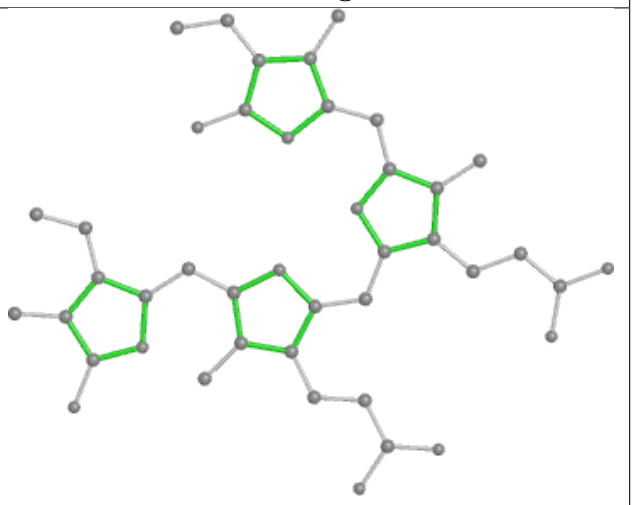

Rings

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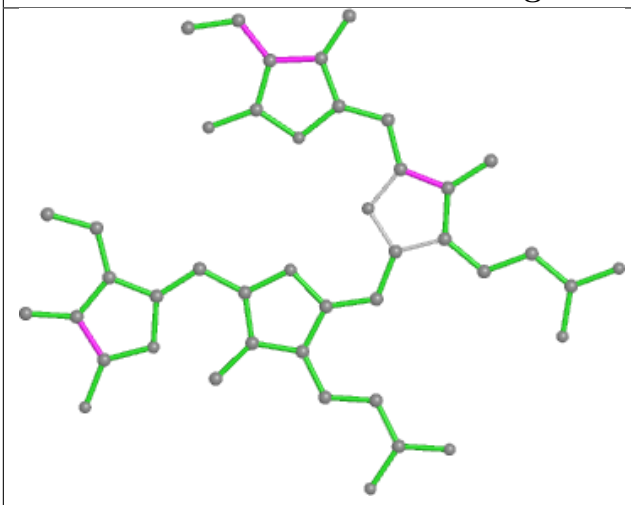

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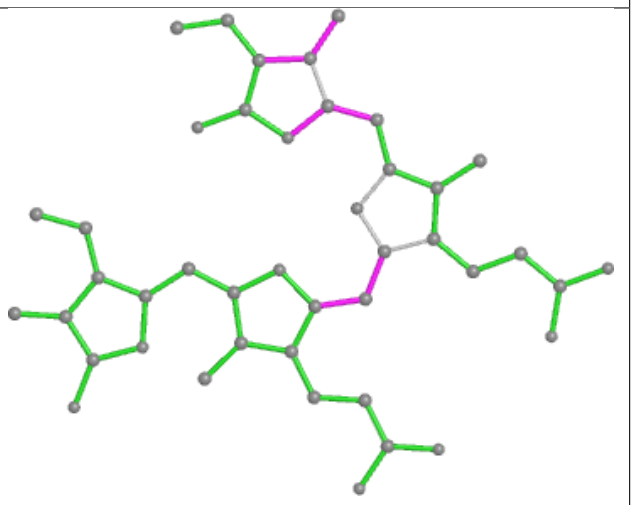

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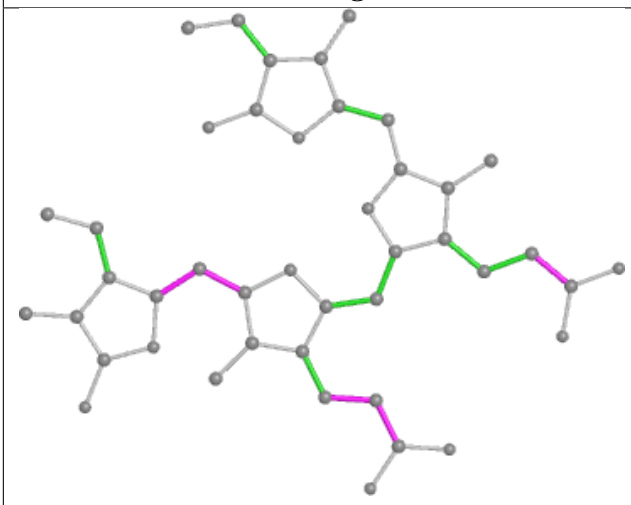

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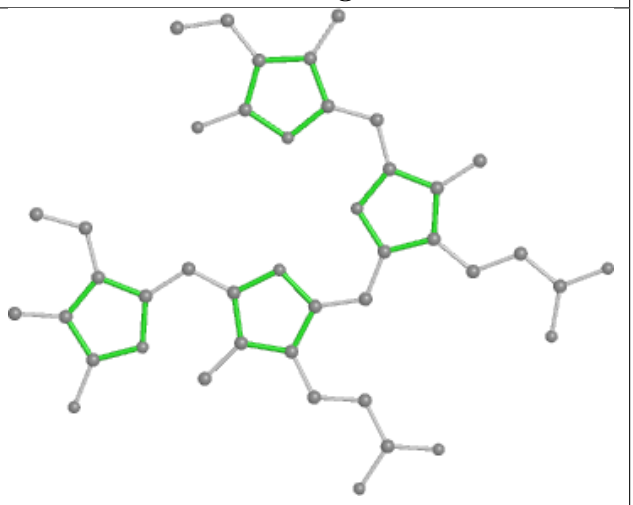

Rings

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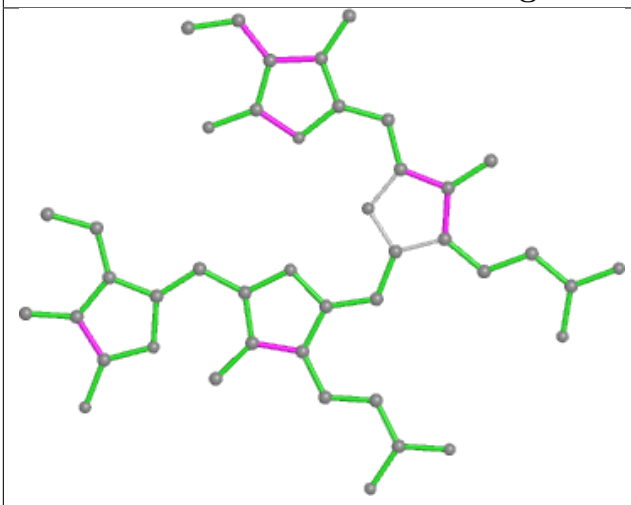

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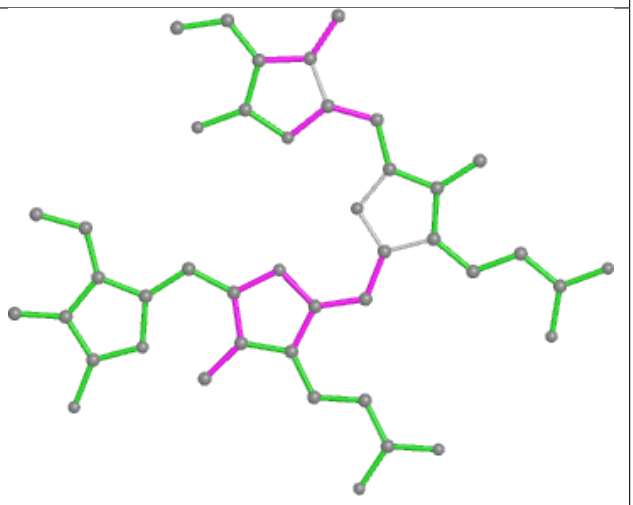

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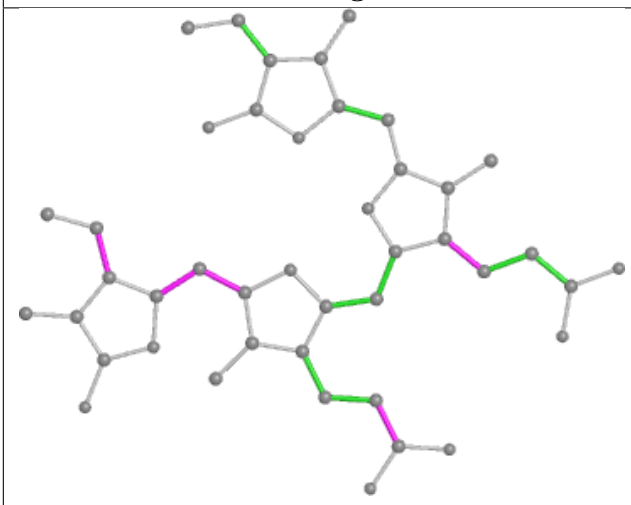

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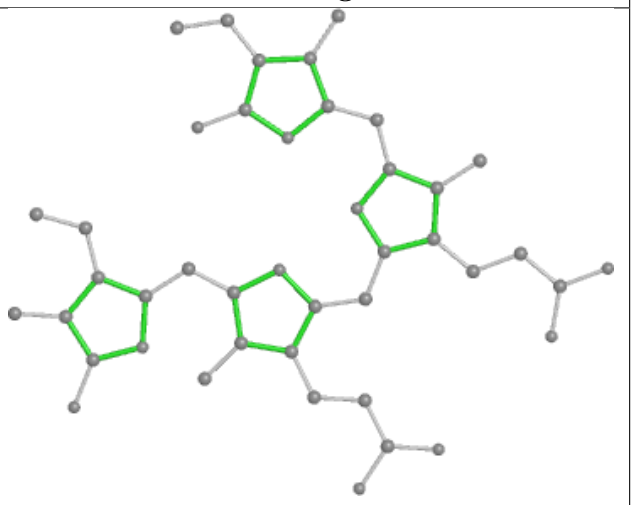
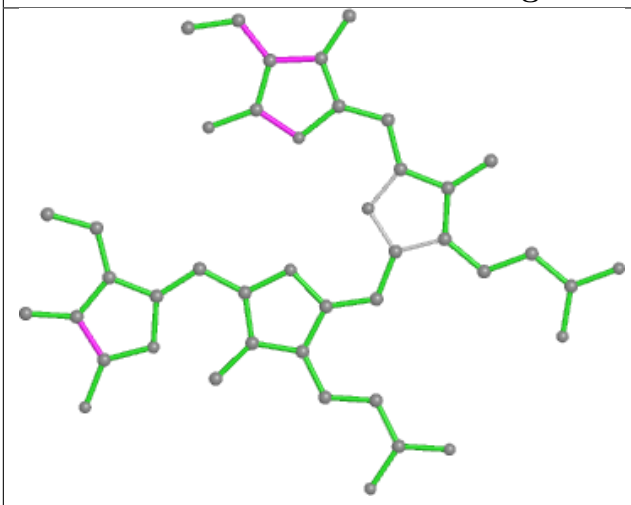


Rings

Ligand PEB cc 201



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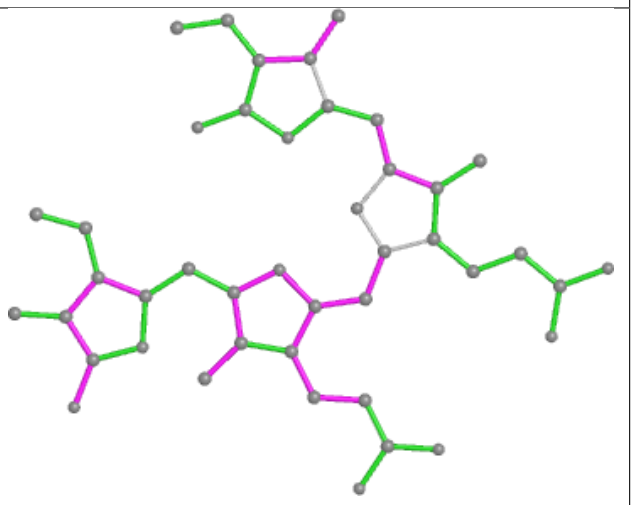

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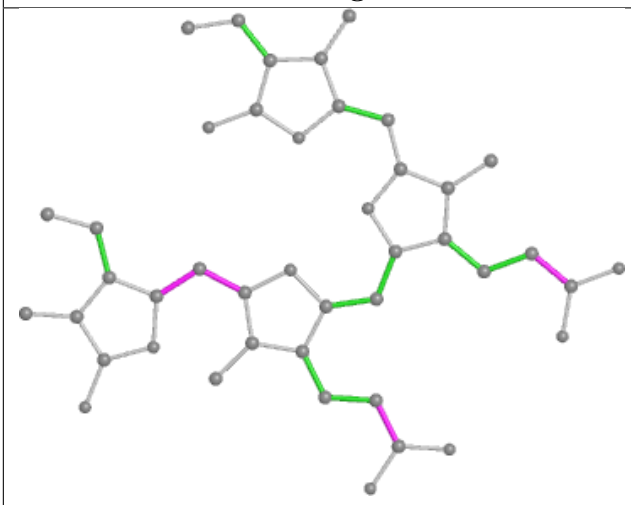

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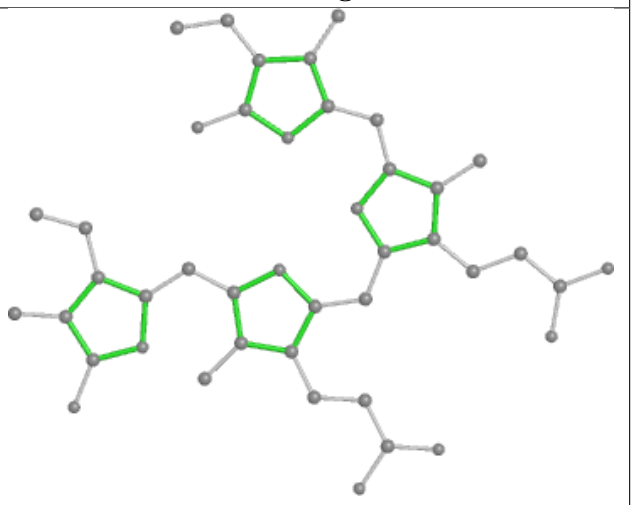
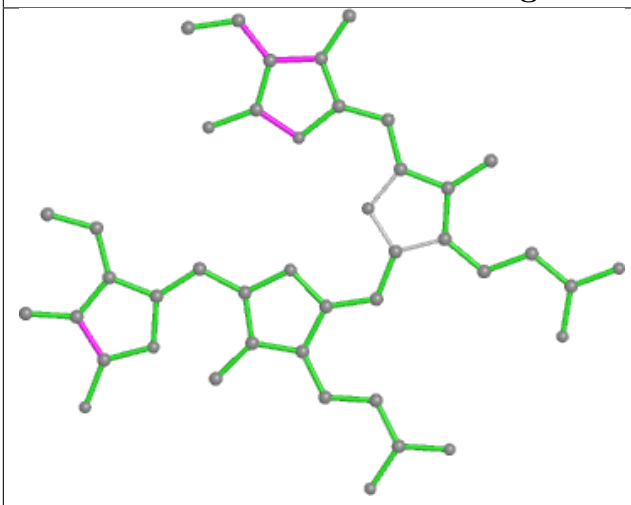


Rings

Ligand PEB a9 602



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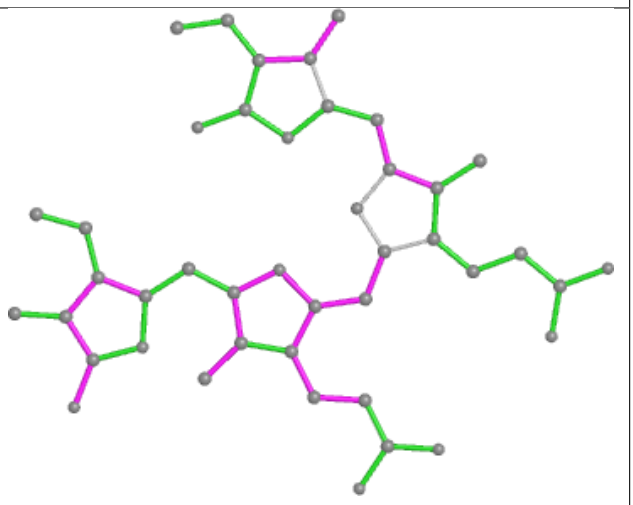

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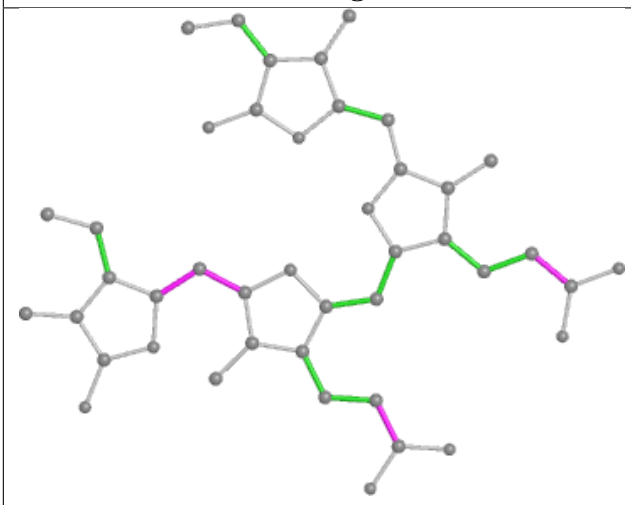

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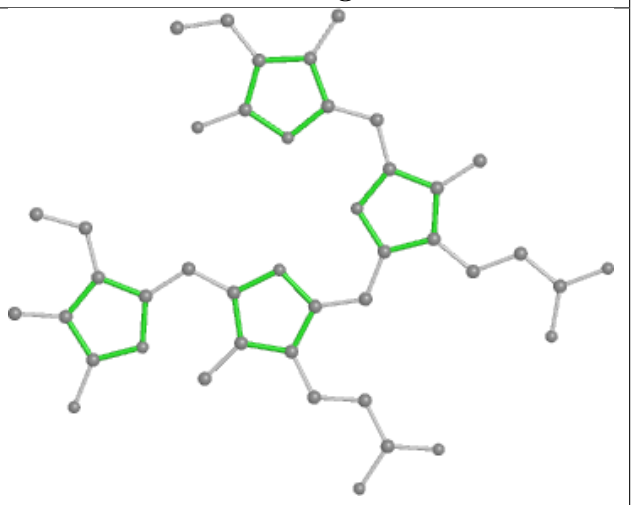
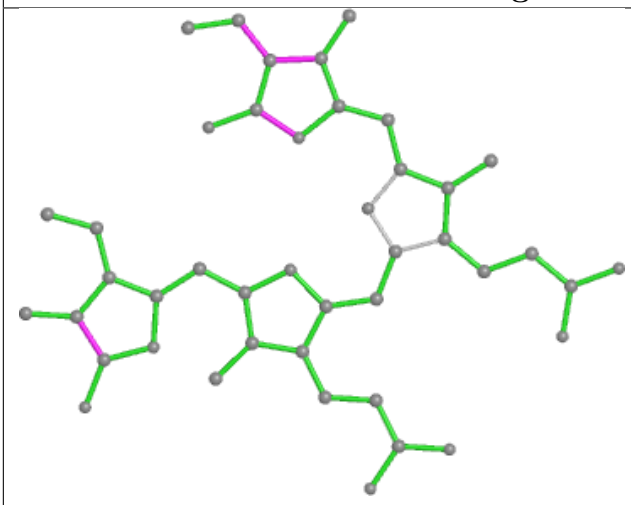


Rings

Ligand PEB M4 202



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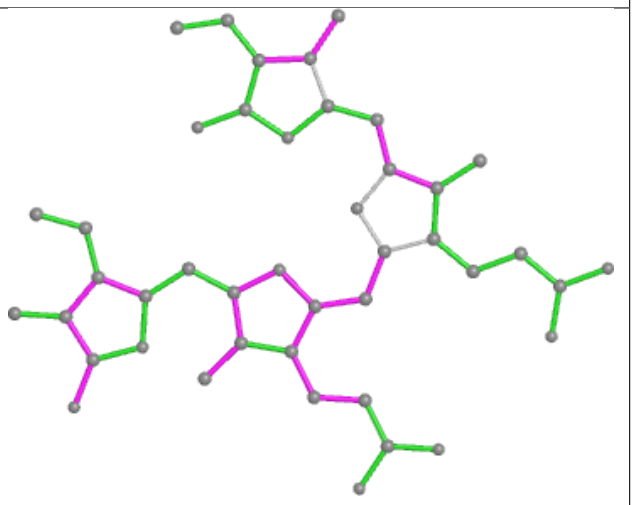

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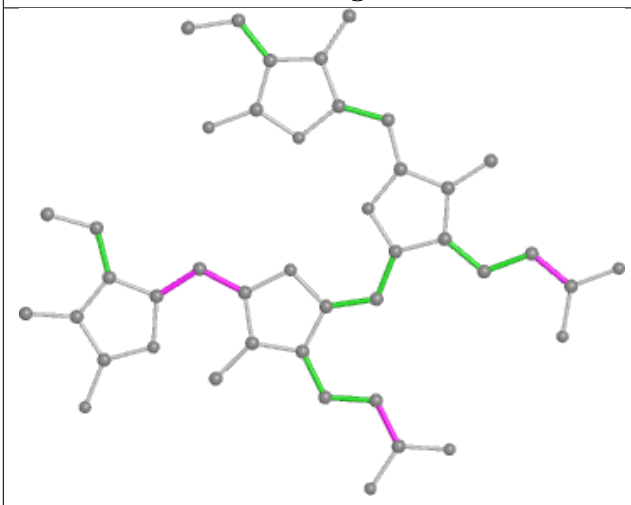

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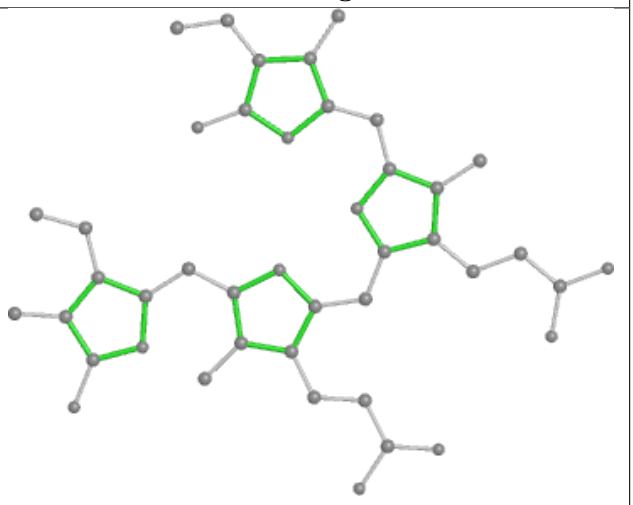
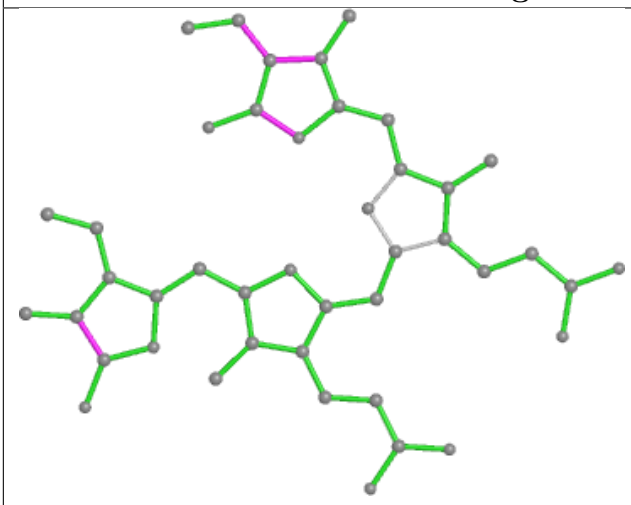


Rings

Ligand PEB c6 1003



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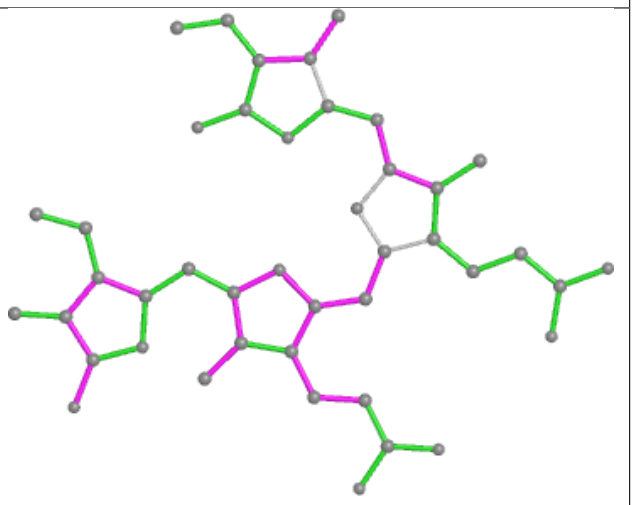
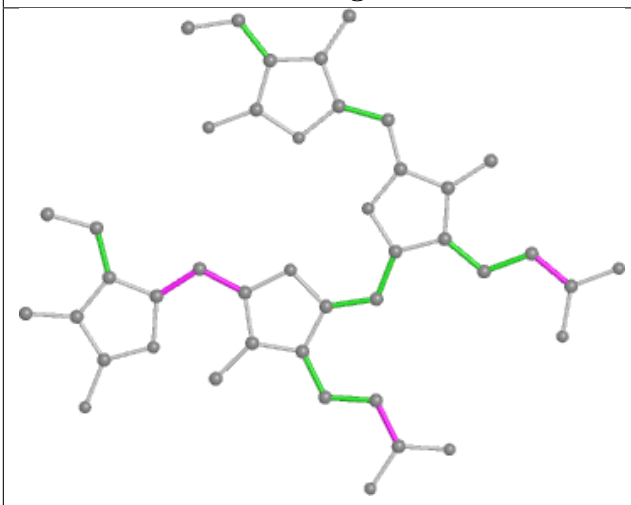


Bond angles



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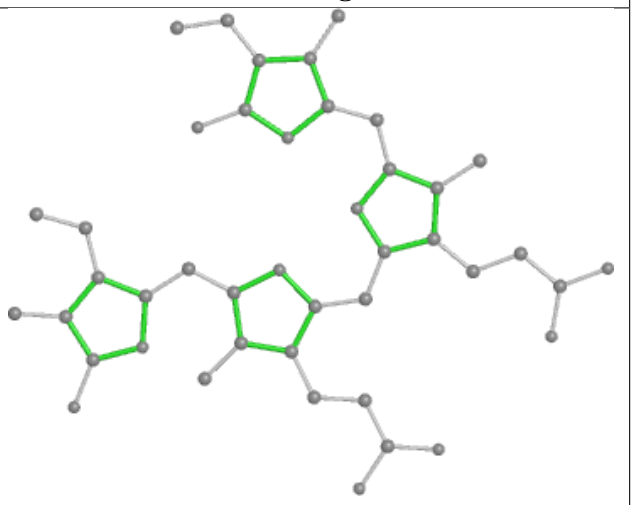
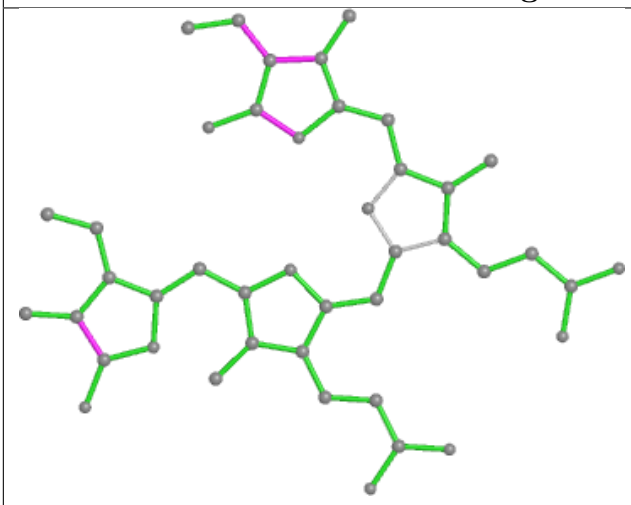


Rings

Ligand PEB ae 201



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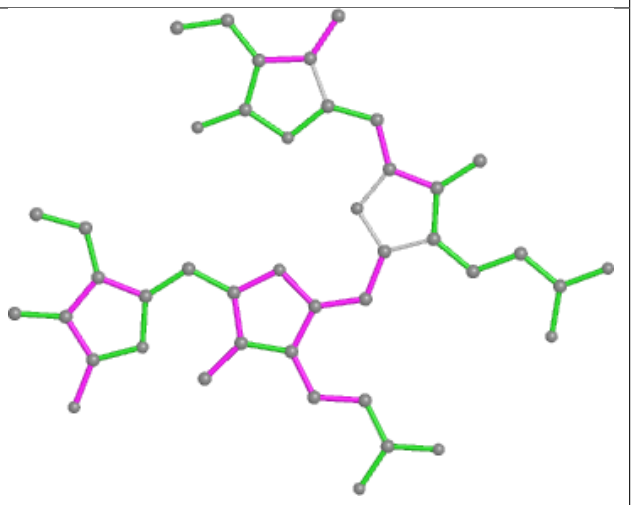

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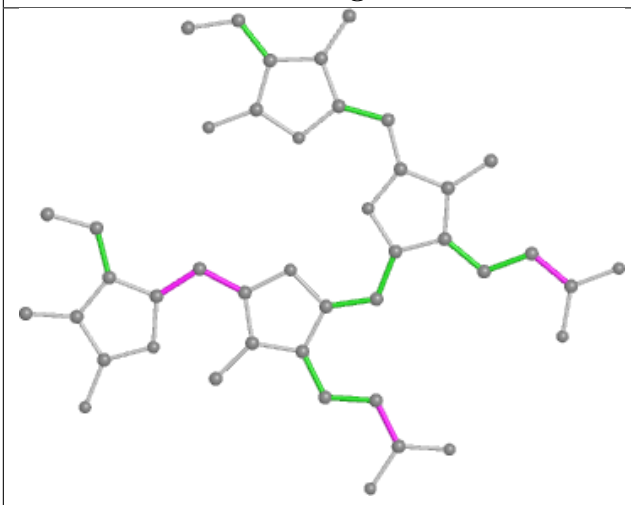
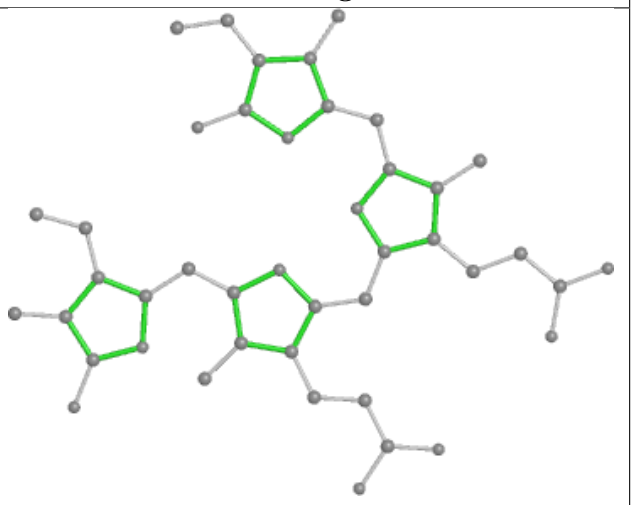
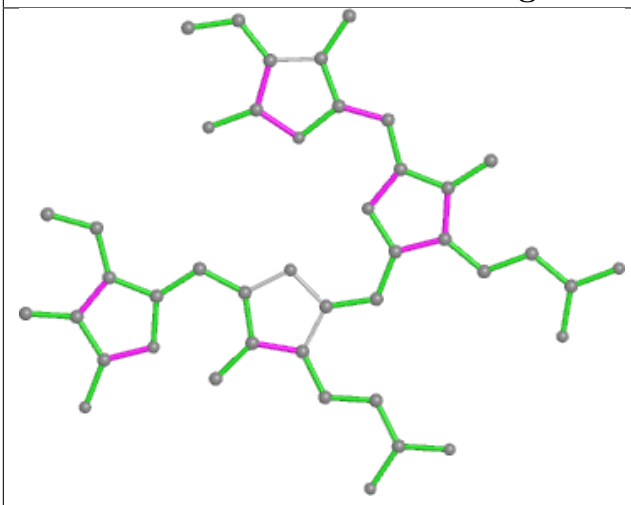


Torsions



Rings

Ligand PUB e6 203



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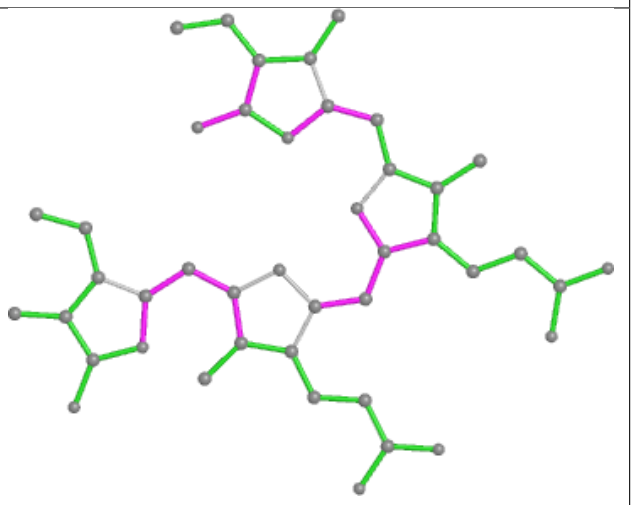

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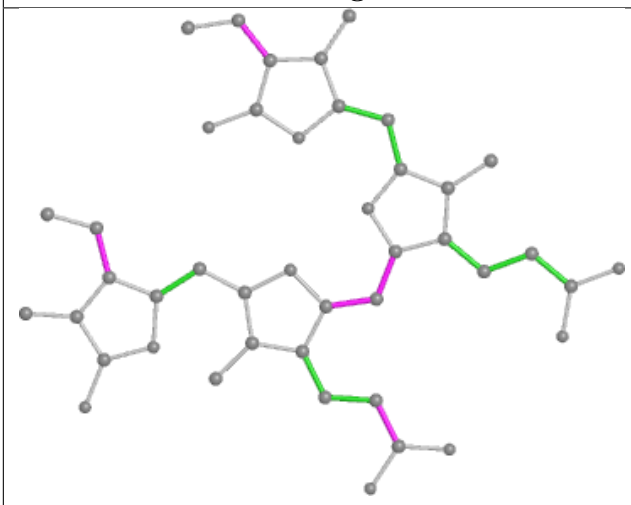

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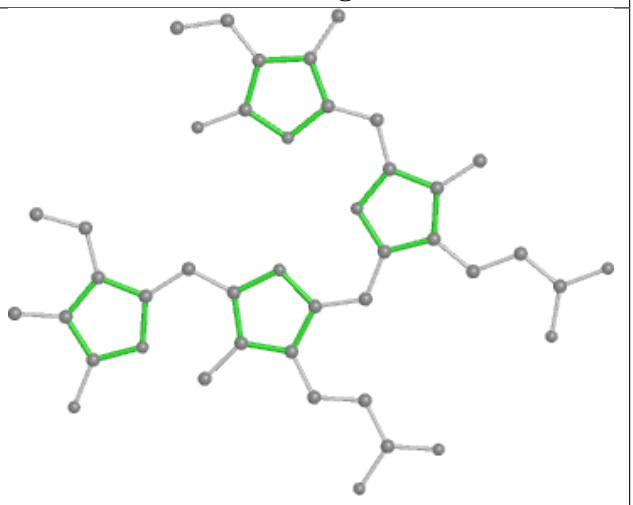

Rings

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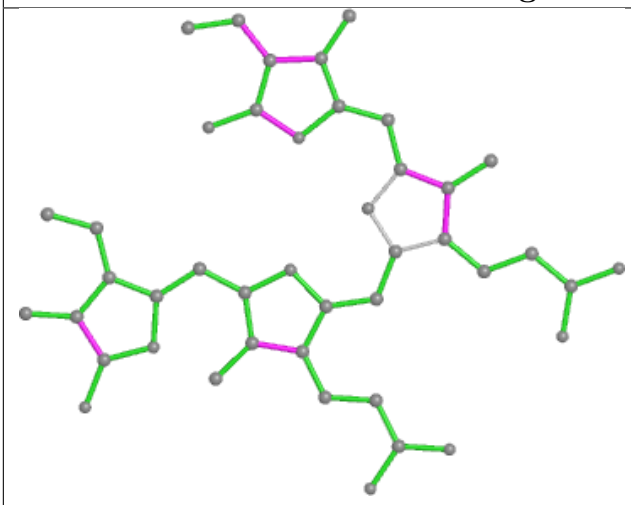

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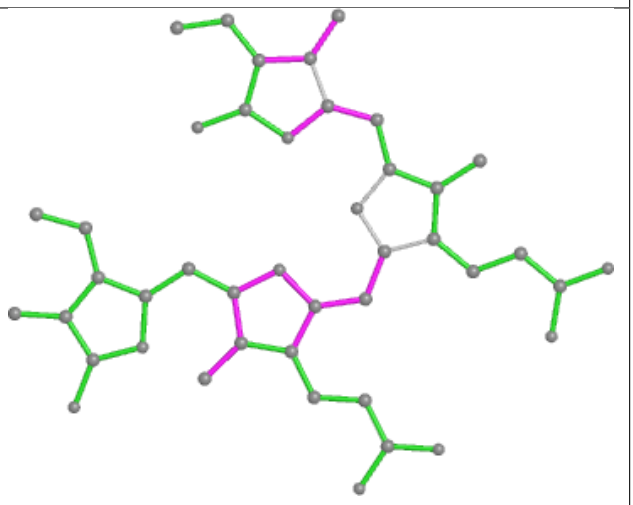

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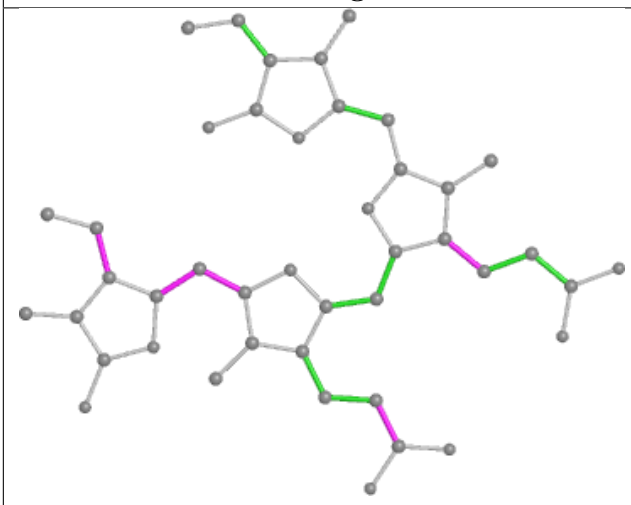

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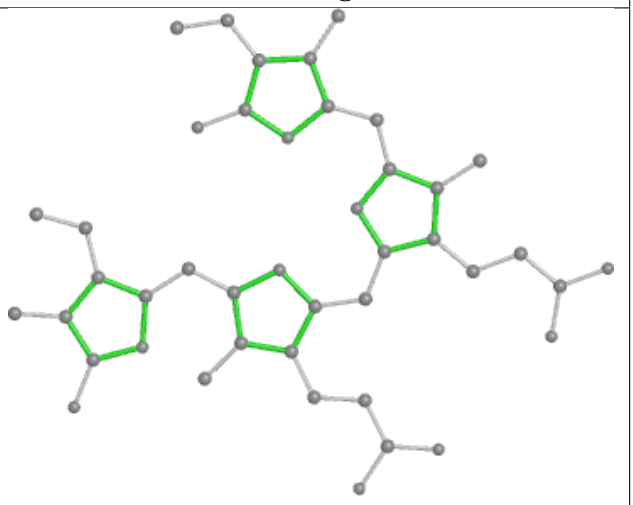

Rings

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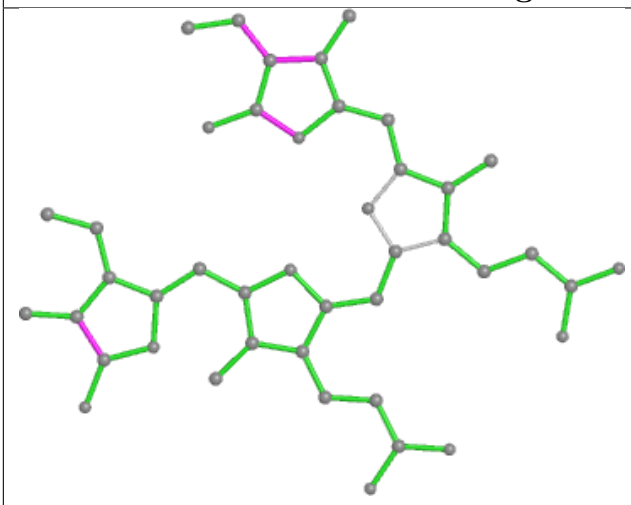

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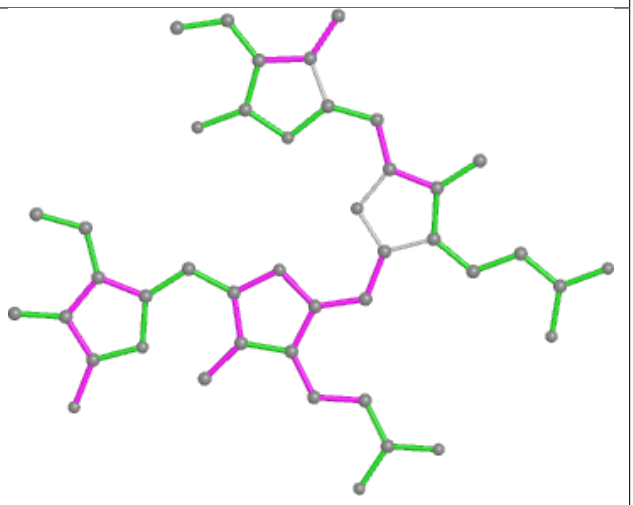

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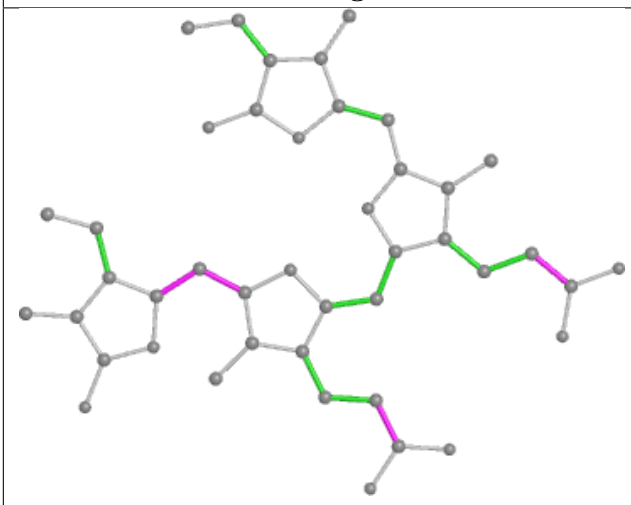

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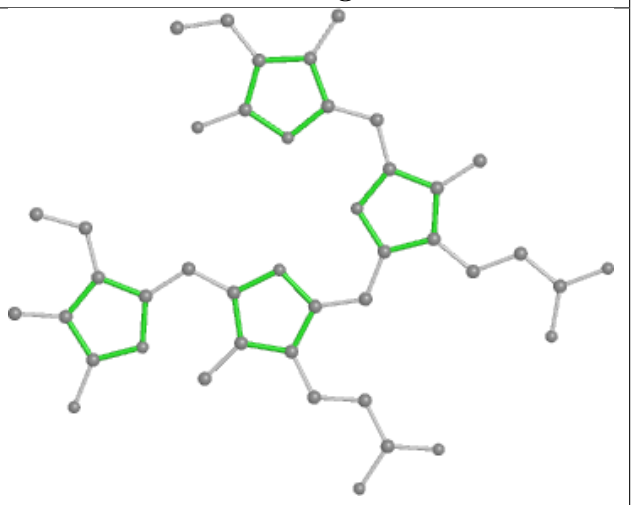

Rings

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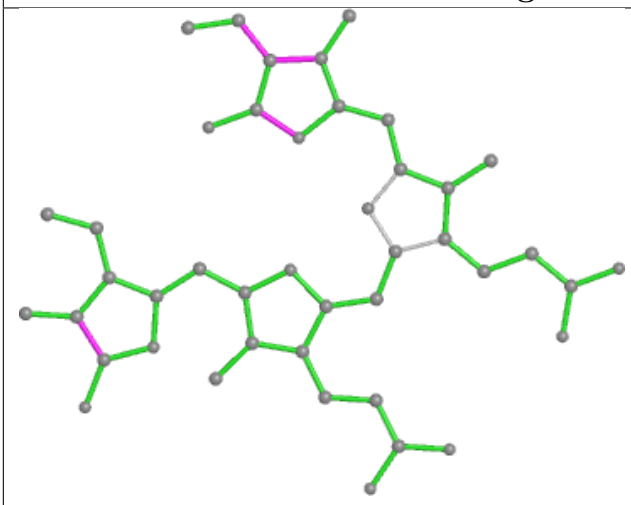

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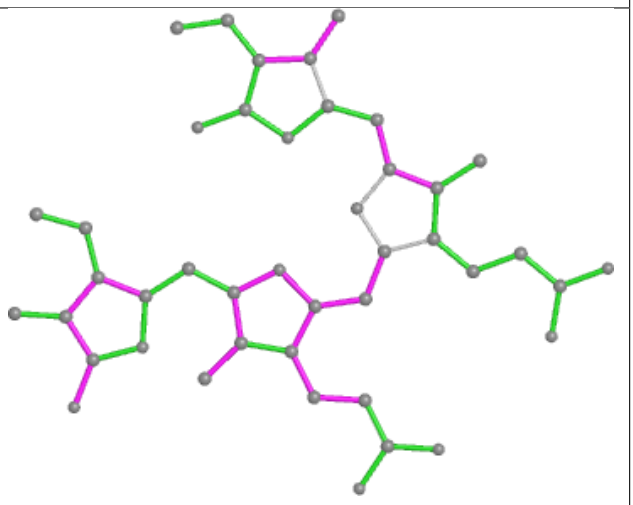

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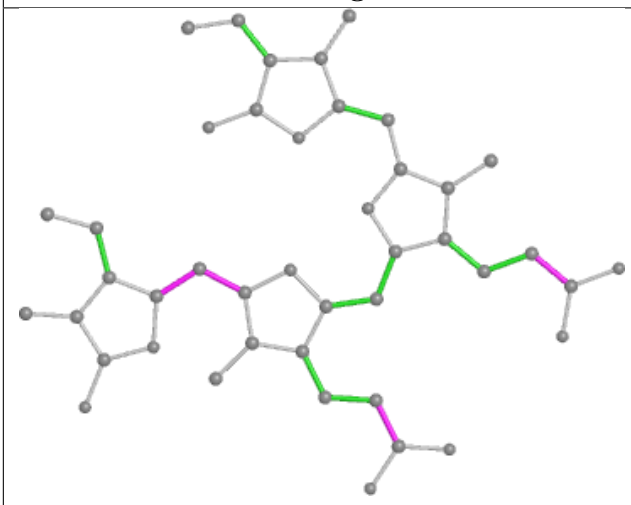

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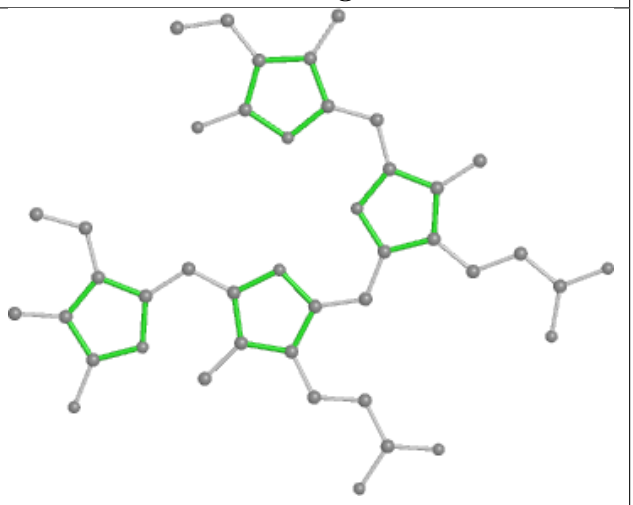

Rings

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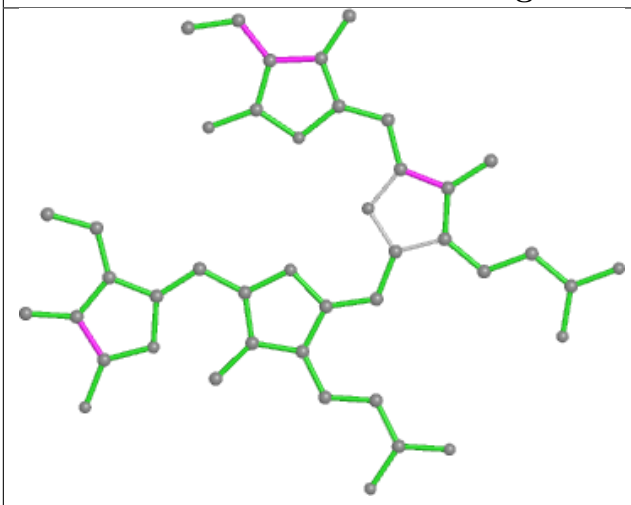

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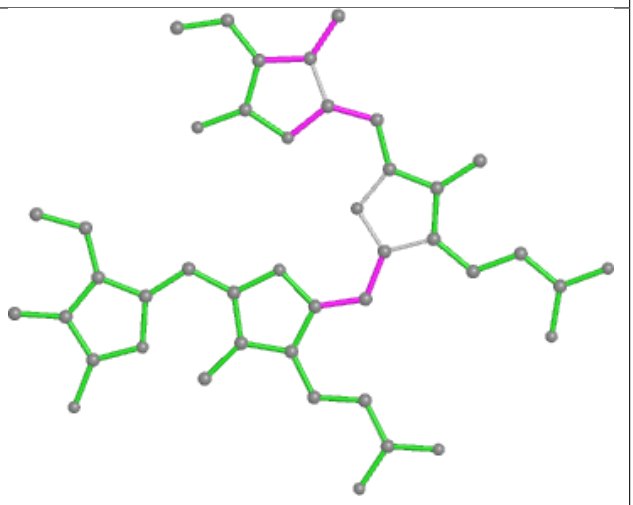

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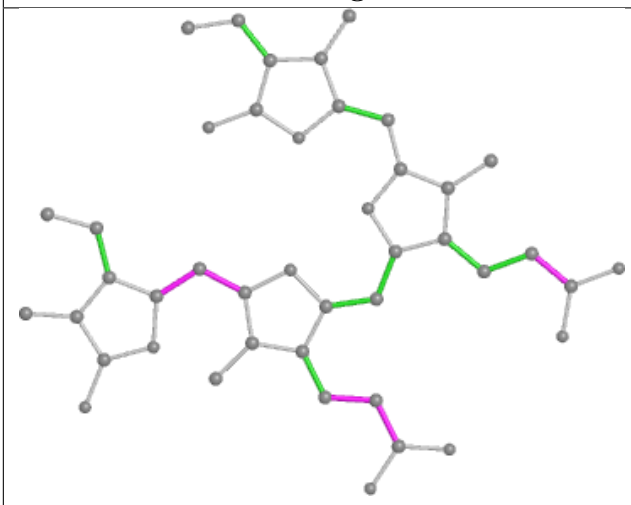

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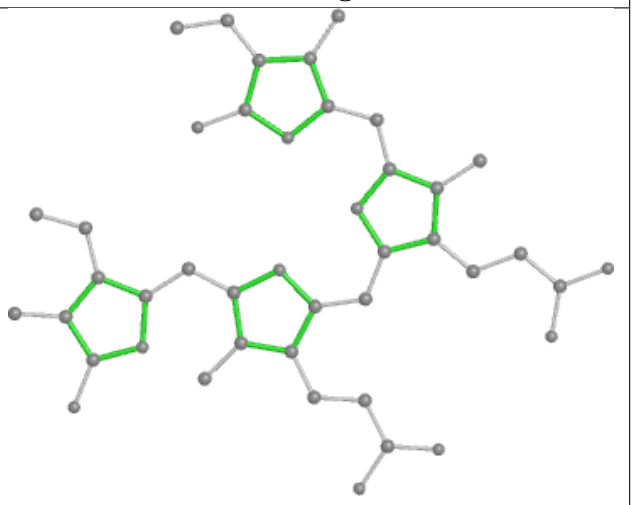

Rings

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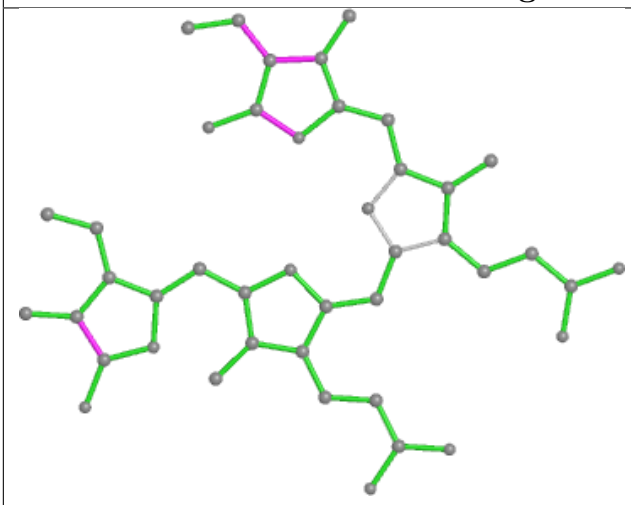

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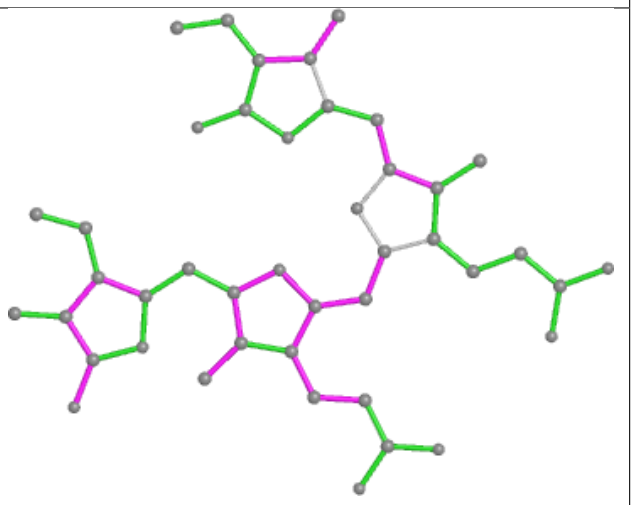

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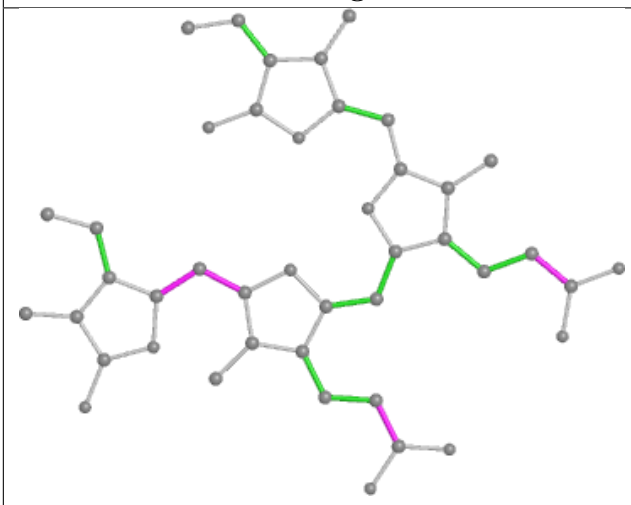

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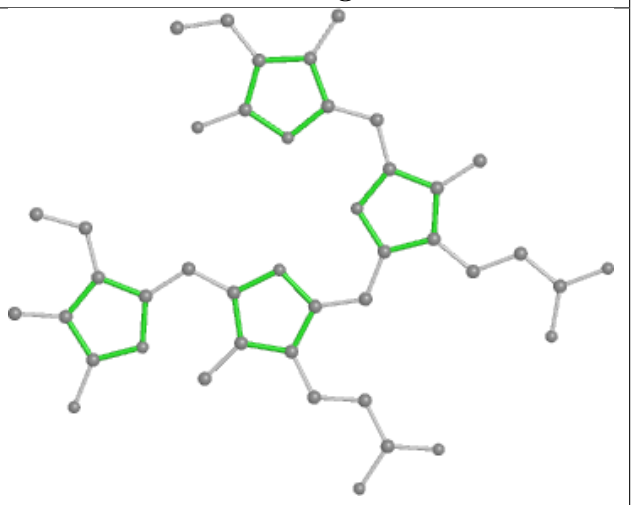

Rings

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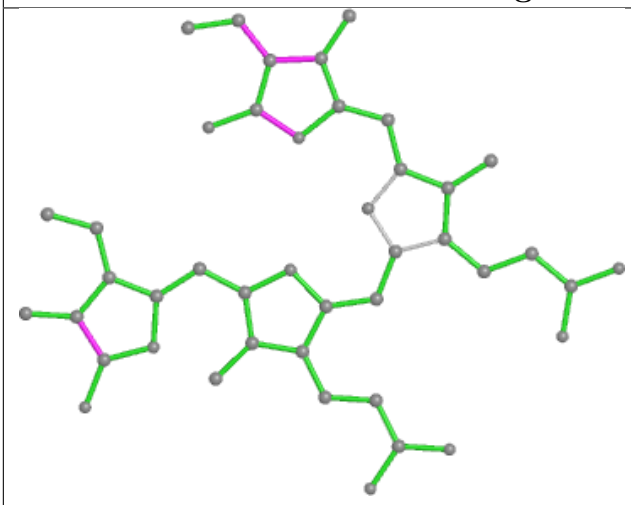

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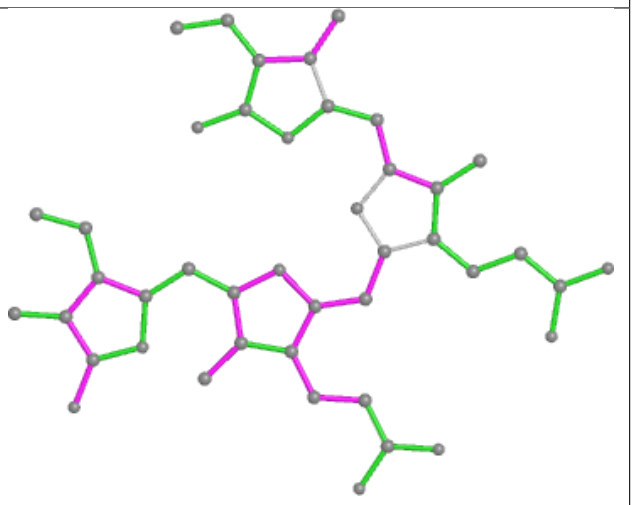

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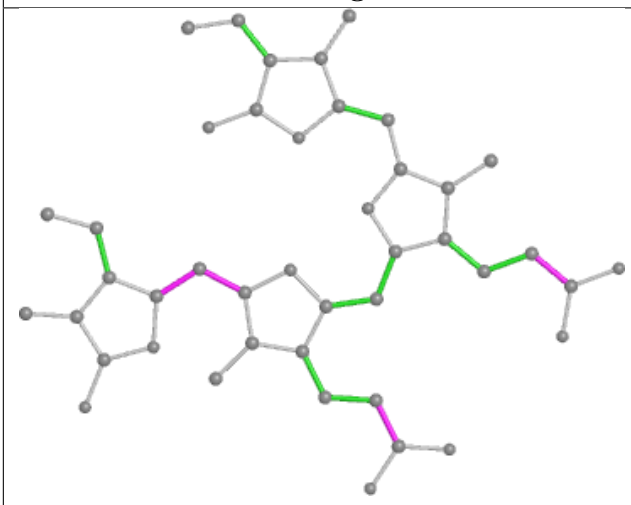

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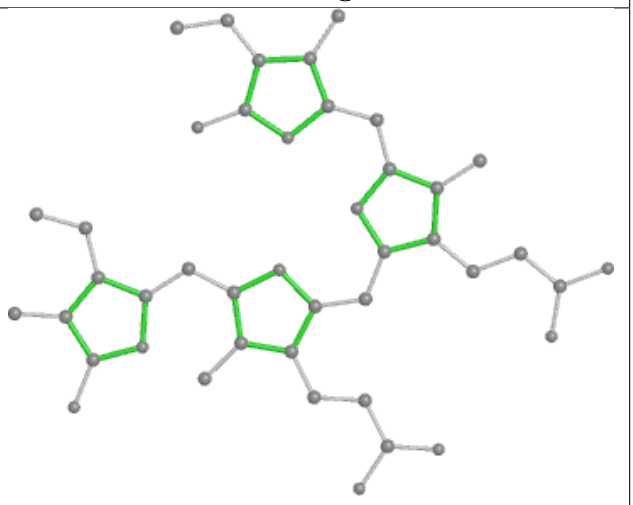

Rings

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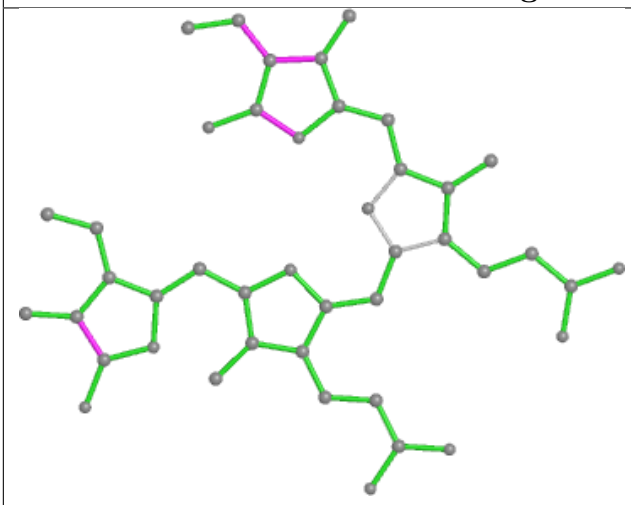

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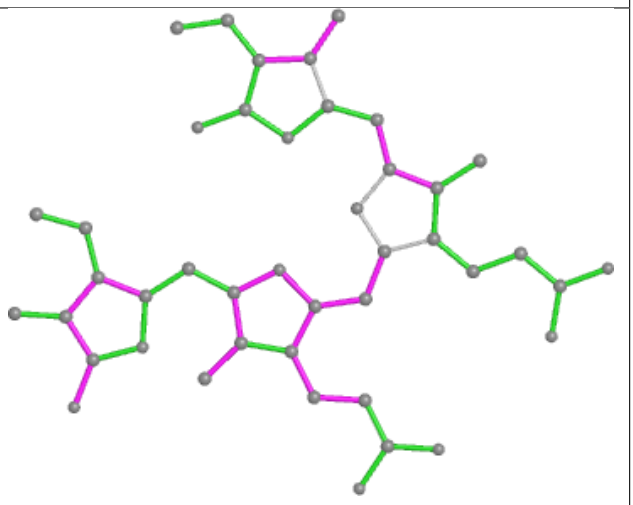

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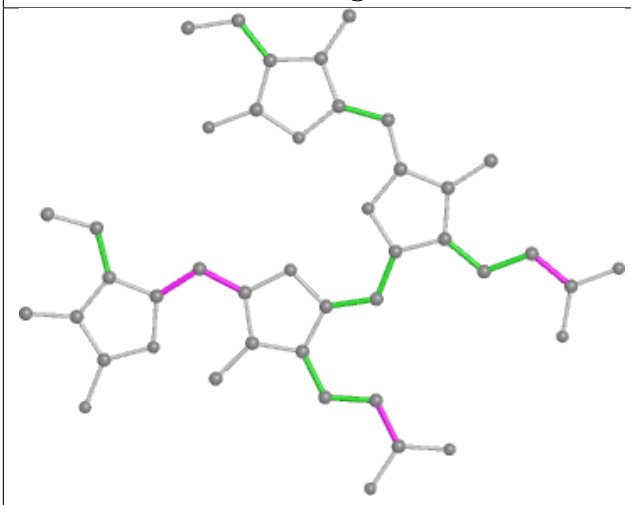

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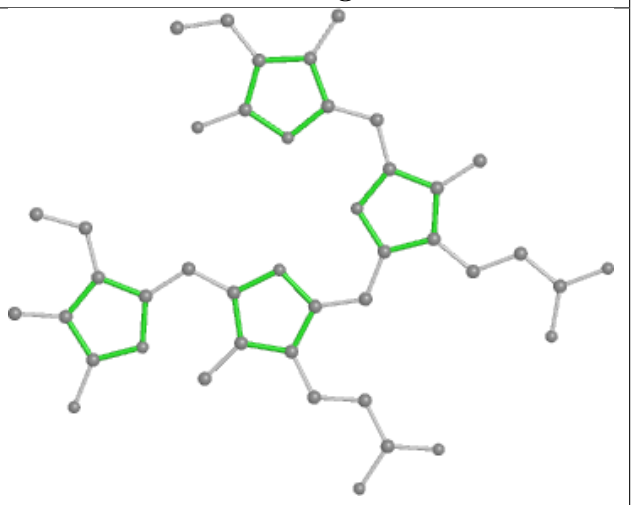

Rings

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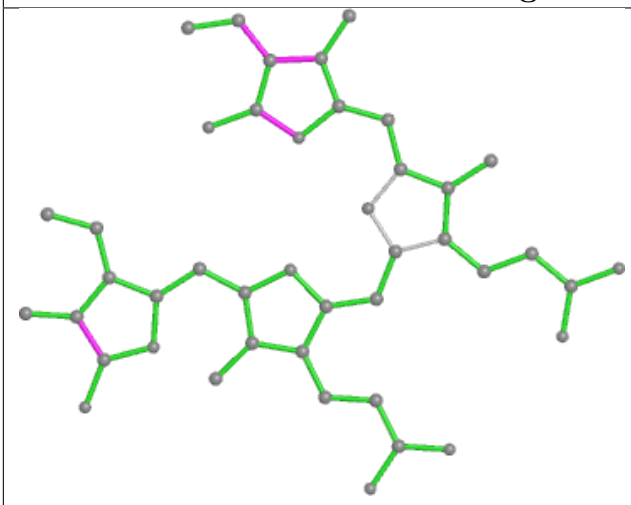

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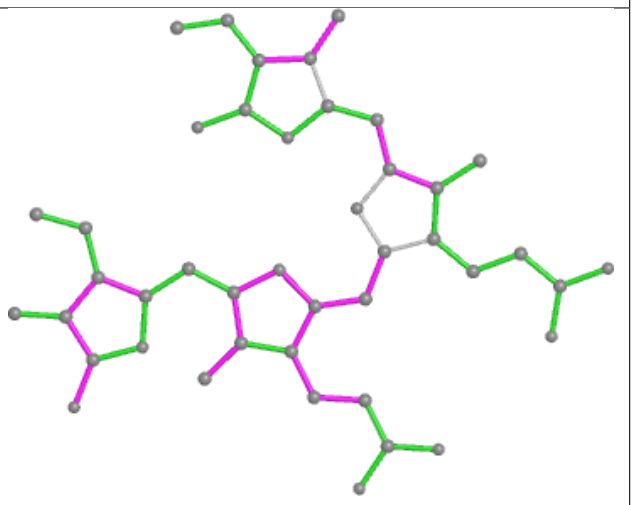

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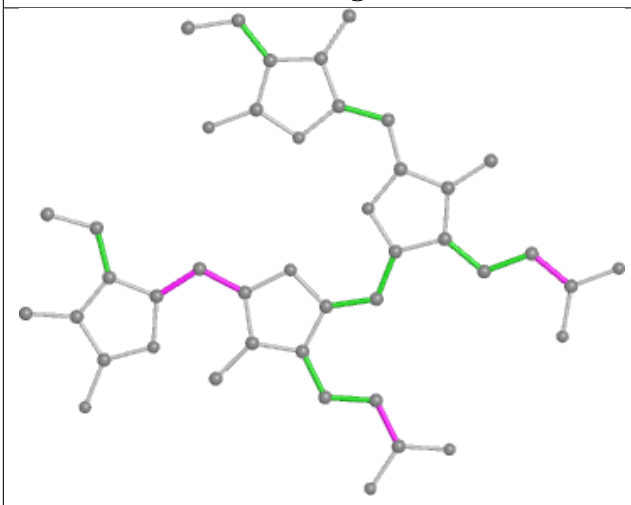

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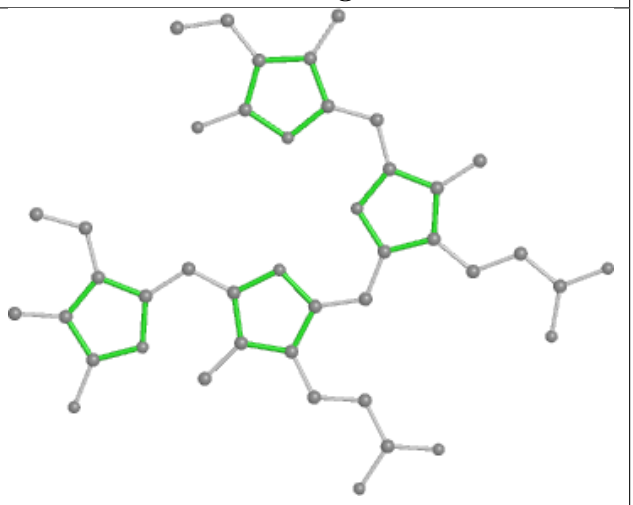

Rings

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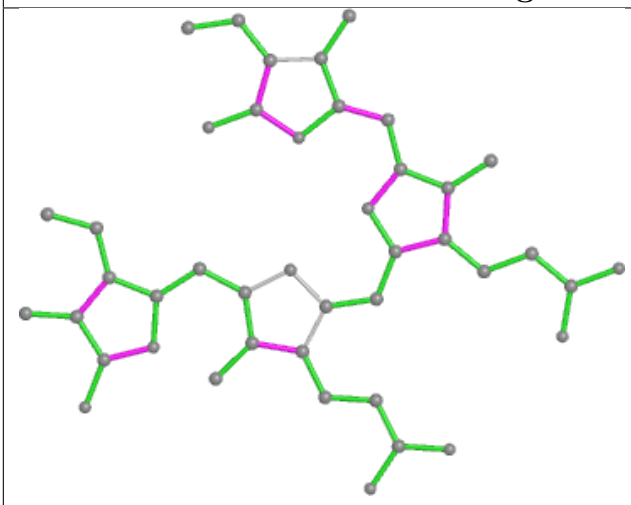

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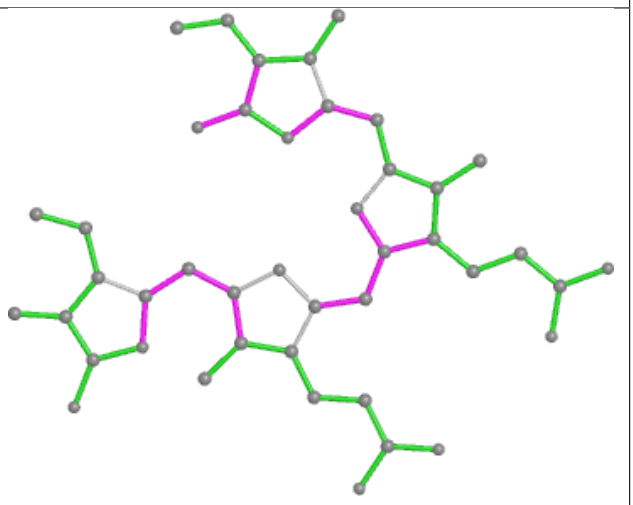

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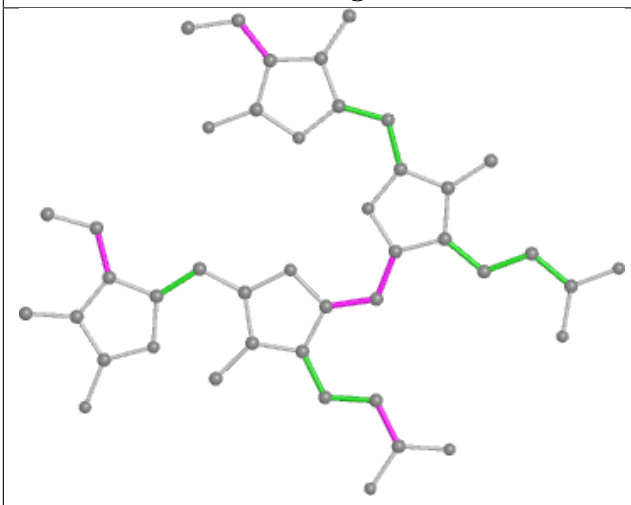

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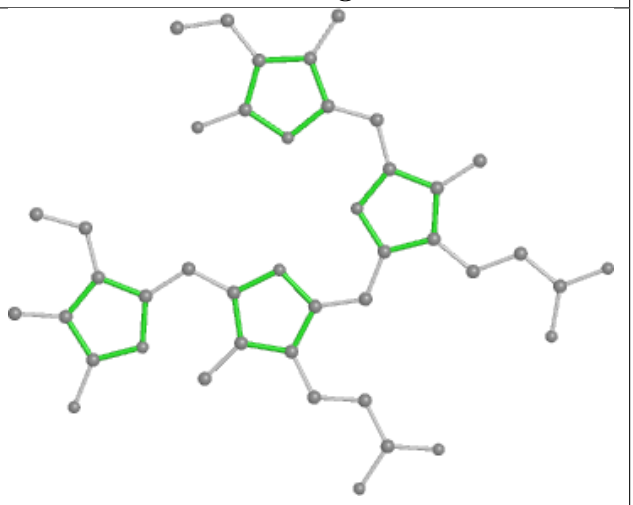

Rings

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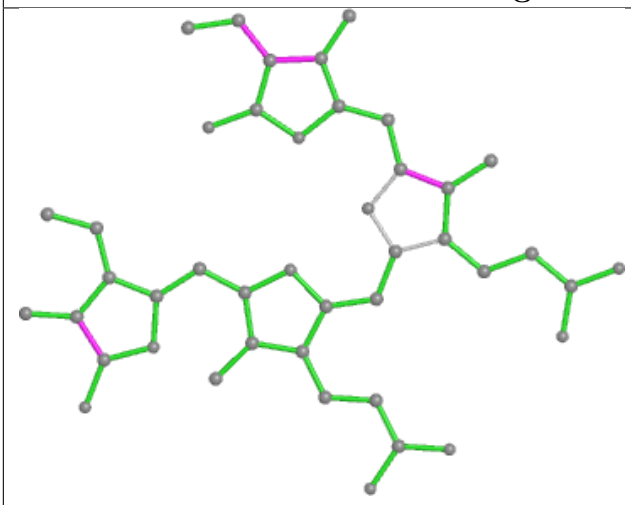

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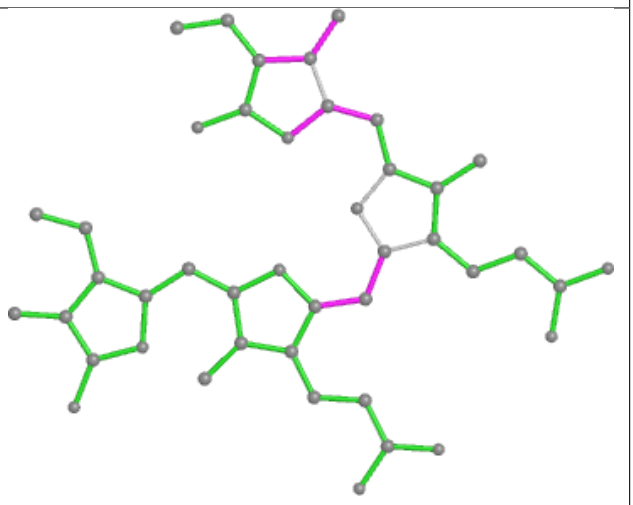

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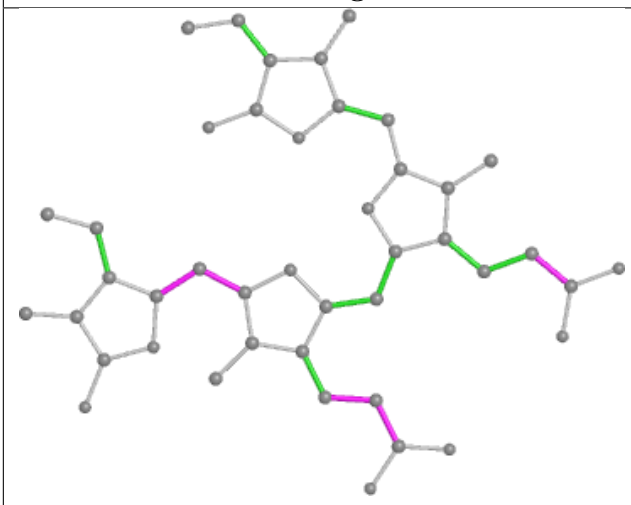

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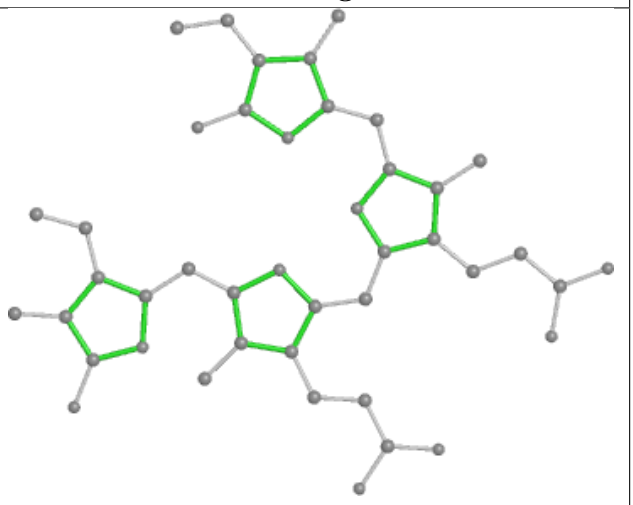

Rings

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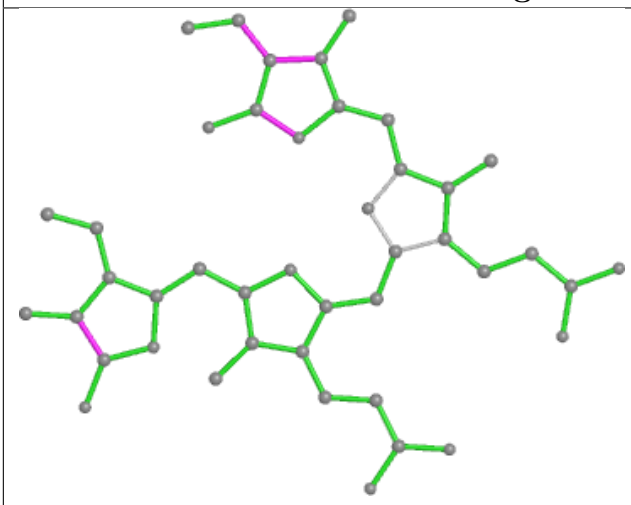

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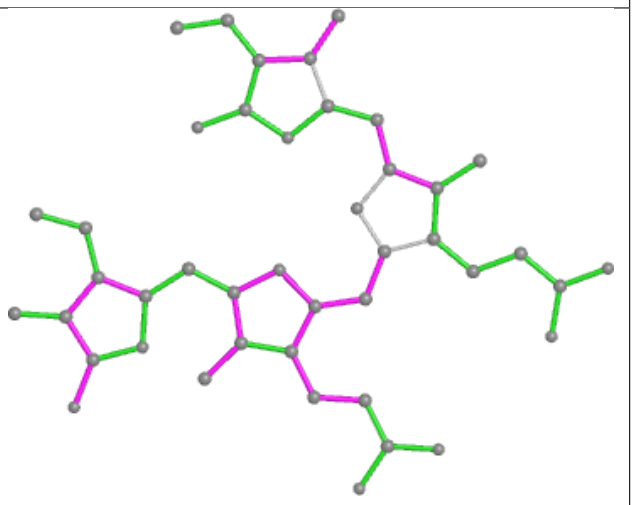

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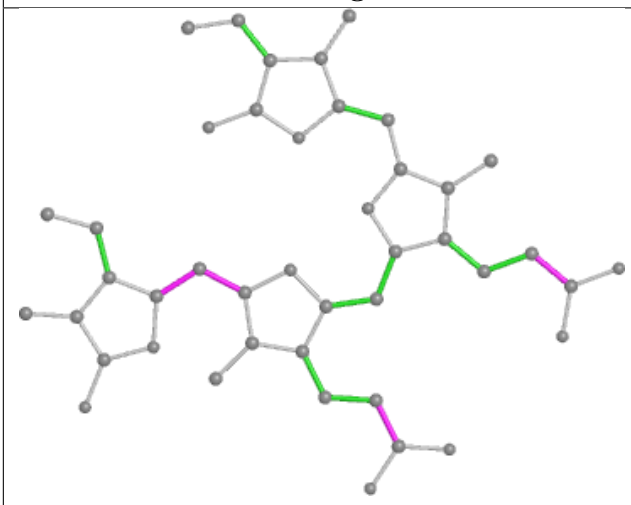

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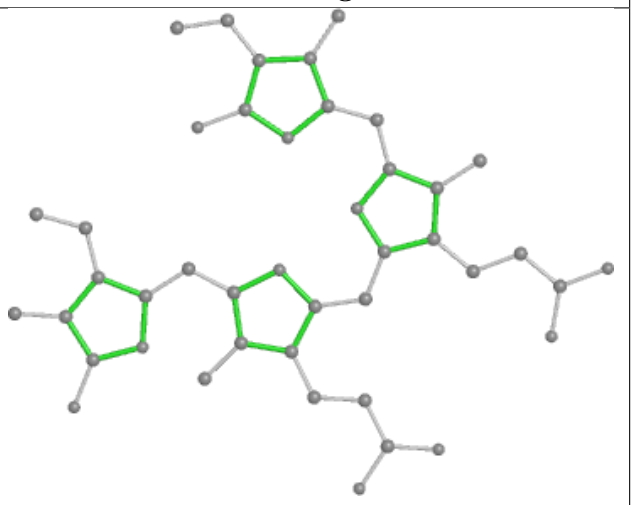
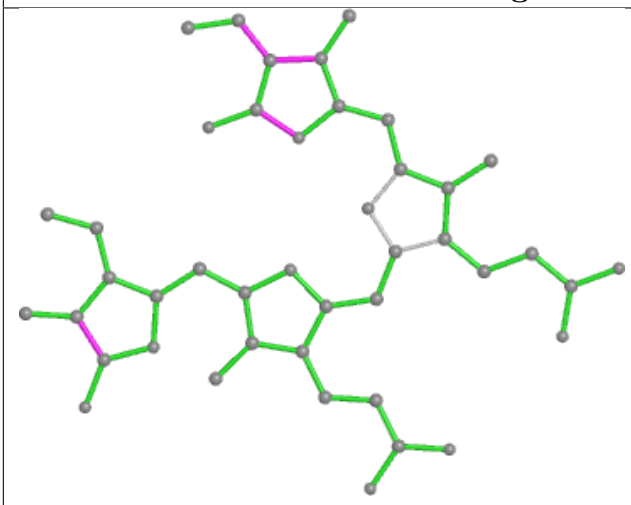


Rings

Ligand PEB jP 1001



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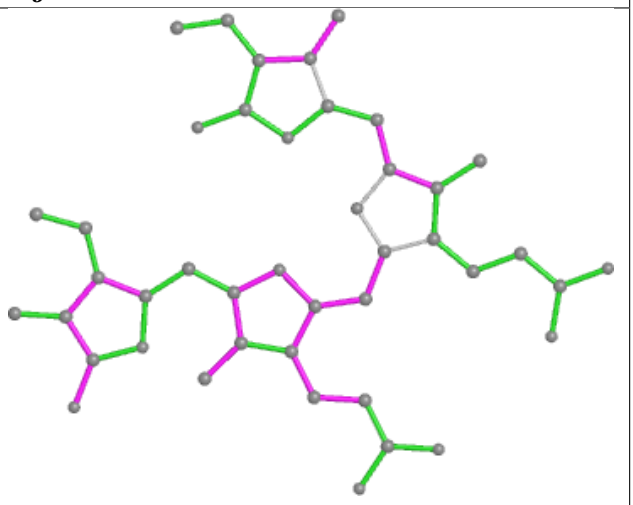
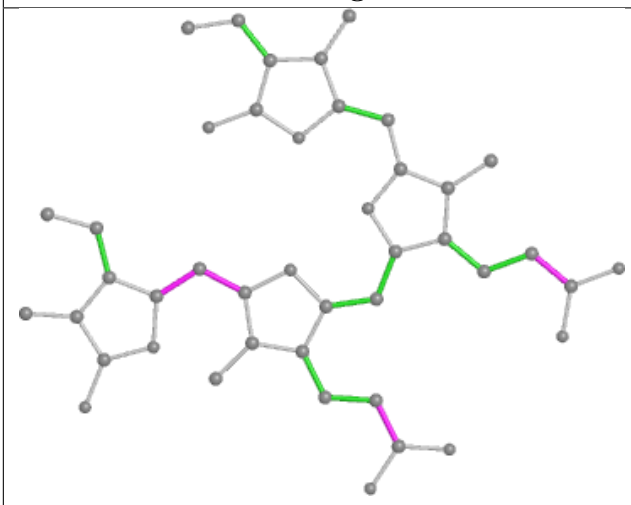
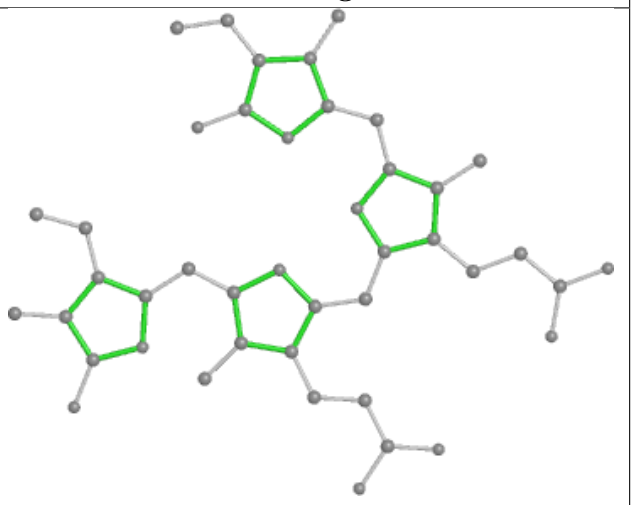


Bond angles

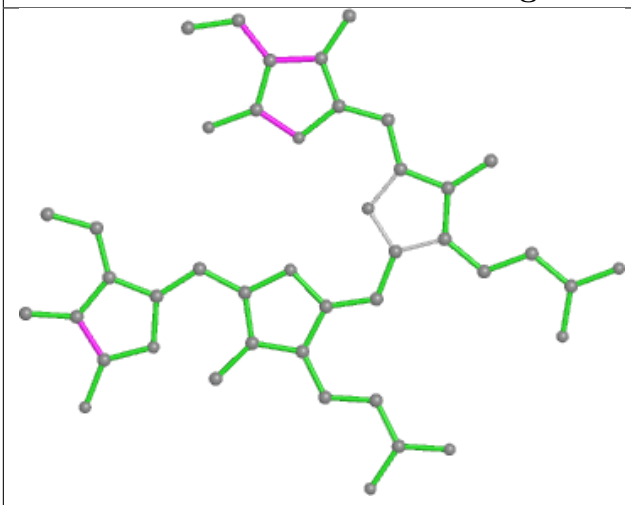


Torsions



Rings

Ligand PEB eb 201



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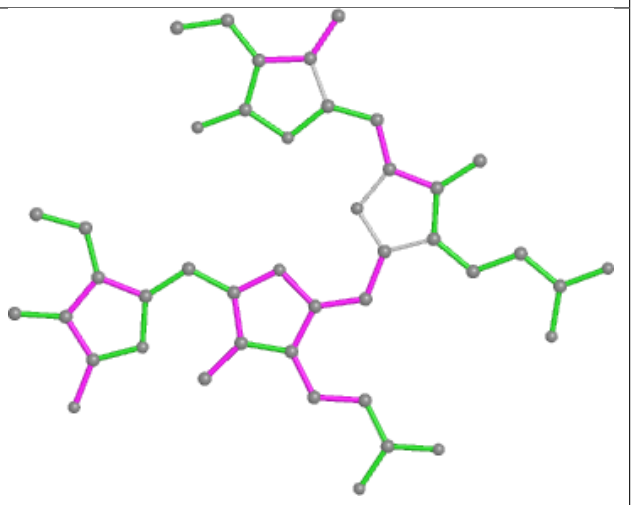

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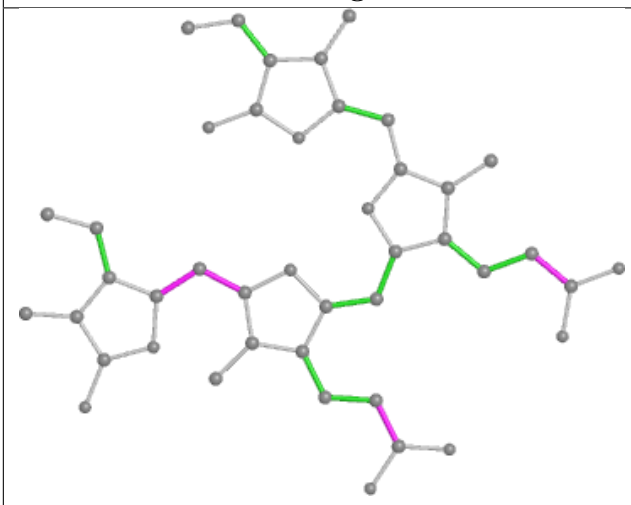

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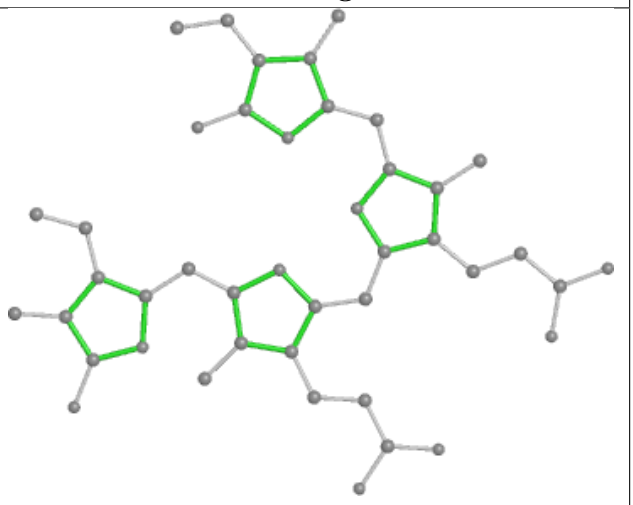

Rings

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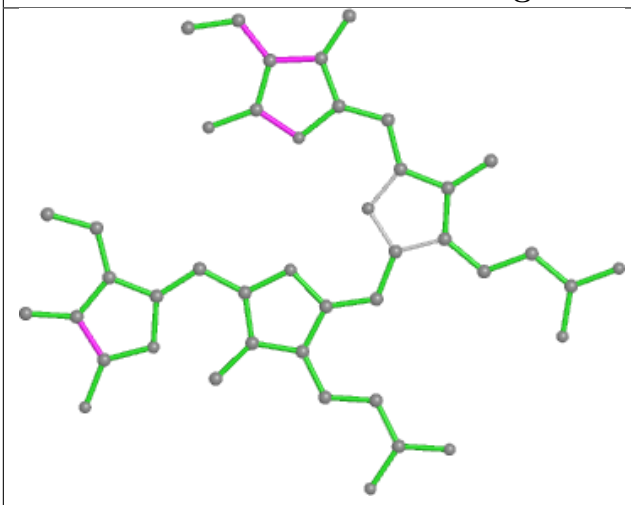

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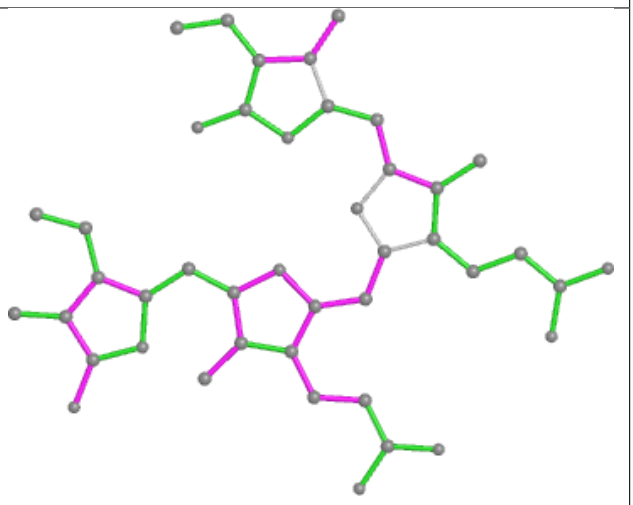

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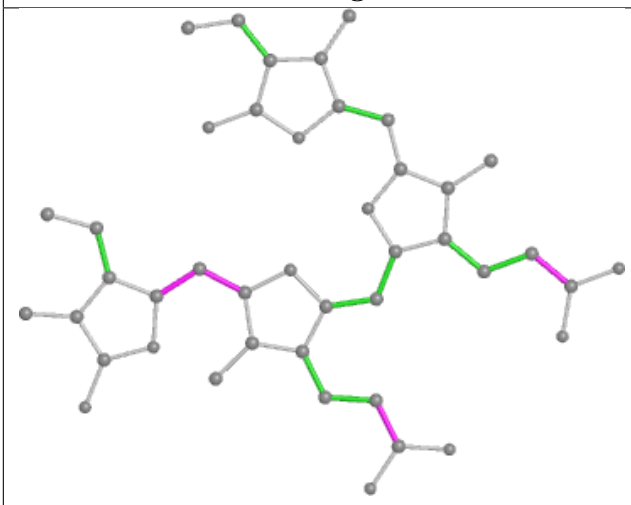

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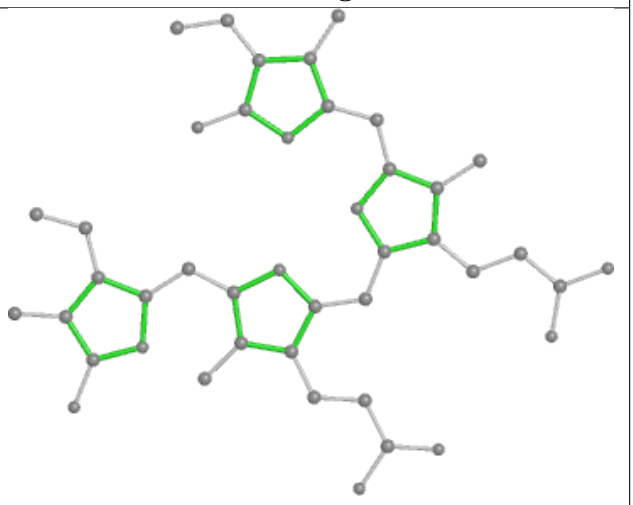
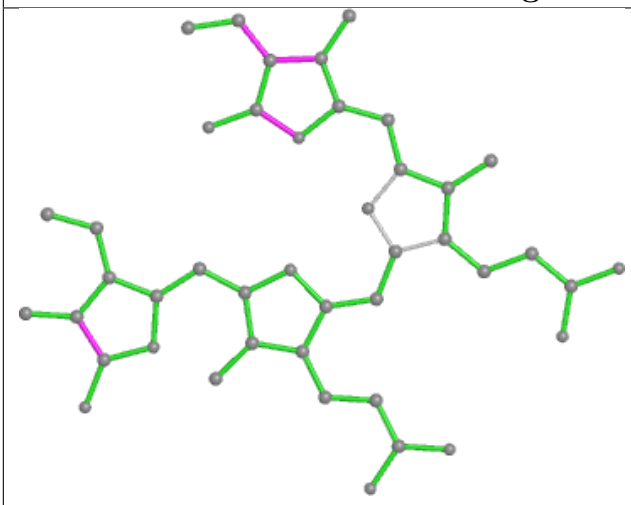


Rings

Ligand PEB as 201



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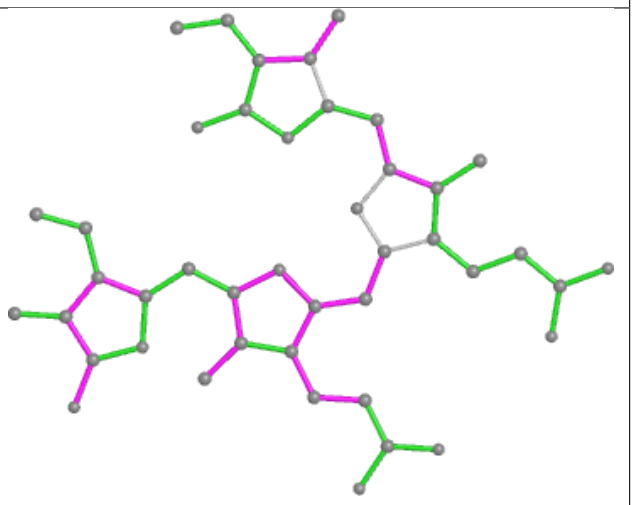

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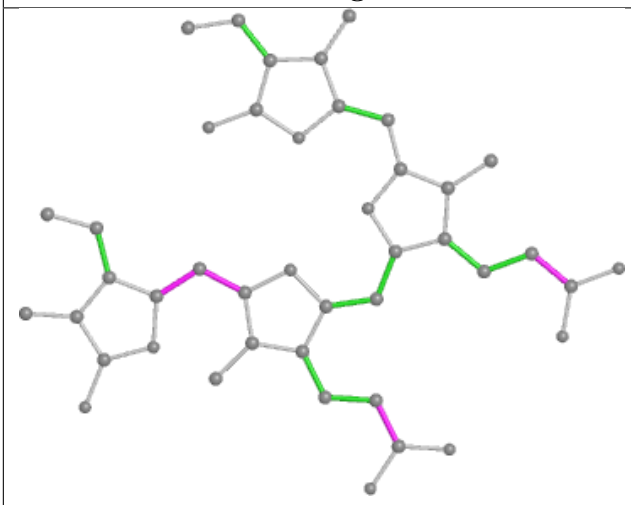

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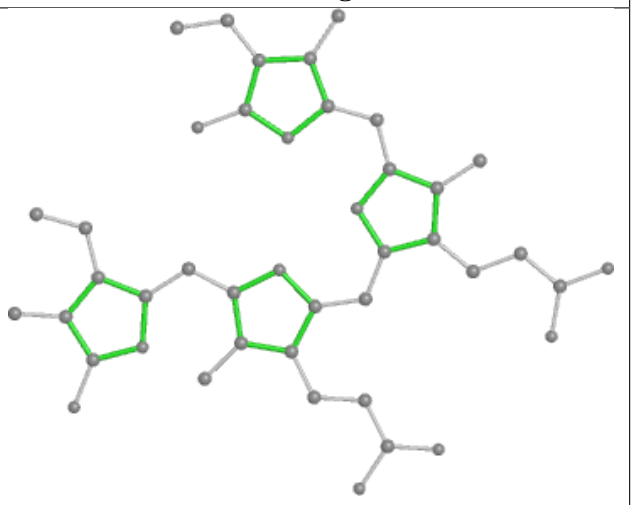

Rings

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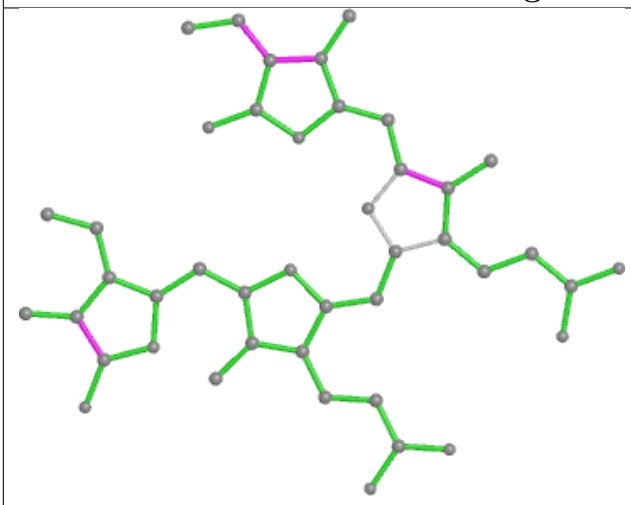

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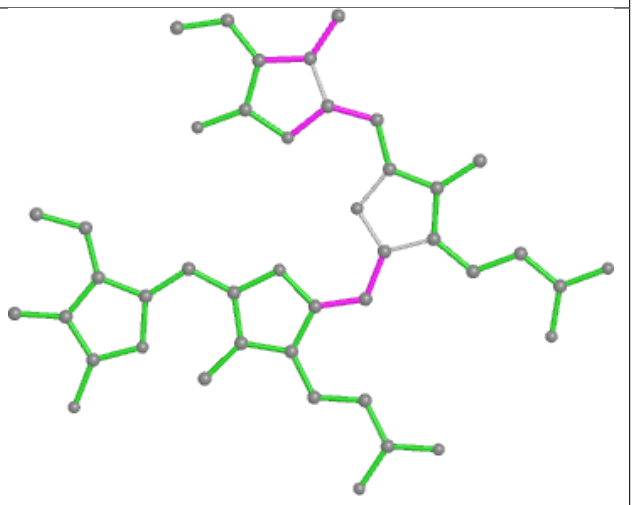

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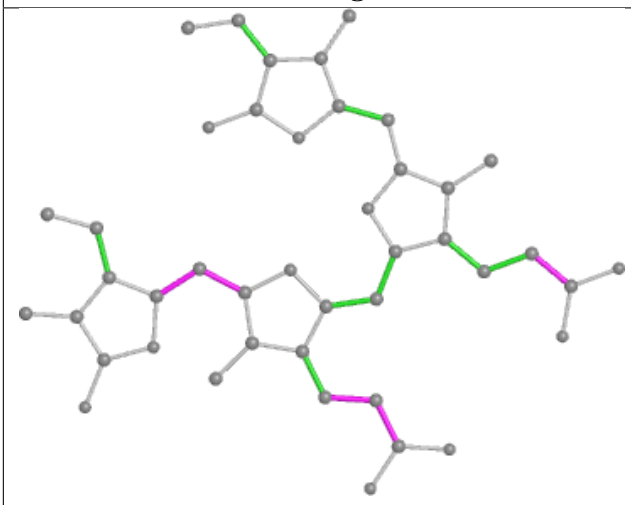

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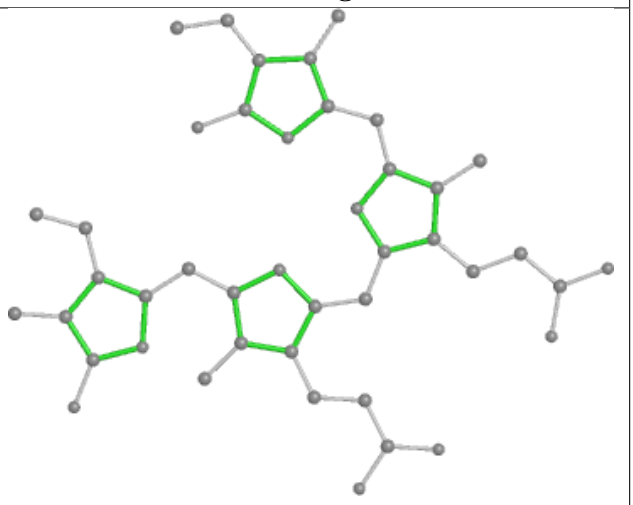

Rings

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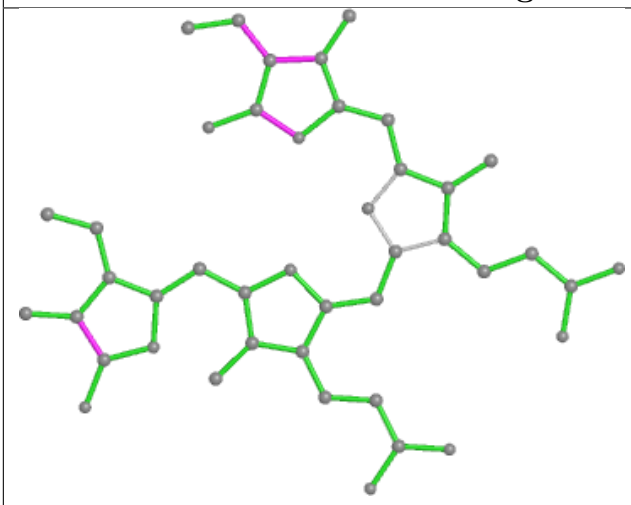

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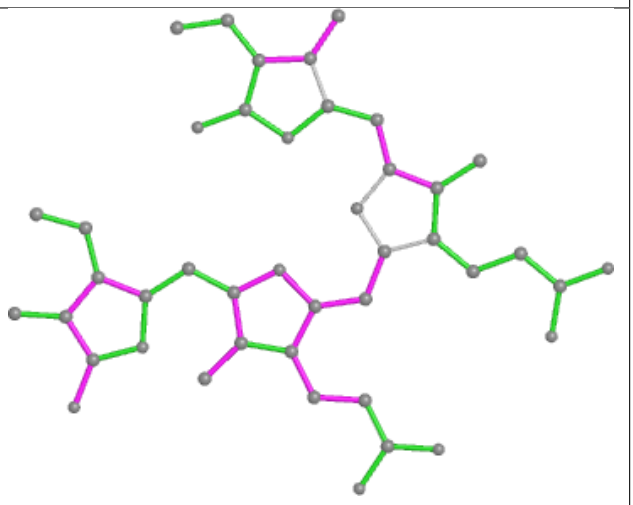

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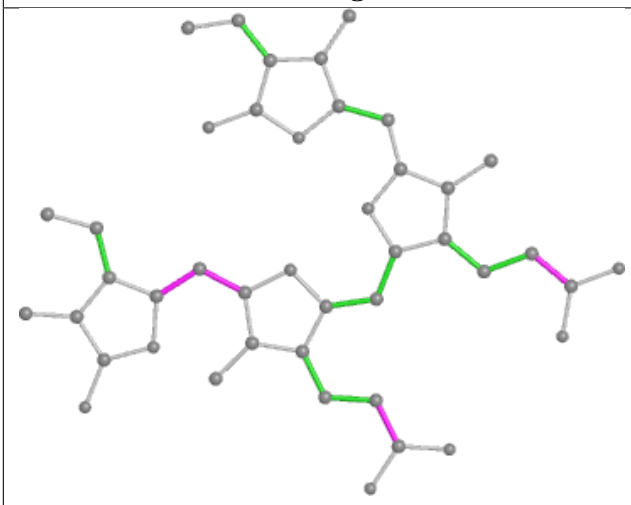

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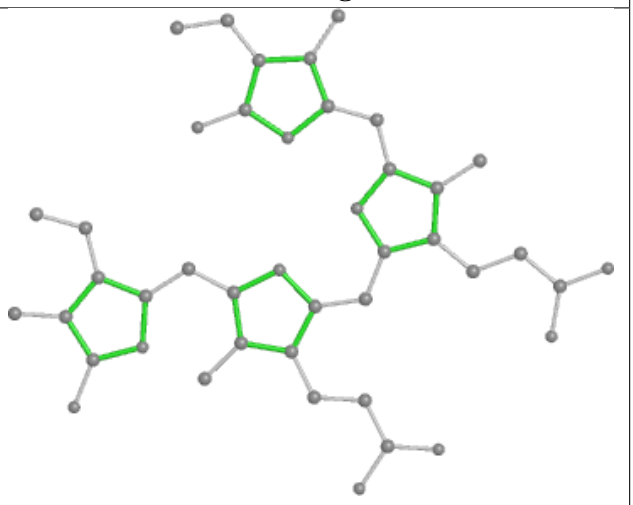

Rings

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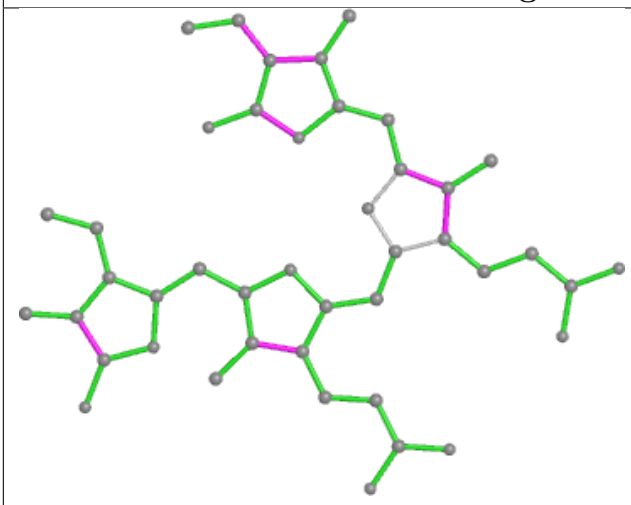

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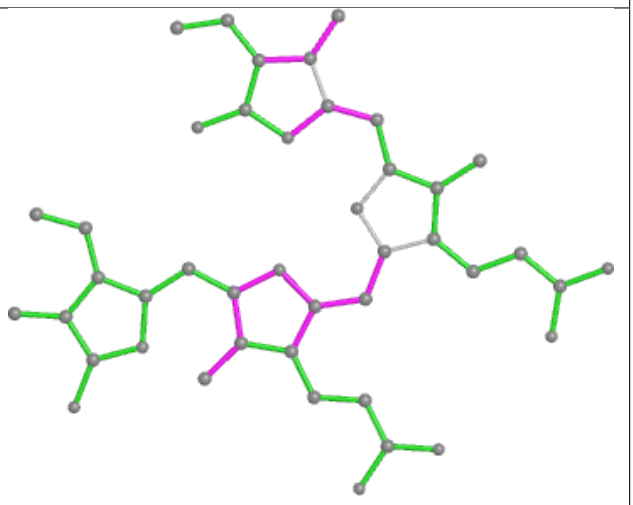

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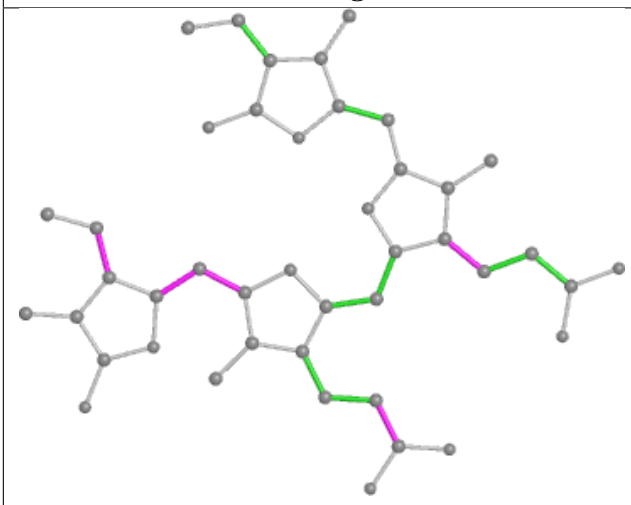

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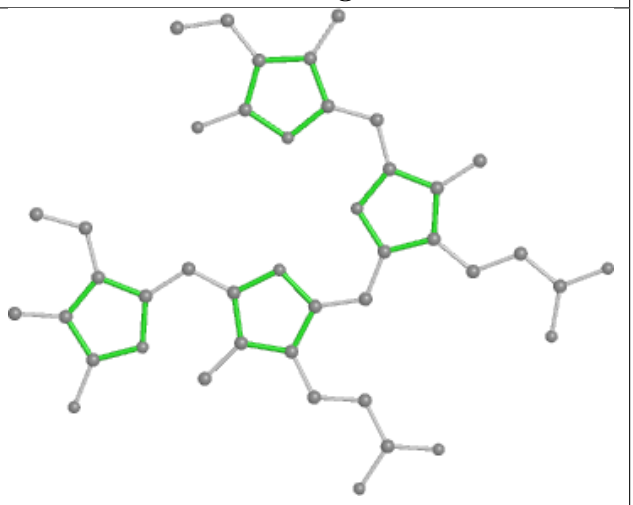

Rings

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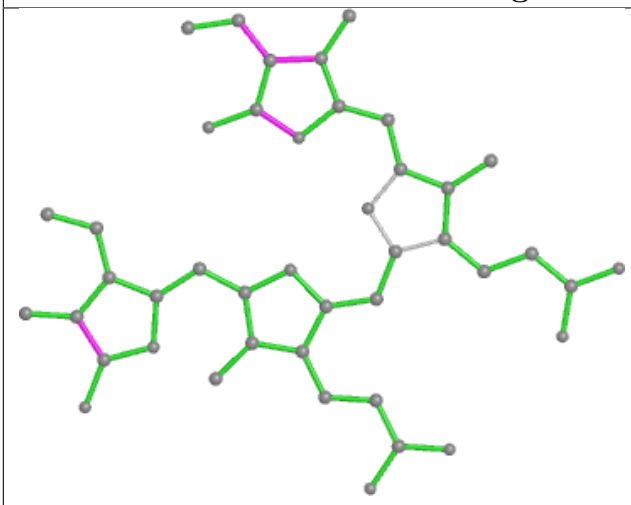

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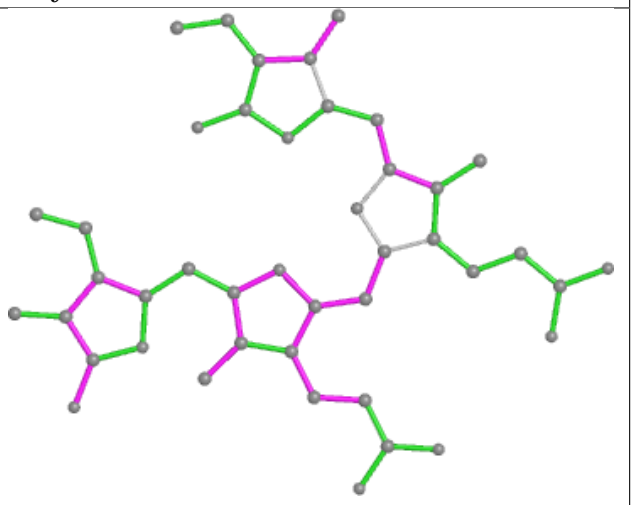

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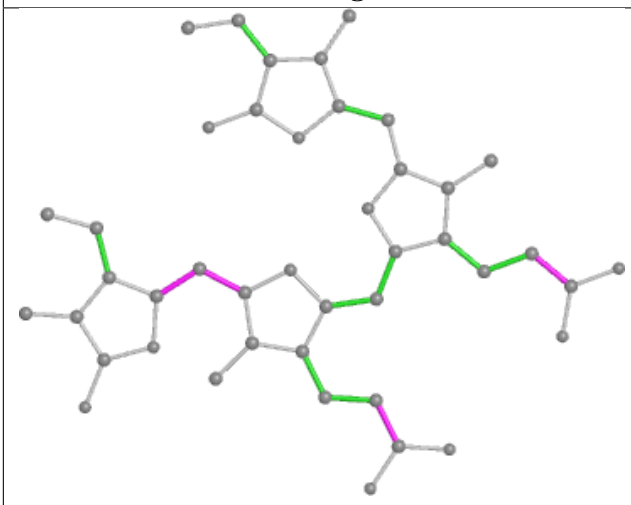

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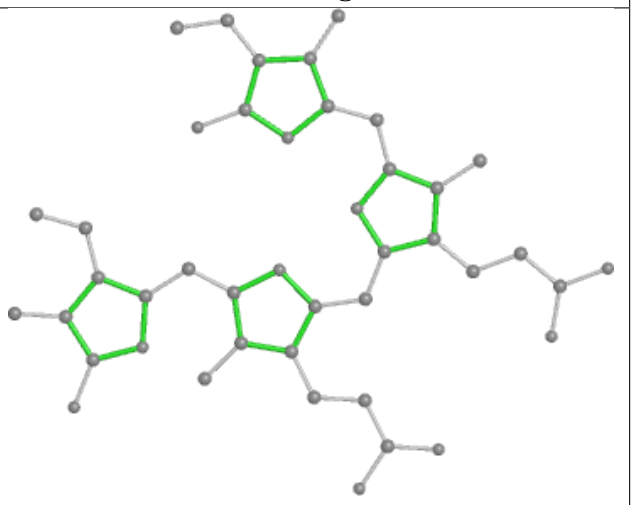

Rings

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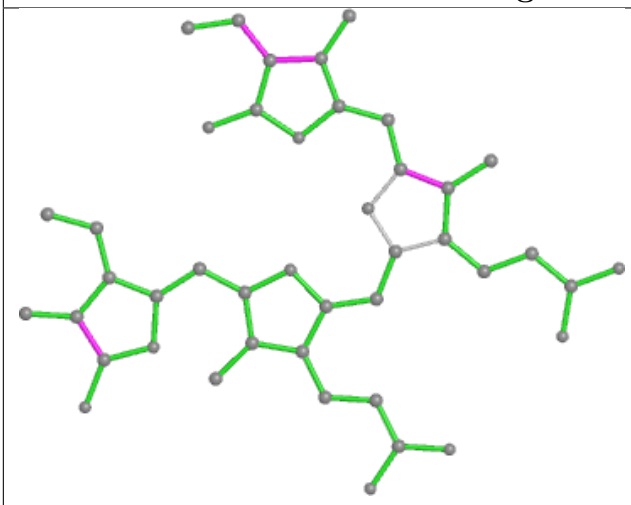

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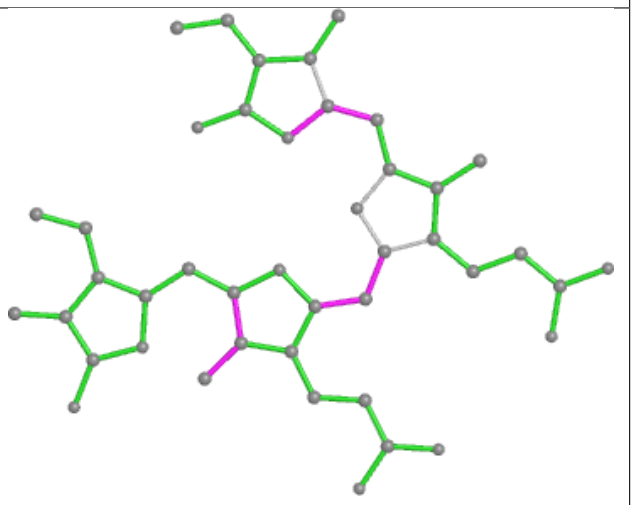

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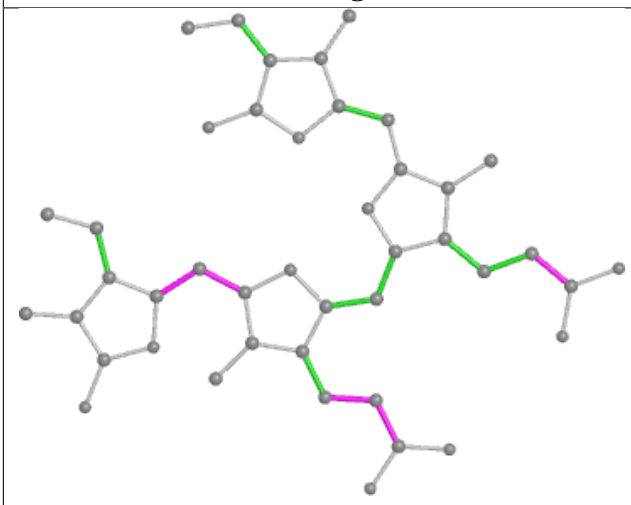

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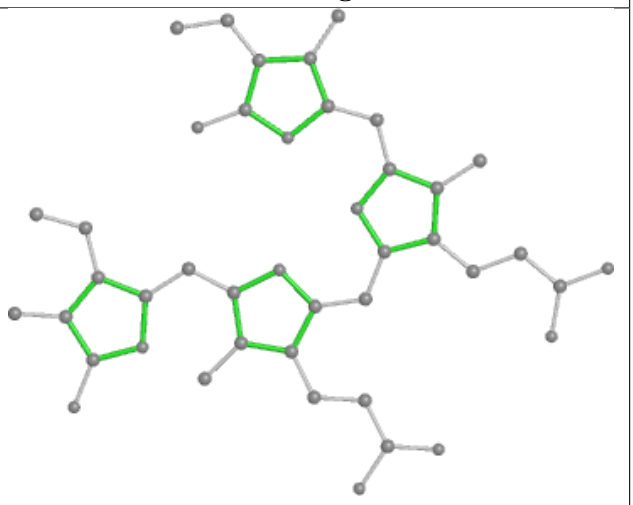

Rings

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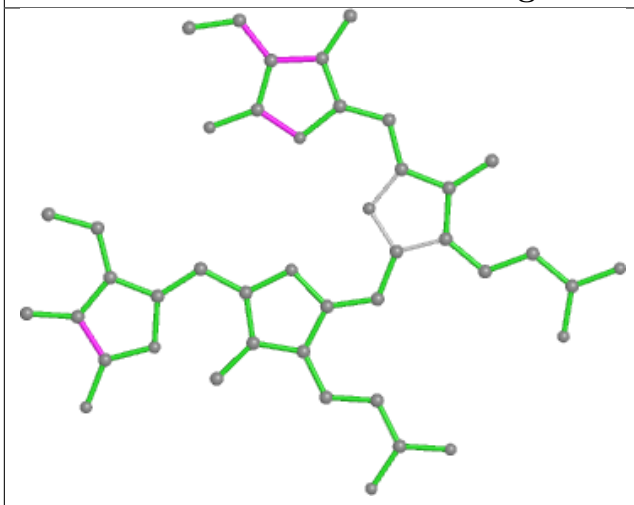

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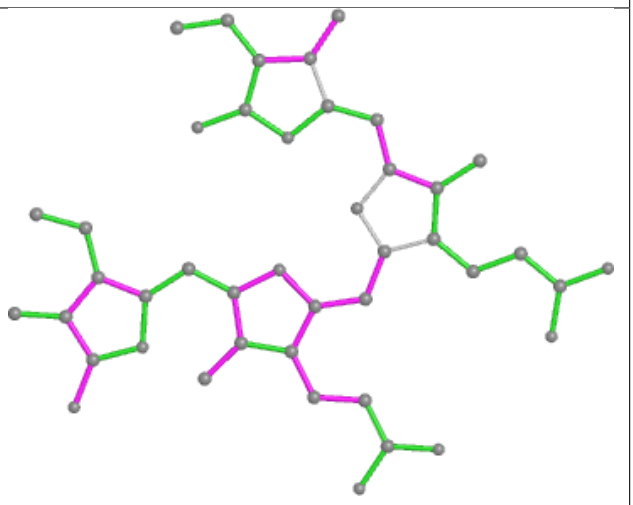

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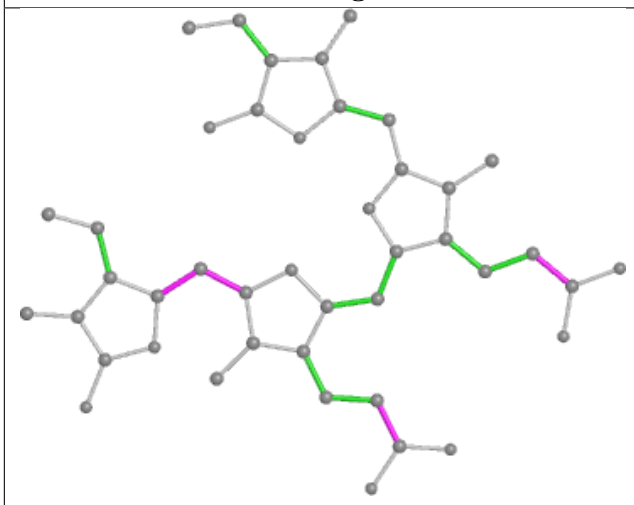

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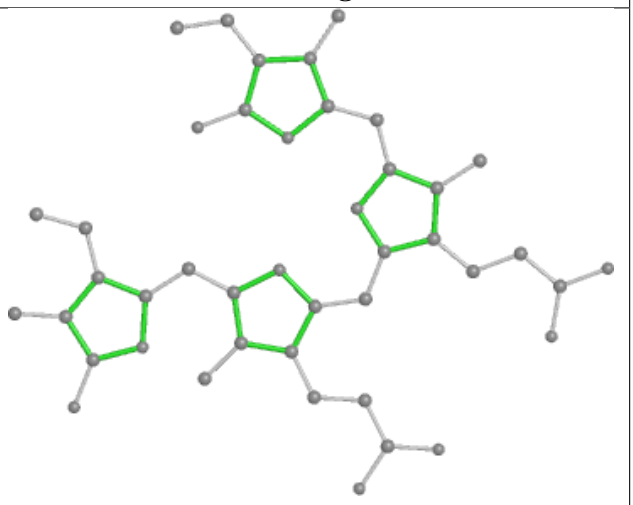

Rings

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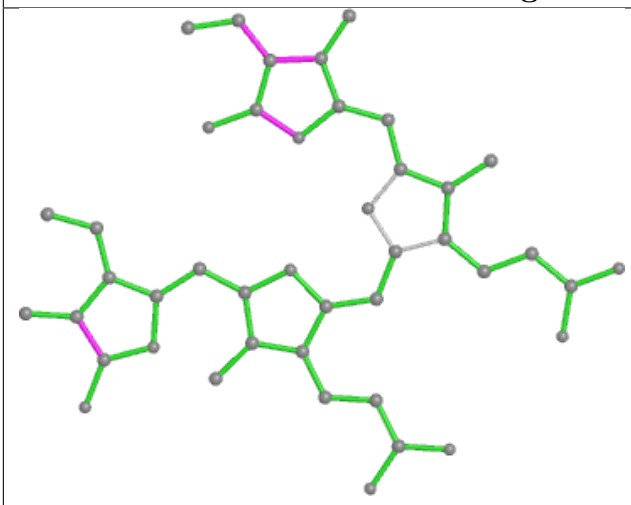

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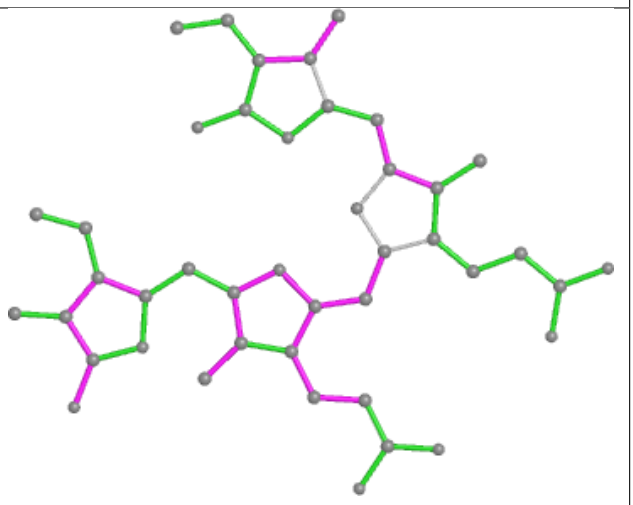

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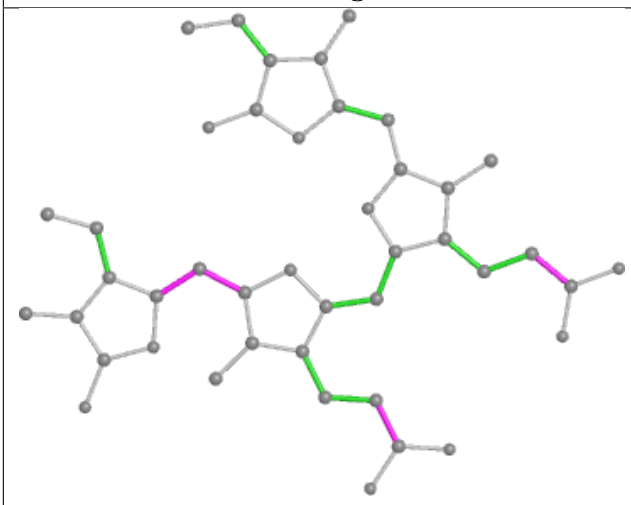

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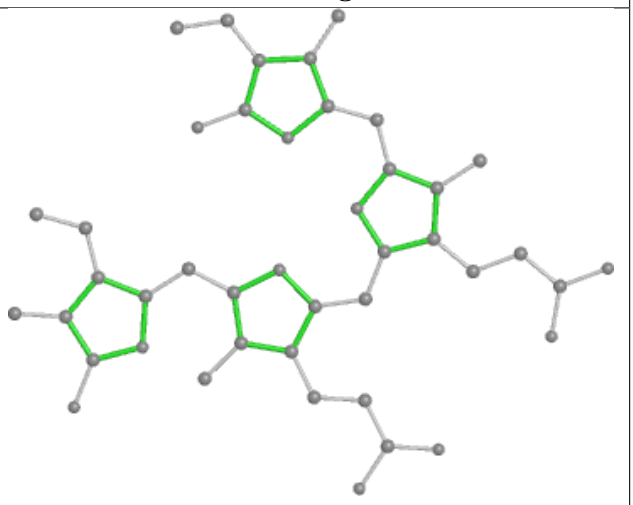

Rings

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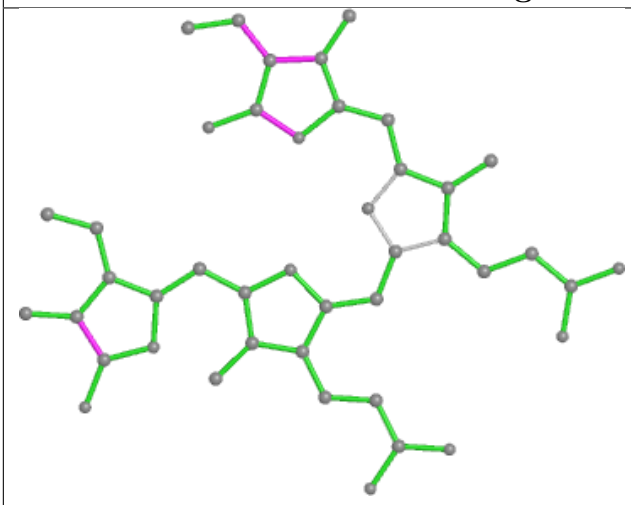

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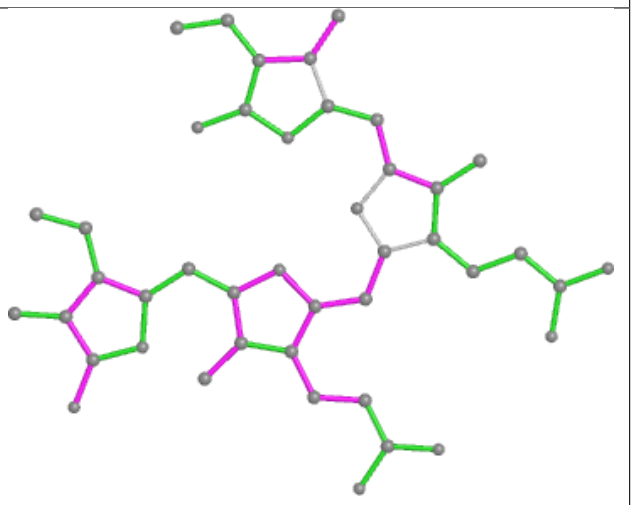

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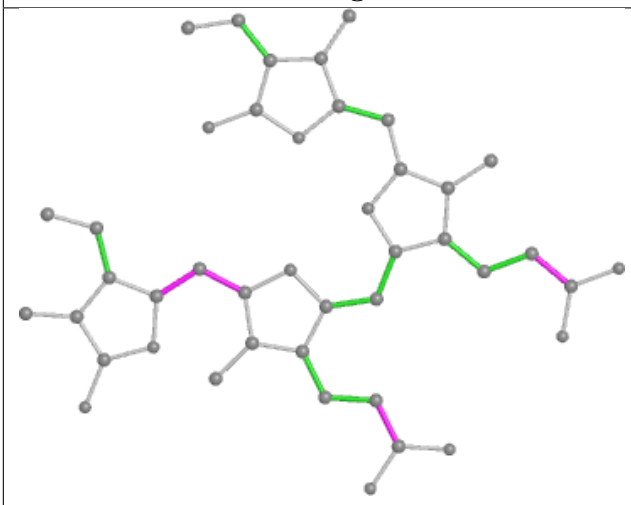

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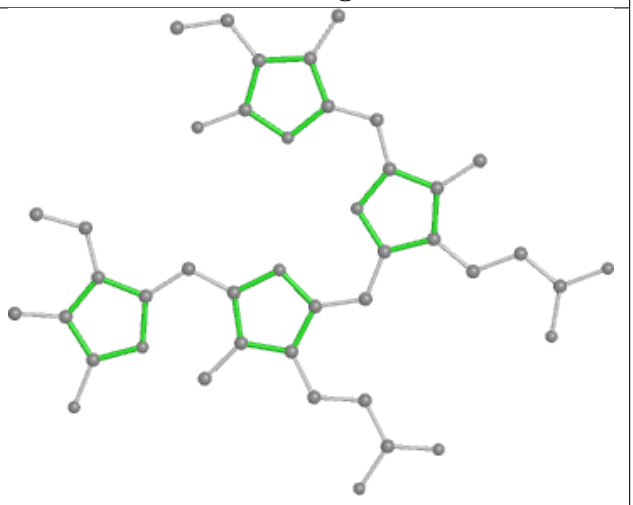

Rings

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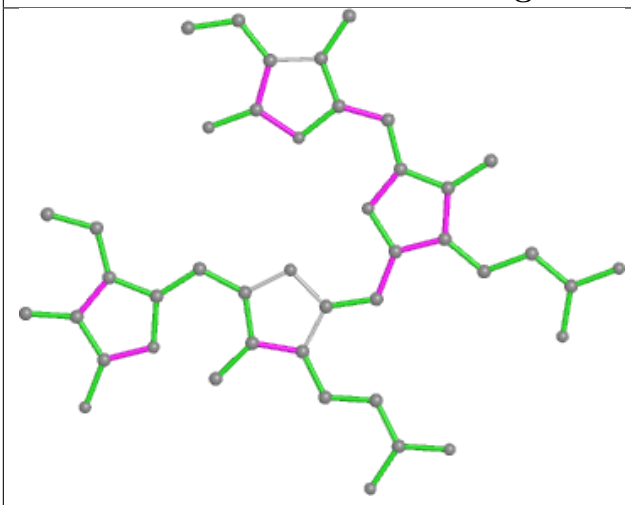

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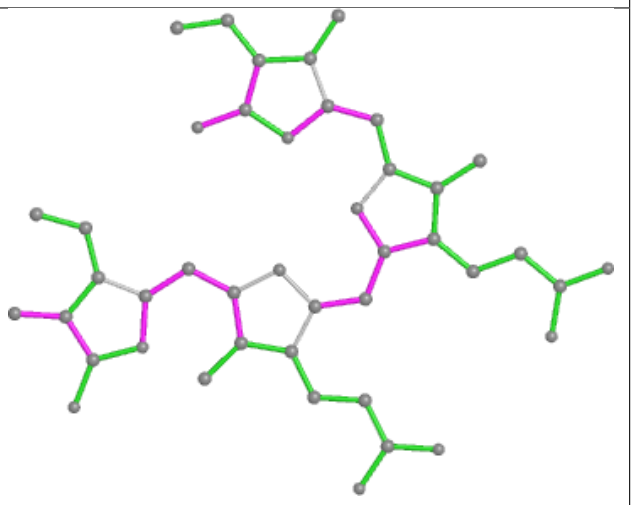

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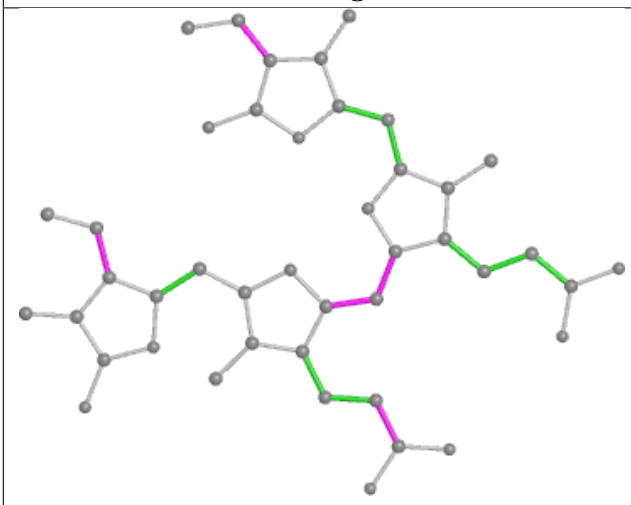

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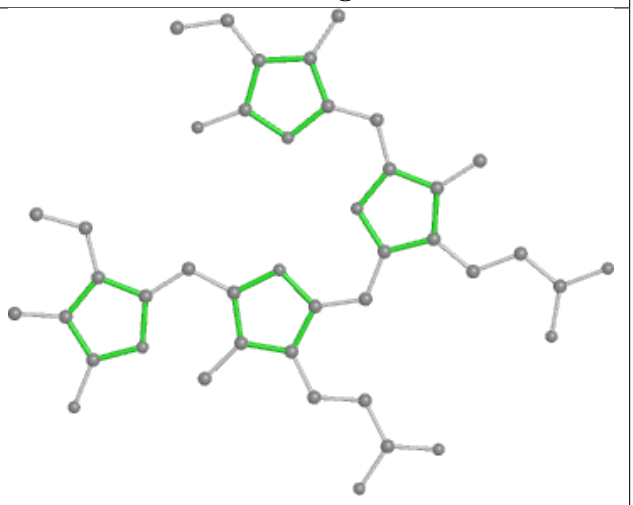
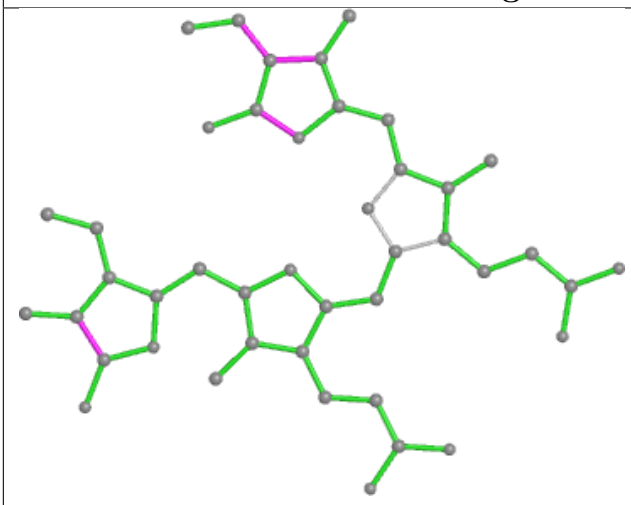


Rings

Ligand PEB kW 1001



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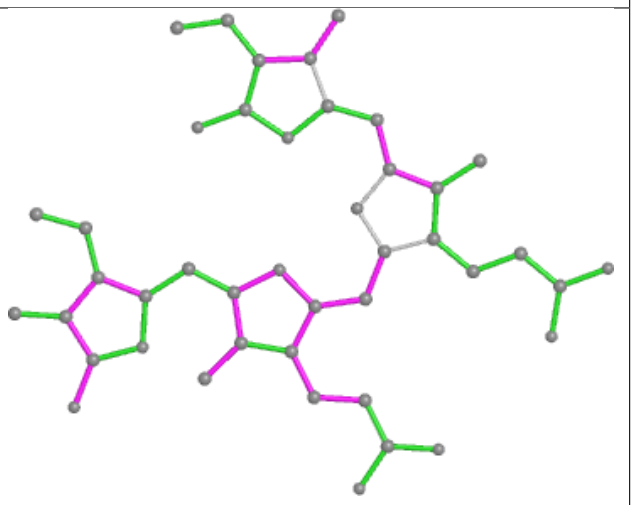

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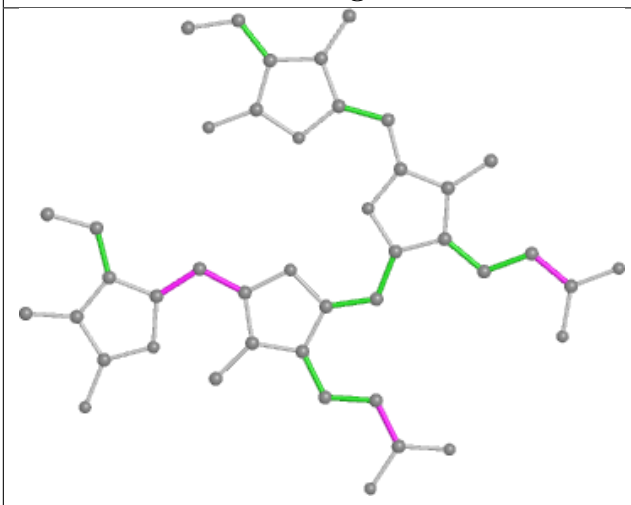
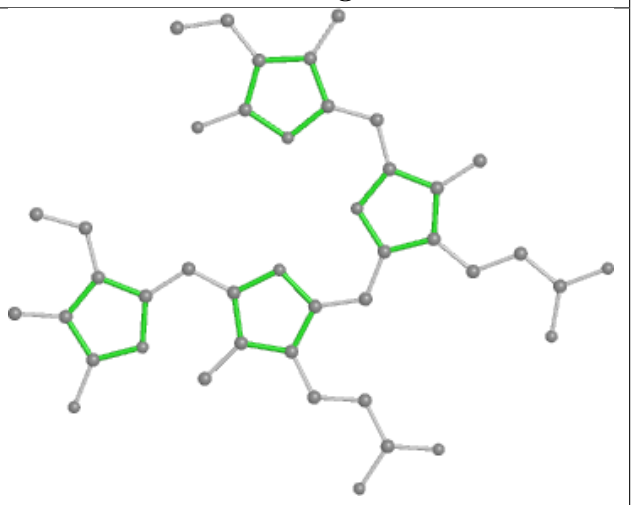
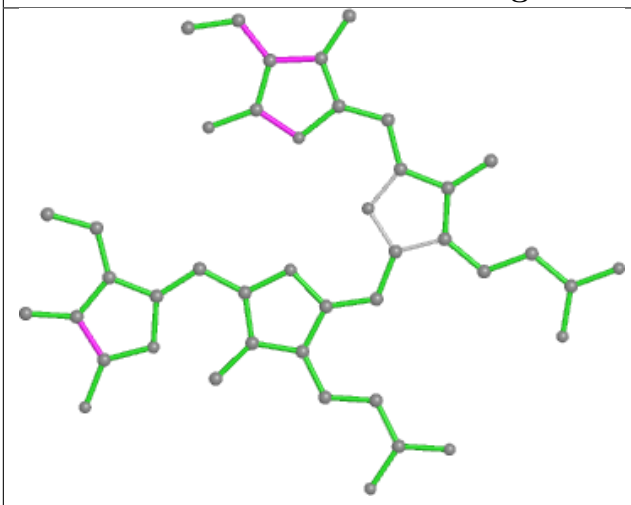


Torsions



Rings

Ligand PEB ay 1001



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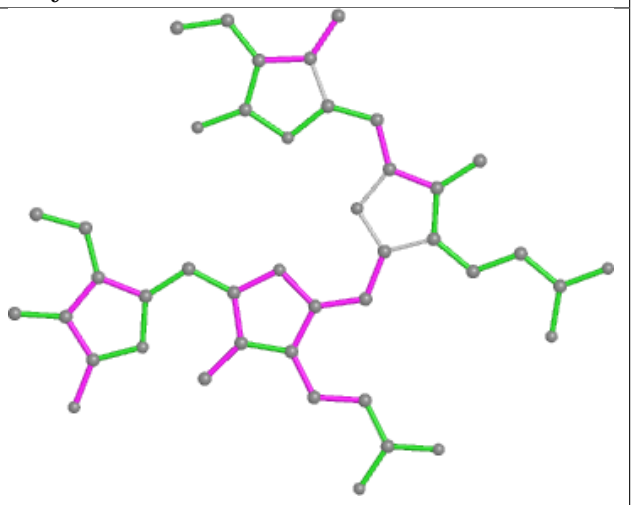

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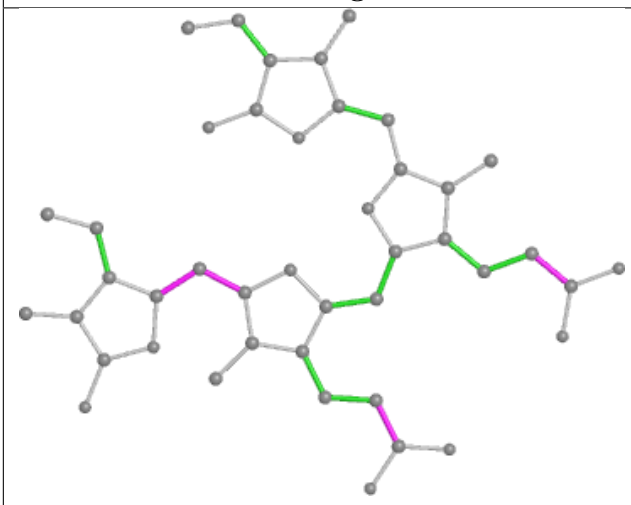

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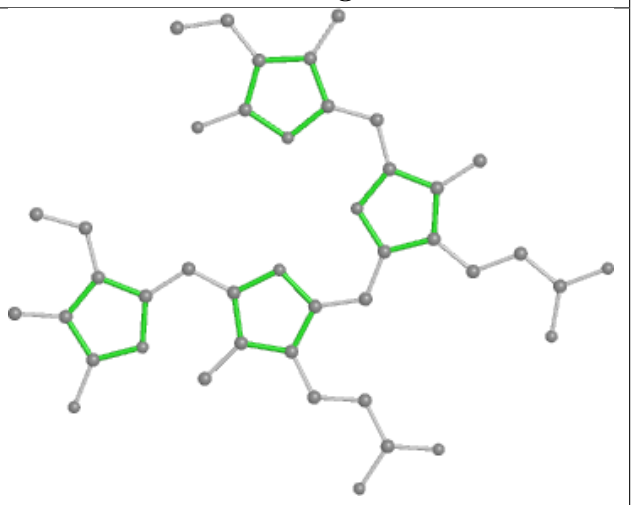
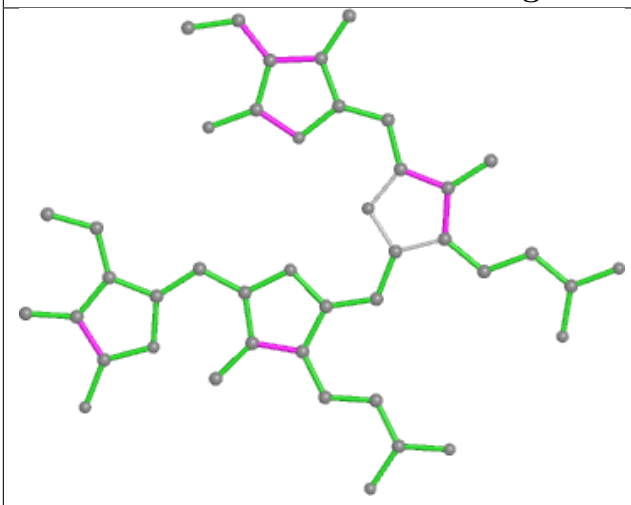


Rings

Ligand PEB dj 202



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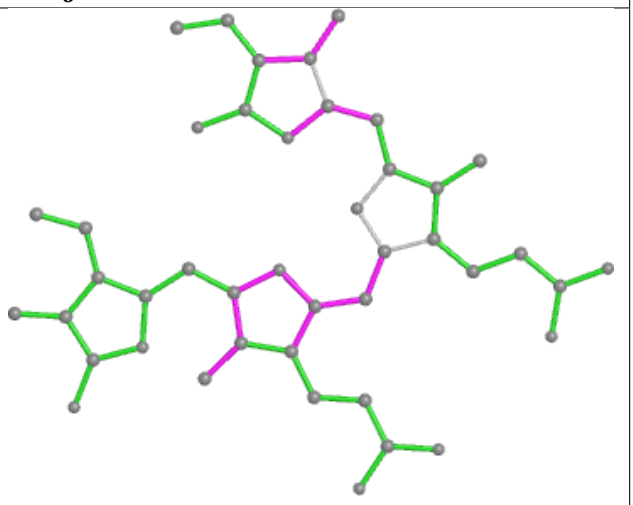

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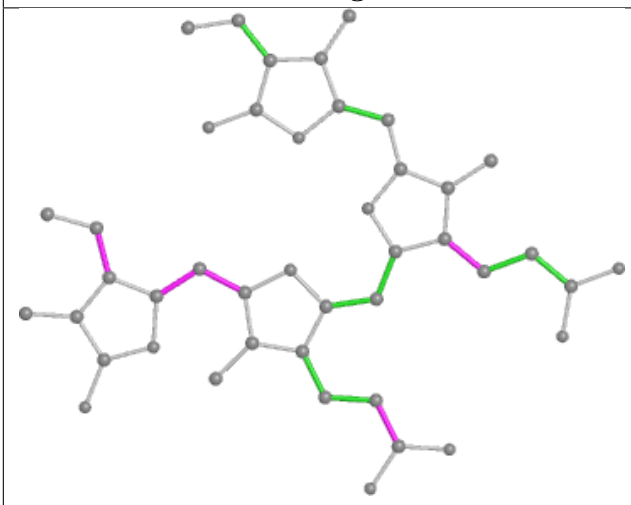

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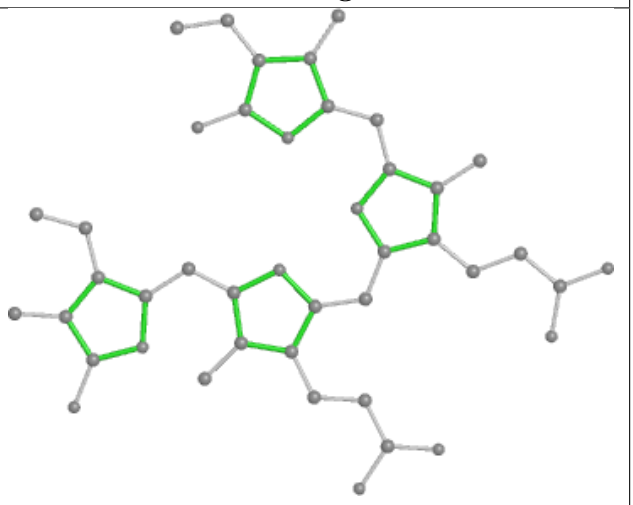

Rings

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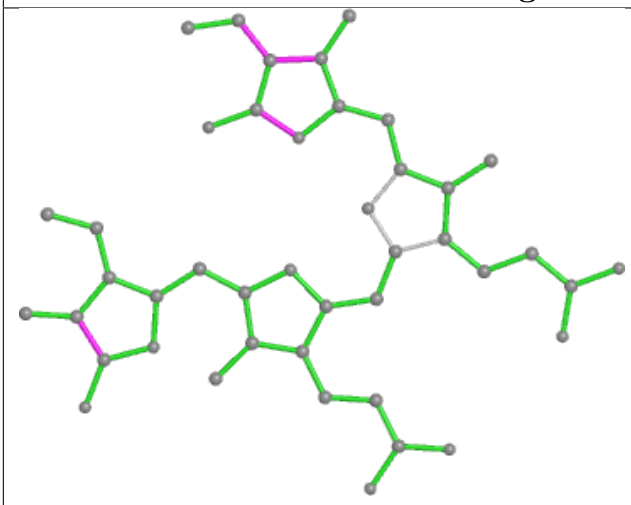

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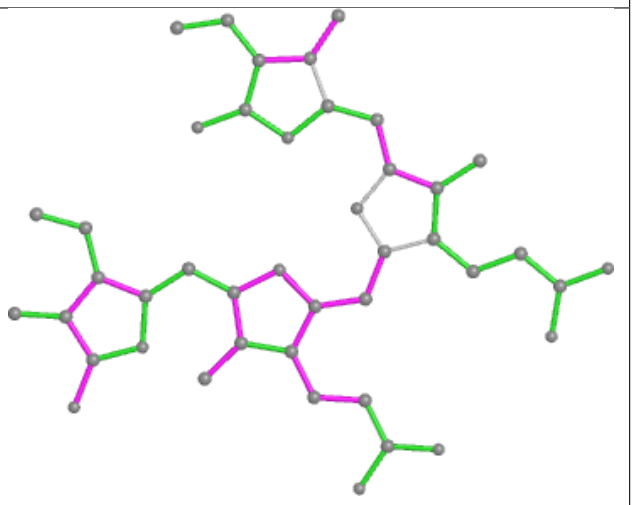

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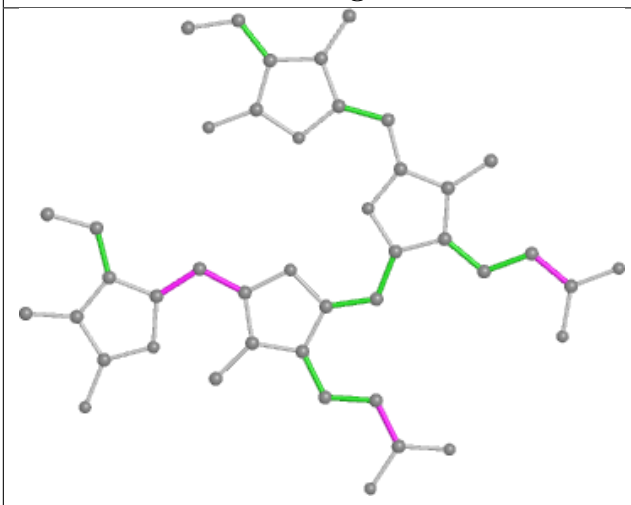

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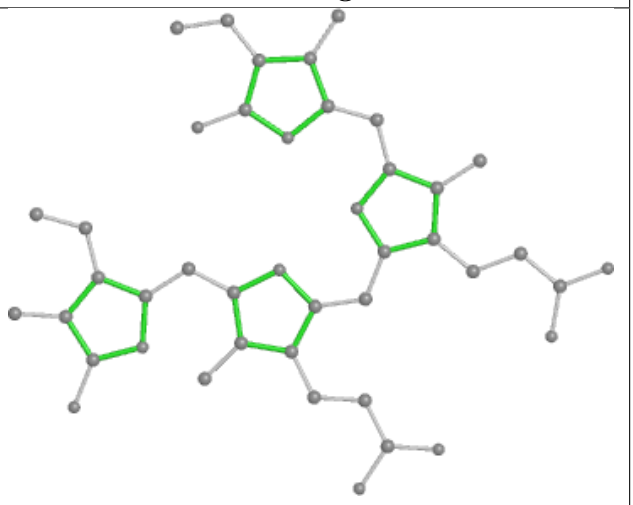
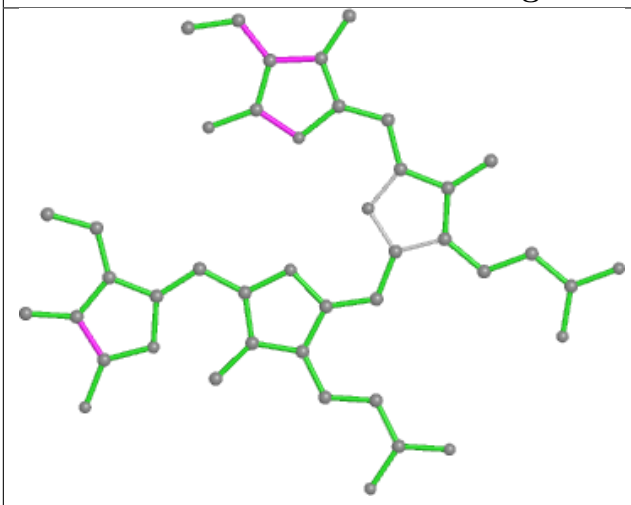


Rings

Ligand PEB I8 201



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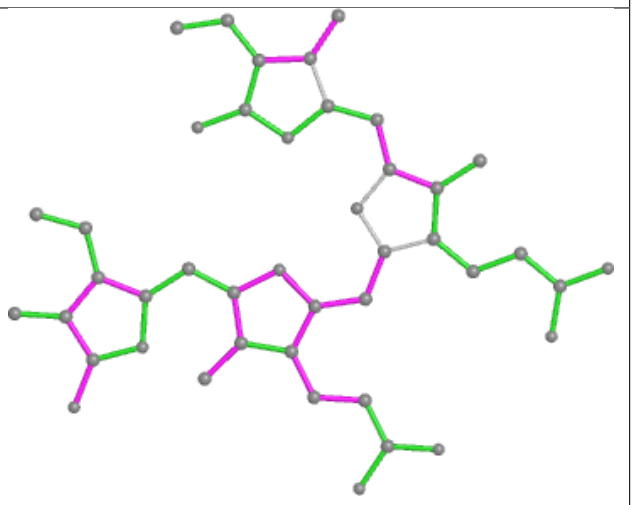

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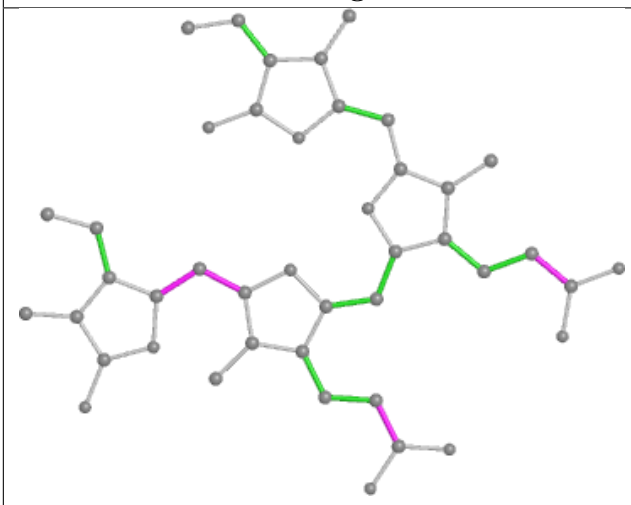

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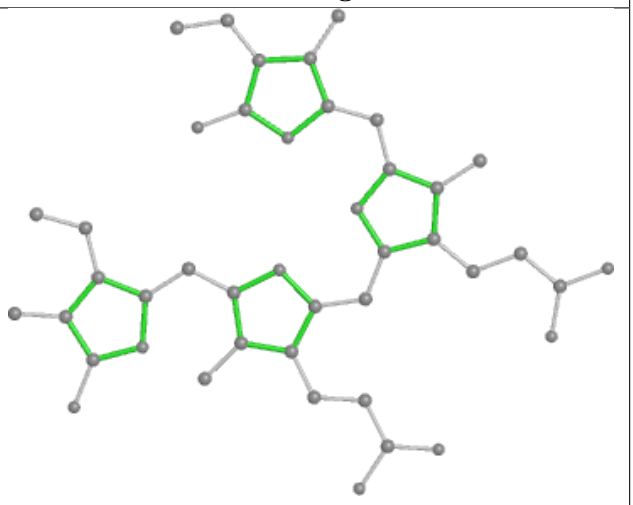

Rings

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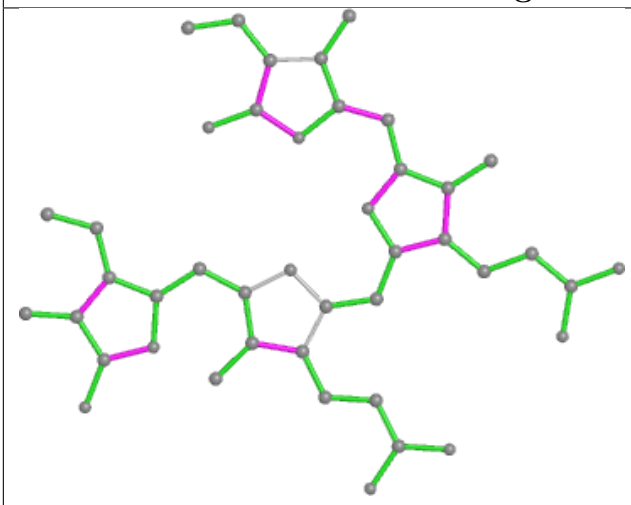

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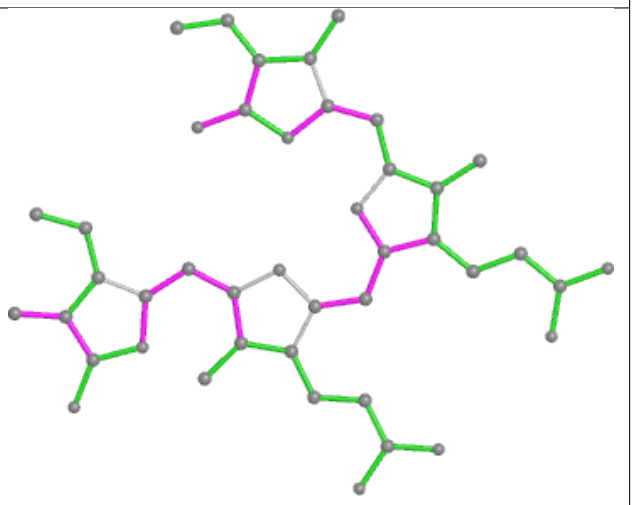

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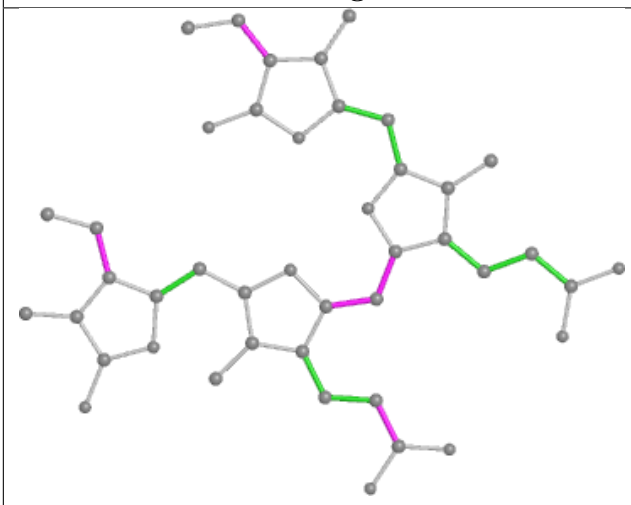

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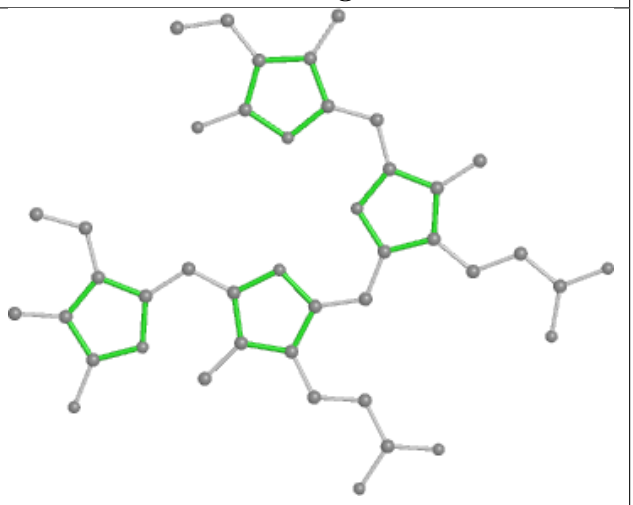

Rings

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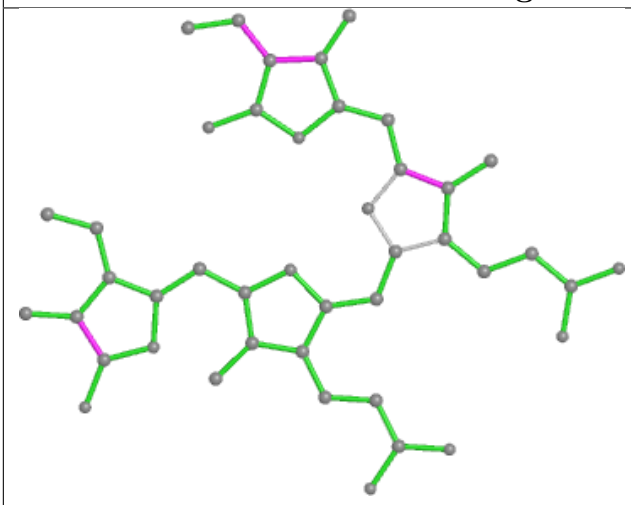

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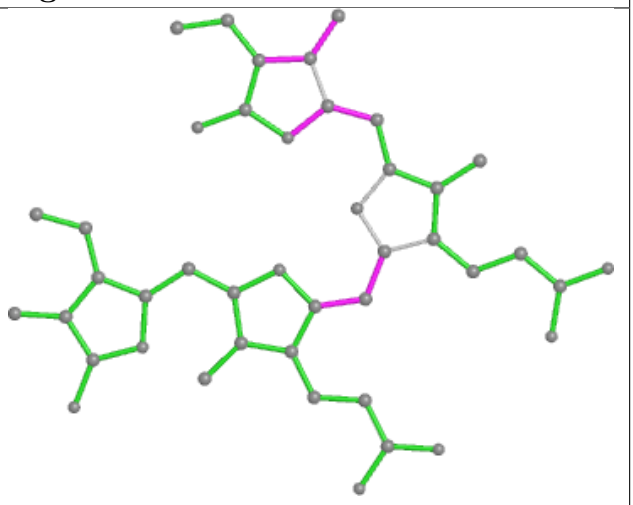

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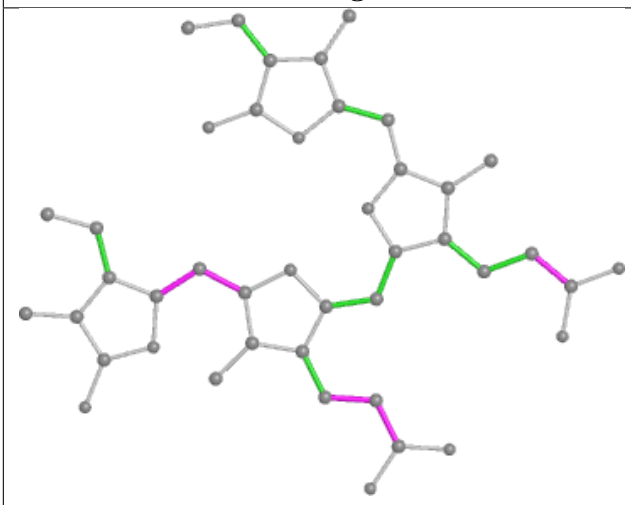

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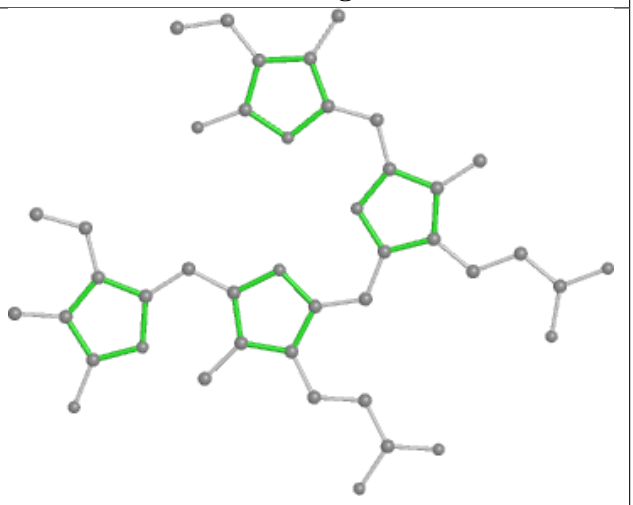

Rings

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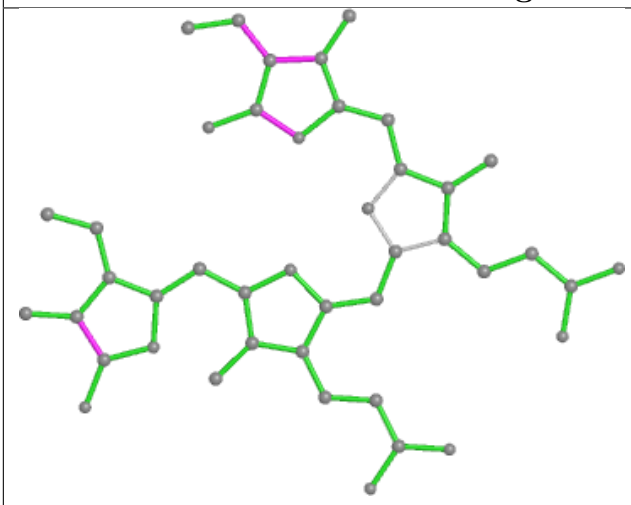

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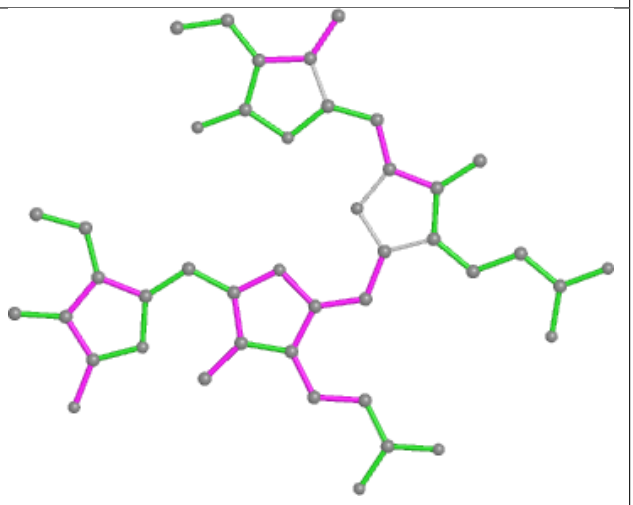

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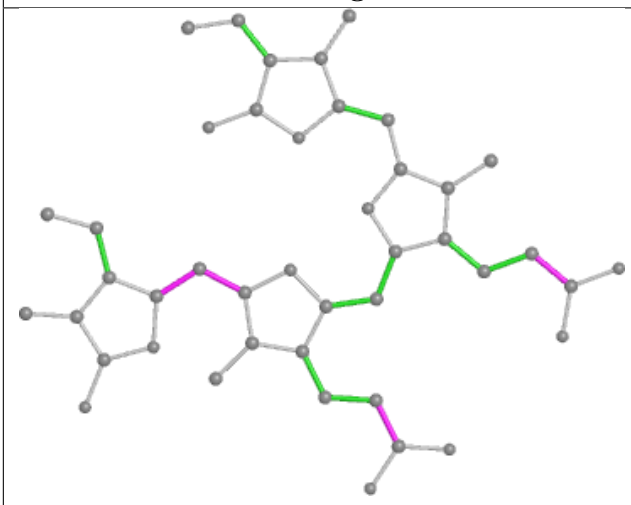

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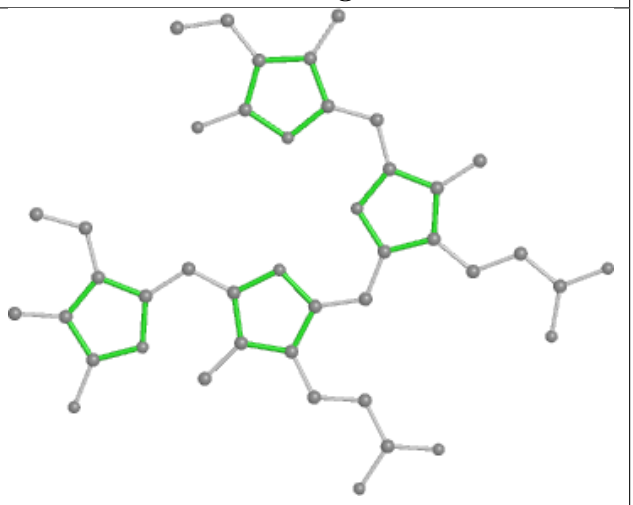
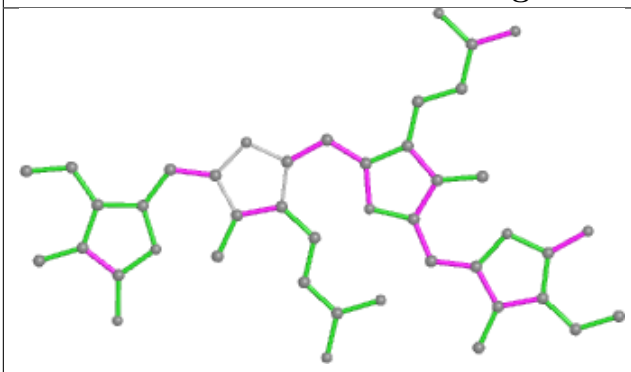


Rings

Ligand CYC K1 201



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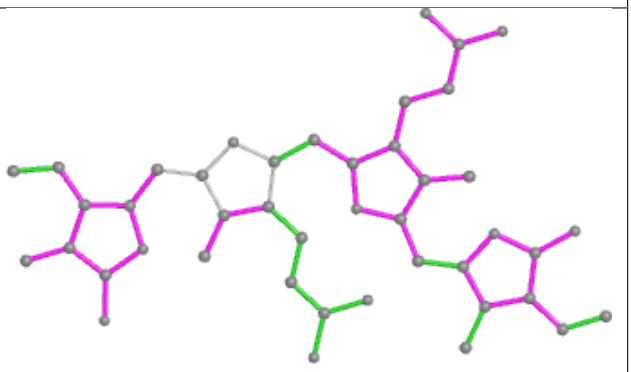

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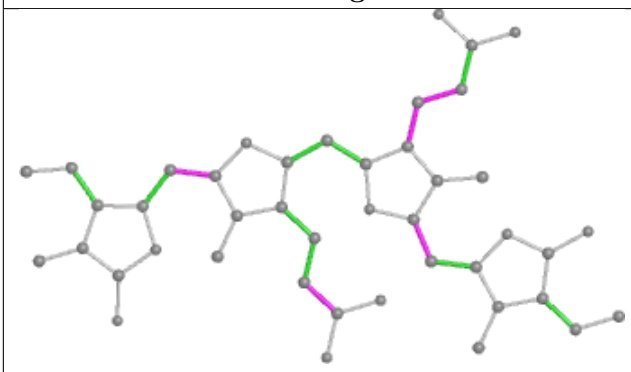

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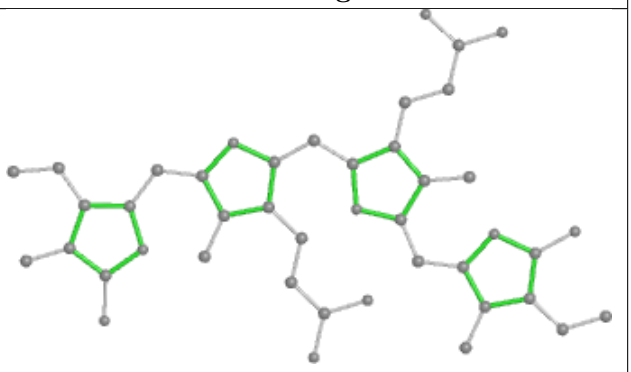

Rings

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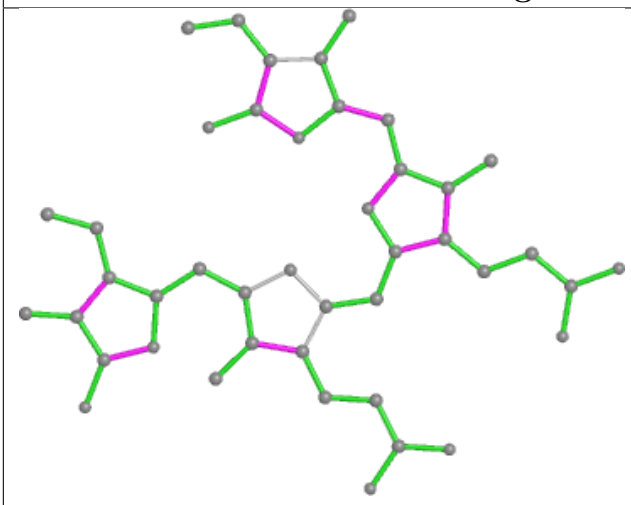

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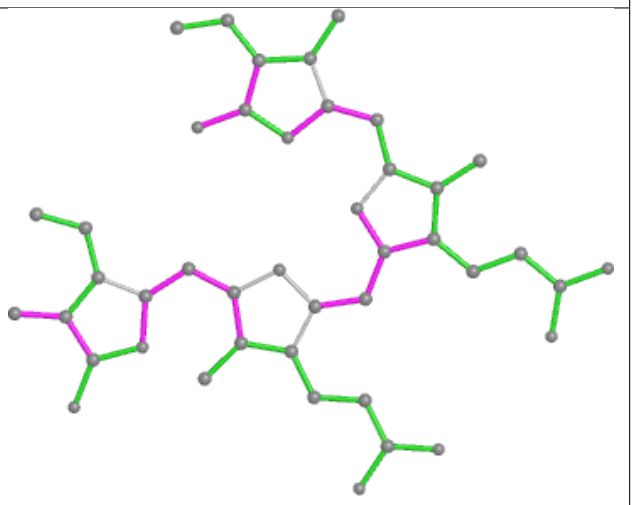

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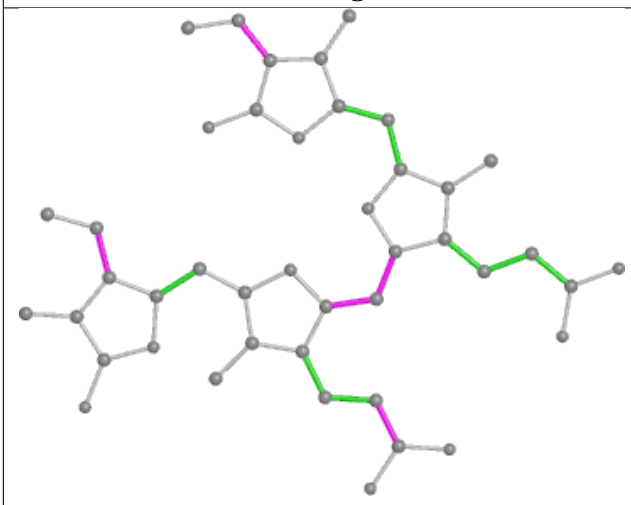

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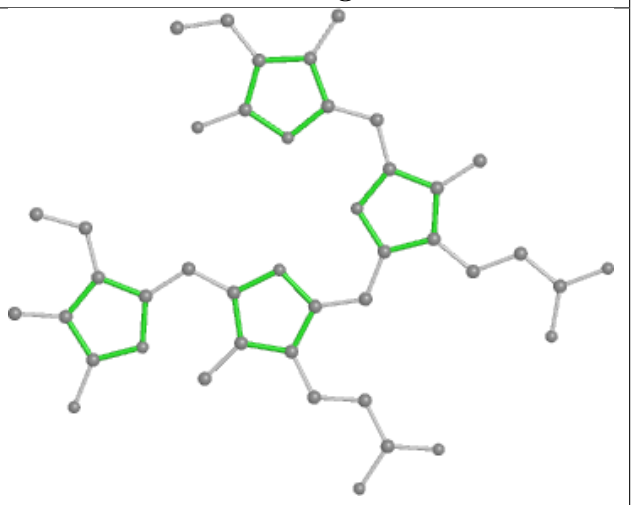

Rings

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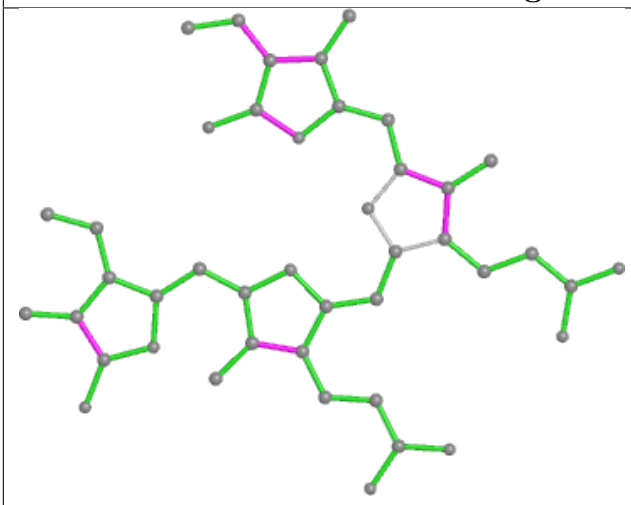

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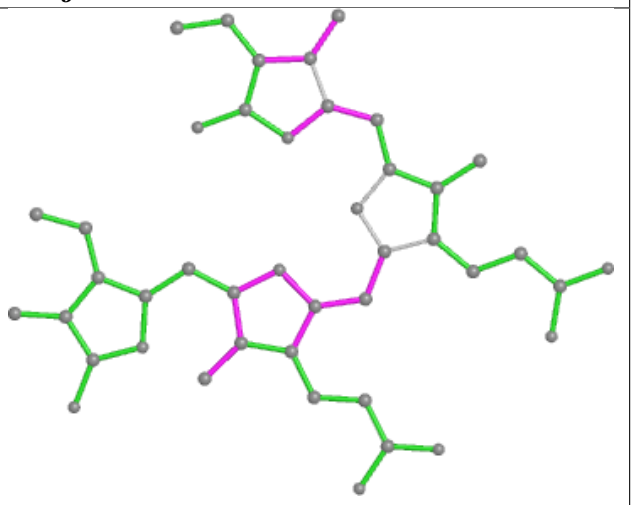

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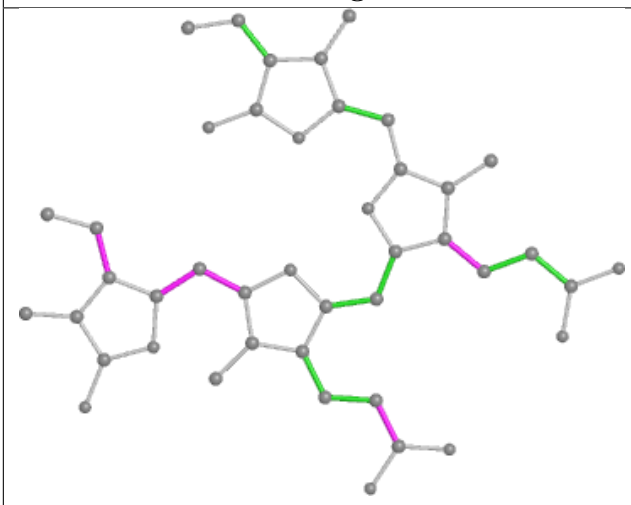

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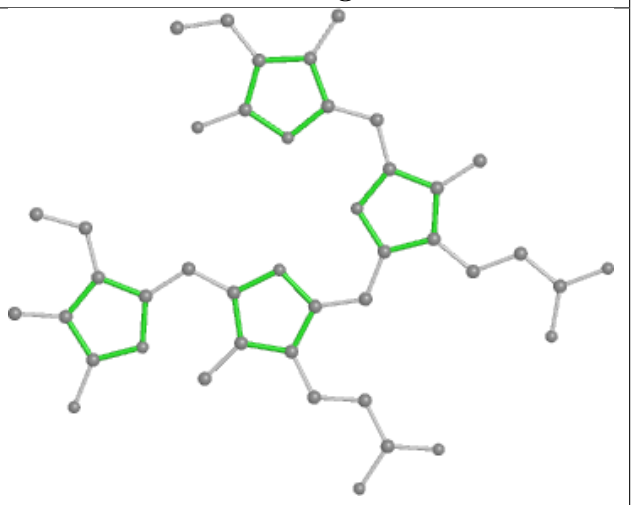

Rings

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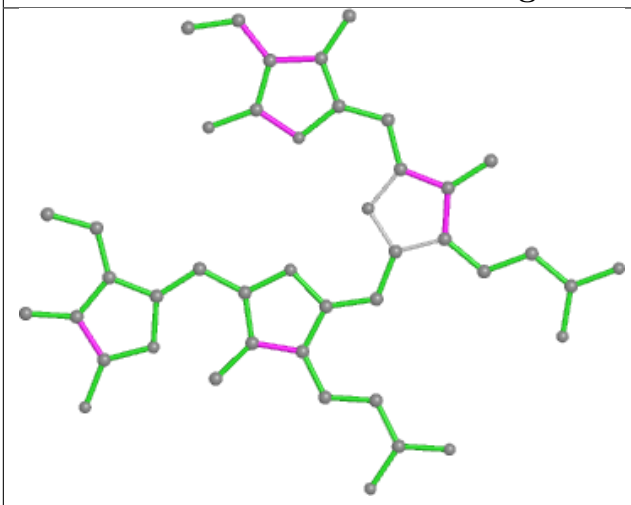

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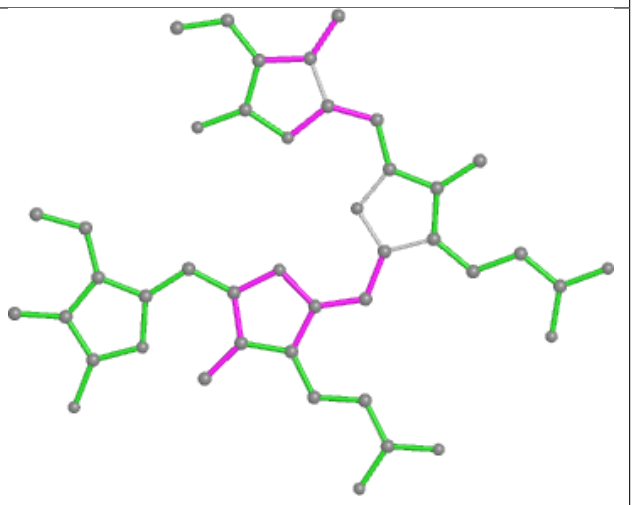

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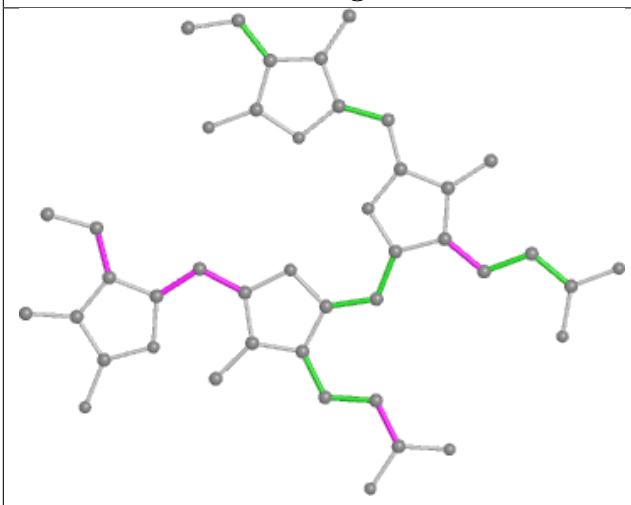

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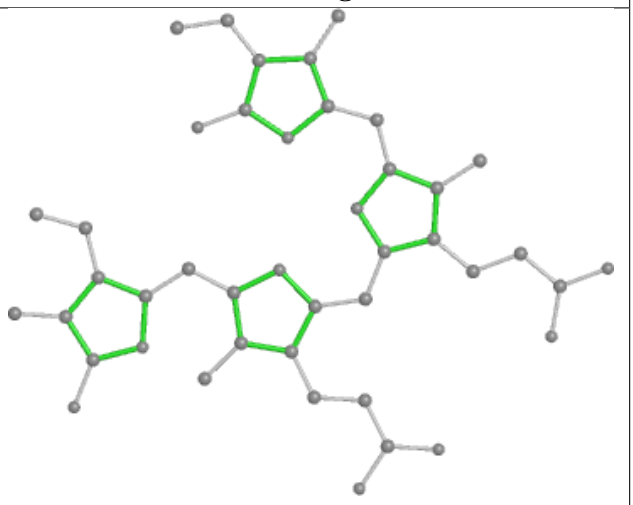

Rings

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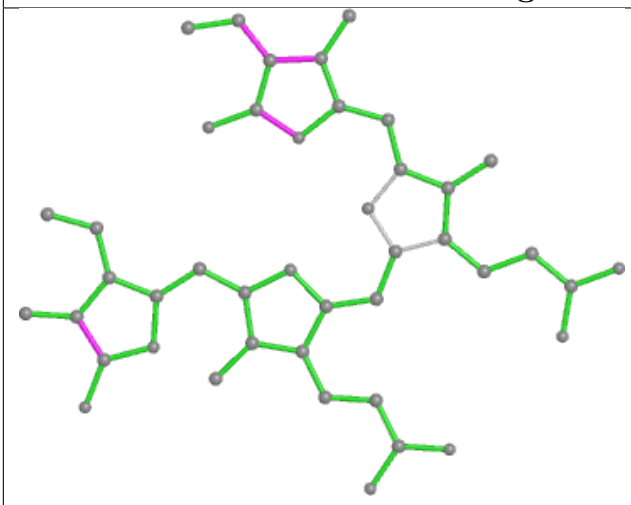

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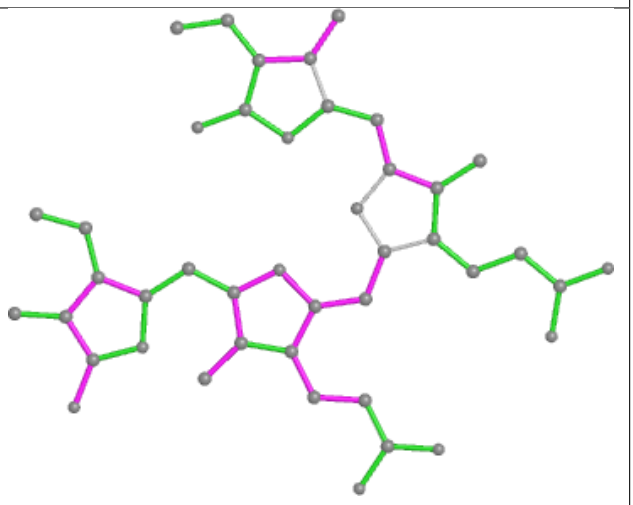

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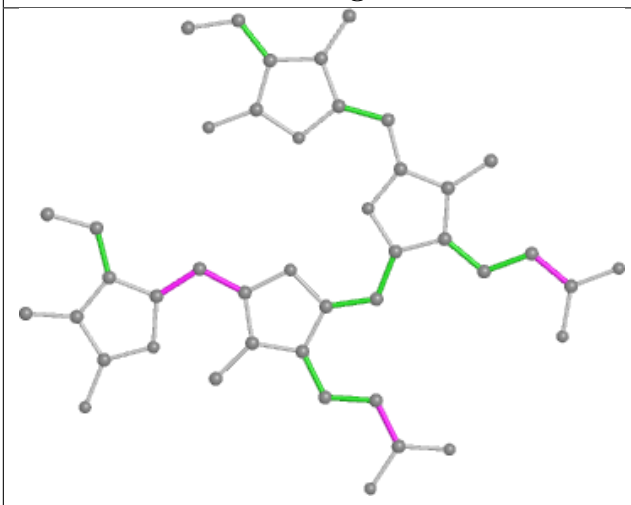

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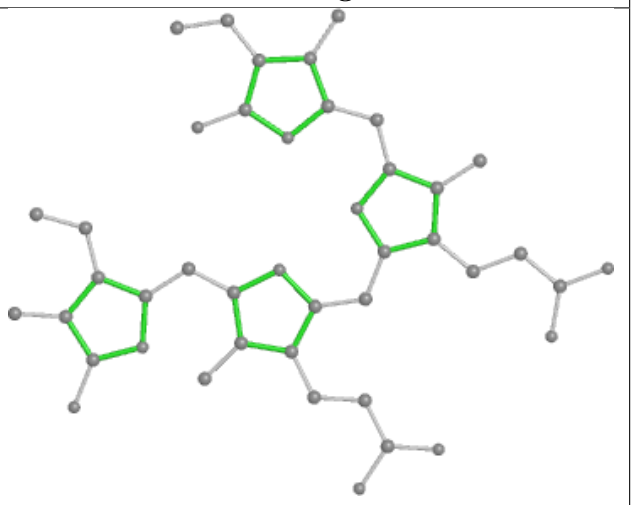
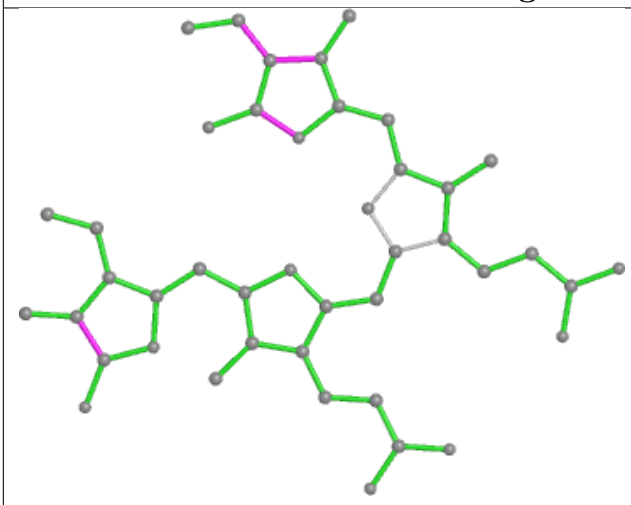


Rings

Ligand PEB p9 202



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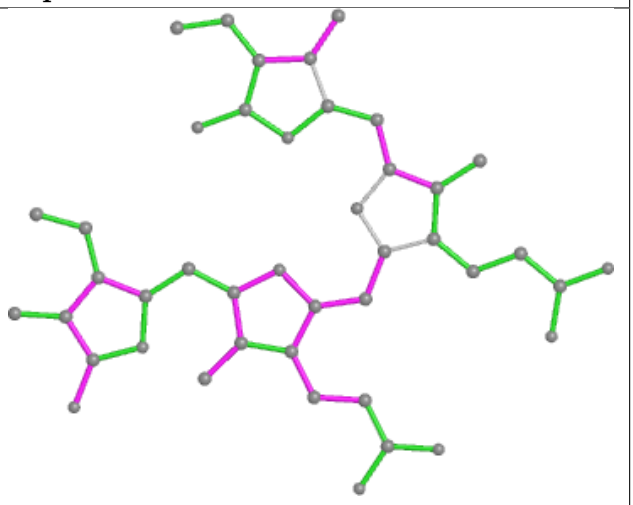

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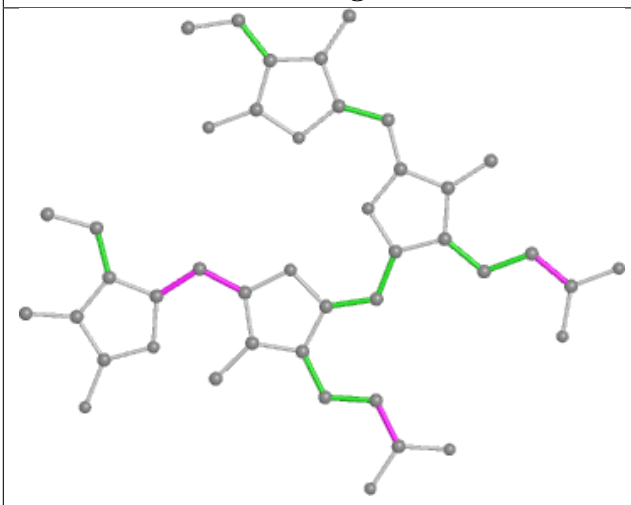

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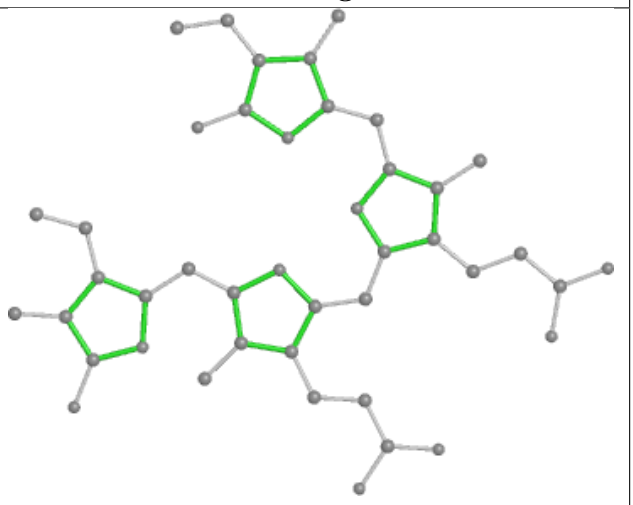
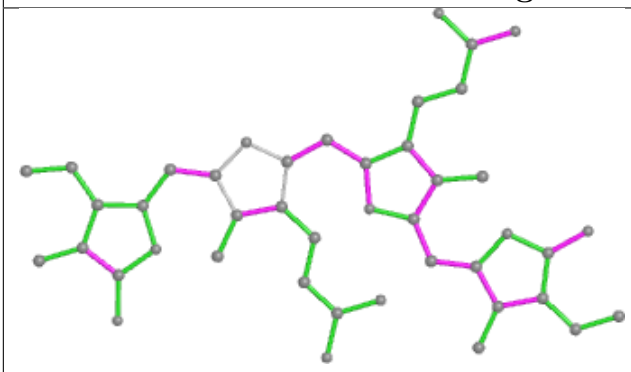
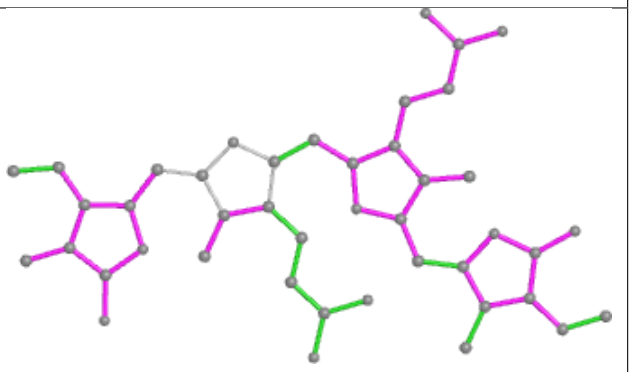


Rings

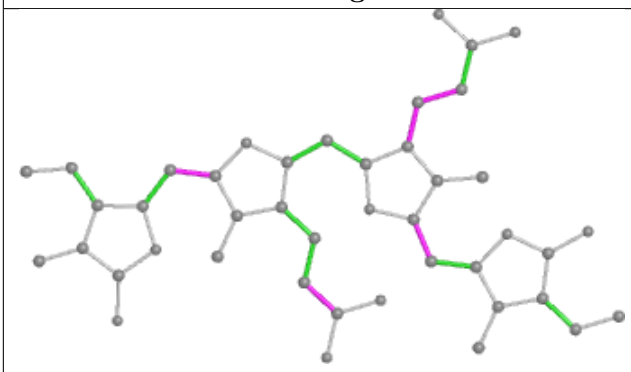
Ligand CYC d2 101



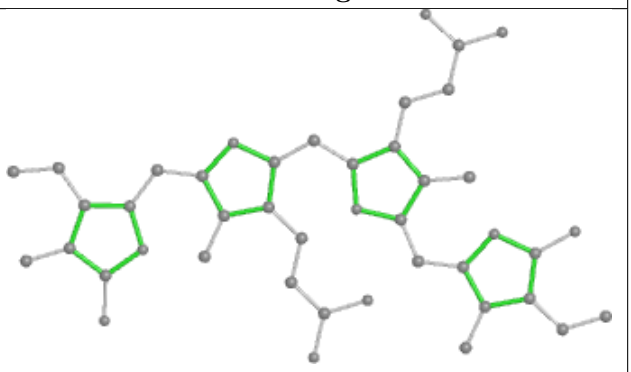
Bond lengths



Bond angles

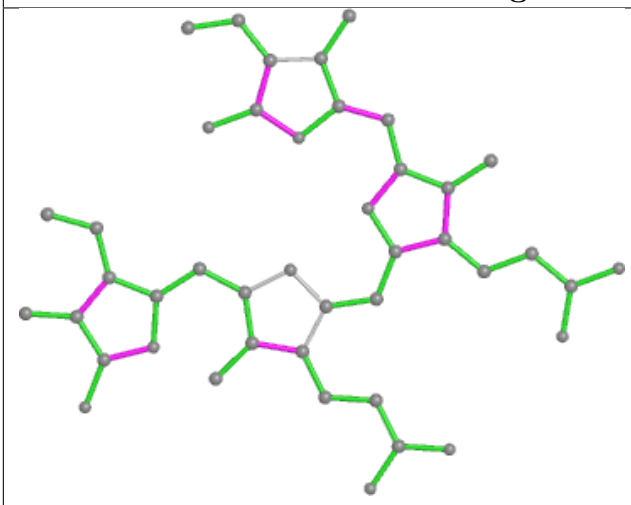


Torsions



Rings

Ligand PUB M8 203



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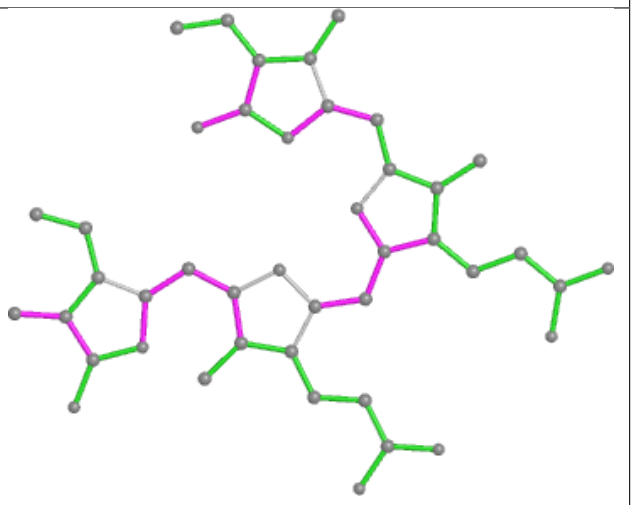

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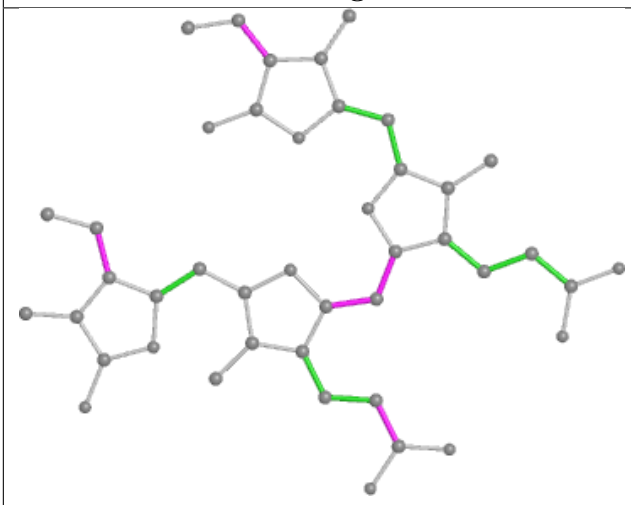

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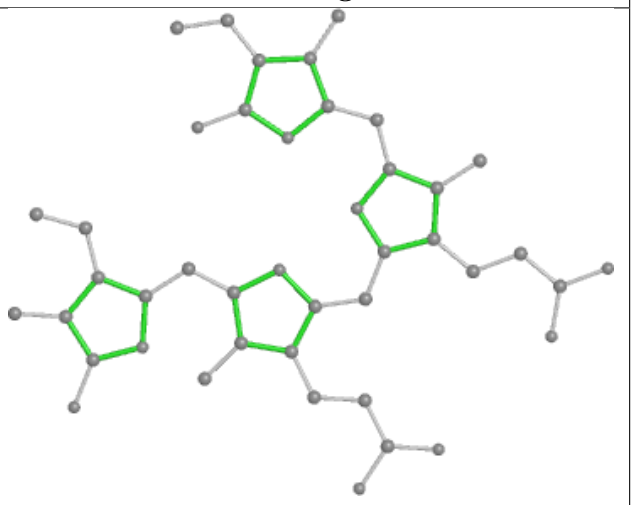

Rings

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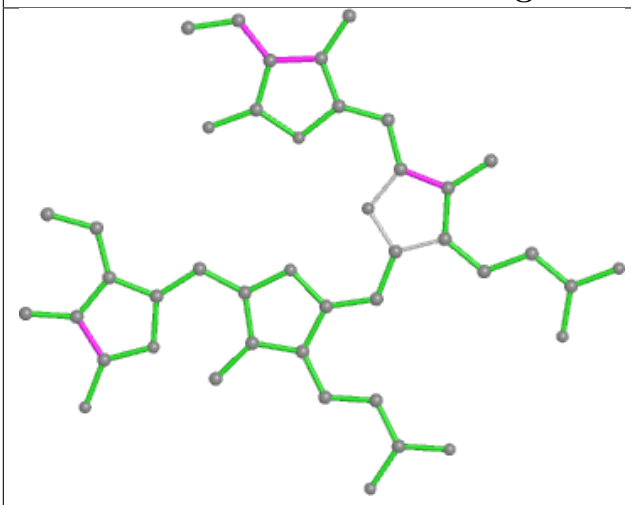

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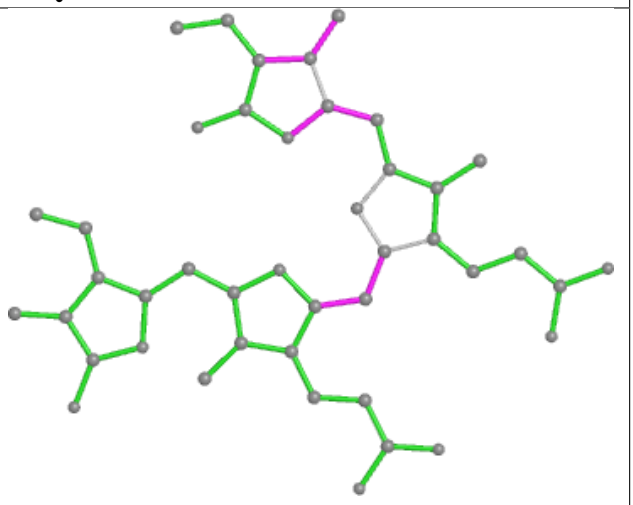

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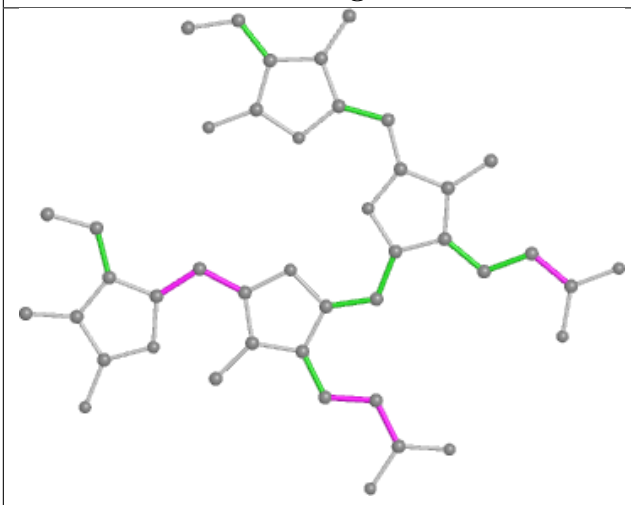

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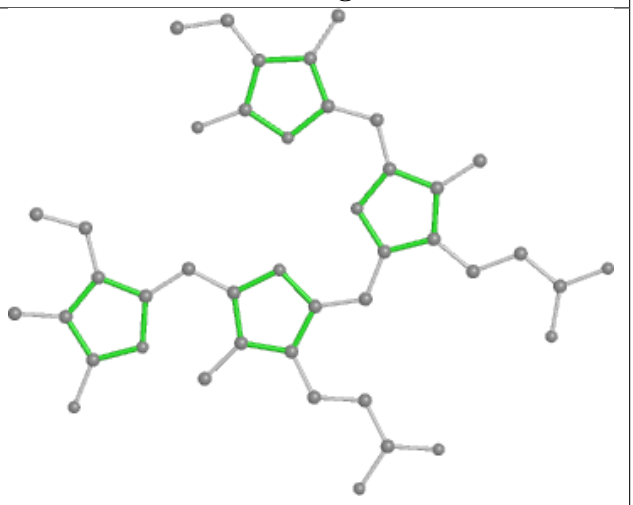

Rings

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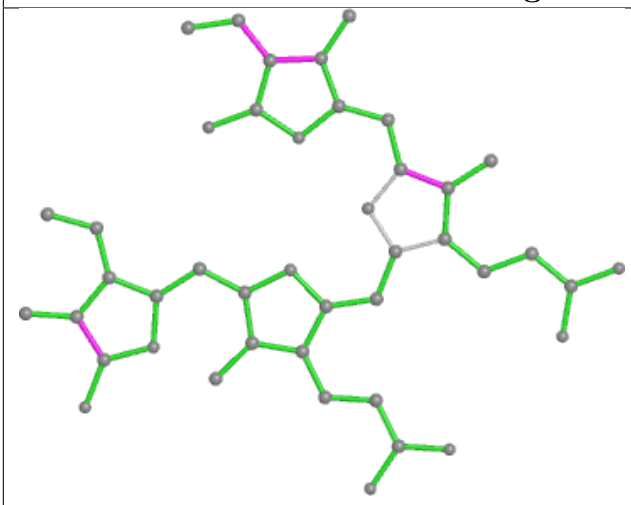

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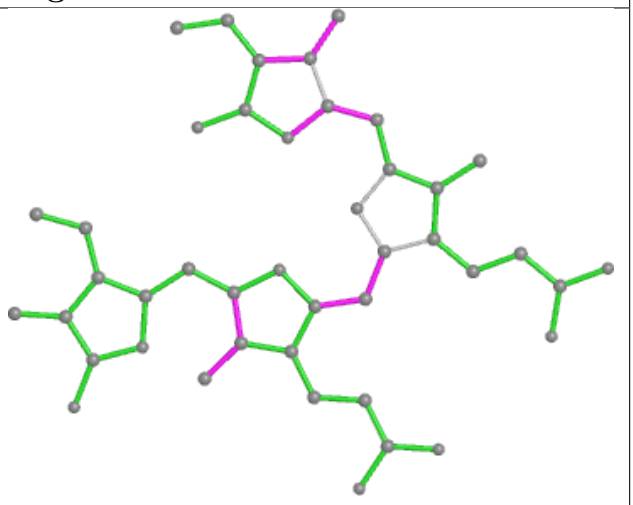

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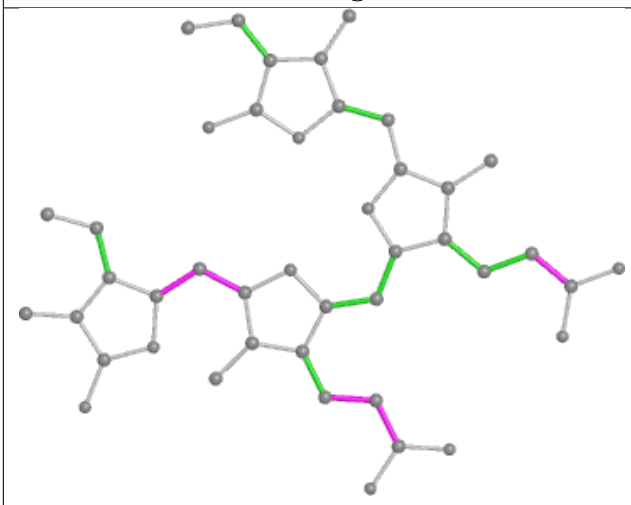

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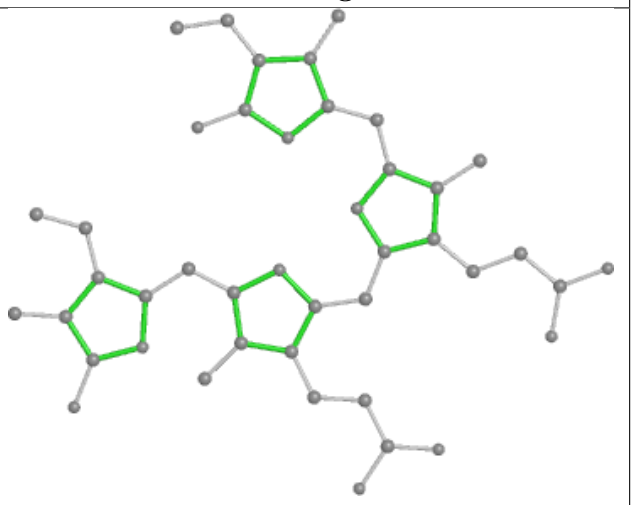

Rings

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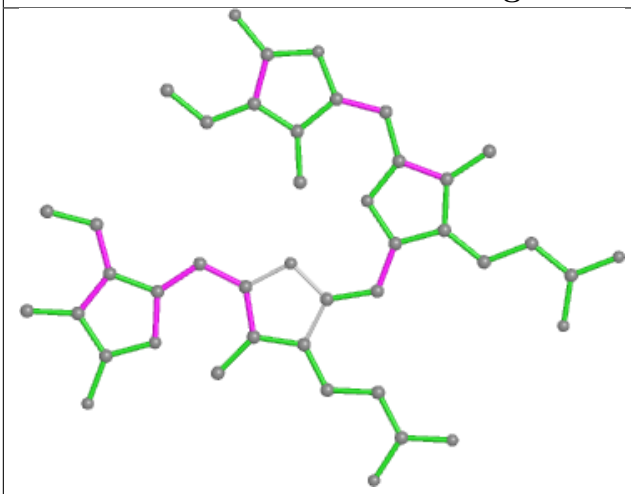

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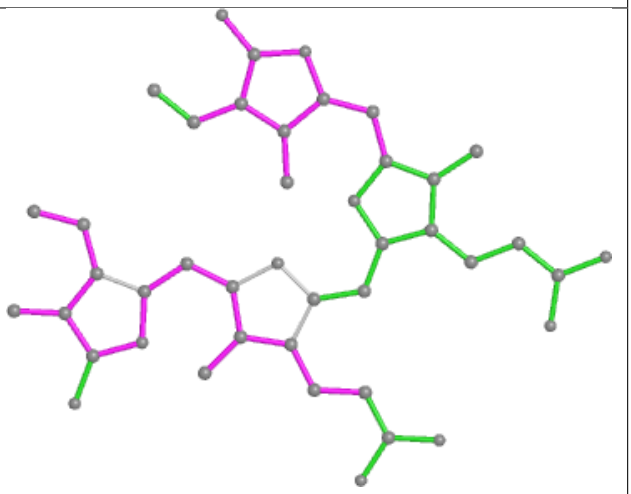

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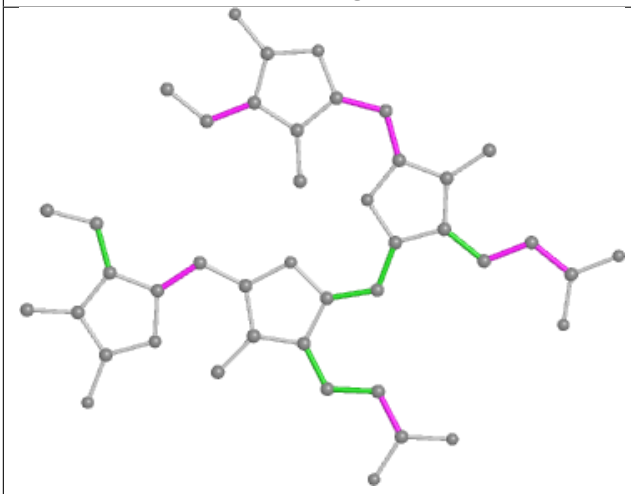

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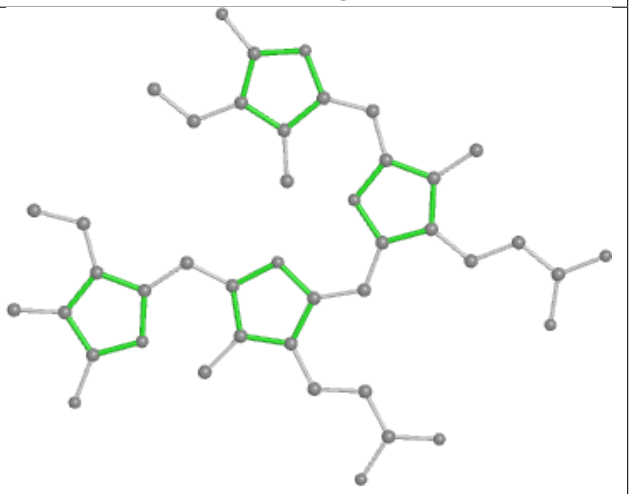

Rings

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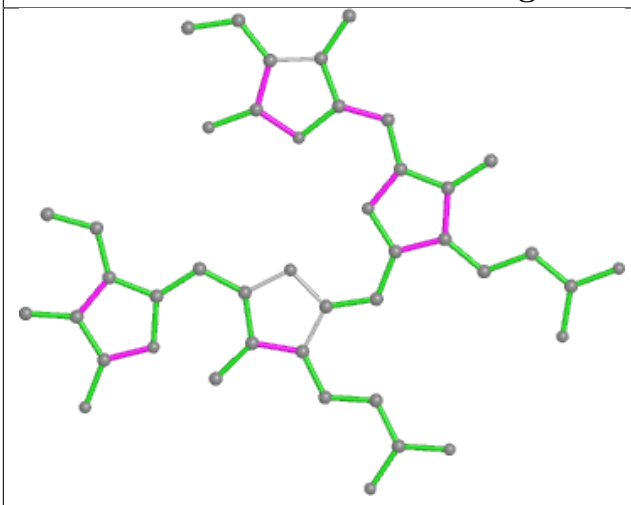

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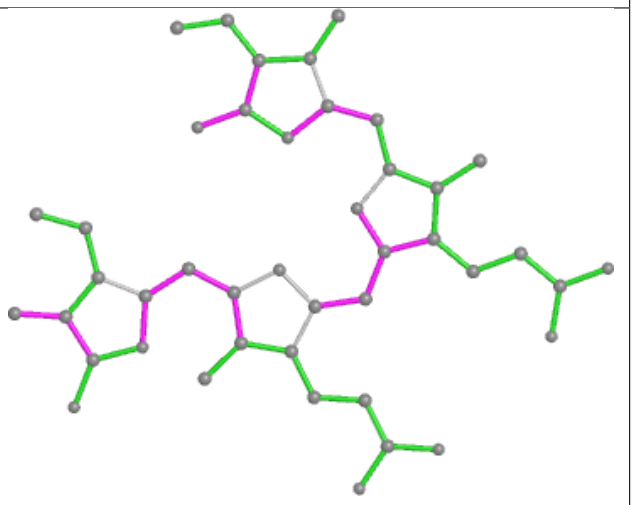

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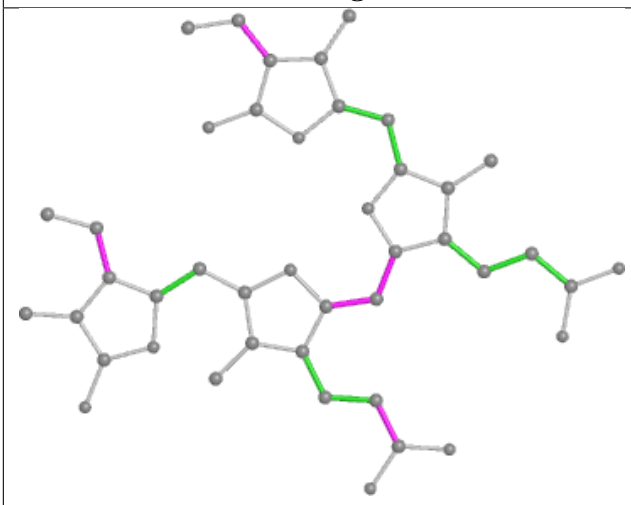

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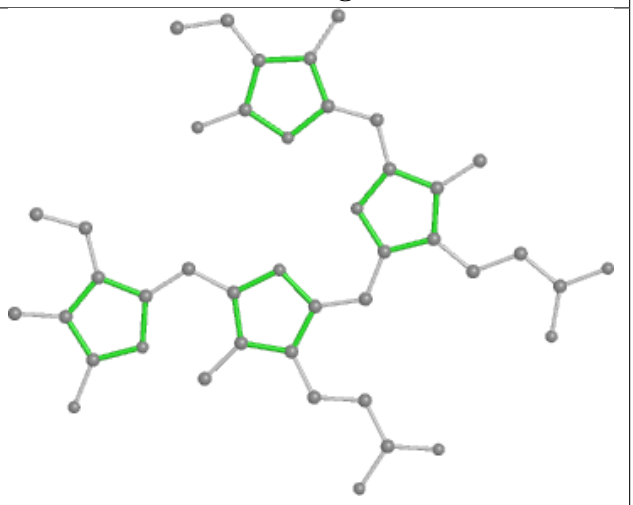
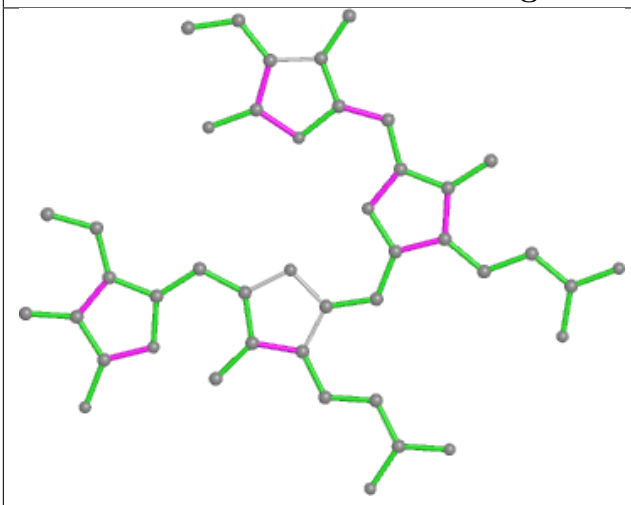


Rings

Ligand PUB fu 202



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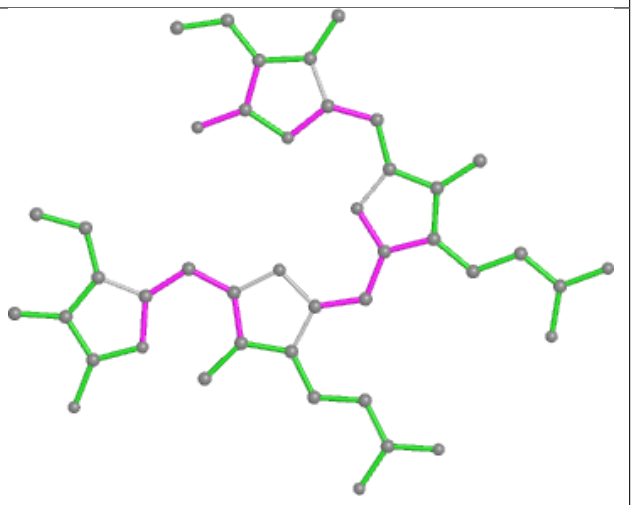

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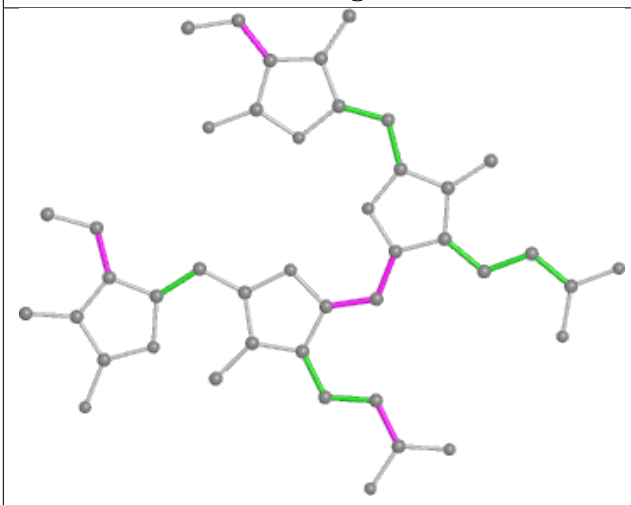

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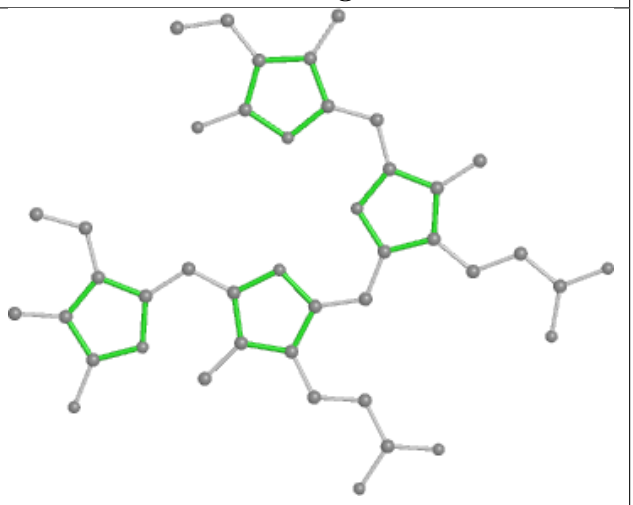

Rings

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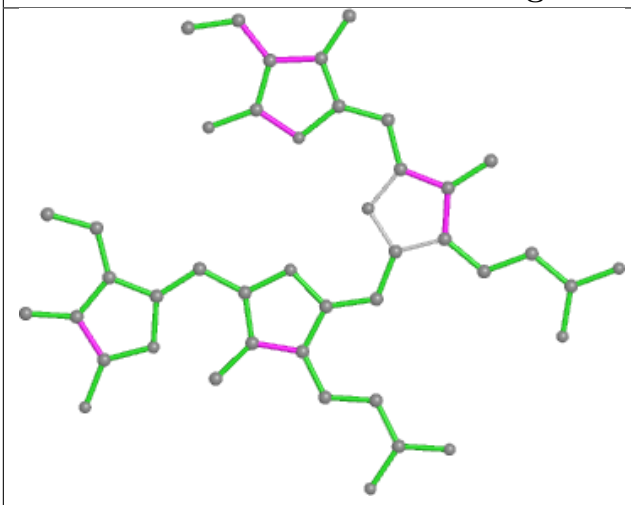

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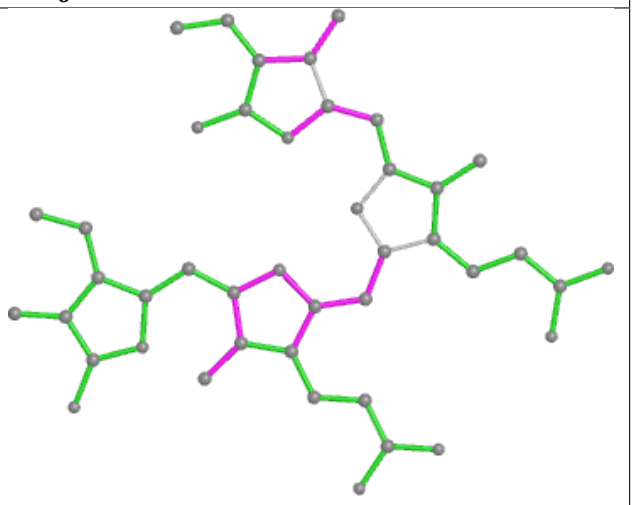

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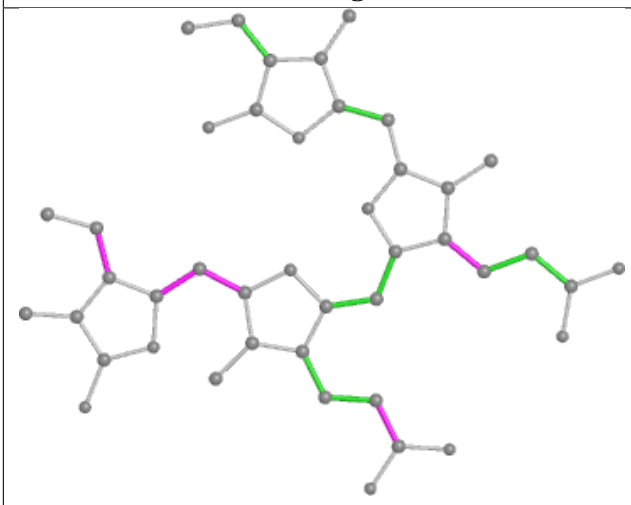

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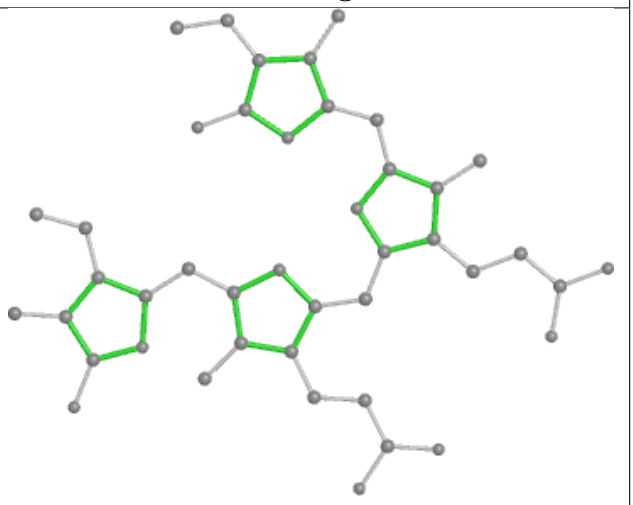
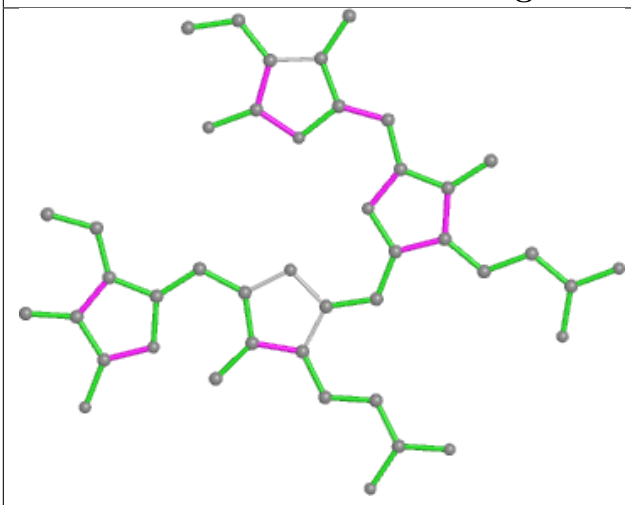


Rings

Ligand PUB F7 202



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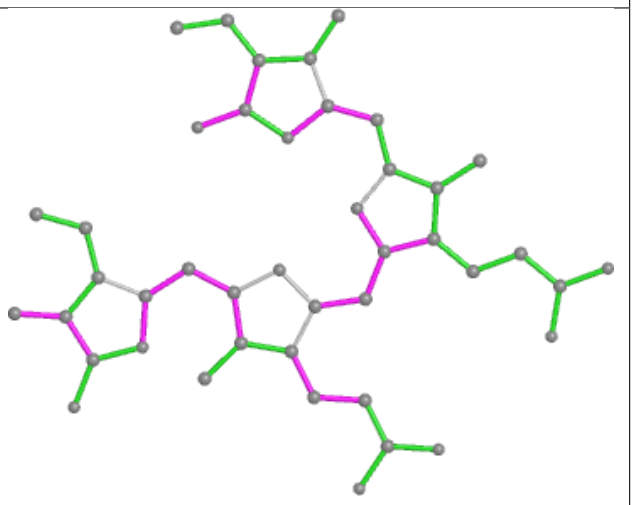

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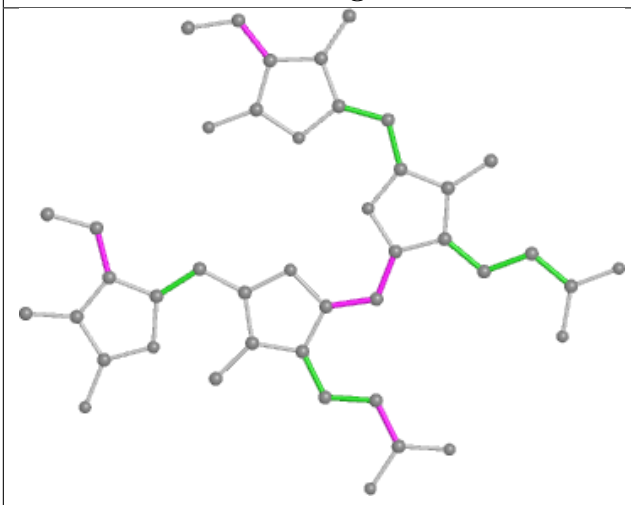

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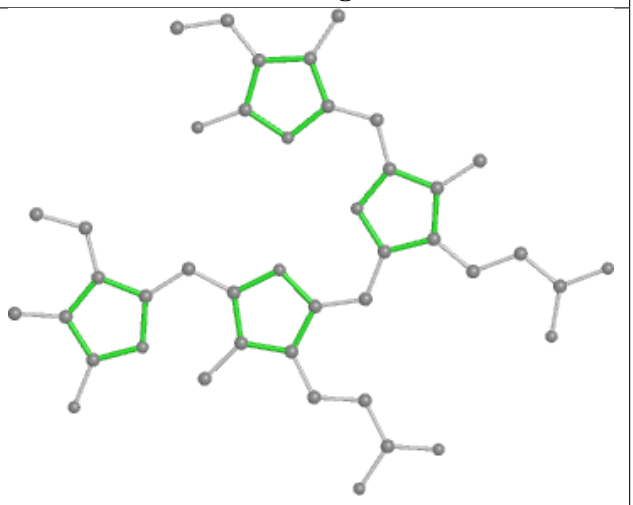

Rings

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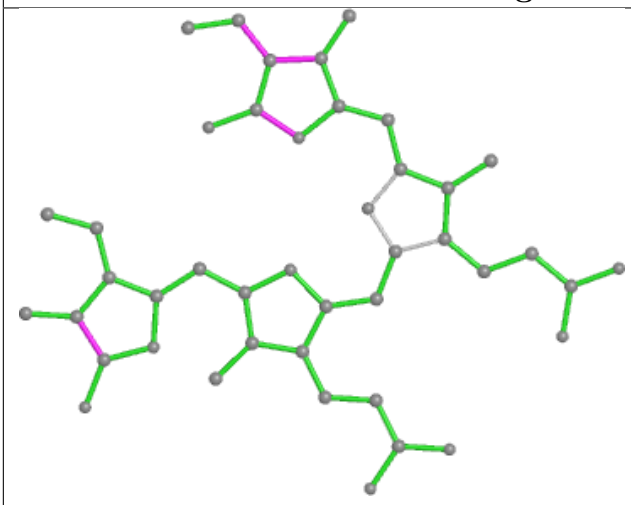

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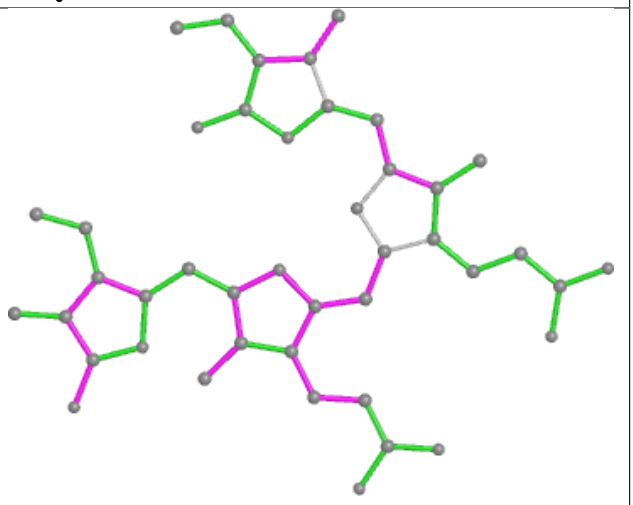

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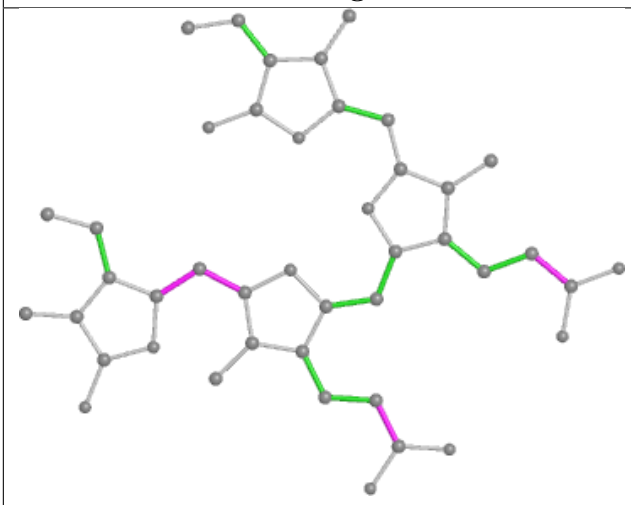

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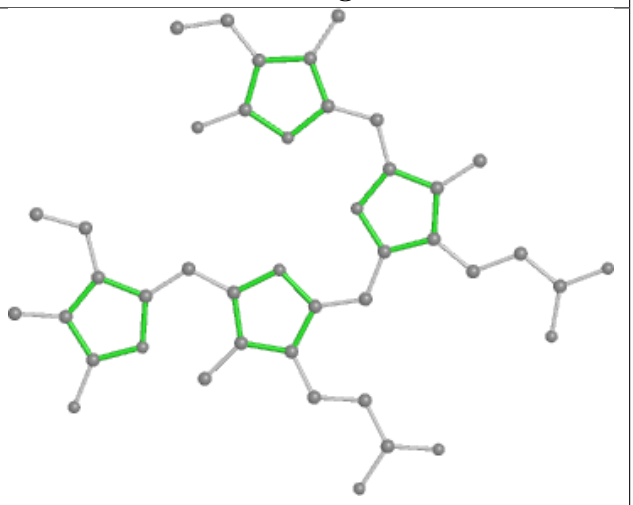

Rings

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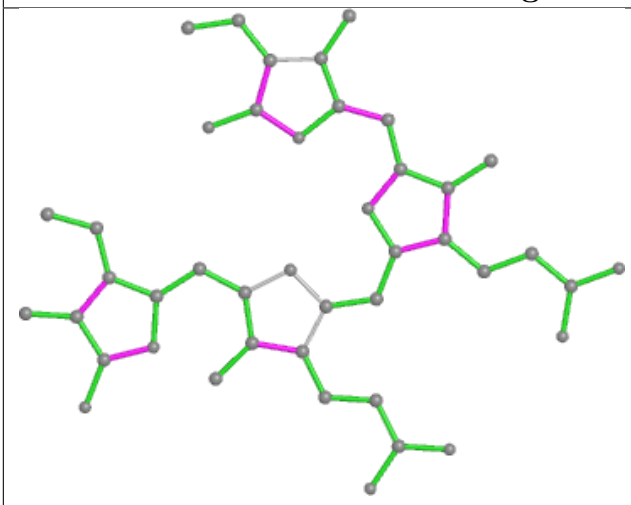

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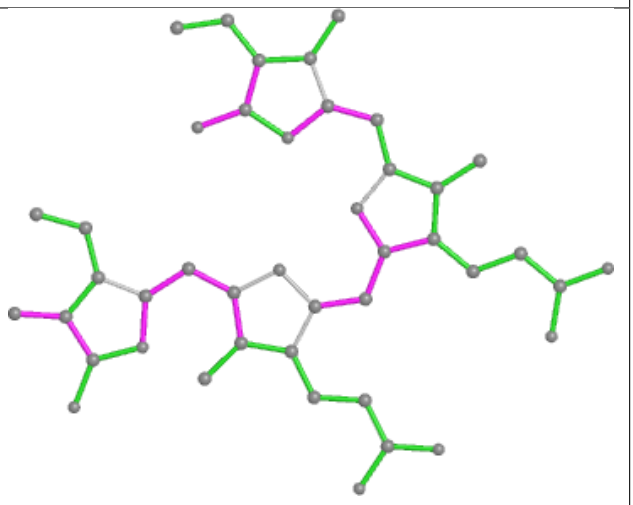

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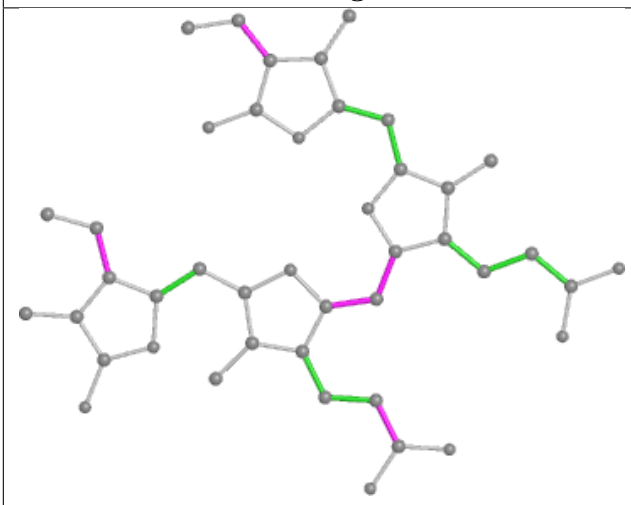

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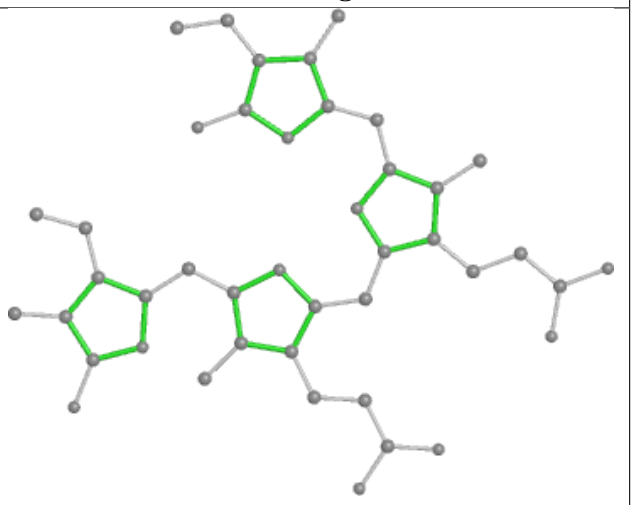
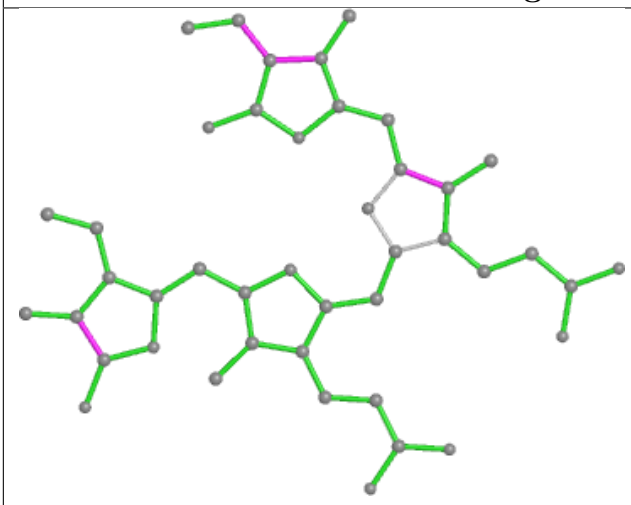


Rings

Ligand PEB ef 202



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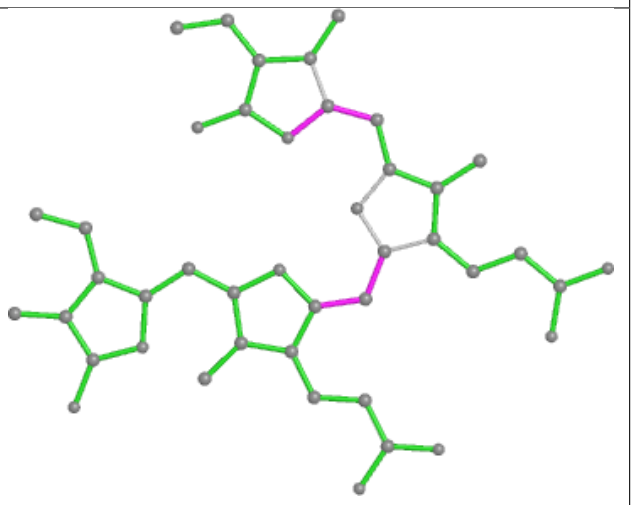
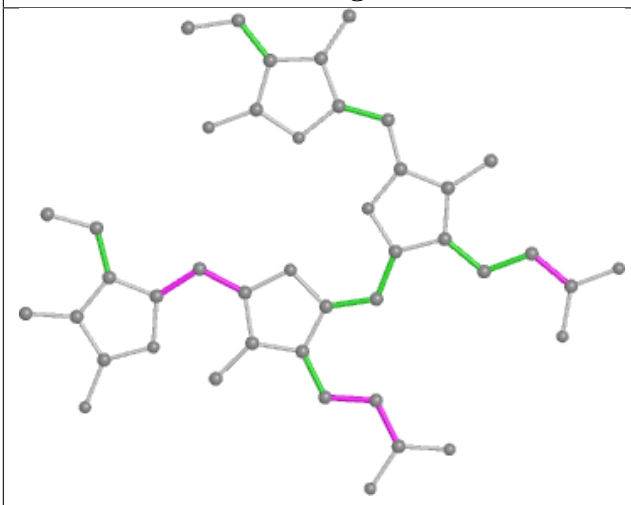


Bond angles



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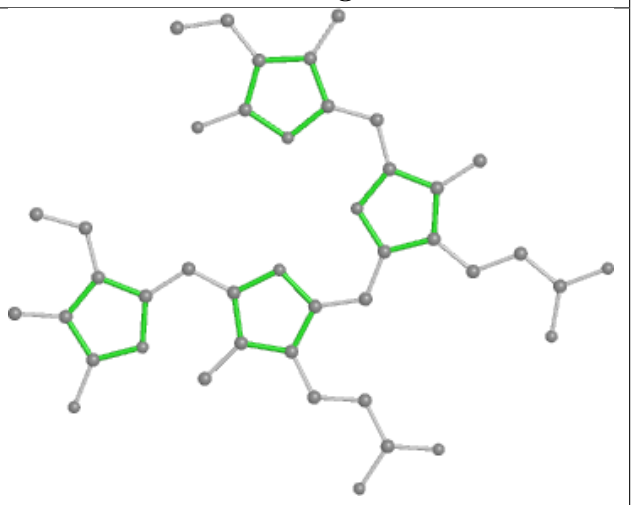

Rings

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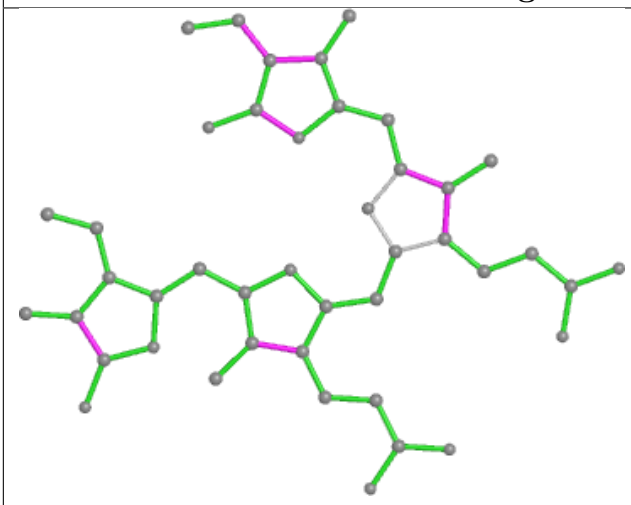

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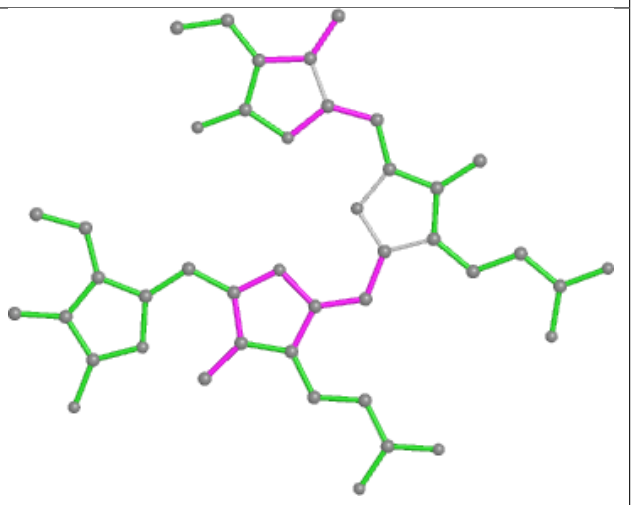
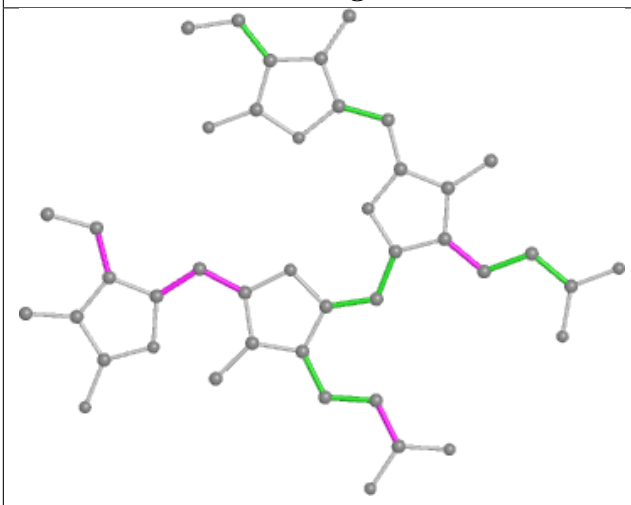


Bond angles



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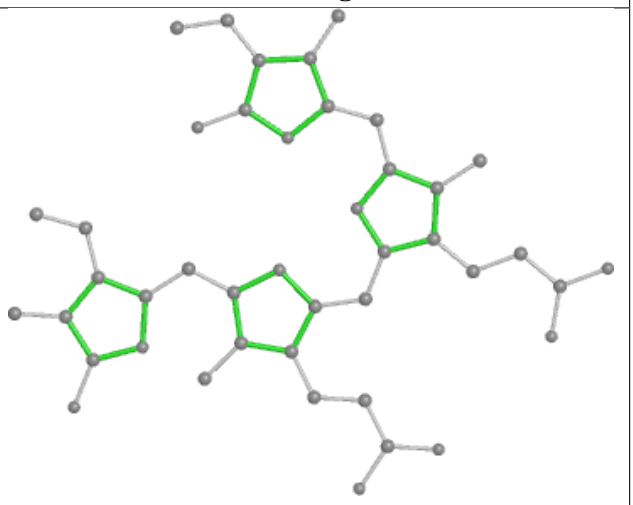
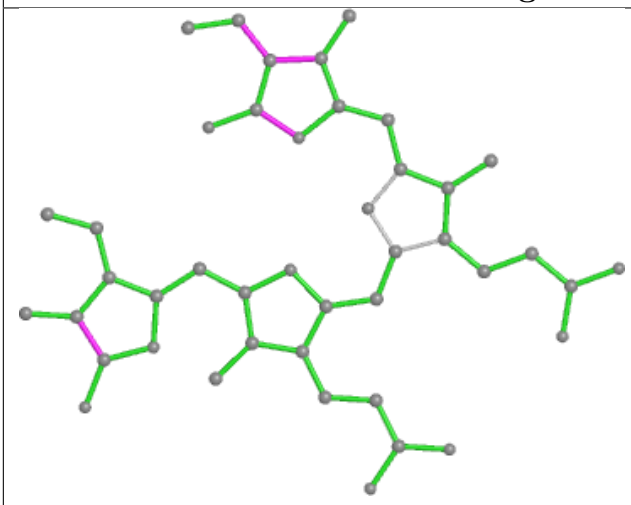
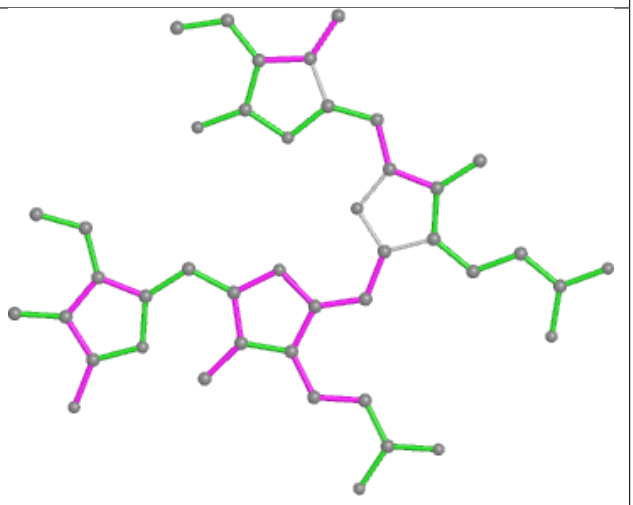


Rings

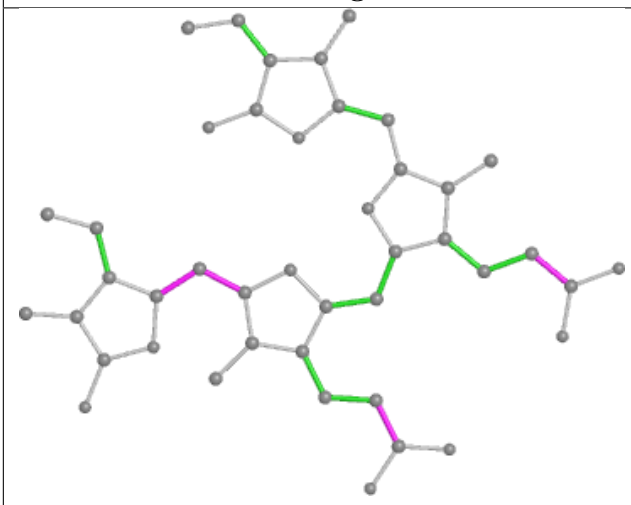
Ligand PEB d8 302



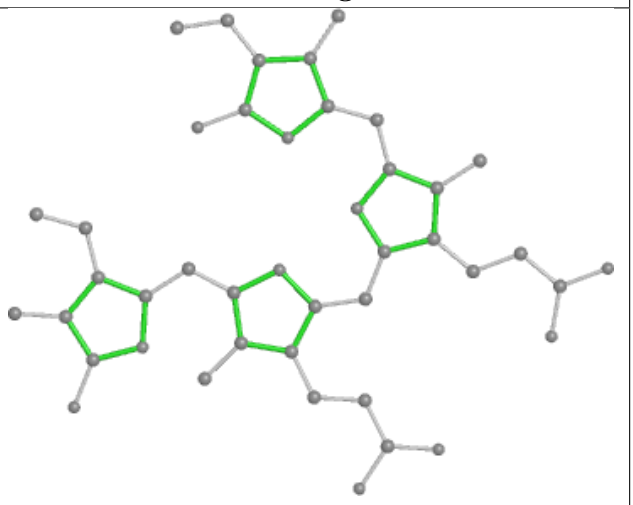
Bond lengths



Bond angles

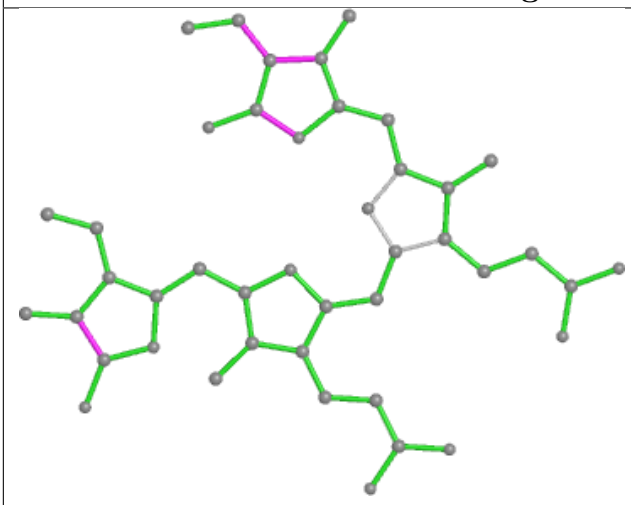


Torsions



Rings

Ligand PEB r9 202



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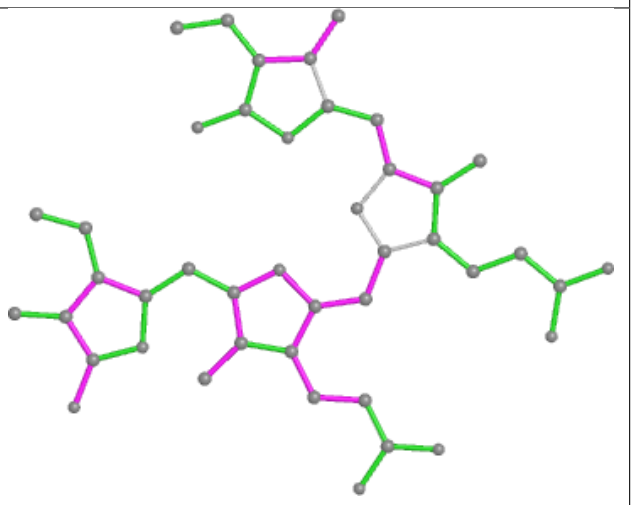

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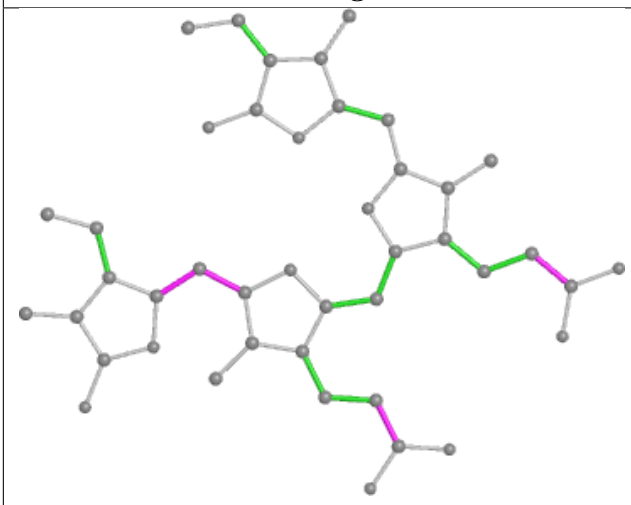

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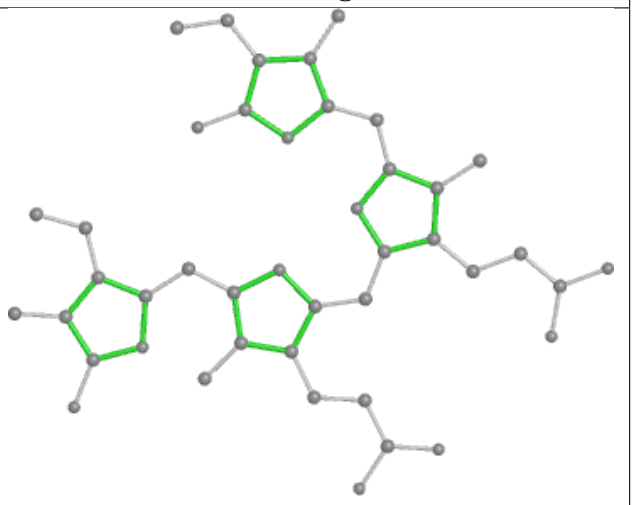
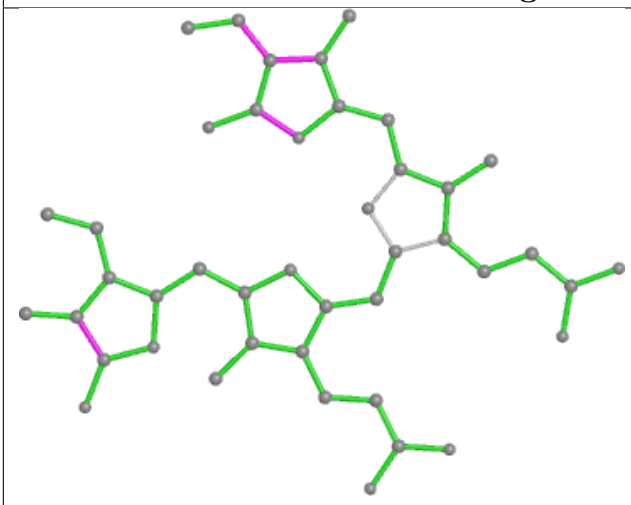


Rings

Ligand PEB o6 202



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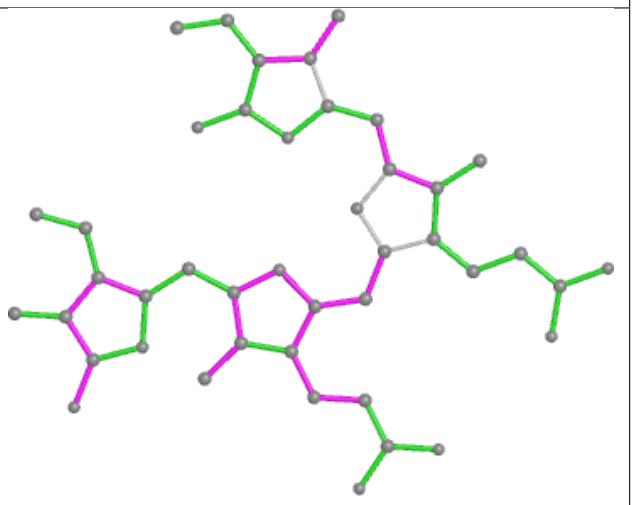

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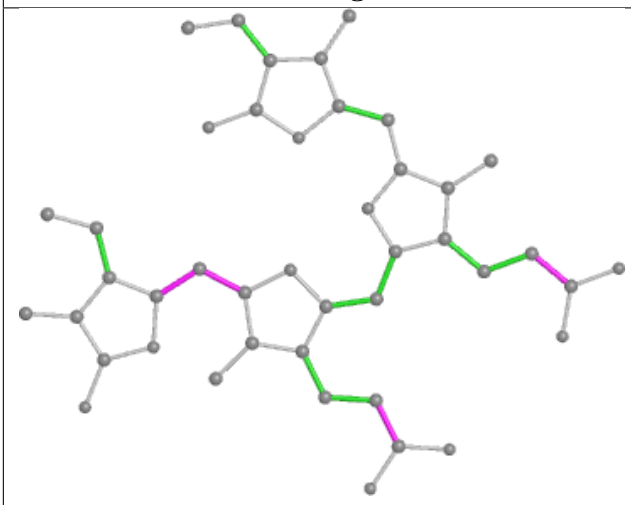

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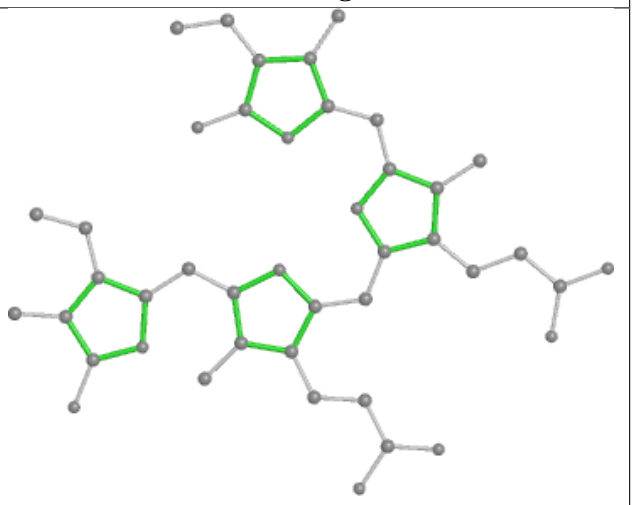
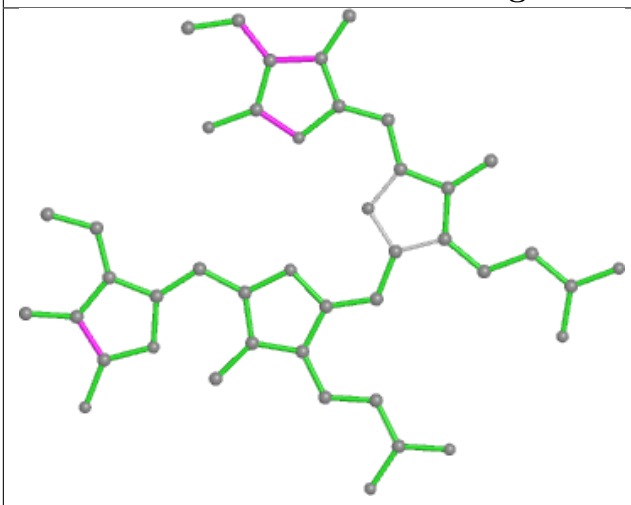


Rings

Ligand PEB Z9 1007



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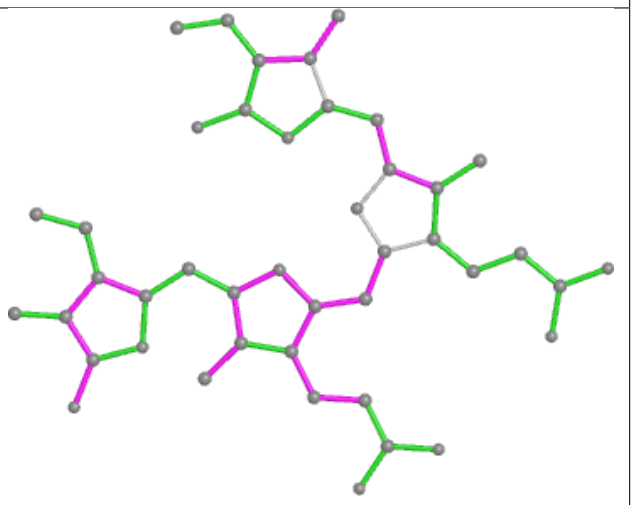

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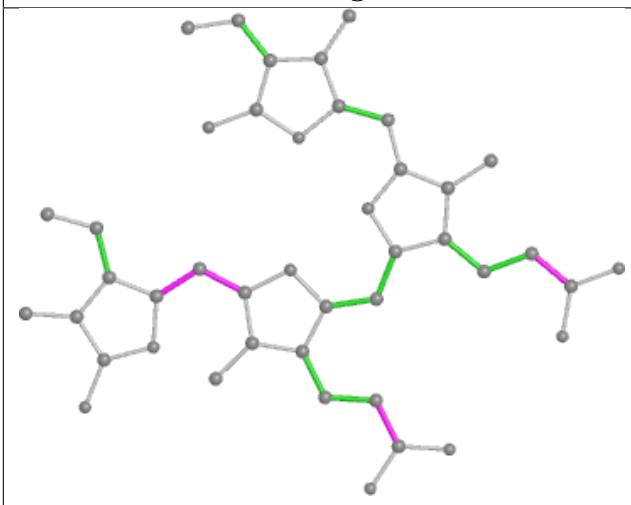

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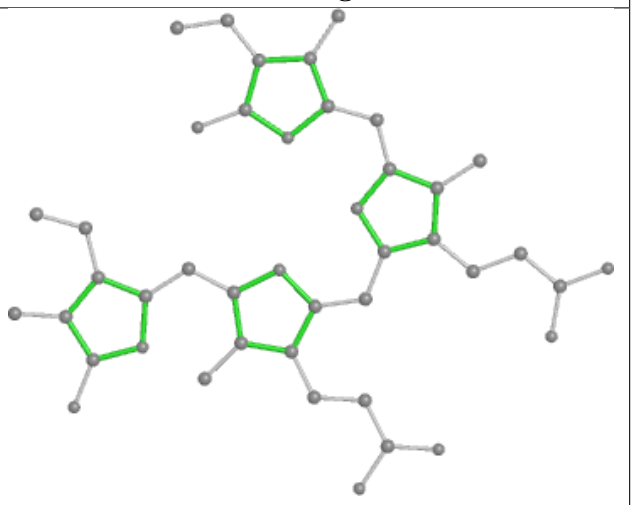
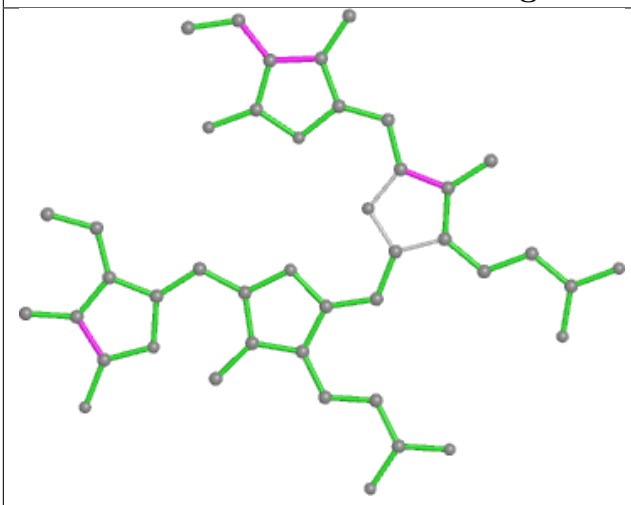


Rings

Ligand PEB de 202



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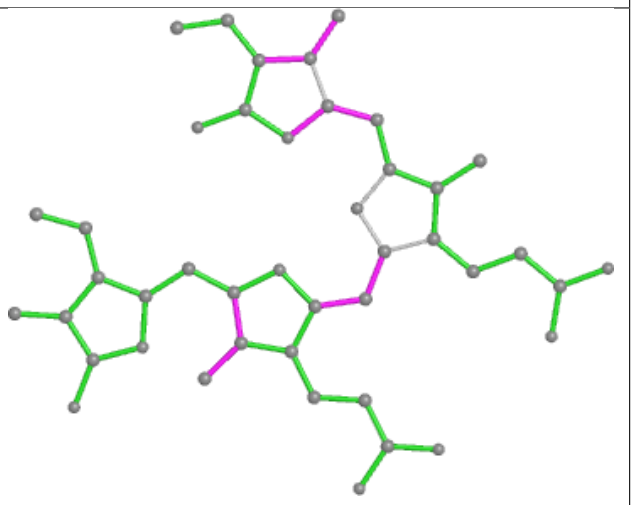

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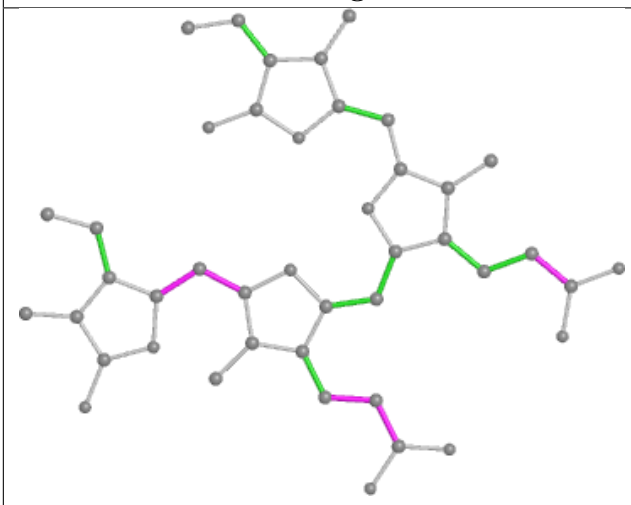

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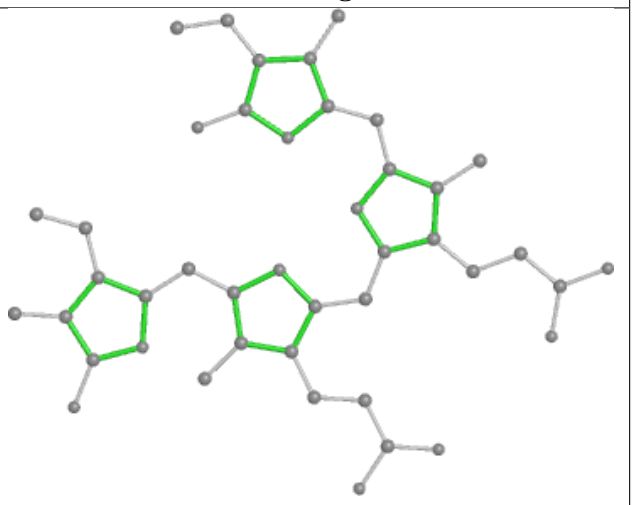
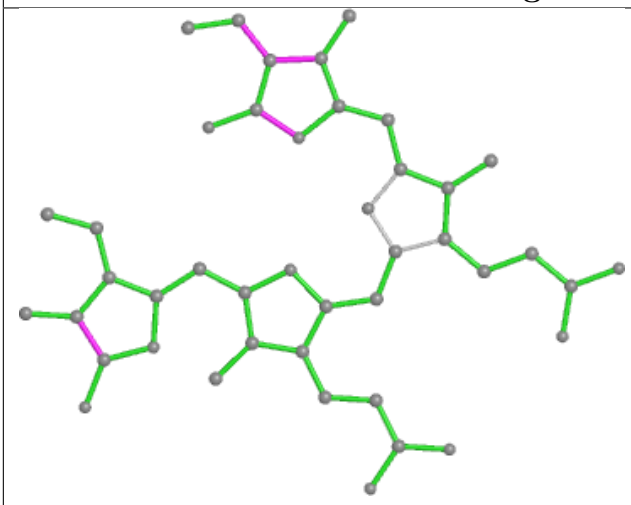


Rings

Ligand PEB ly 402



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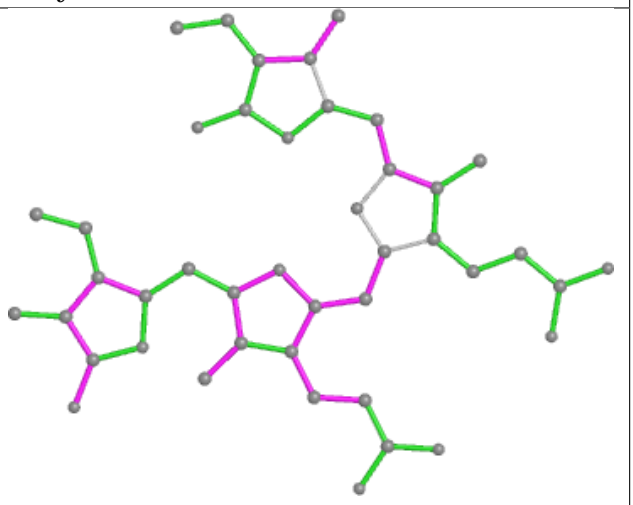

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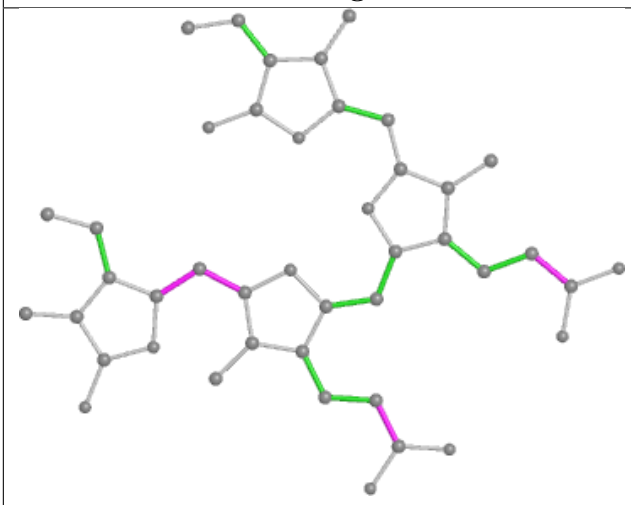

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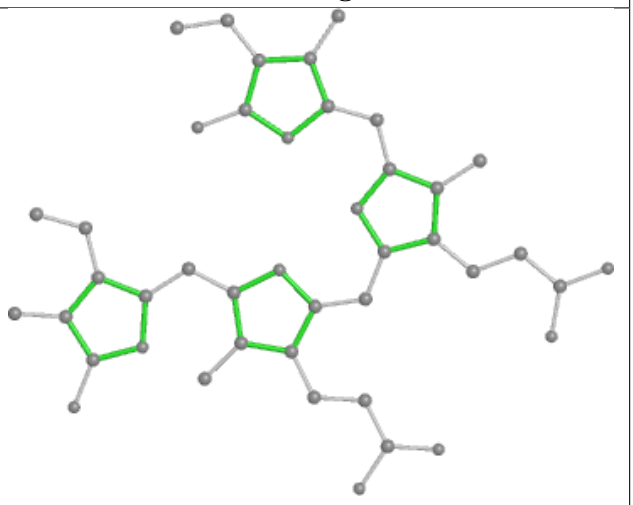

Rings

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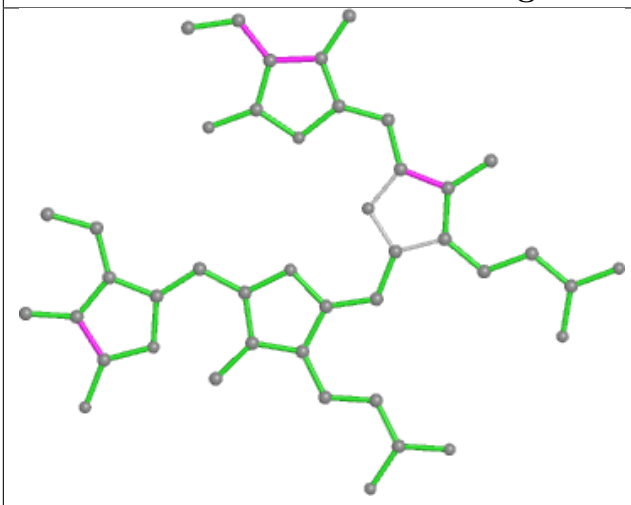

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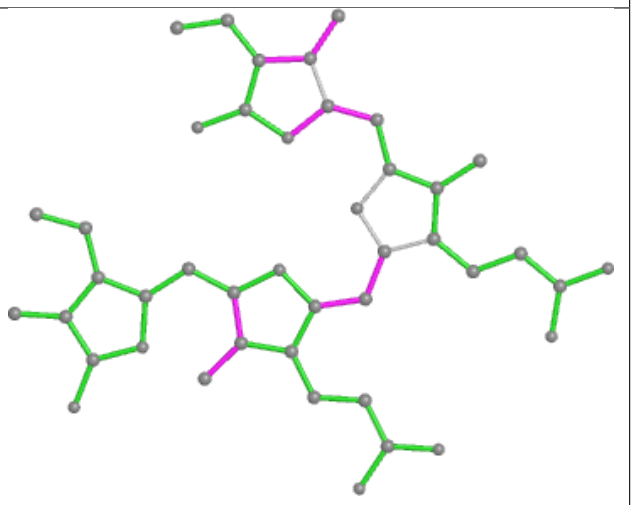

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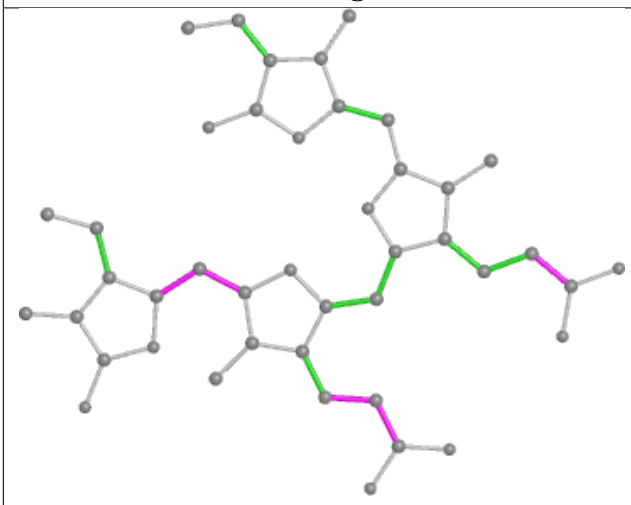

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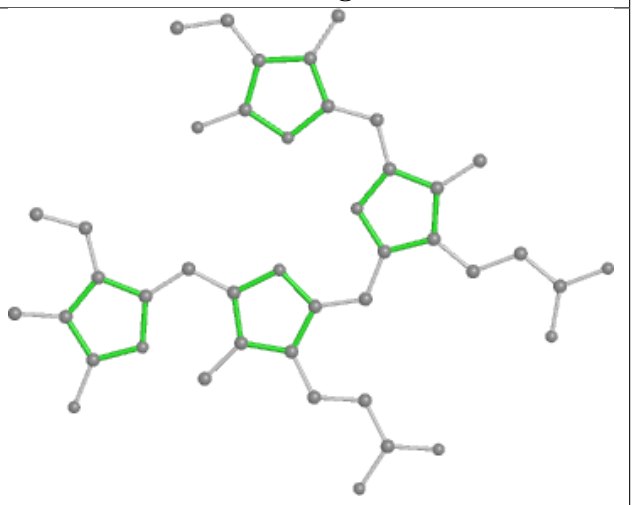

Rings

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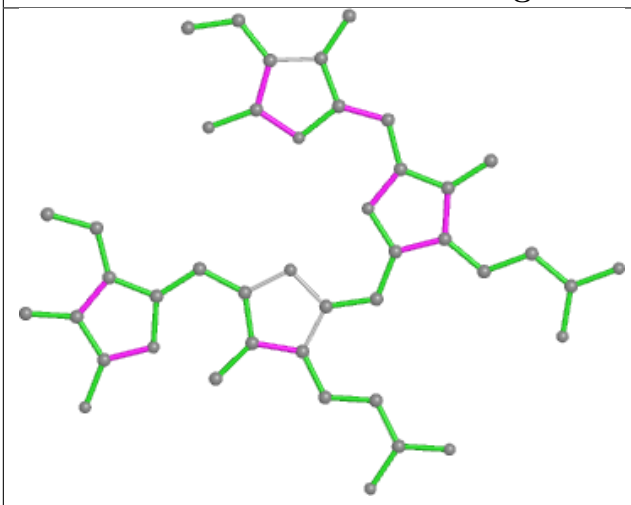

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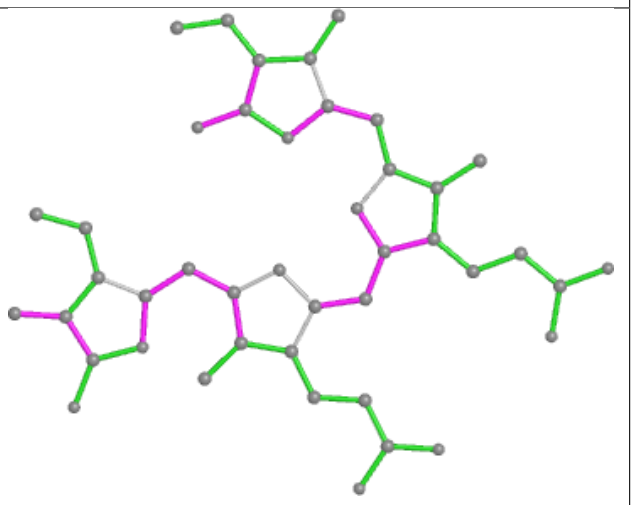

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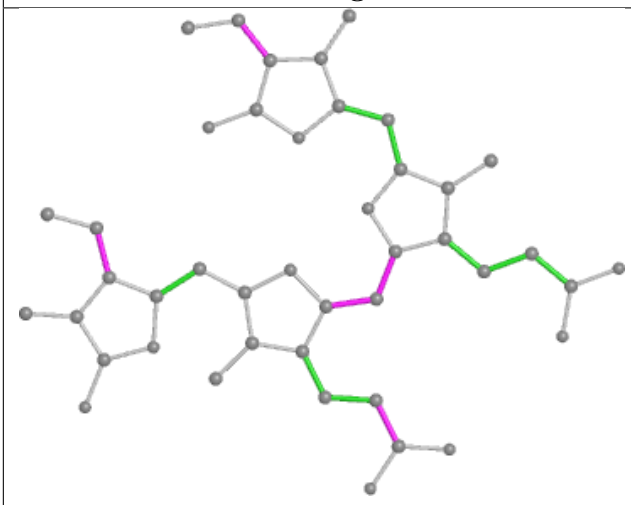

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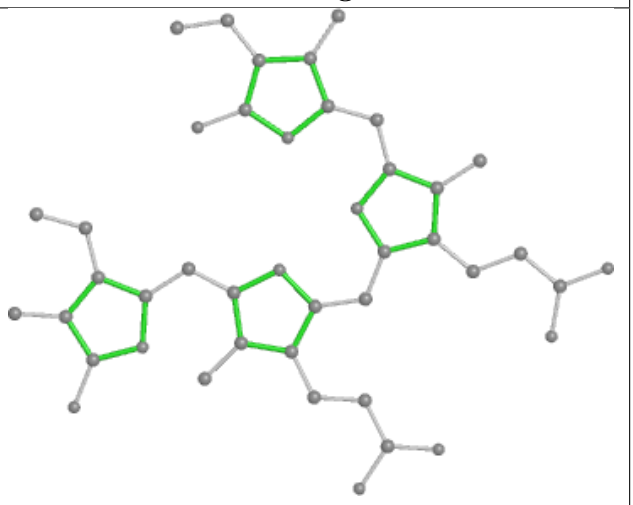

Rings

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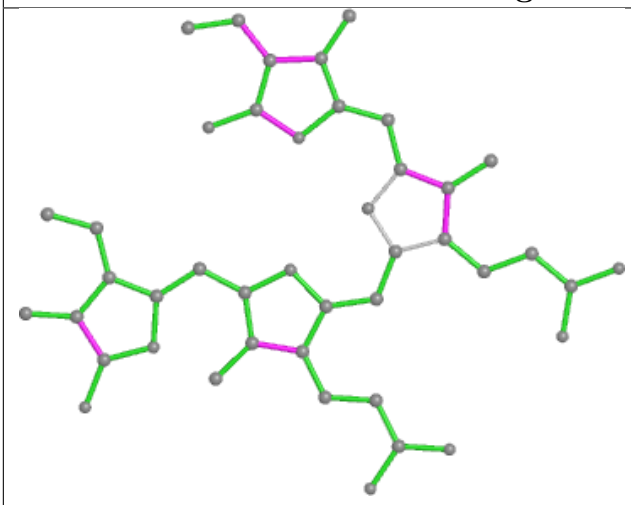

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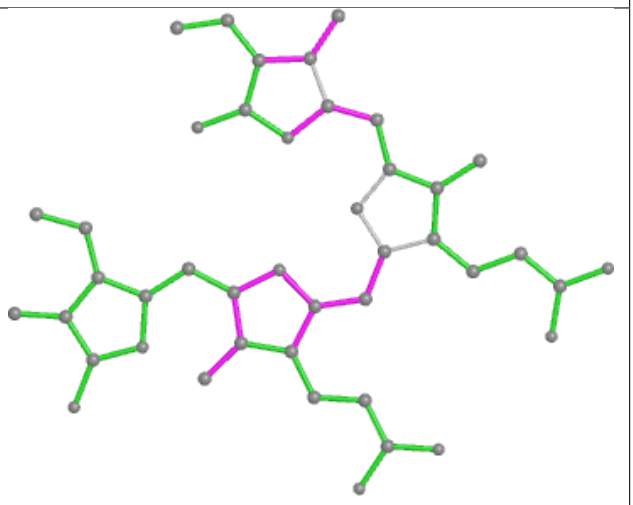

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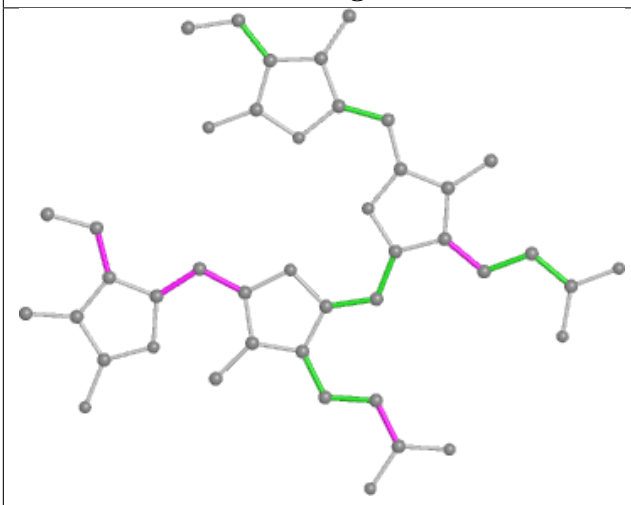

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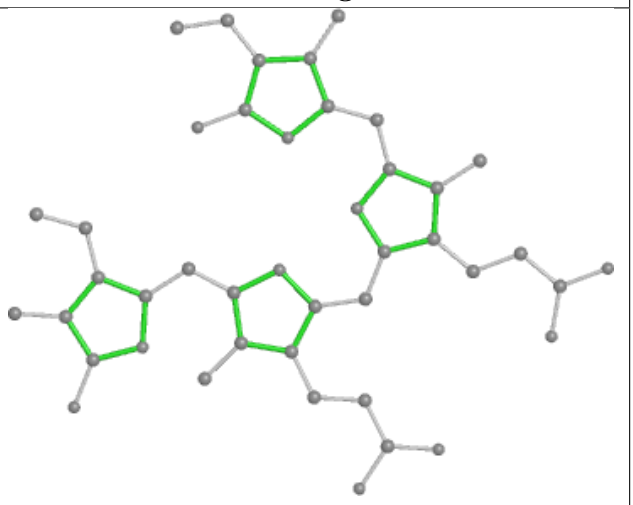
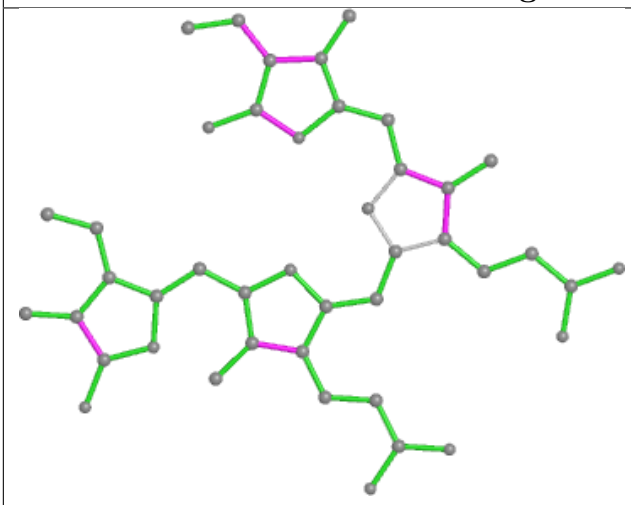


Rings

Ligand PEB gk 202



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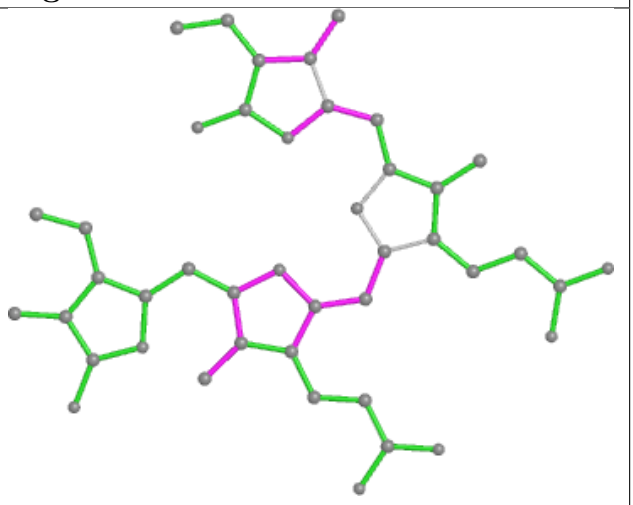

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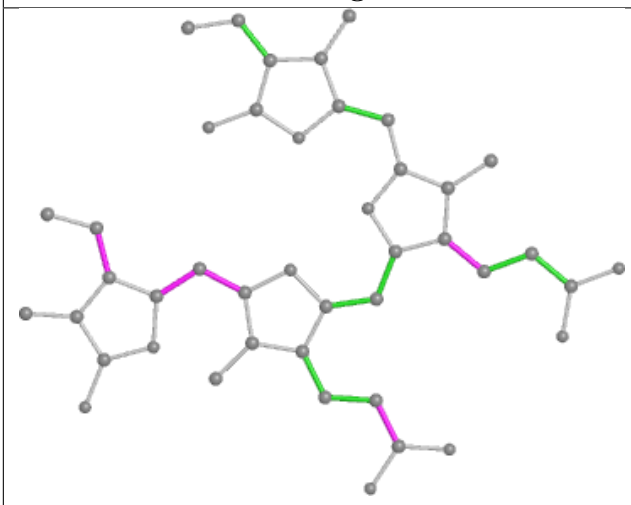

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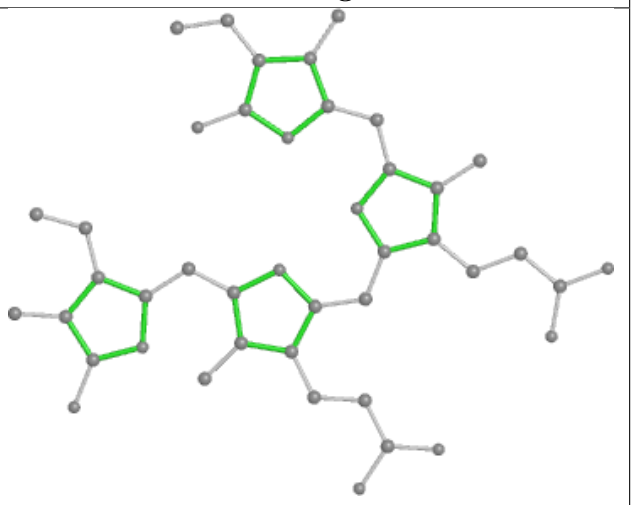
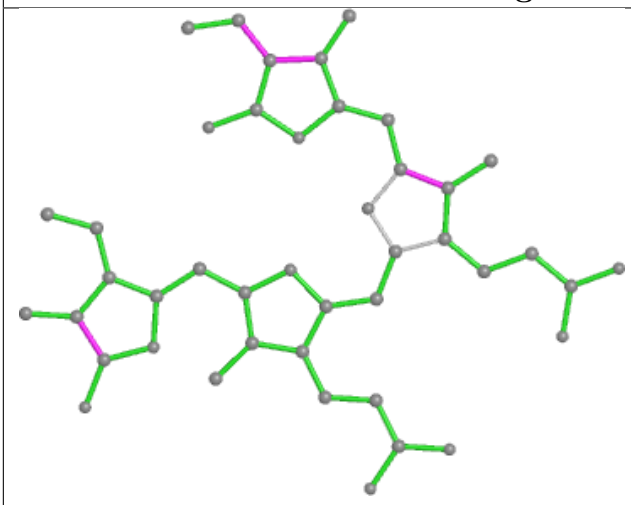


Rings

Ligand PEB O5 202



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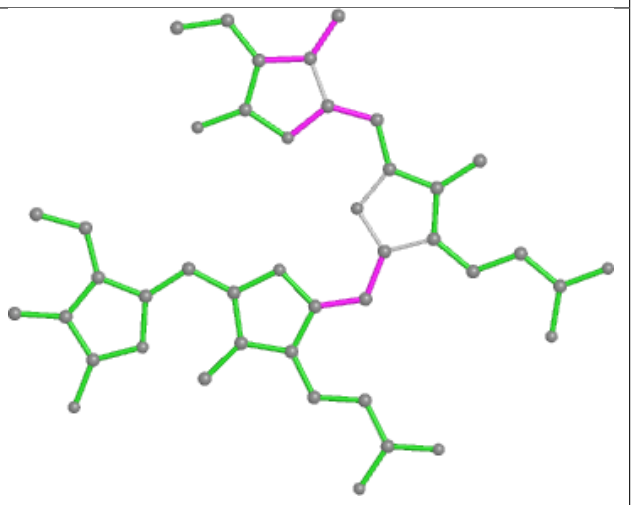

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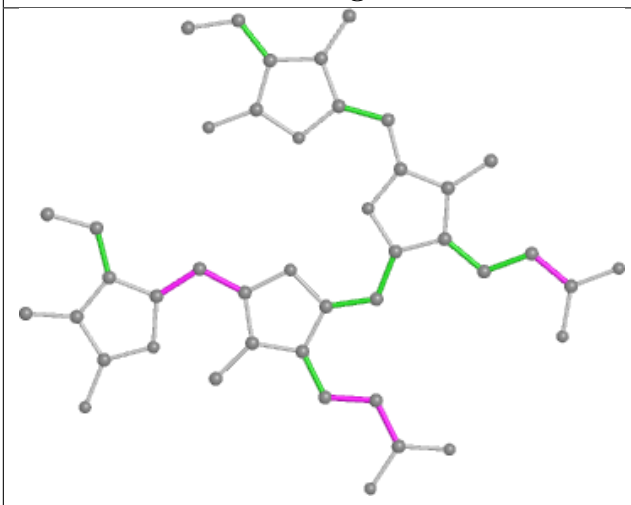

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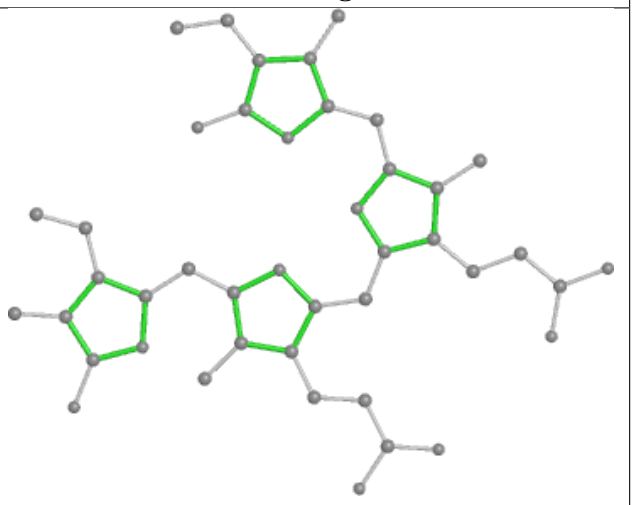

Rings

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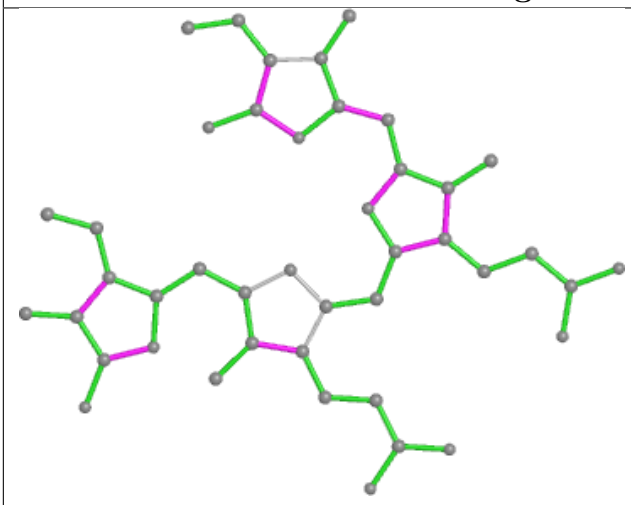

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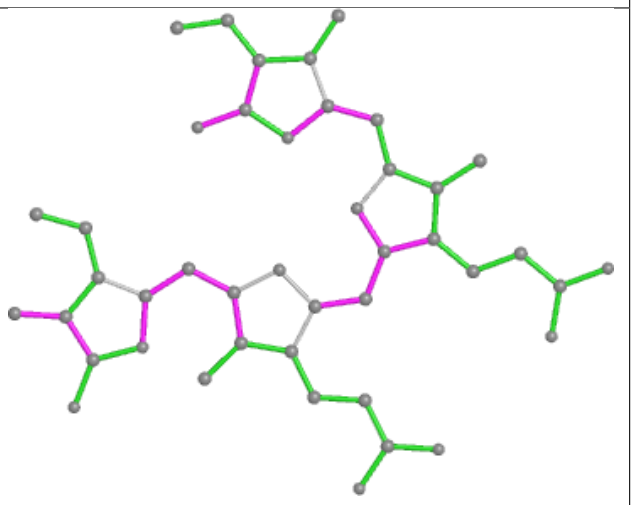

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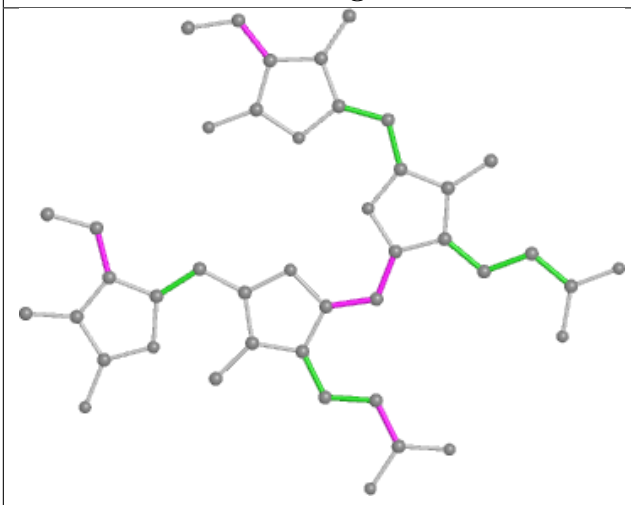

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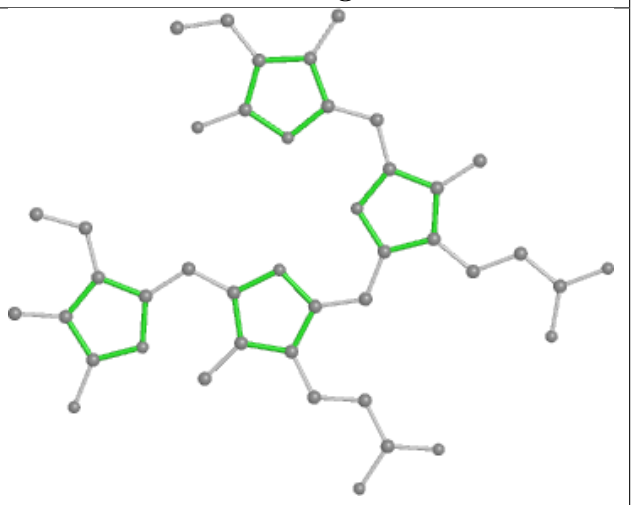
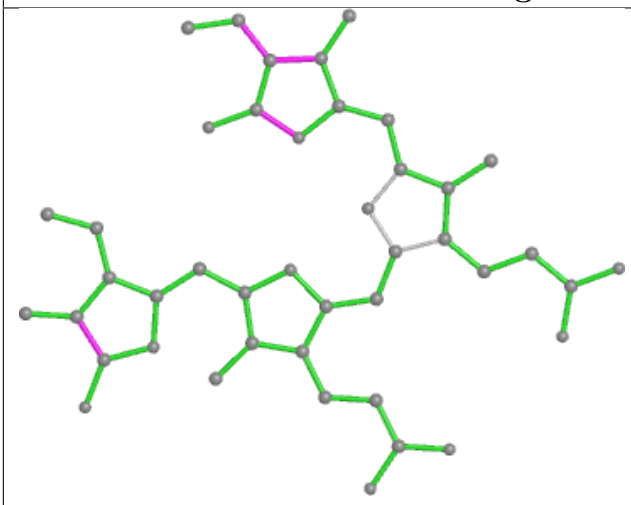


Rings

Ligand PEB G6 201



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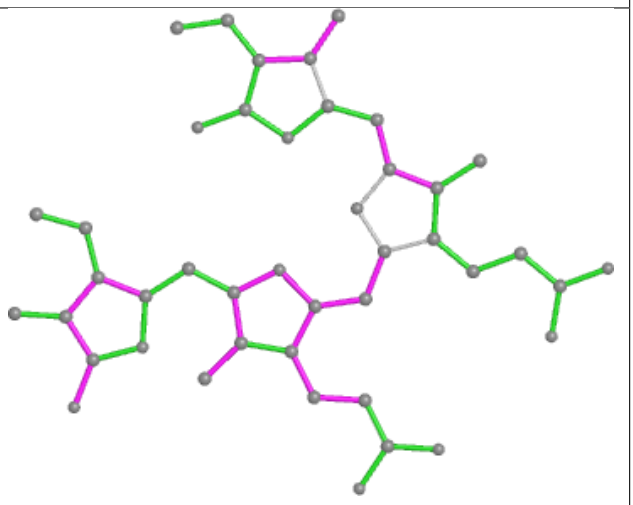

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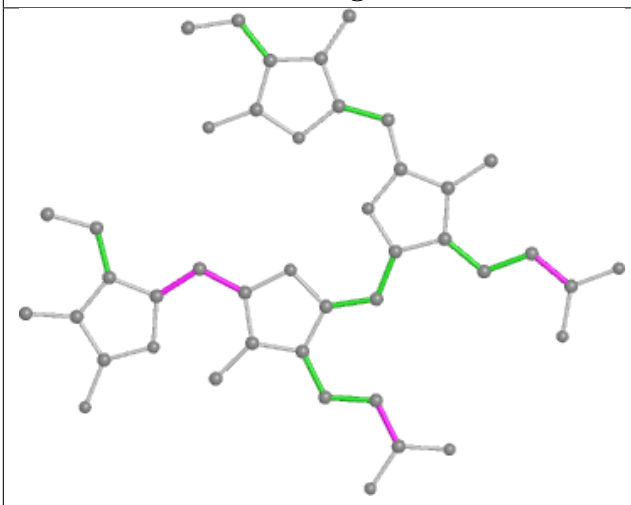

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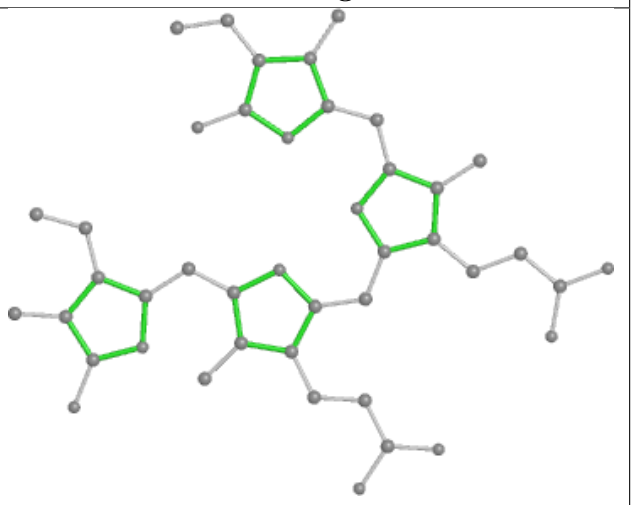
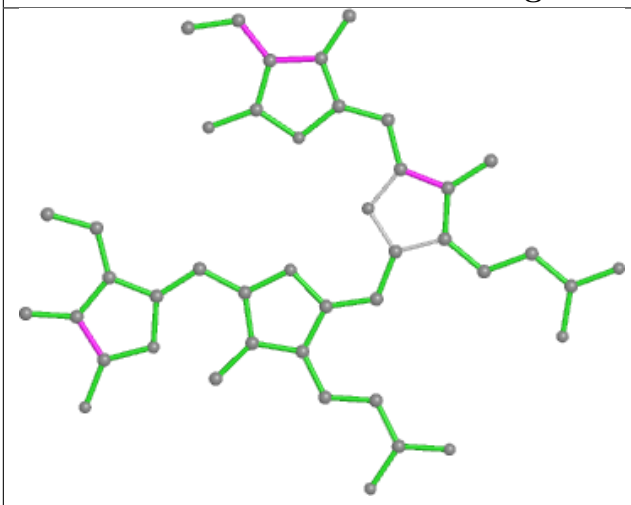


Rings

Ligand PEB lc 202



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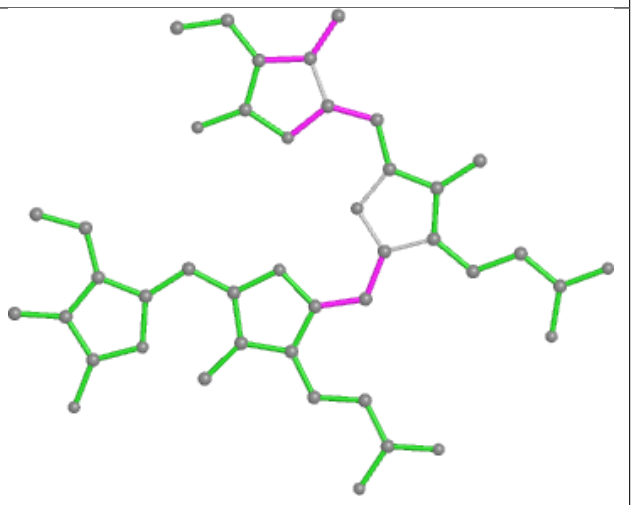
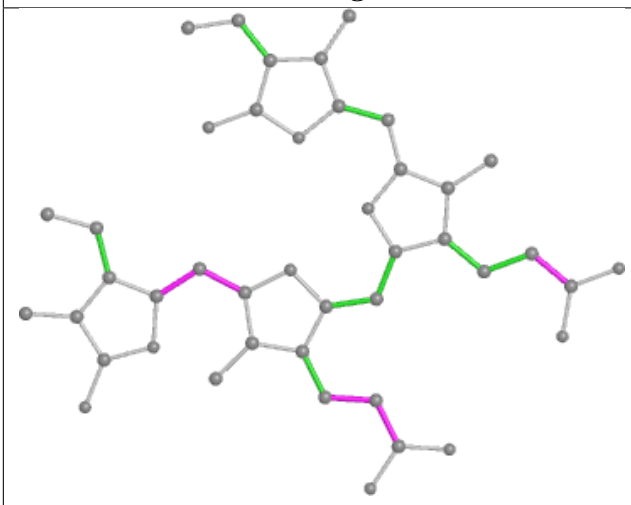
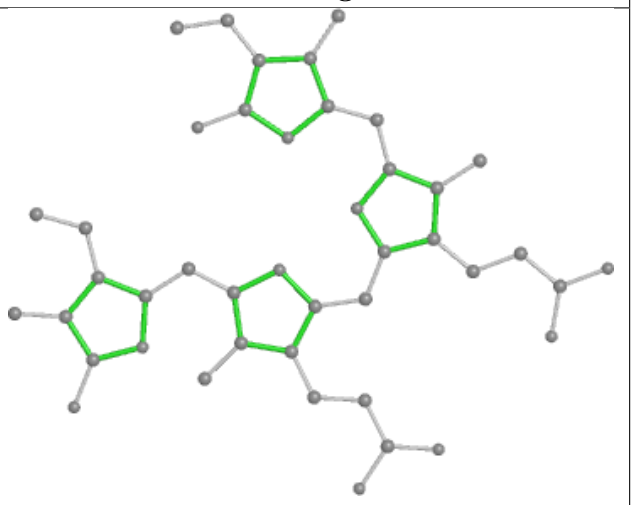


Bond angles

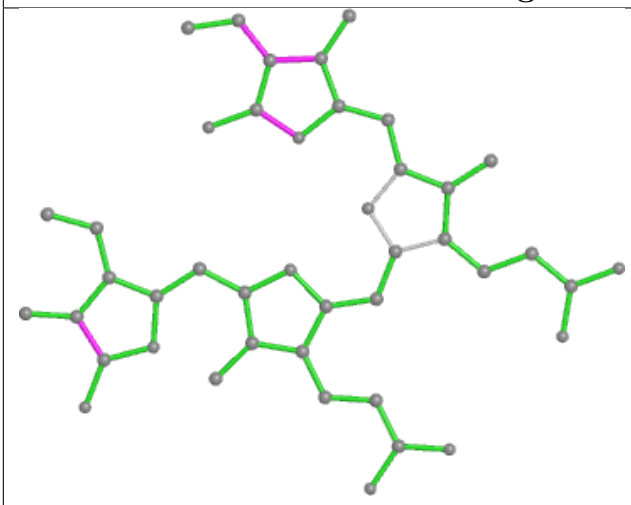


Torsions



Rings

Ligand PEB F5 201



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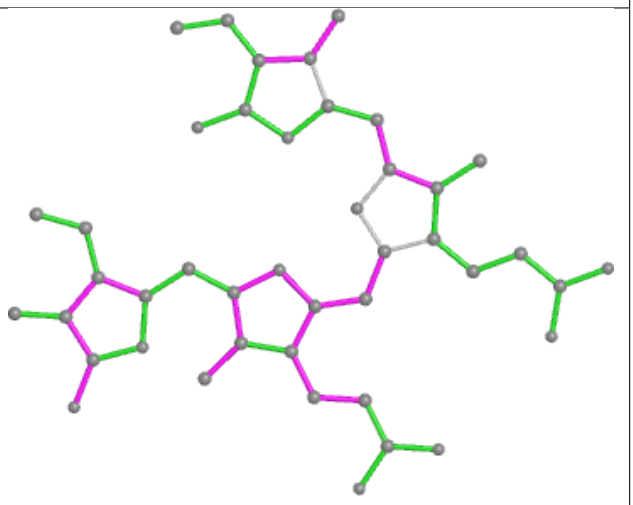

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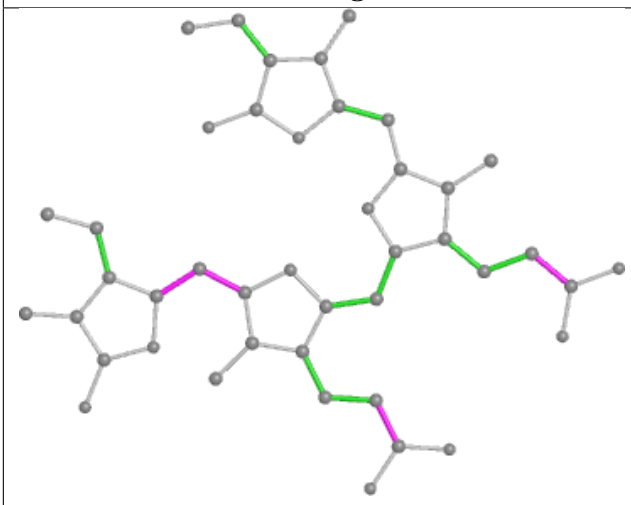

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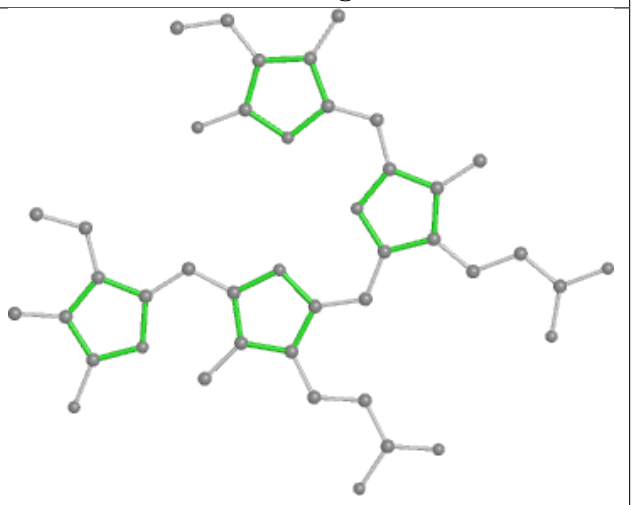
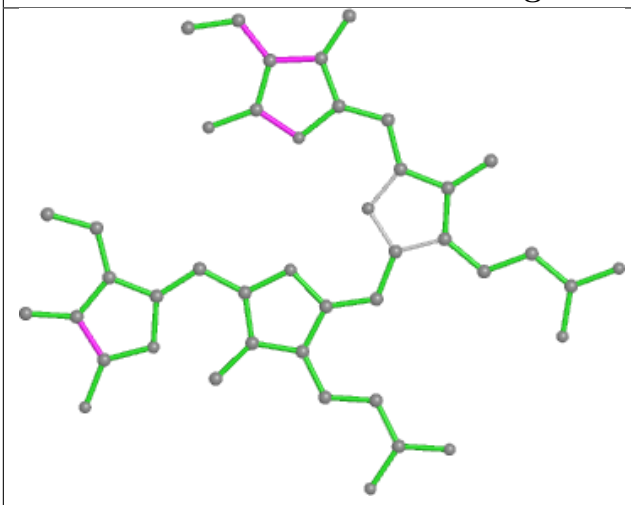


Rings

Ligand PEB al 201



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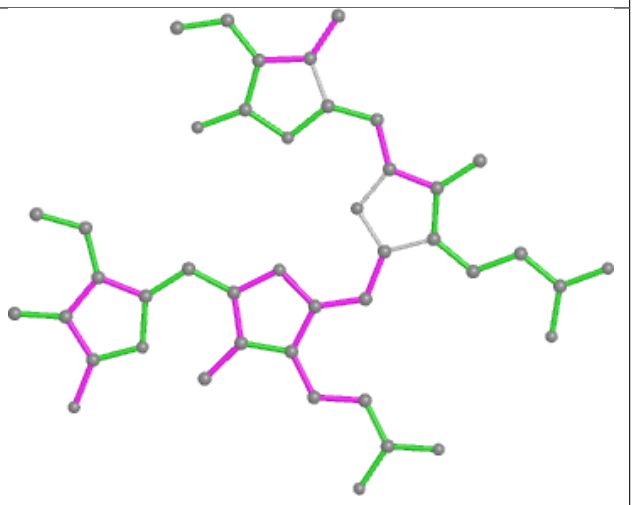

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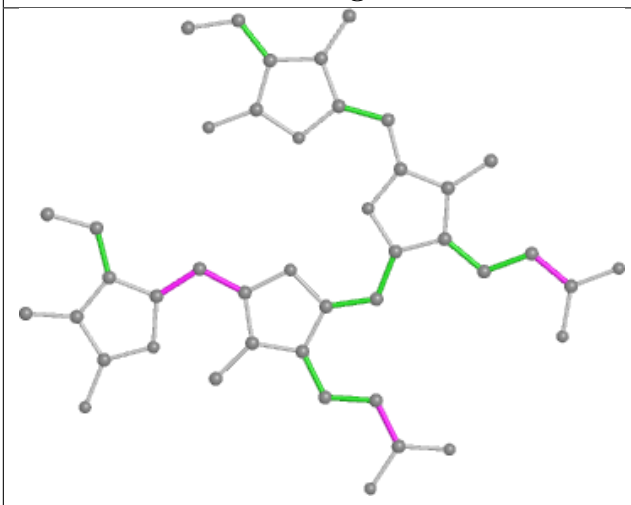

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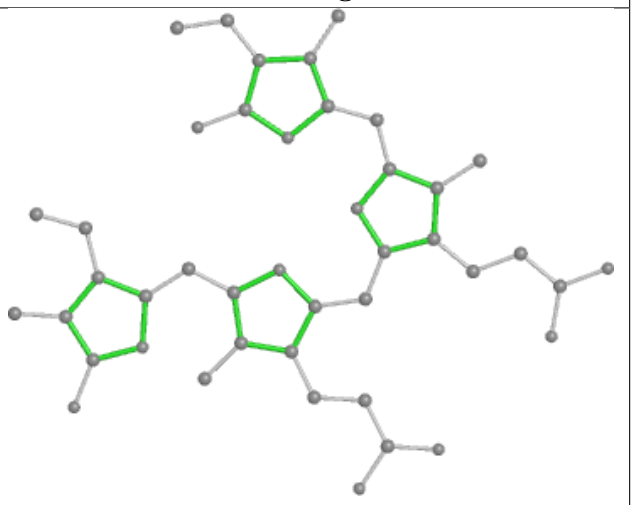
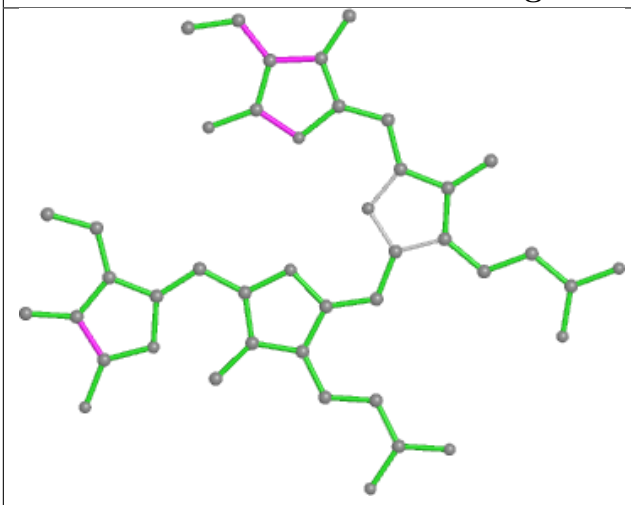


Rings

Ligand PEB lc 201



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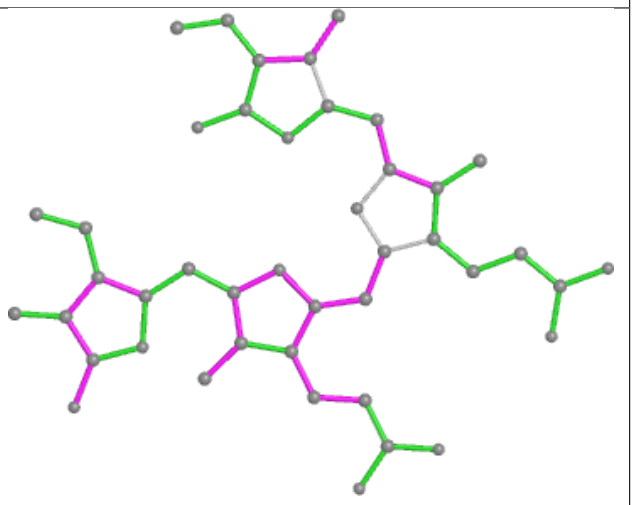

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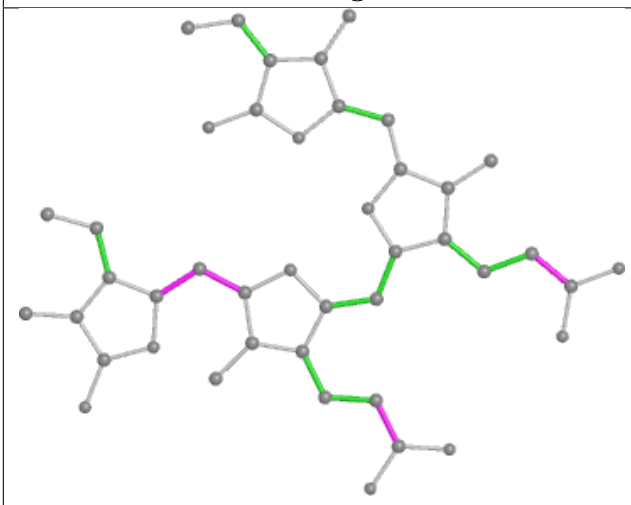

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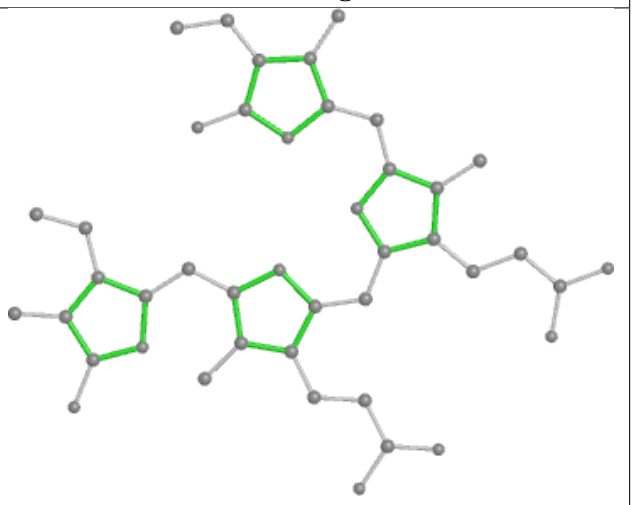
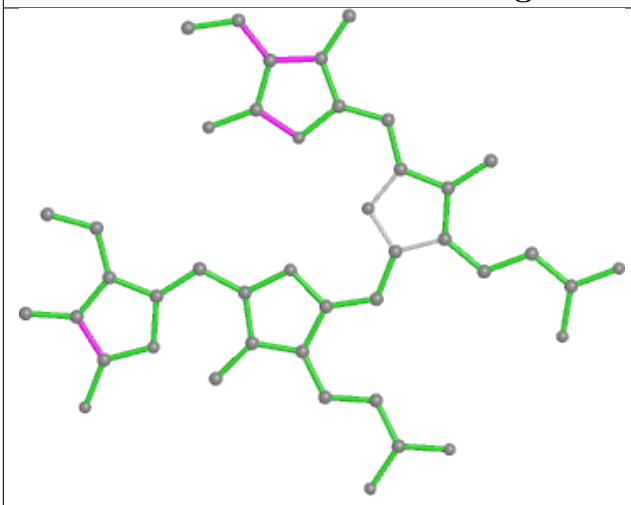


Rings

Ligand PEB G4 201



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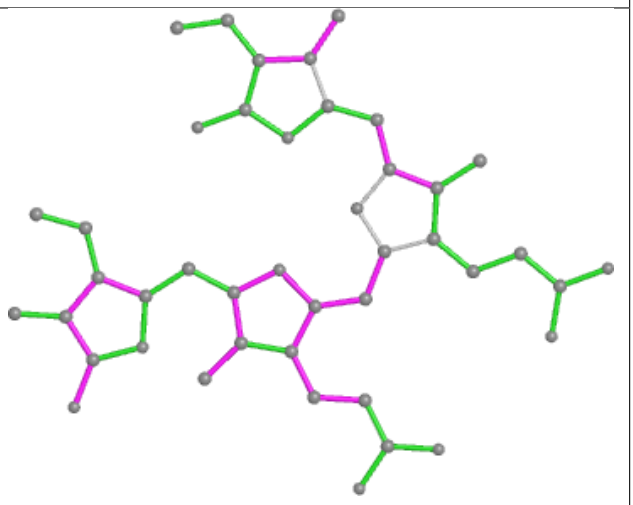

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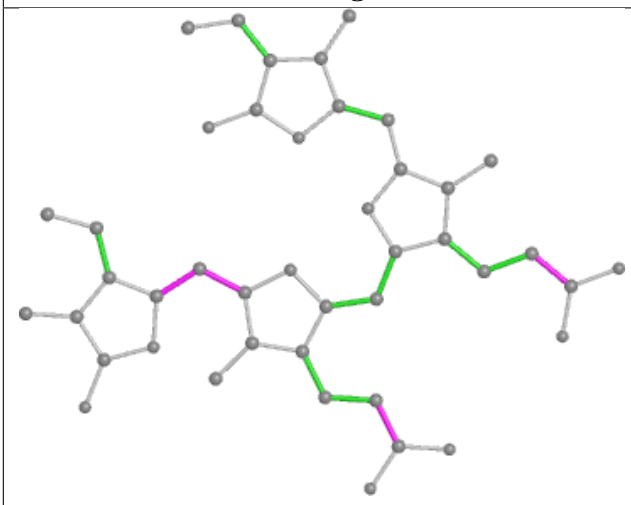

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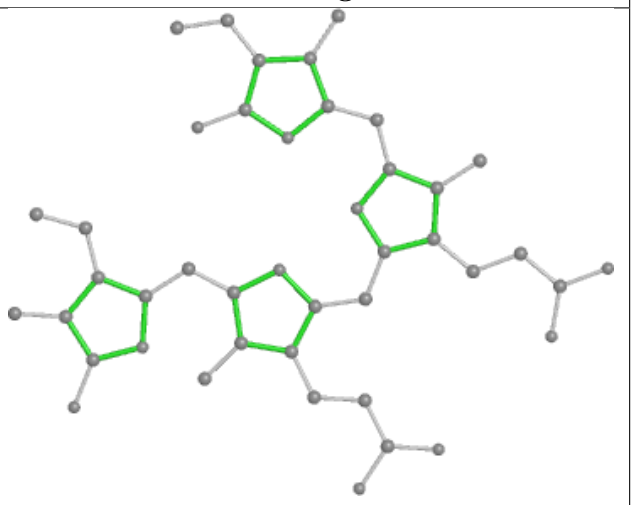
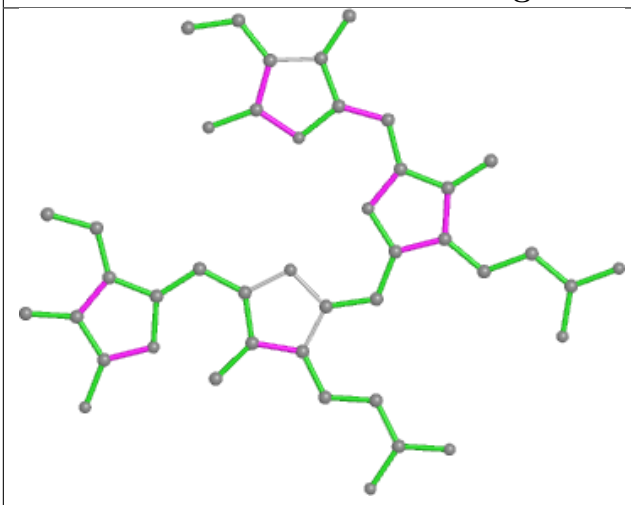


Rings

Ligand PUB R6 203



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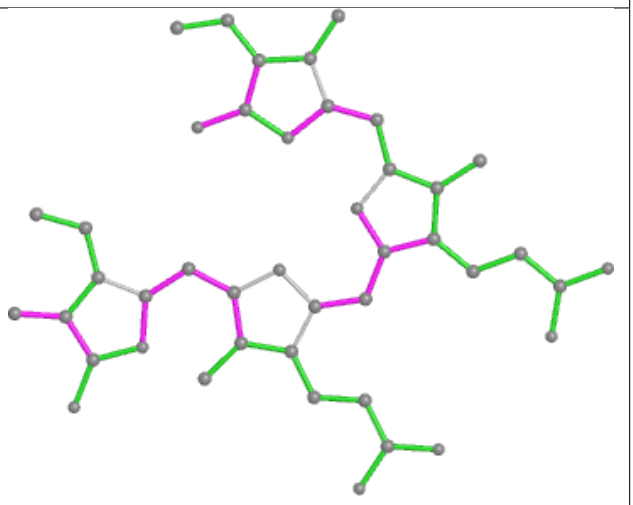

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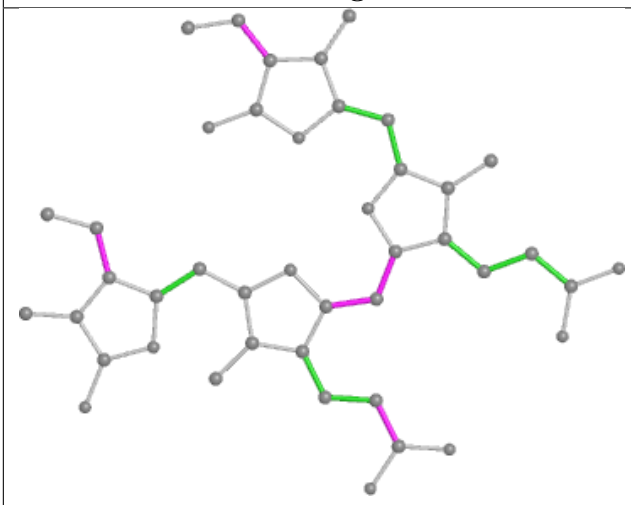

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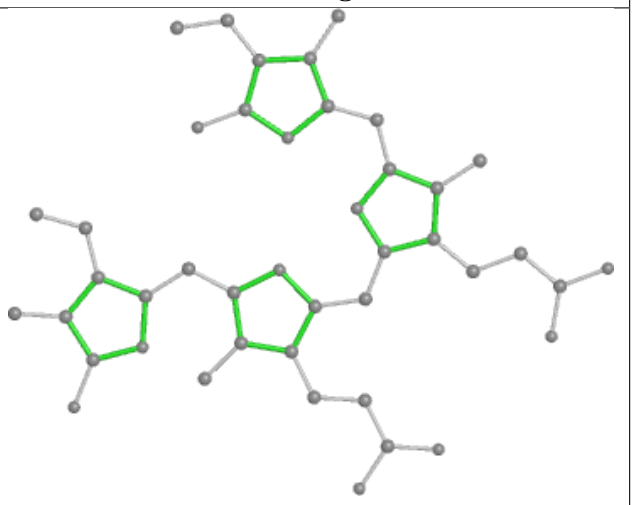

Rings

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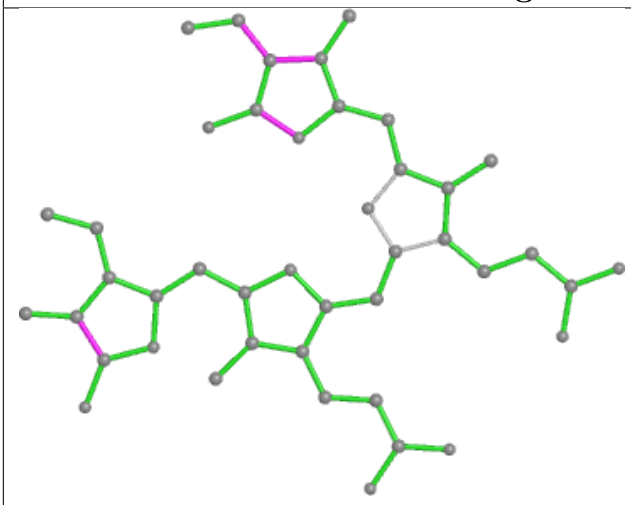

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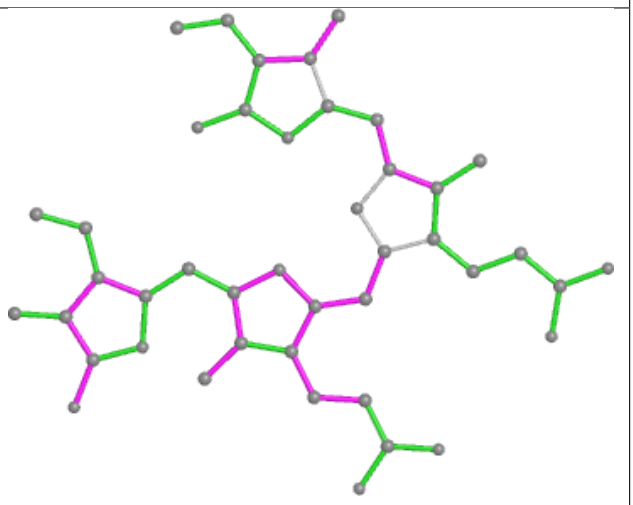

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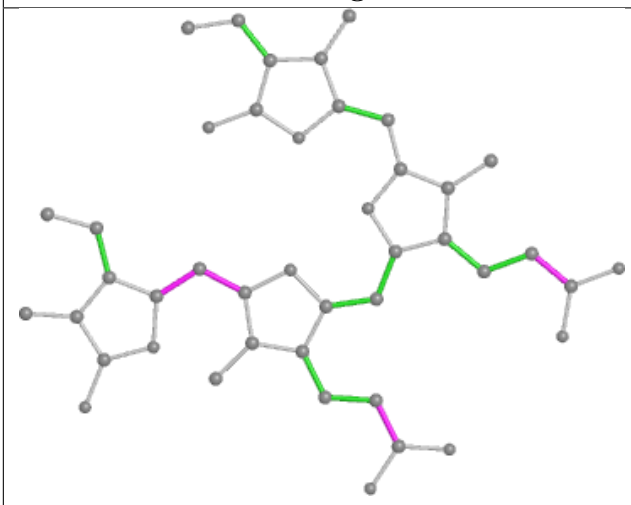

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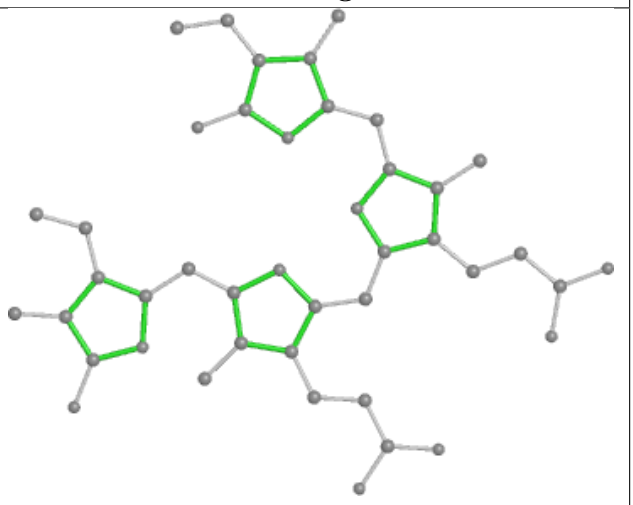
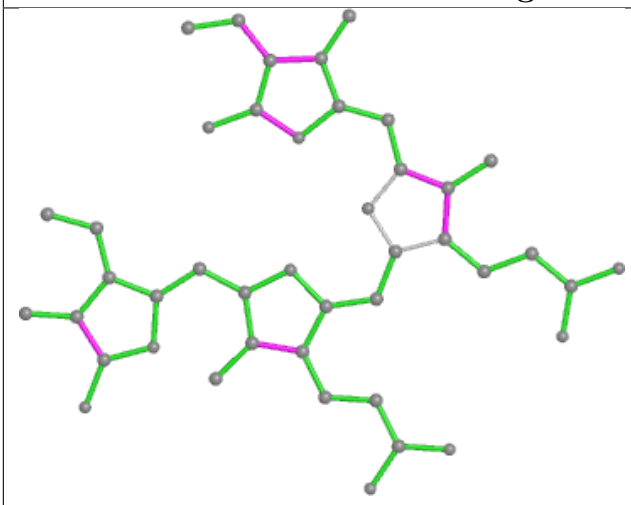


Rings

Ligand PEB hL 202



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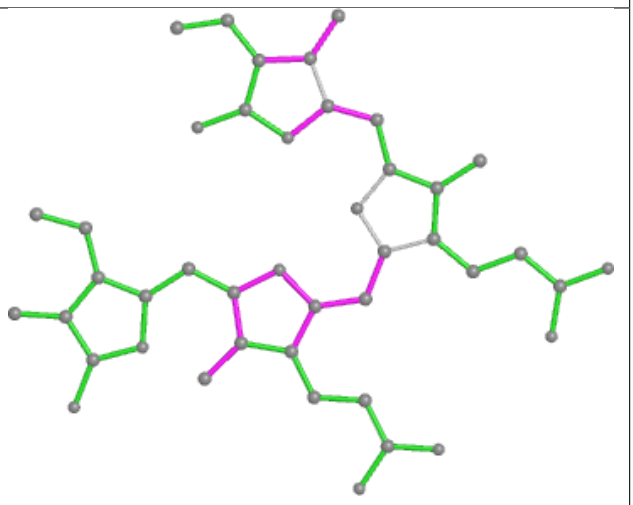

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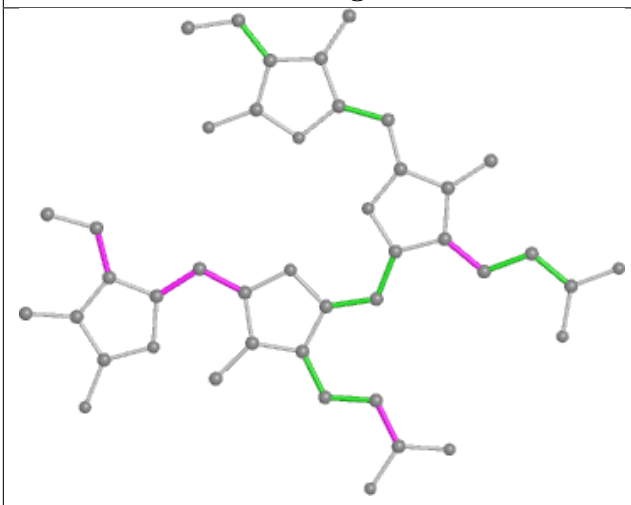

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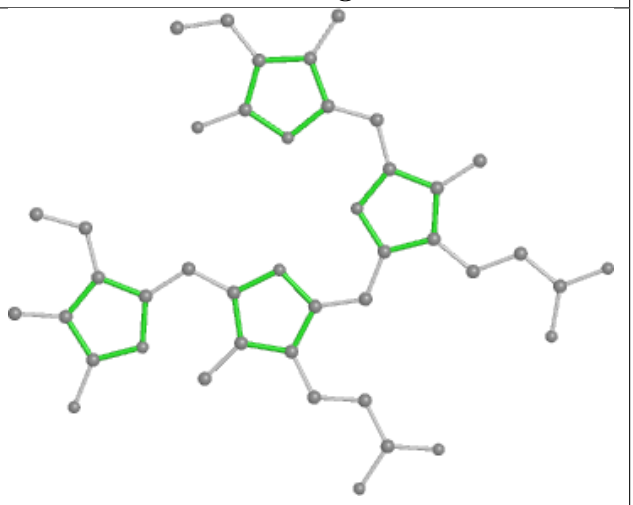
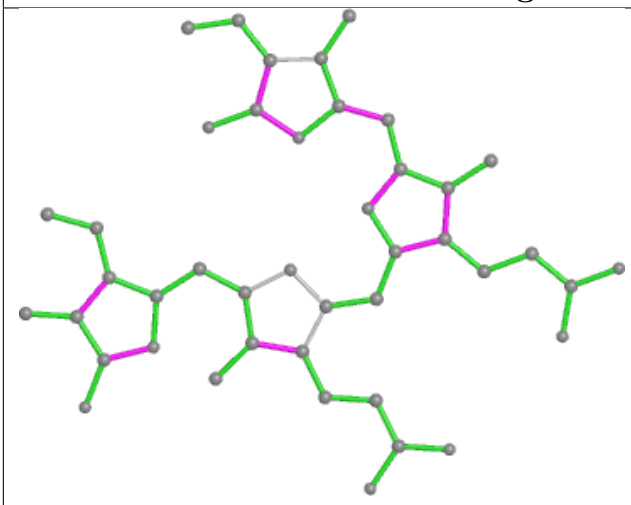


Rings

Ligand PUB n5 203



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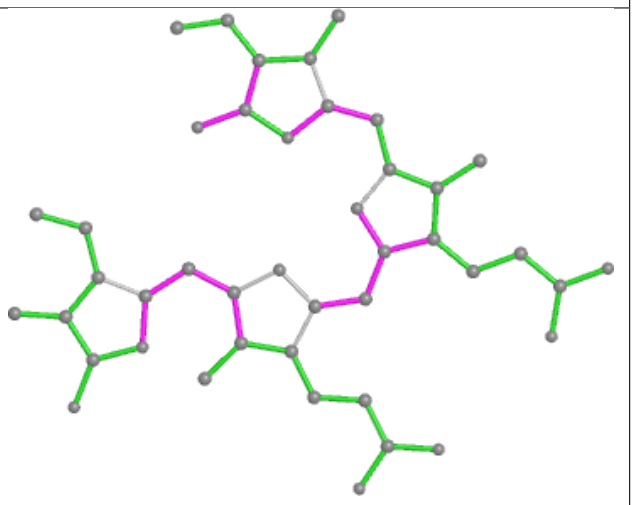

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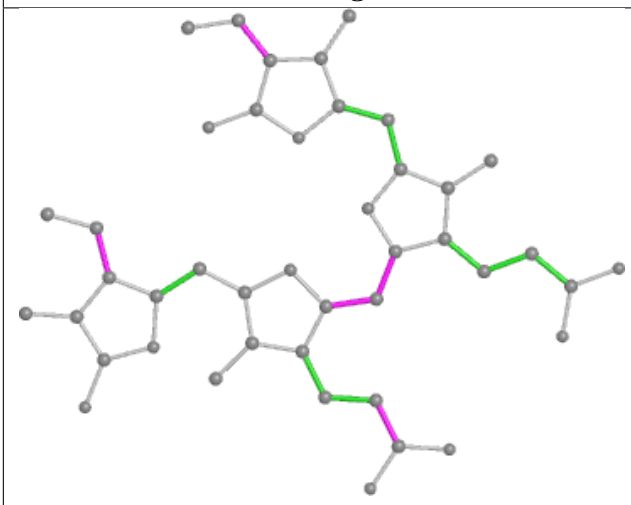

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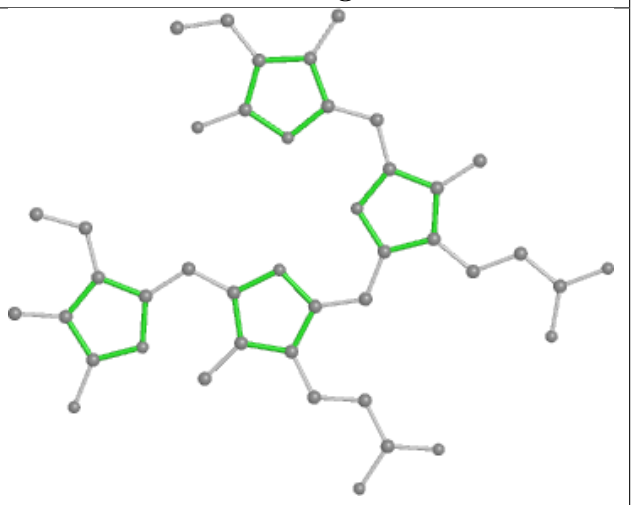
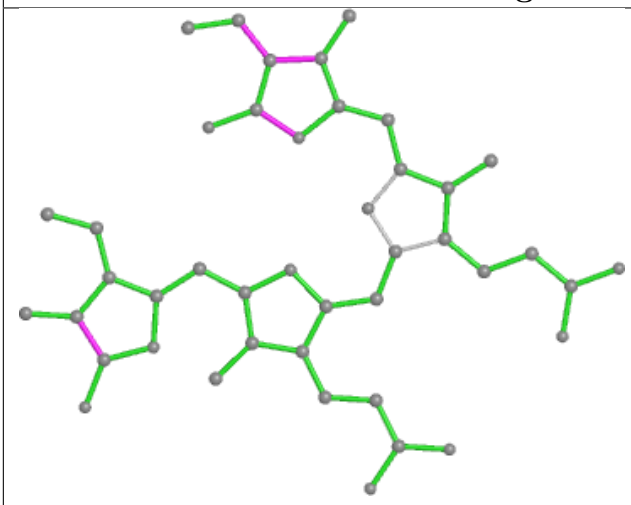


Rings

Ligand PEB w9 202



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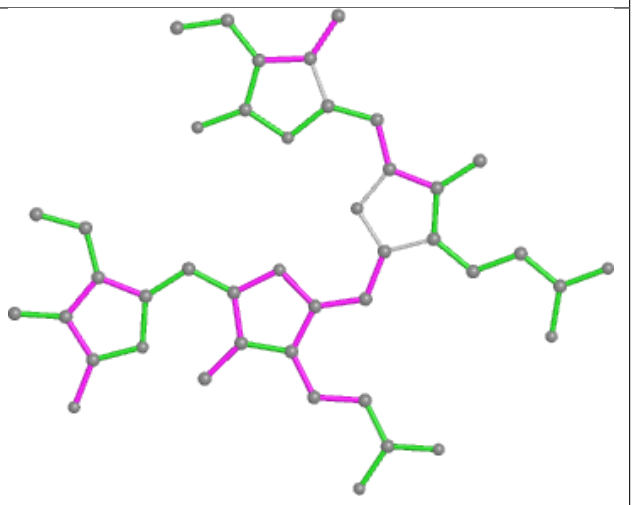

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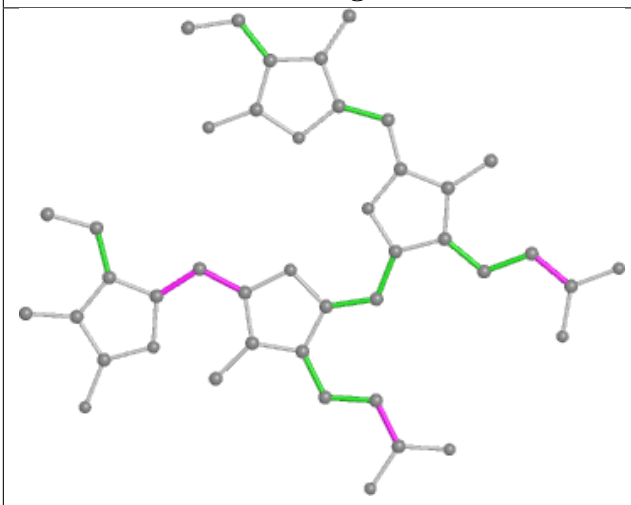

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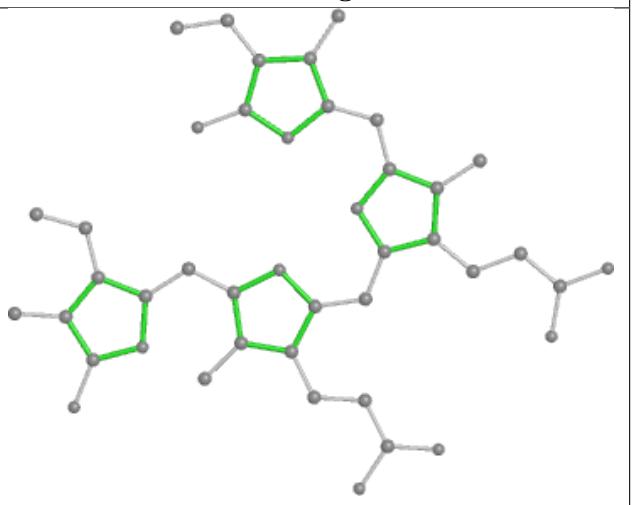
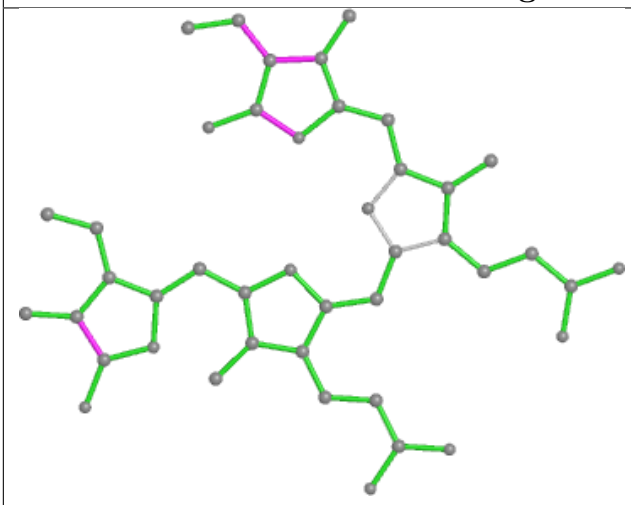


Rings

Ligand PEB h4 202



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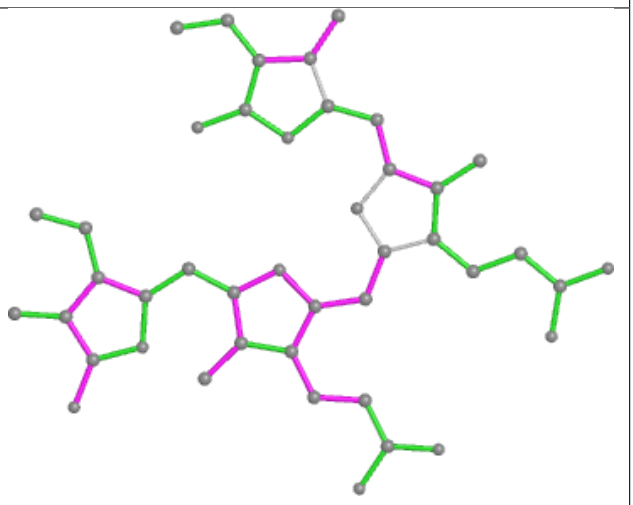

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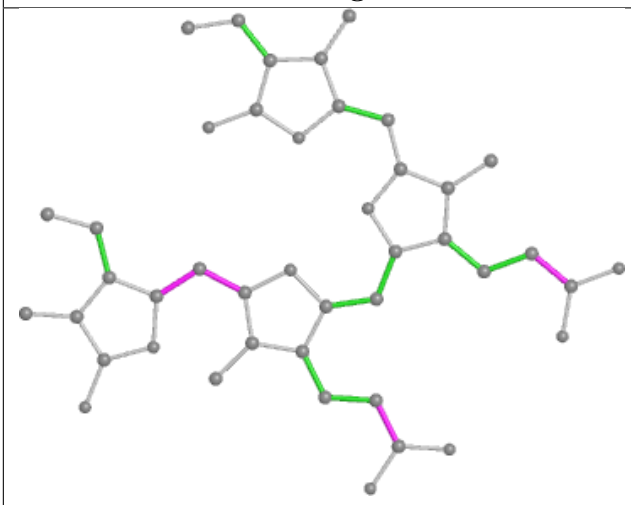

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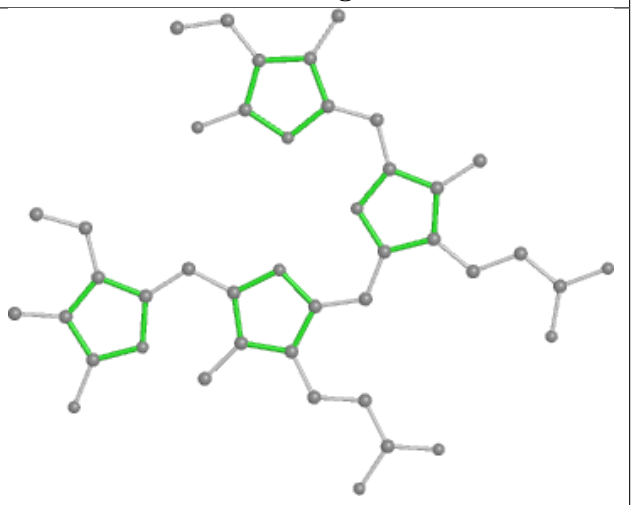
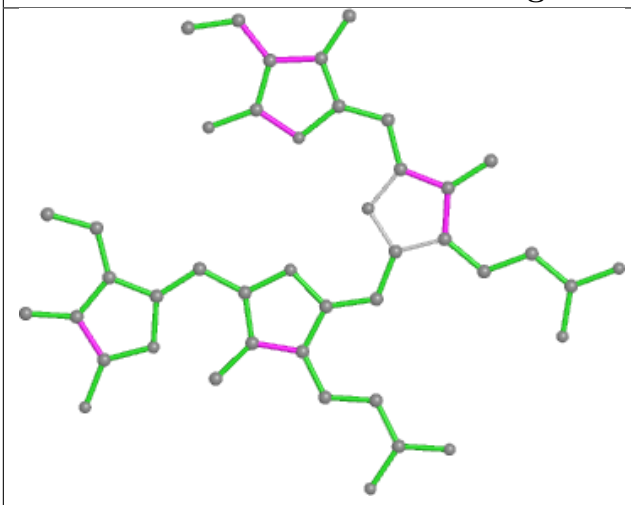


Rings

Ligand PEB lf 202



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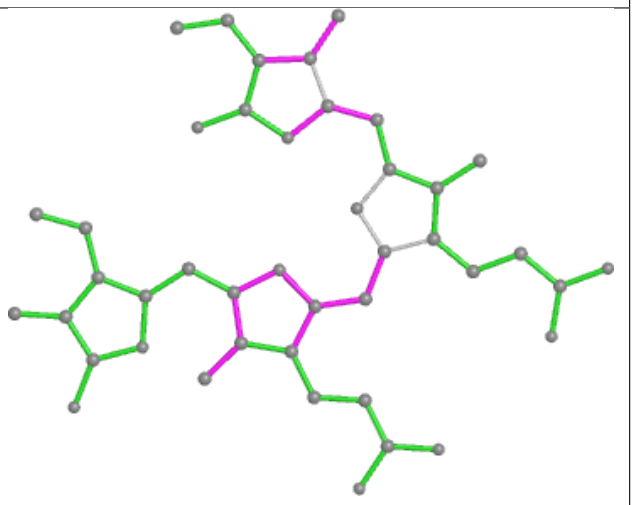

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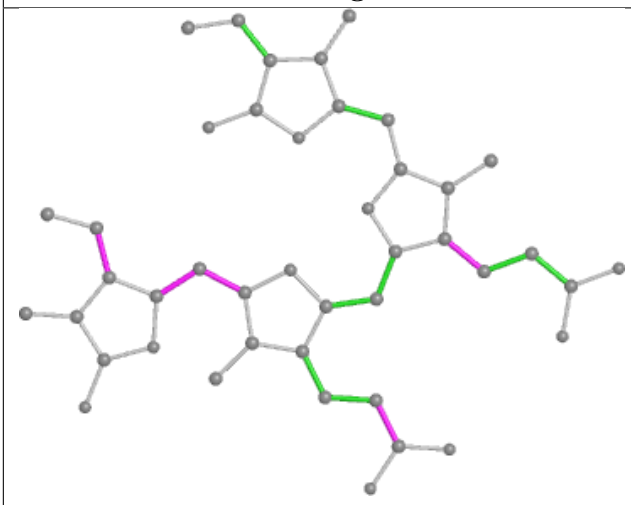

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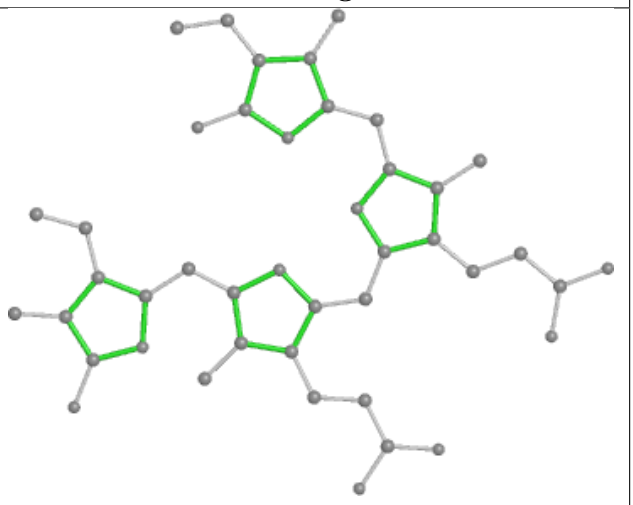
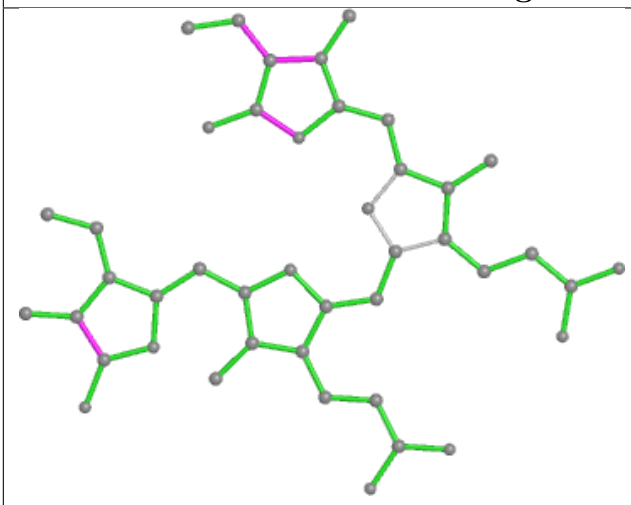


Rings

Ligand PEB D5 201



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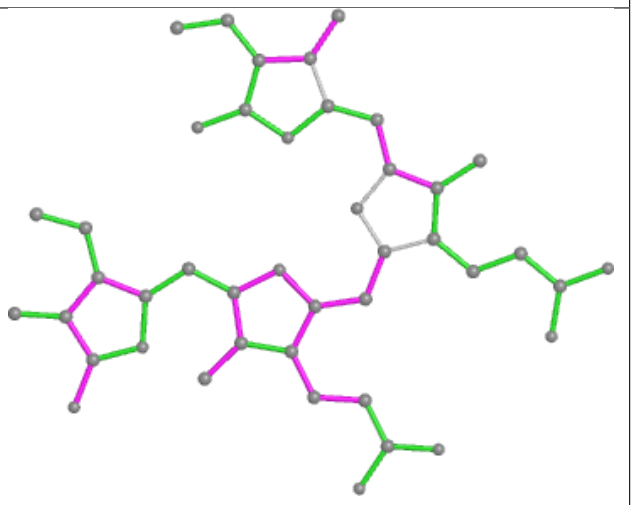

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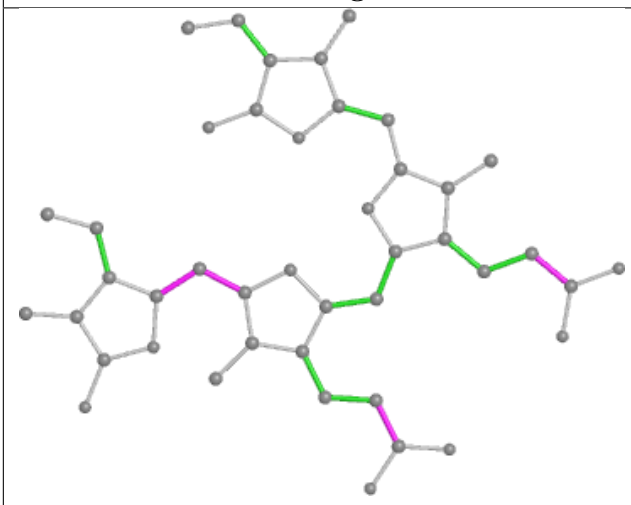

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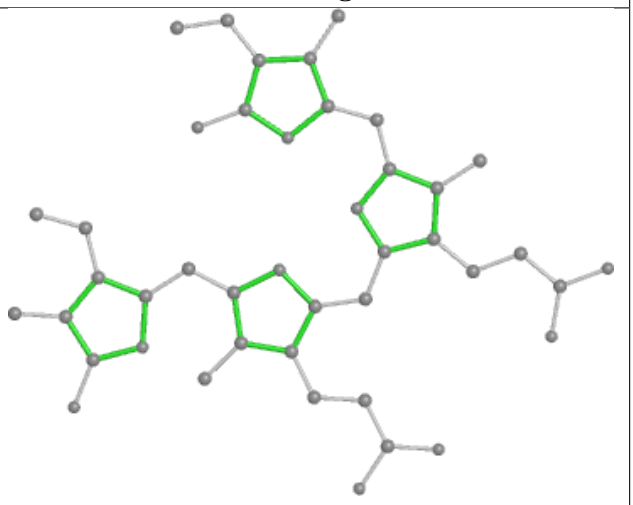
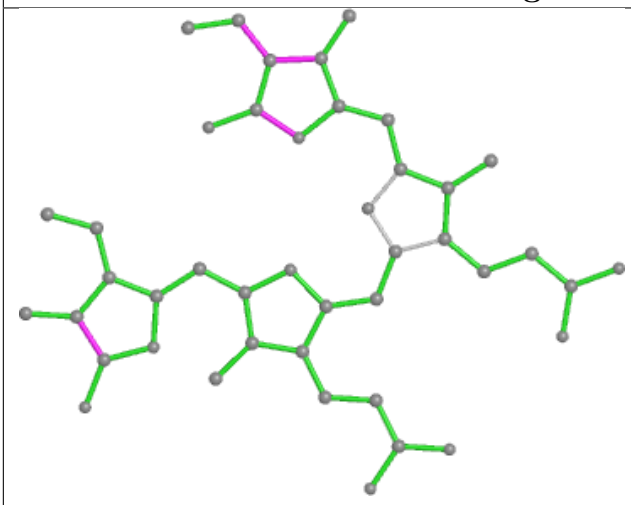


Rings

Ligand PEB j4 201



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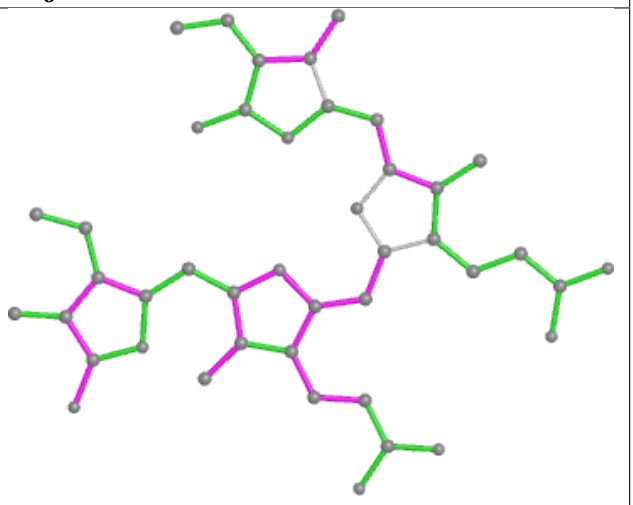

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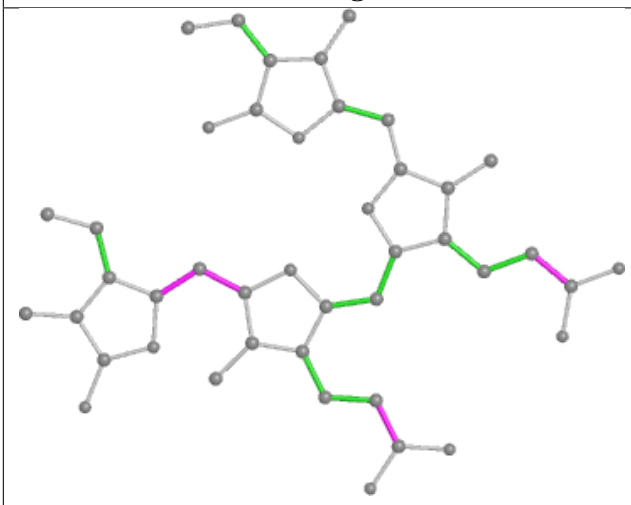
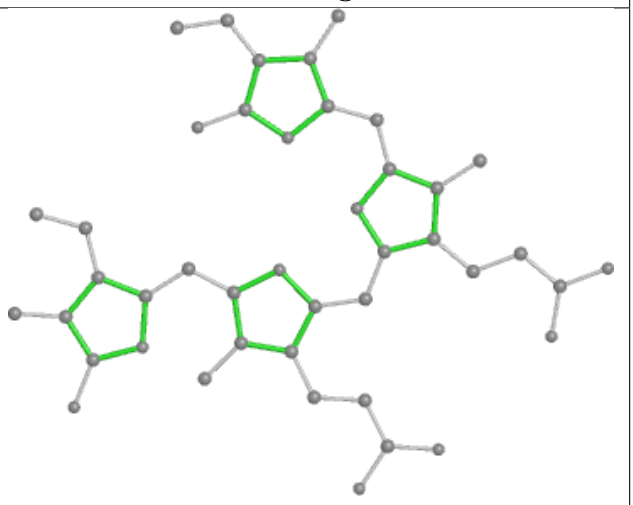
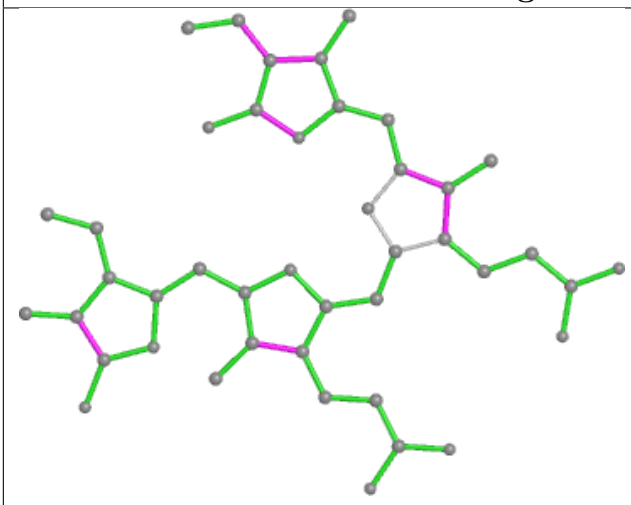


Torsions



Rings

Ligand PEB fm 202



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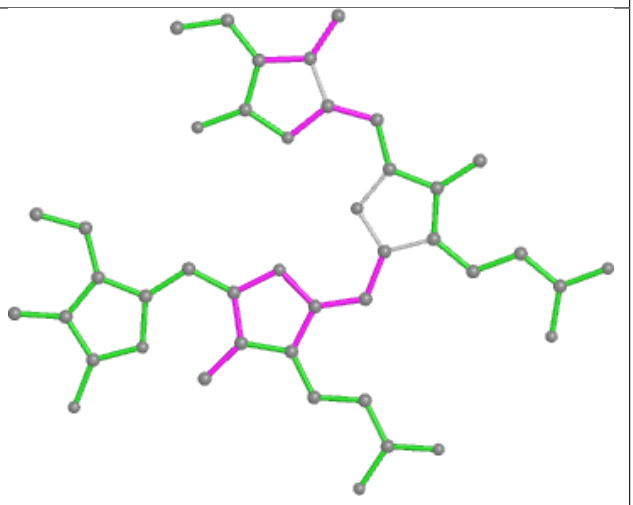

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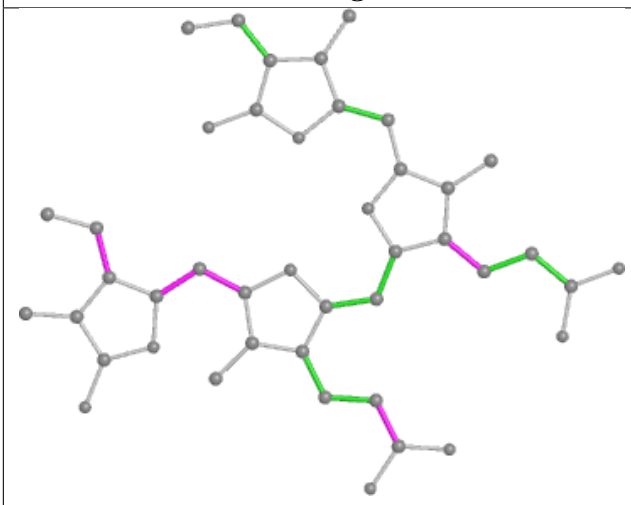

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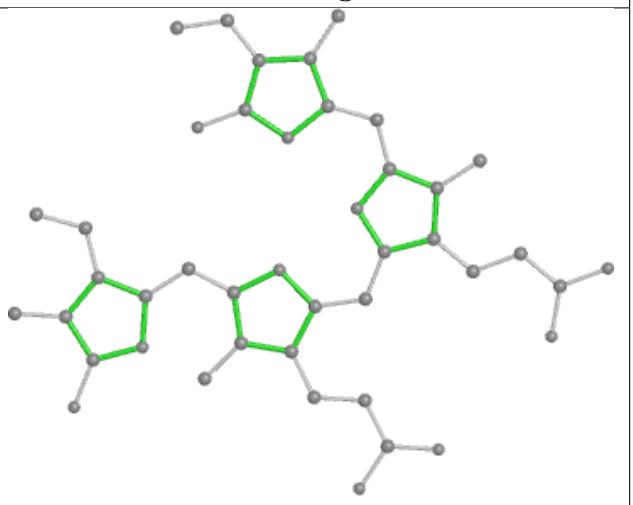
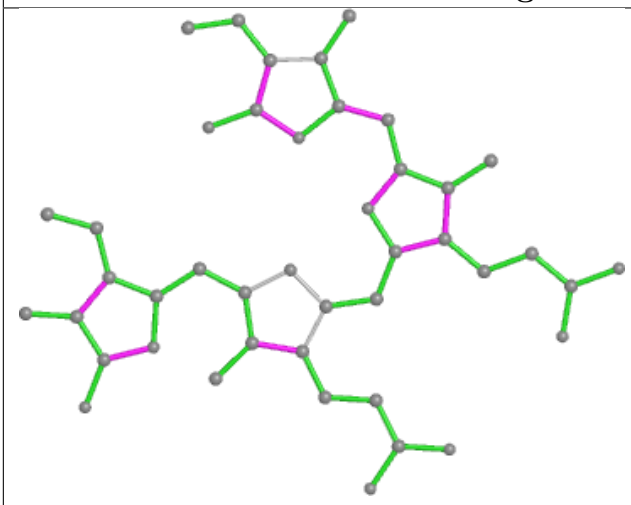


Rings

Ligand PUB eZ 404



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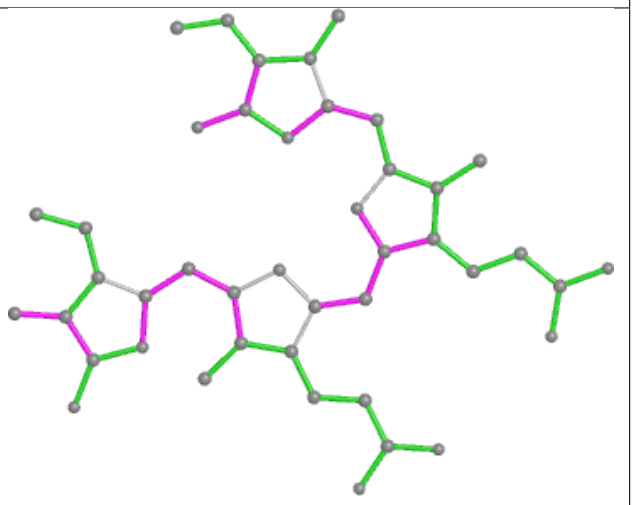

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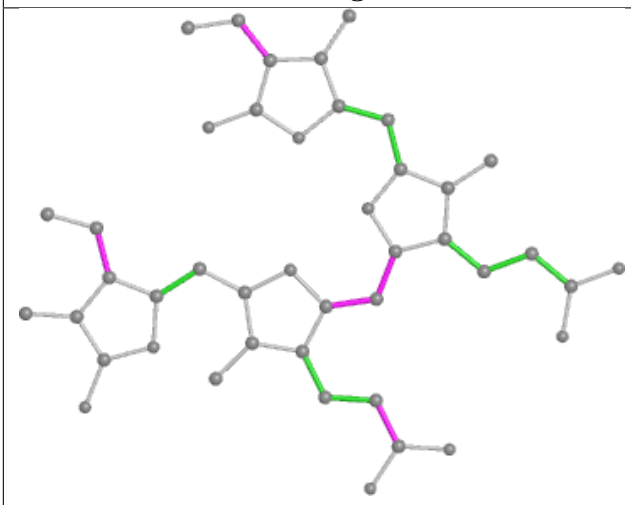

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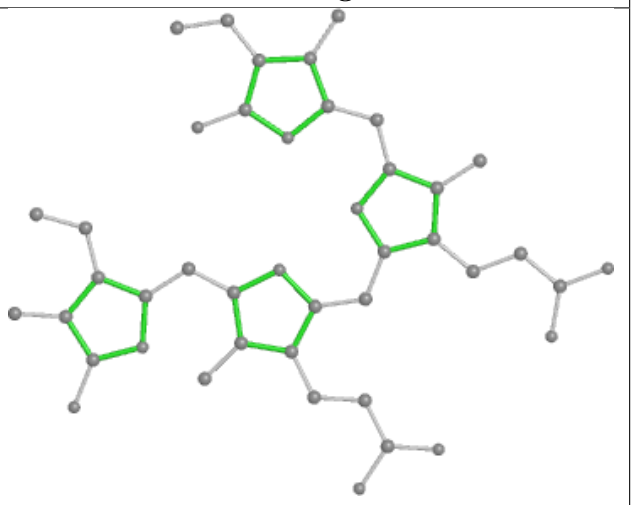
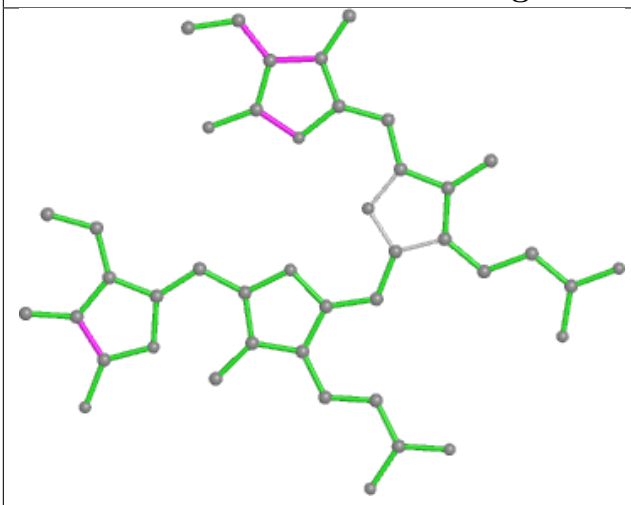


Rings

Ligand PEB e3 1001



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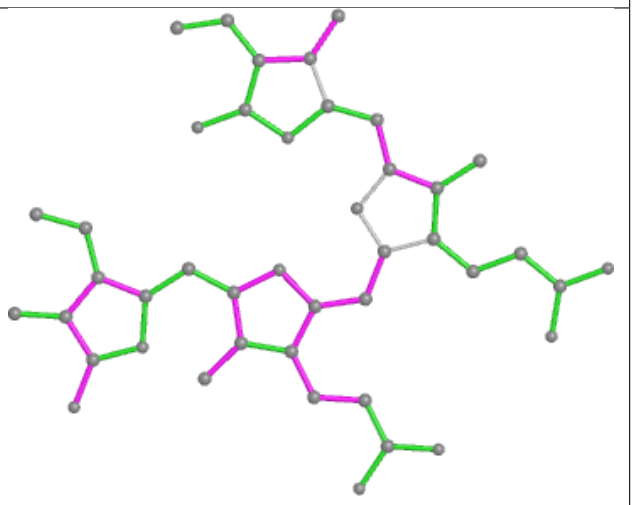

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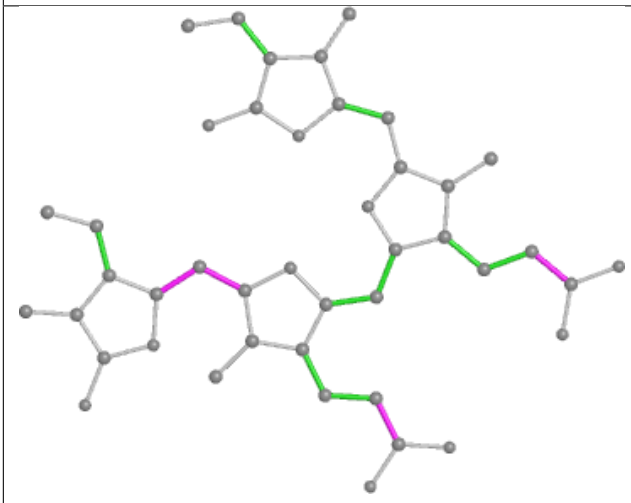

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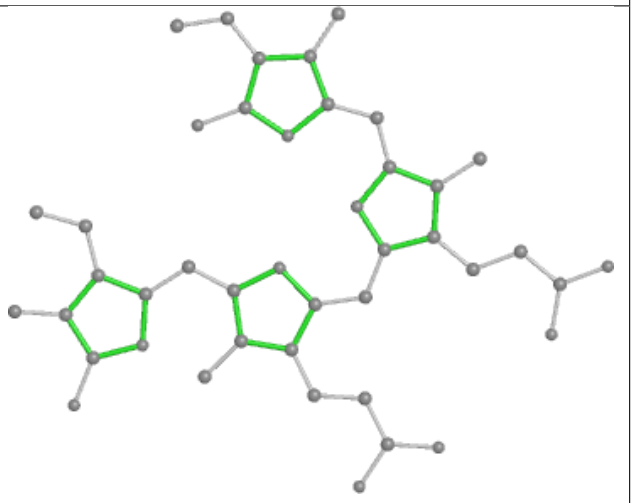
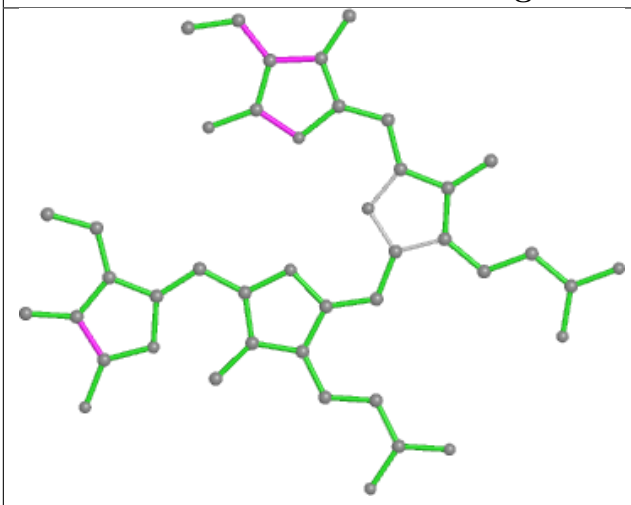


Rings

Ligand PEB G8 202



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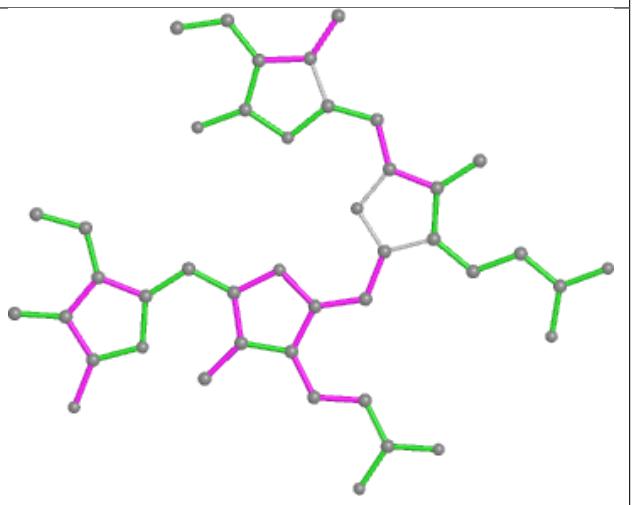

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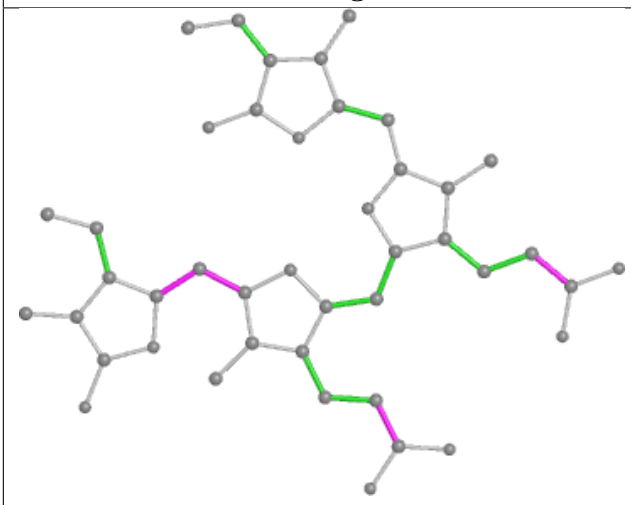

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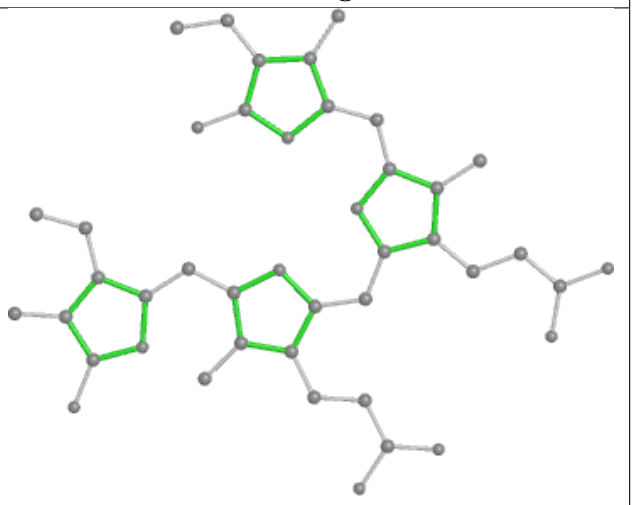

Rings

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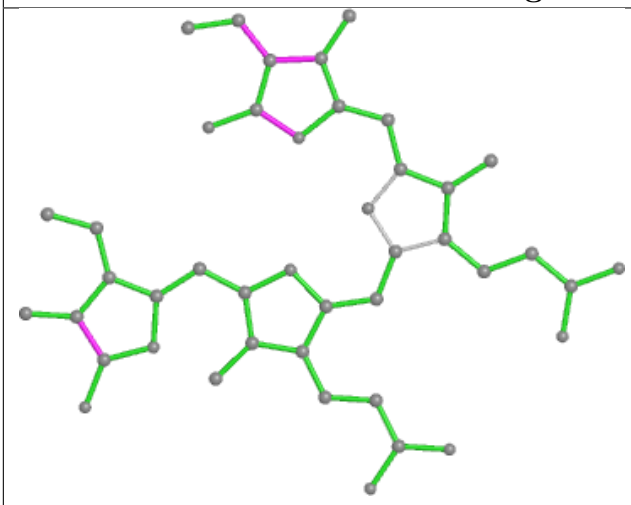

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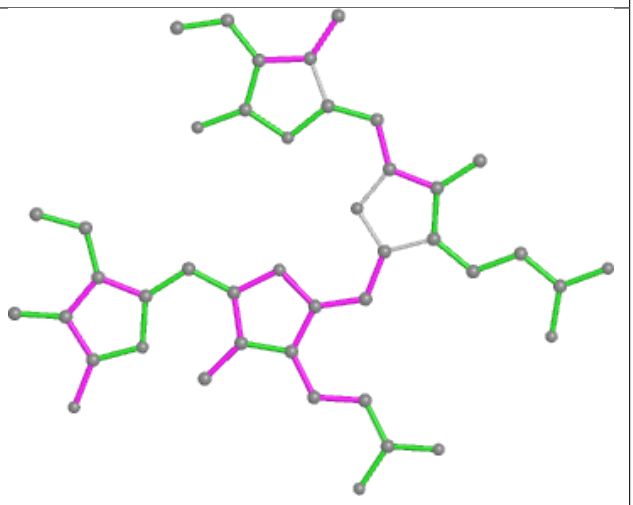

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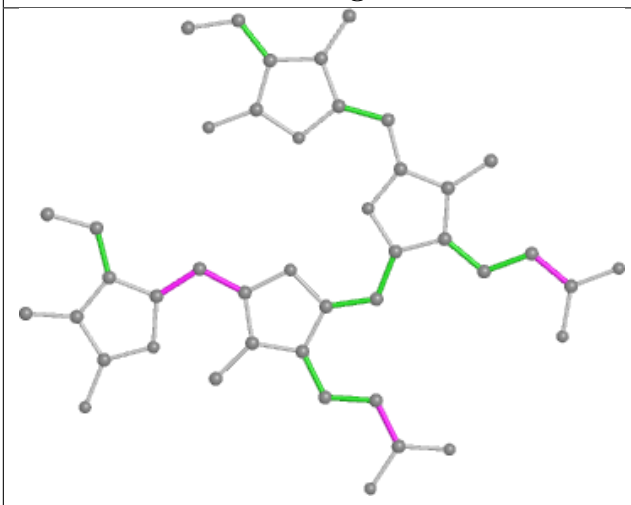

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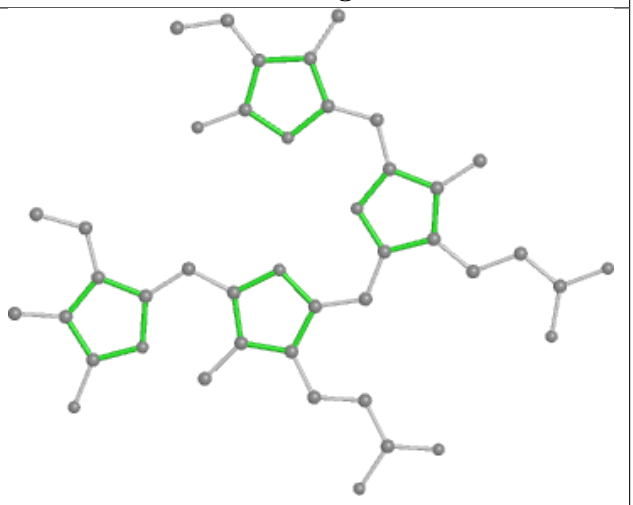

Rings

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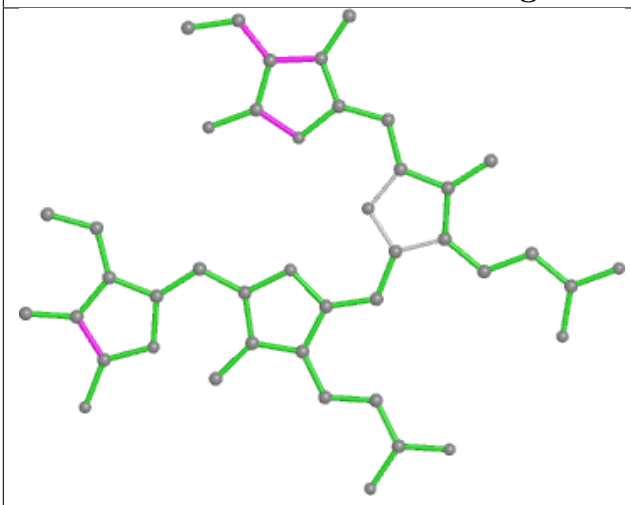

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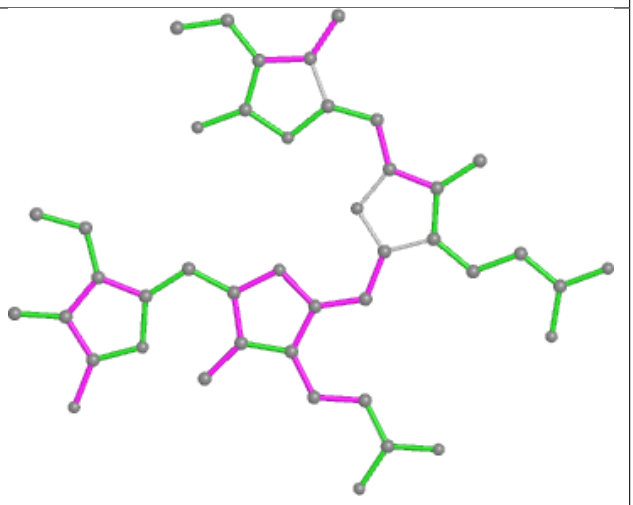

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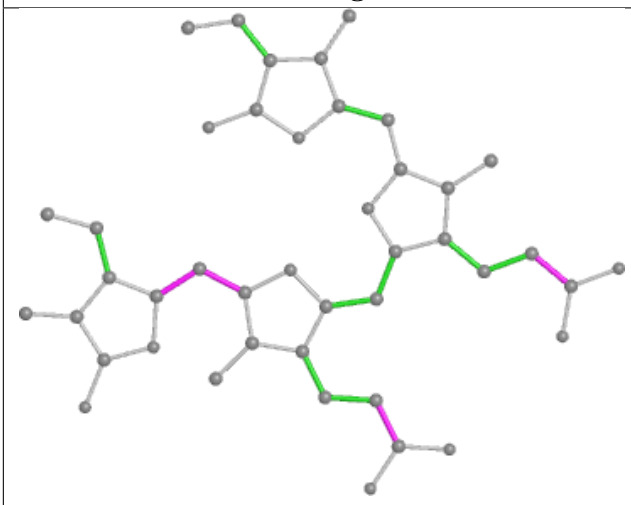

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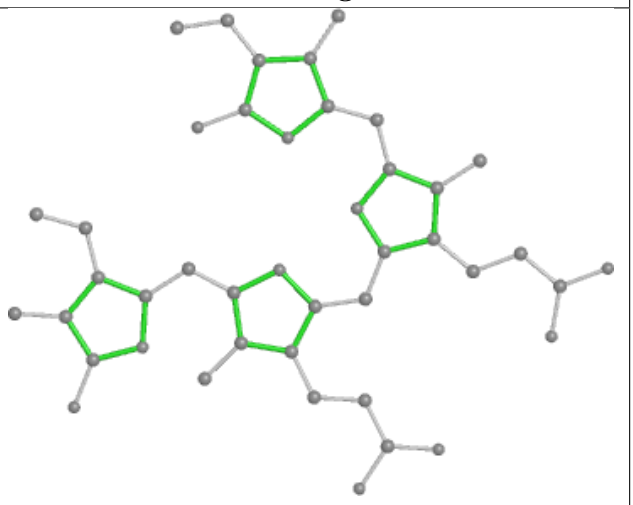

Rings

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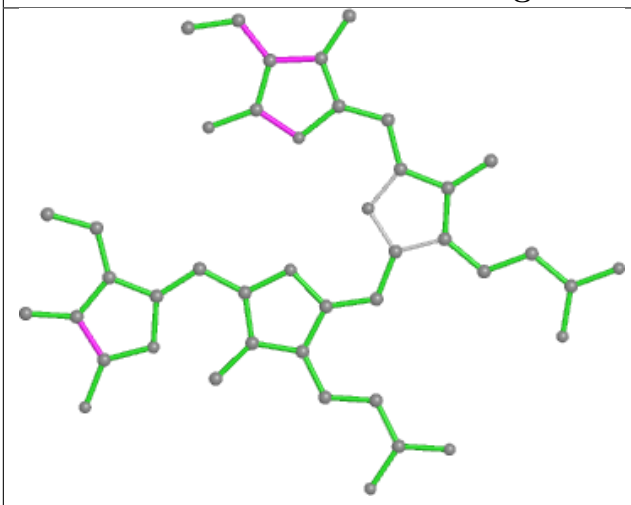

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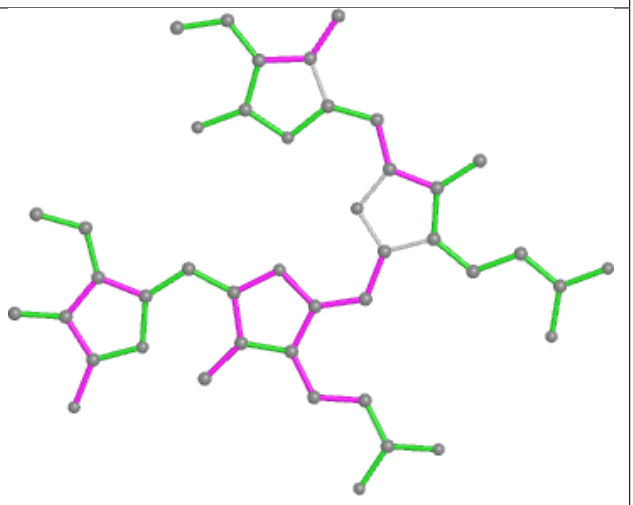

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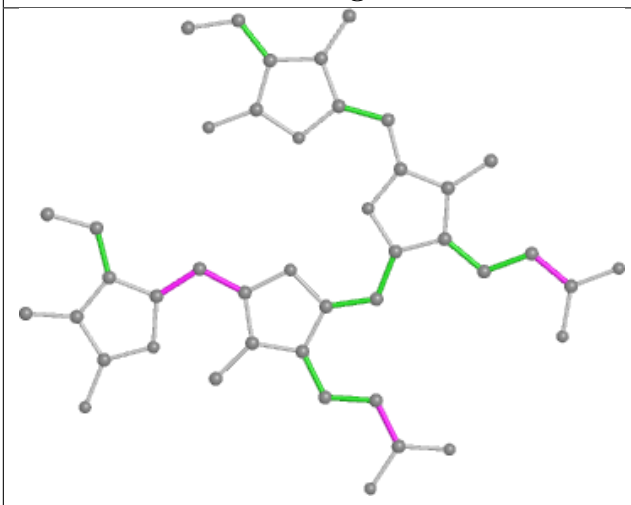

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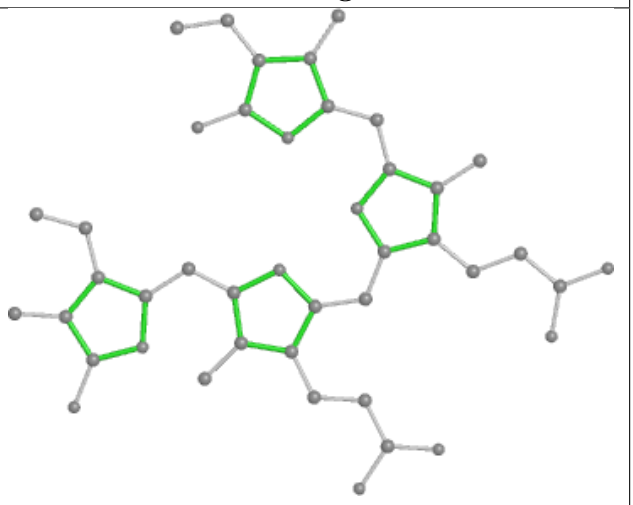

Rings

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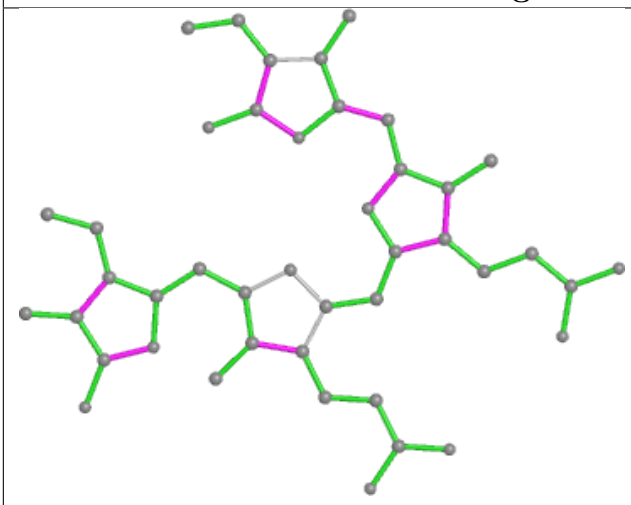

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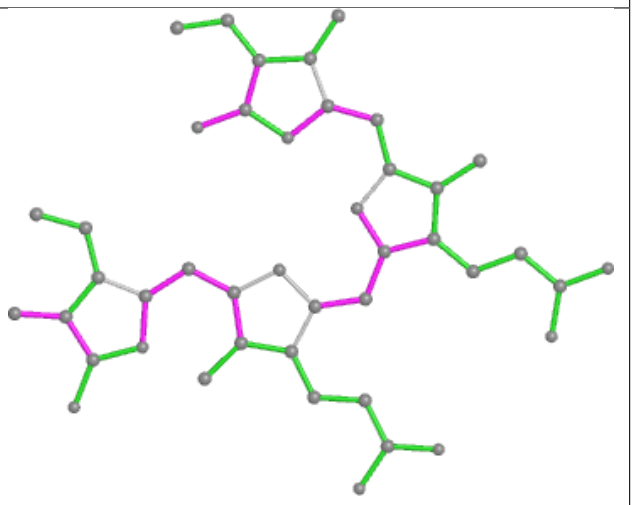

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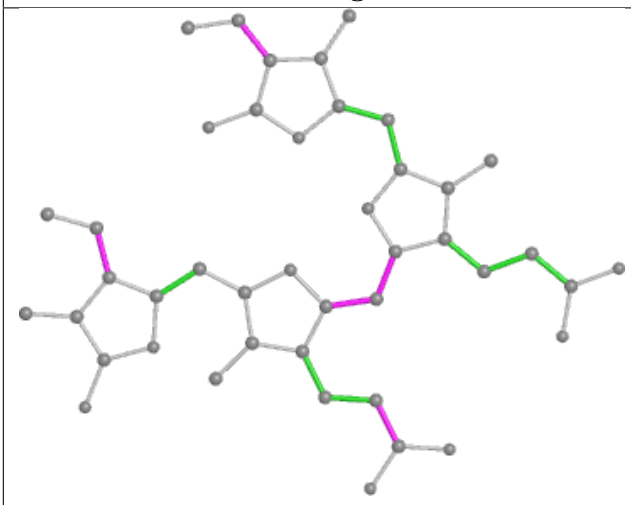

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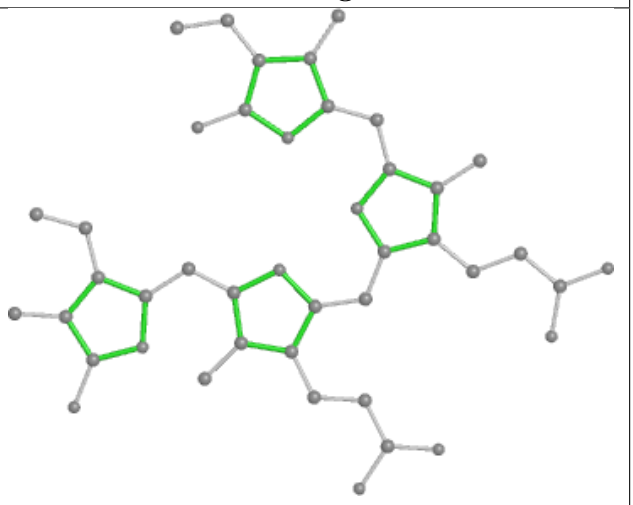

Rings

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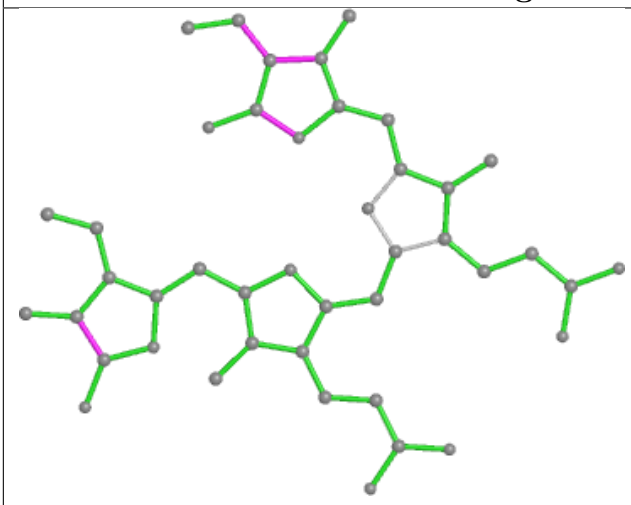

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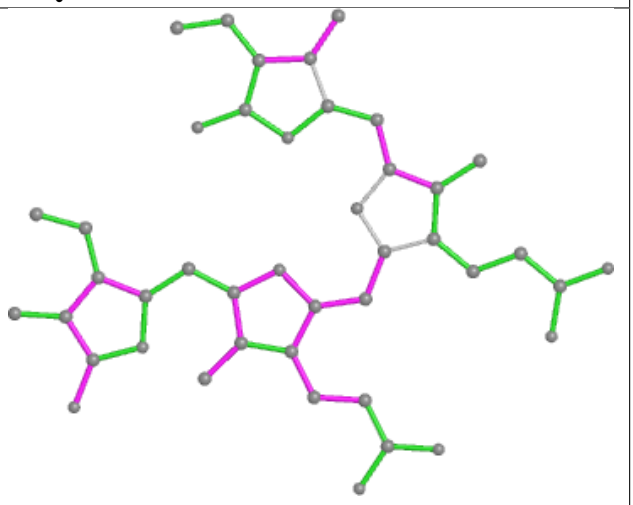

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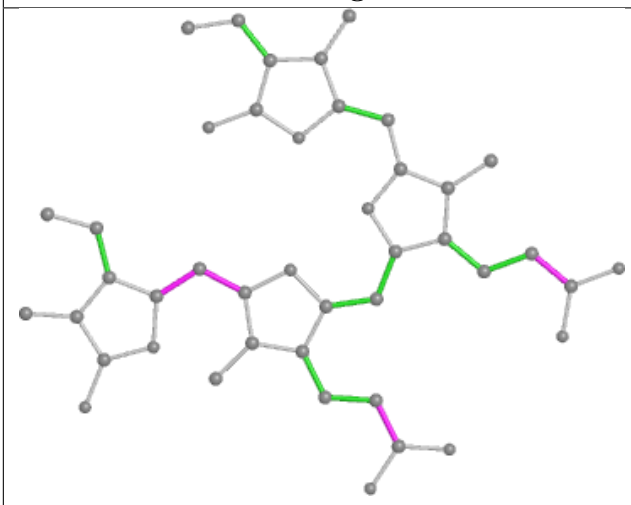

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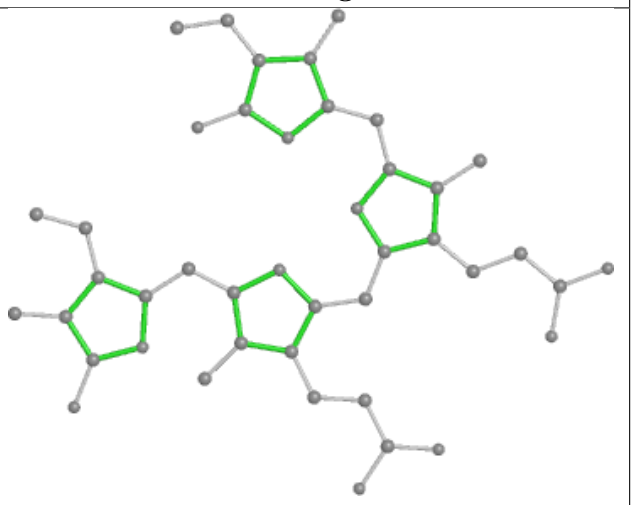
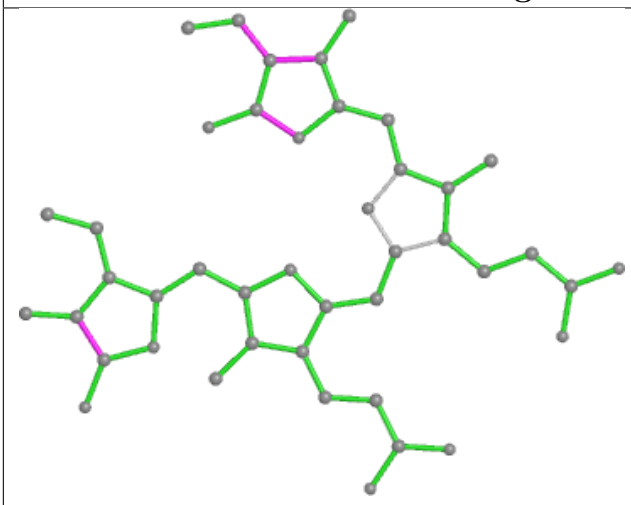


Rings

Ligand PEB hA 201



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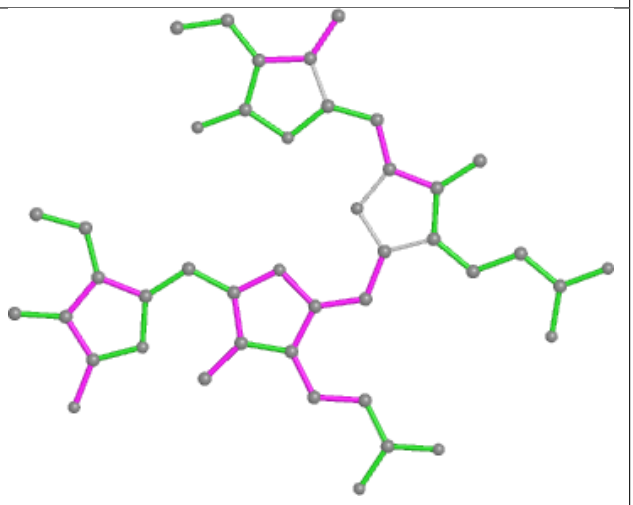

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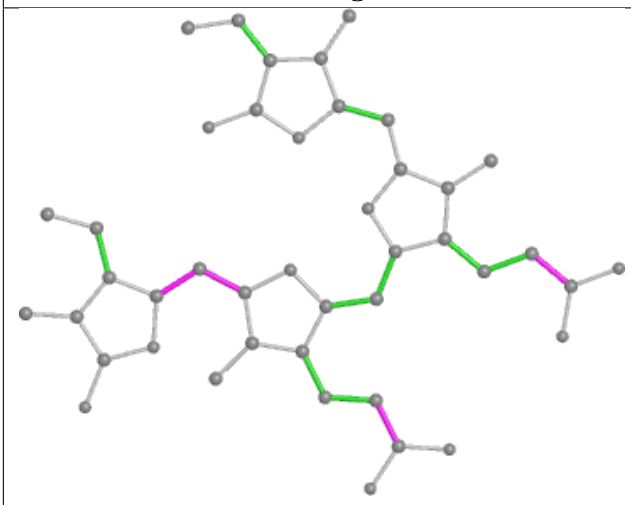

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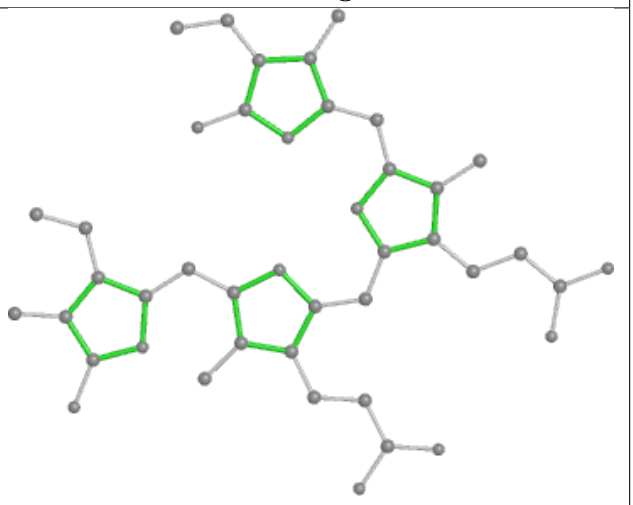

Rings

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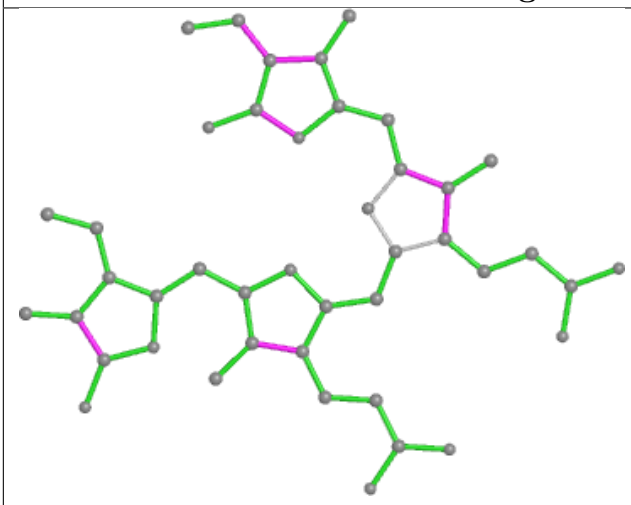

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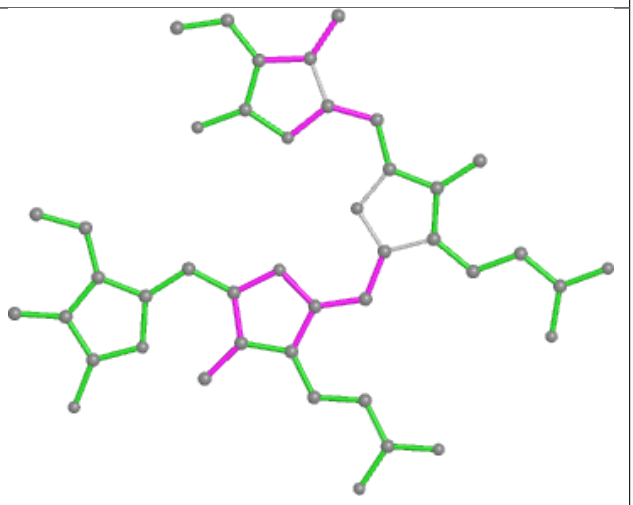

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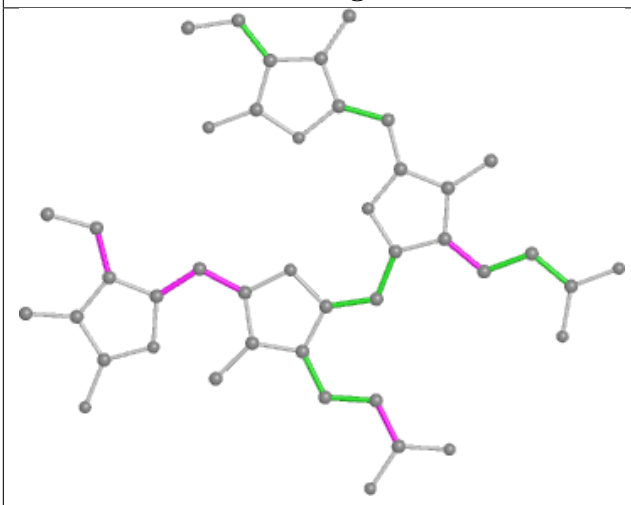

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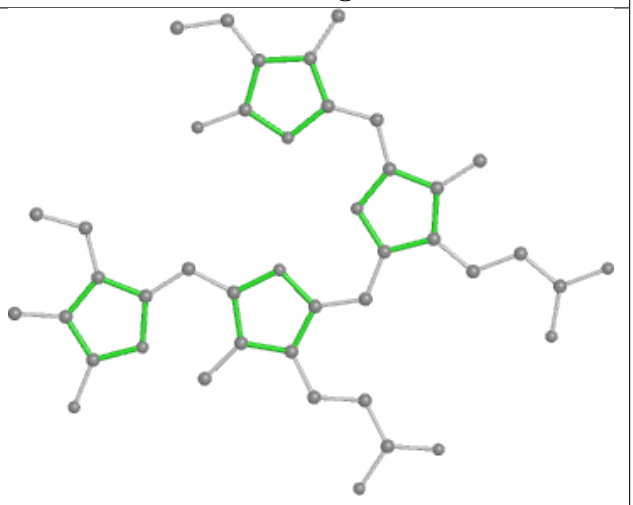

Rings

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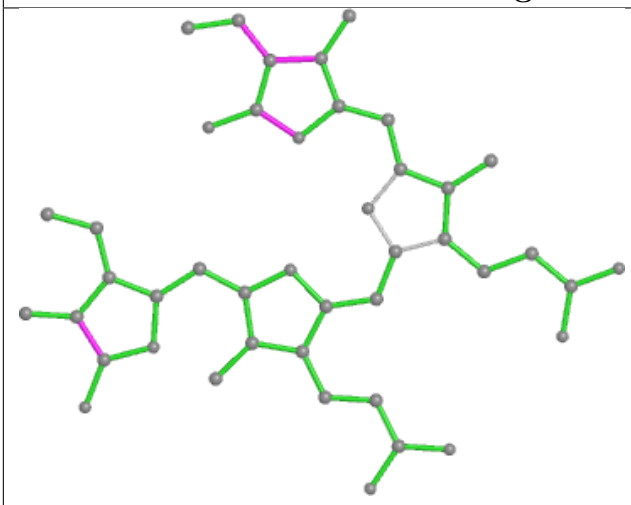

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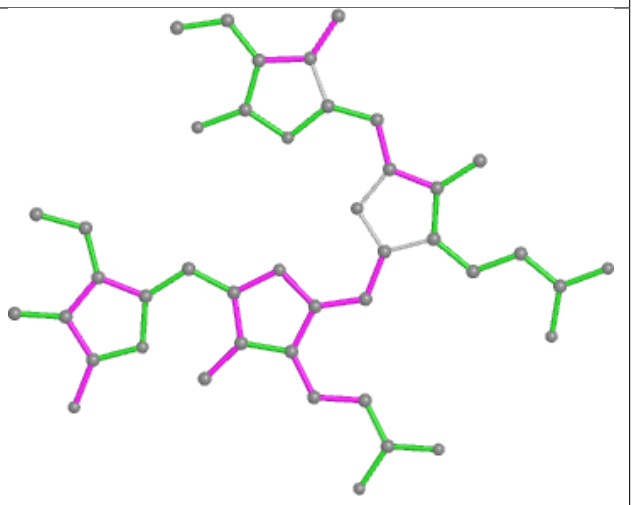

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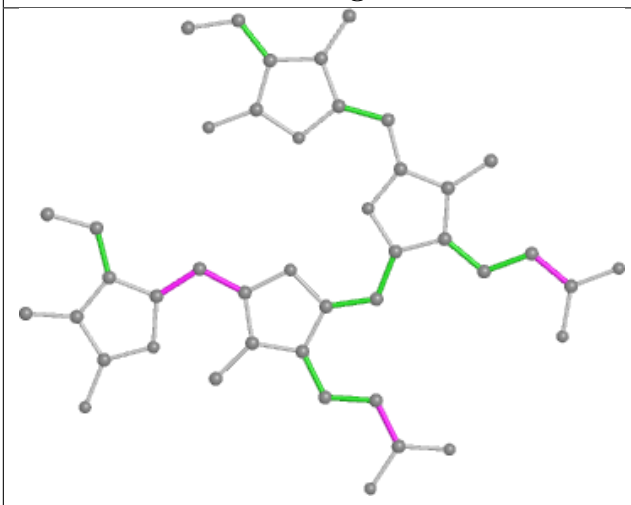

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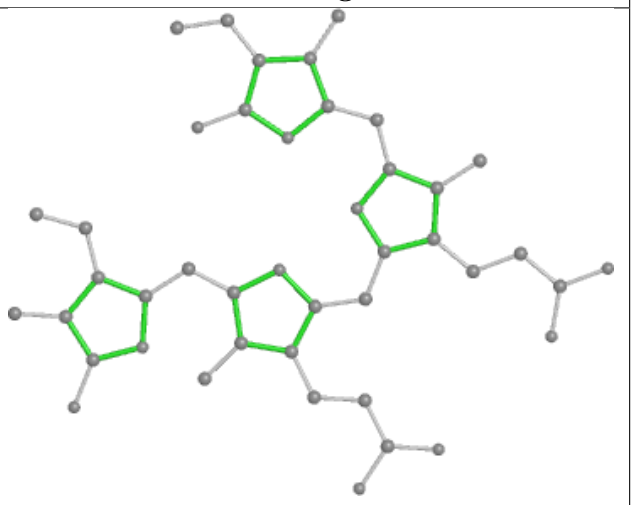
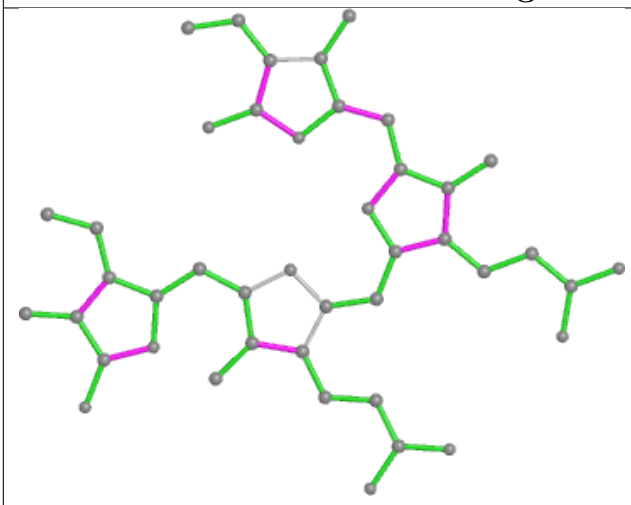


Rings

Ligand PUB x7 203



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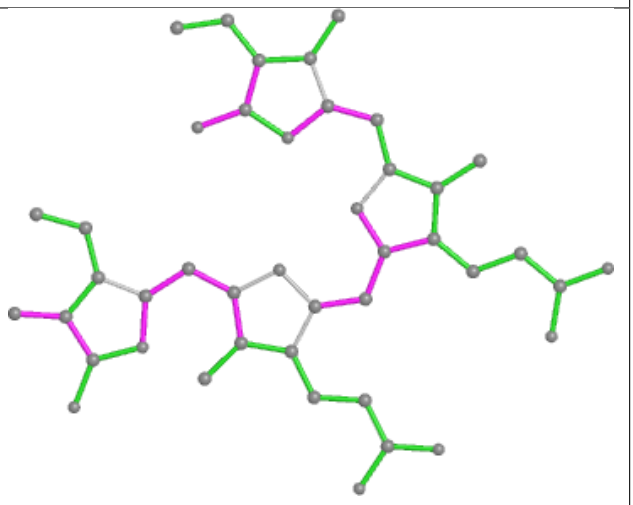

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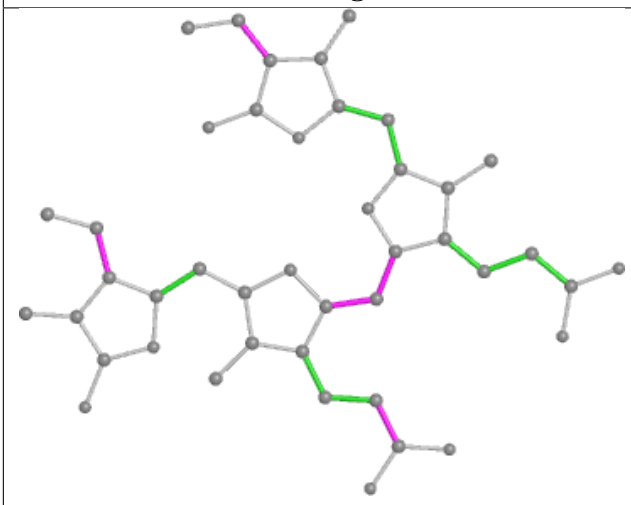

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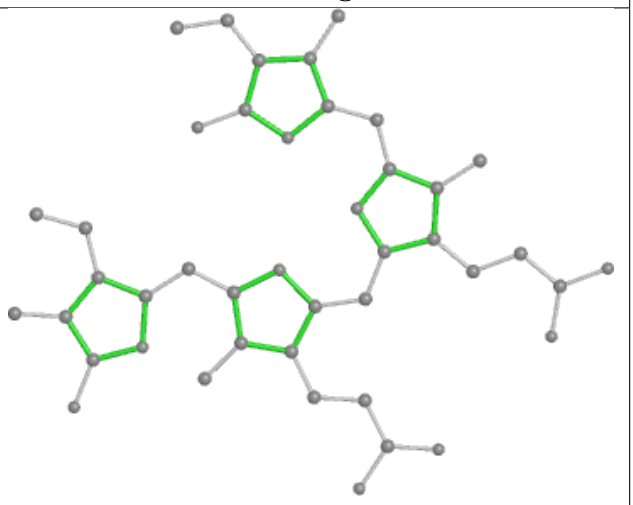
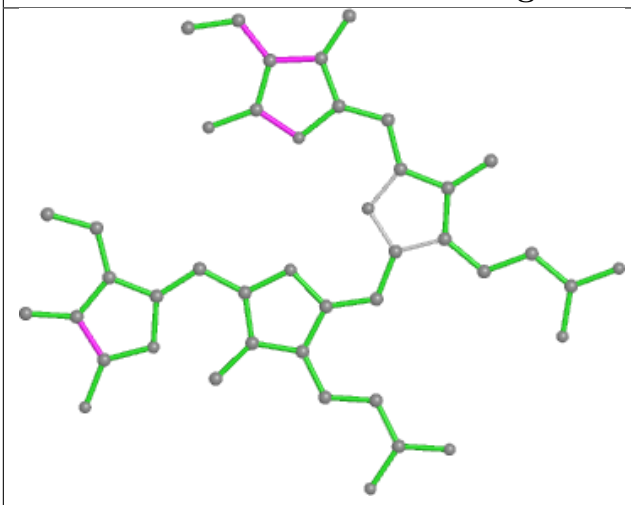


Rings

Ligand PEB eP 202



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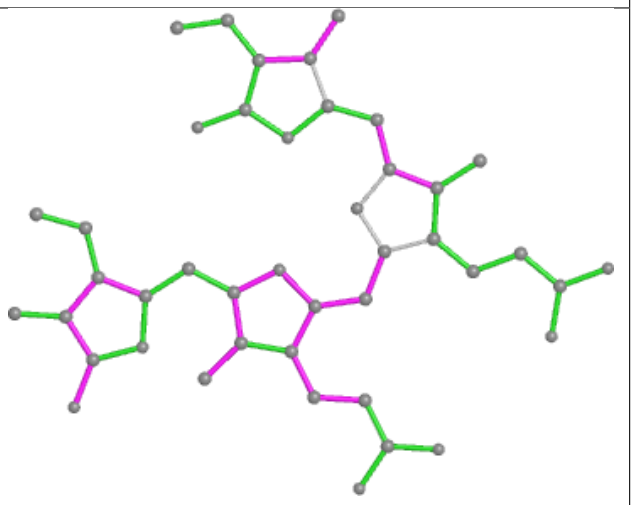
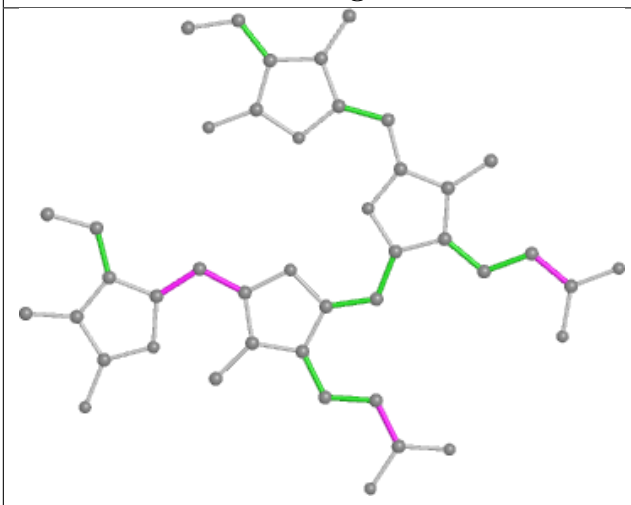
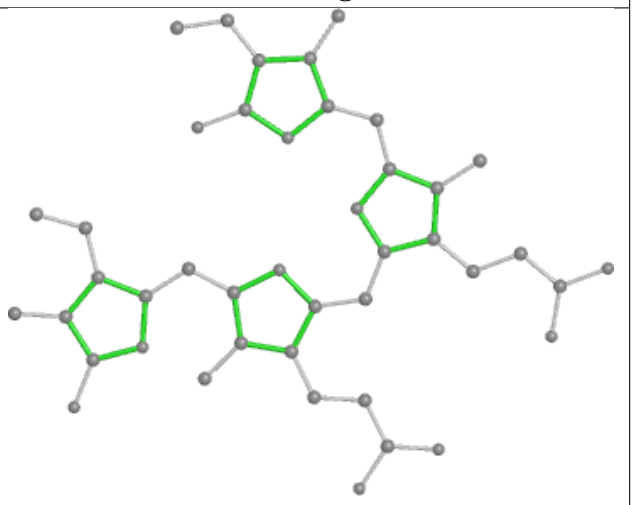


Bond angles

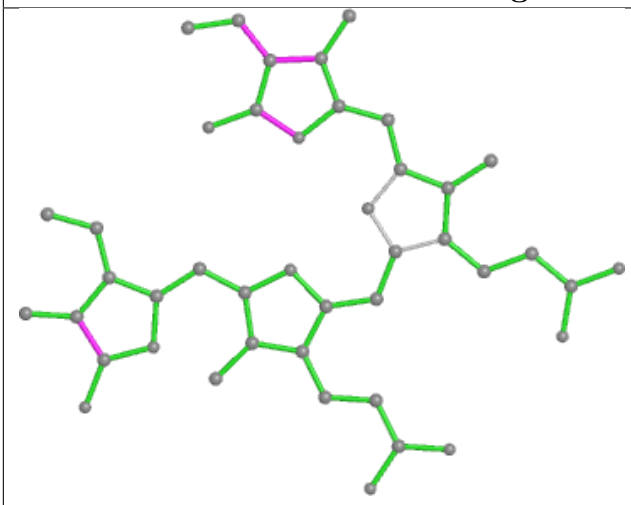


Torsions



Rings

Ligand PEB o2 1002



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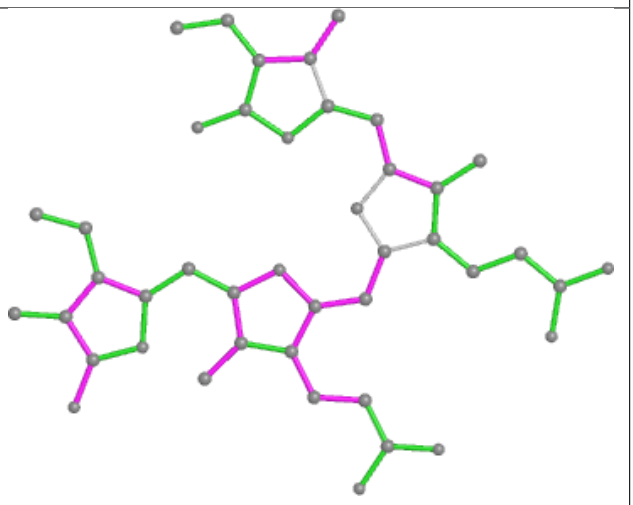

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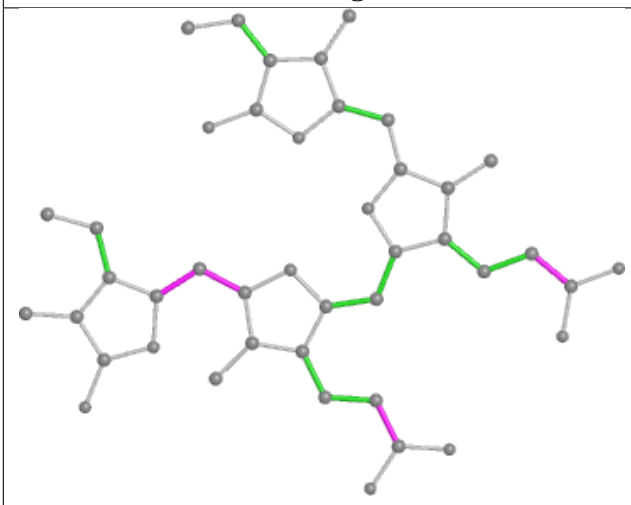

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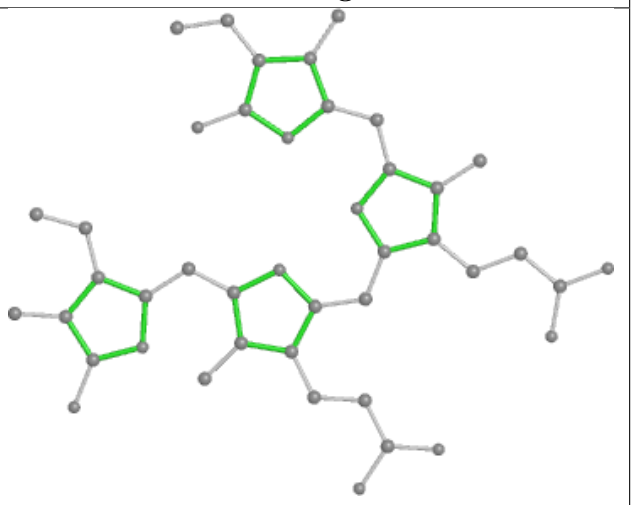
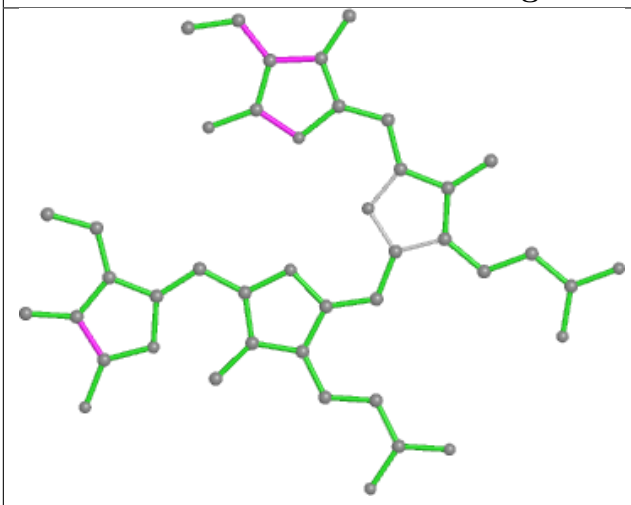


Rings

Ligand PEB r3 201



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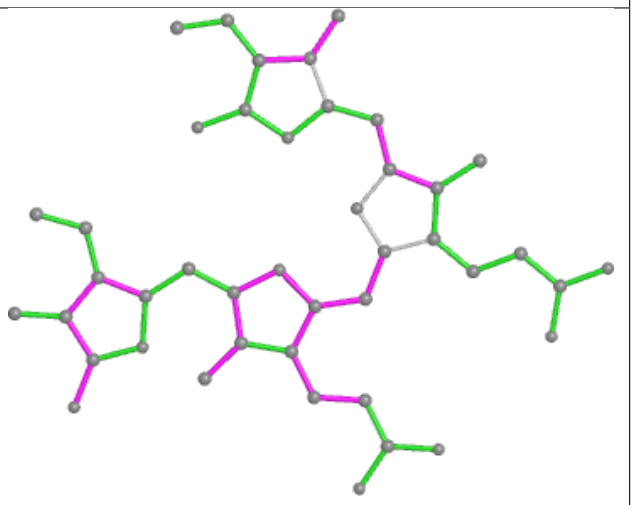

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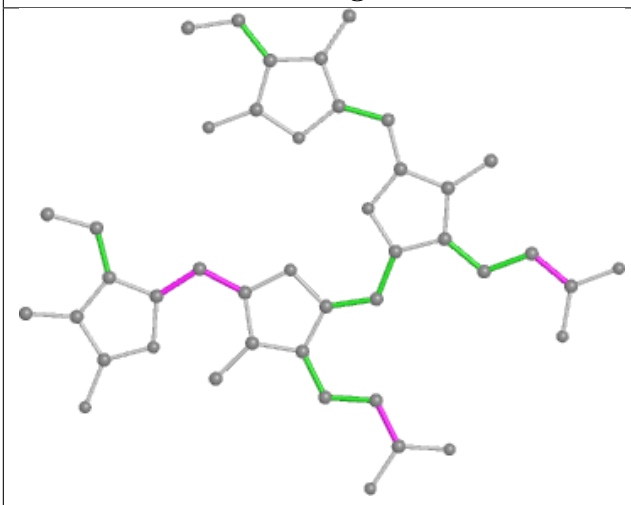

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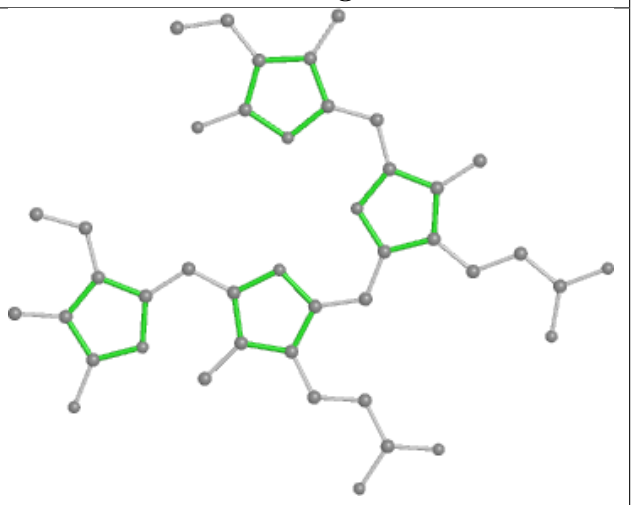
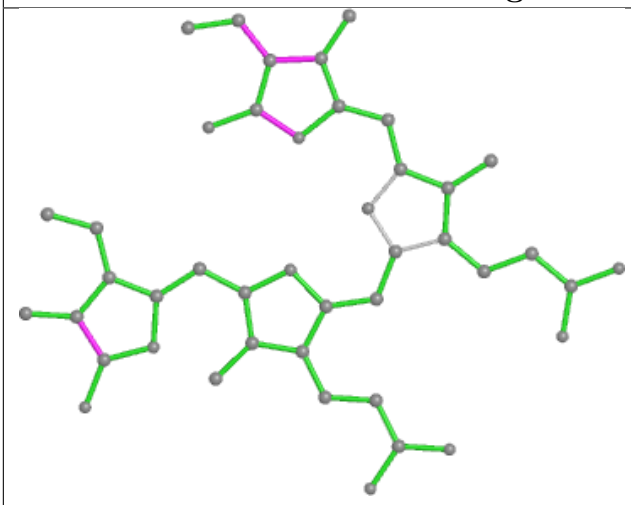


Rings

Ligand PEB U8 1003



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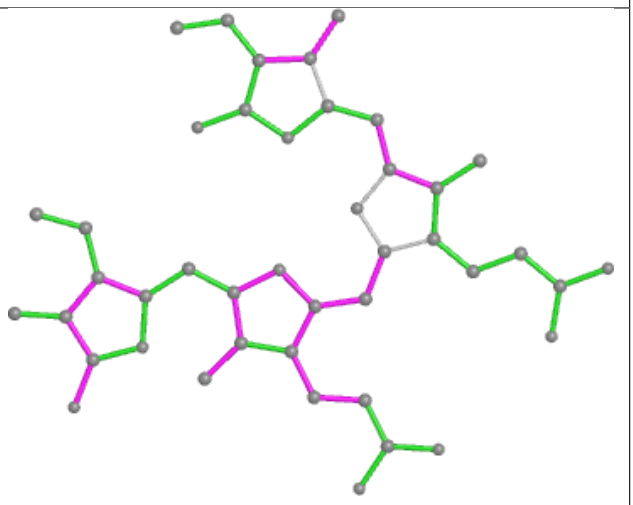

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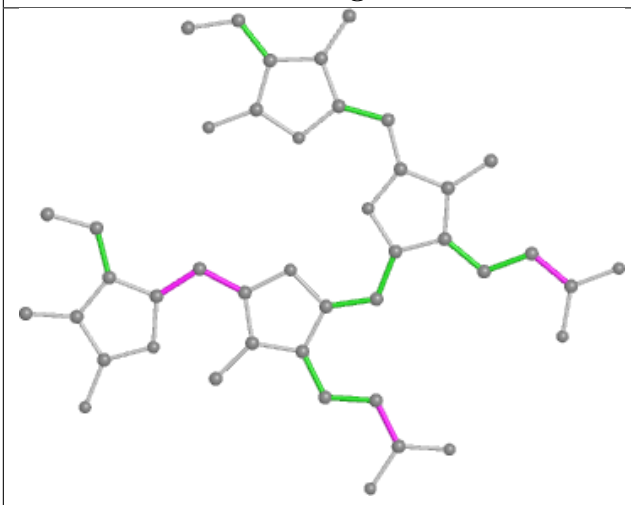

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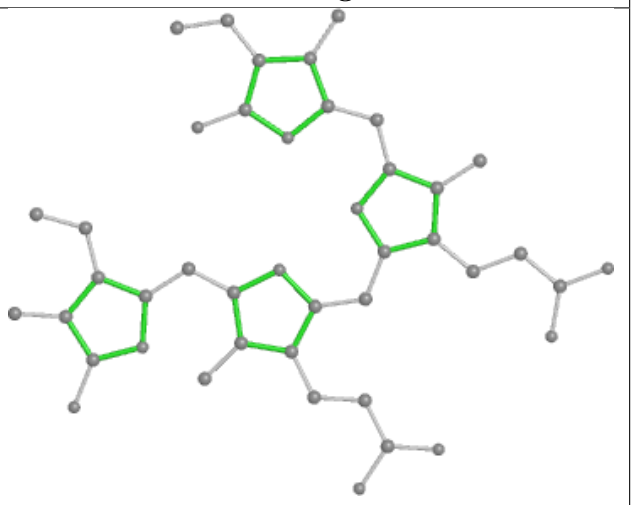

Rings

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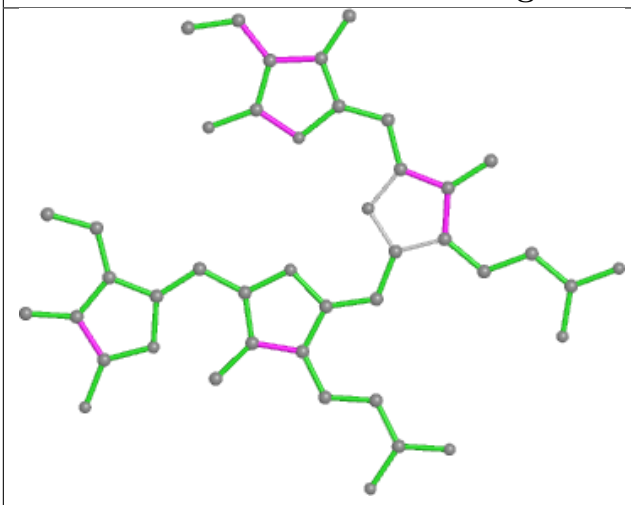

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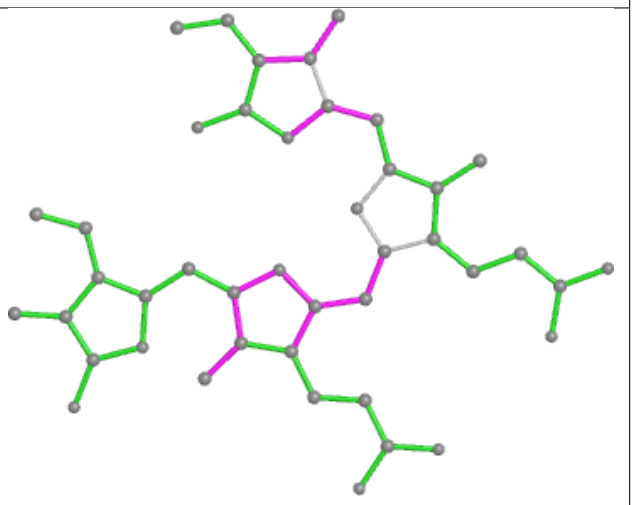

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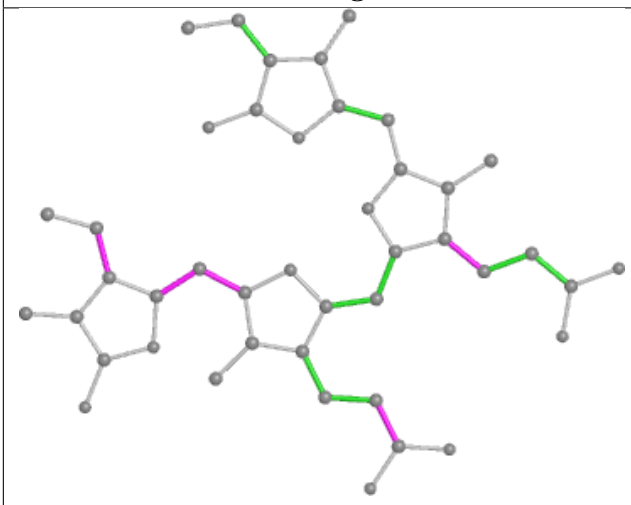

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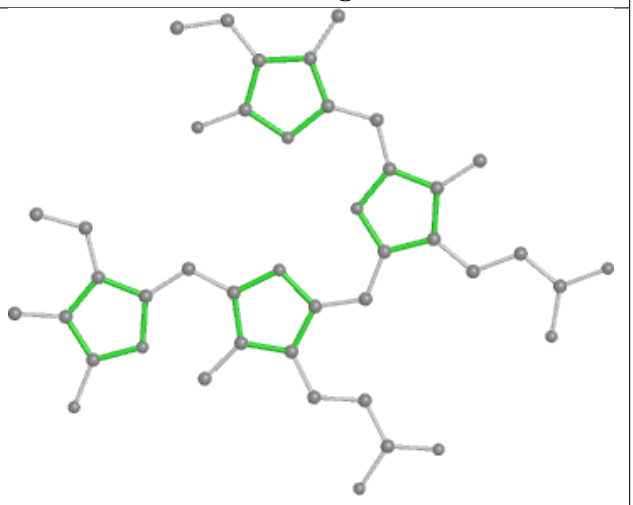
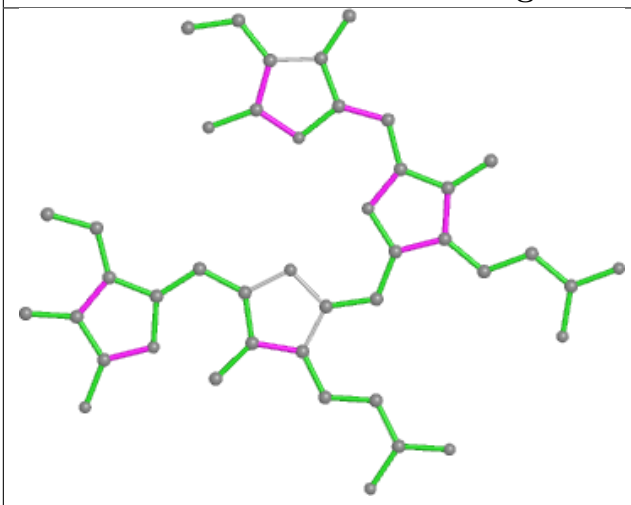


Rings

Ligand PUB h2 203



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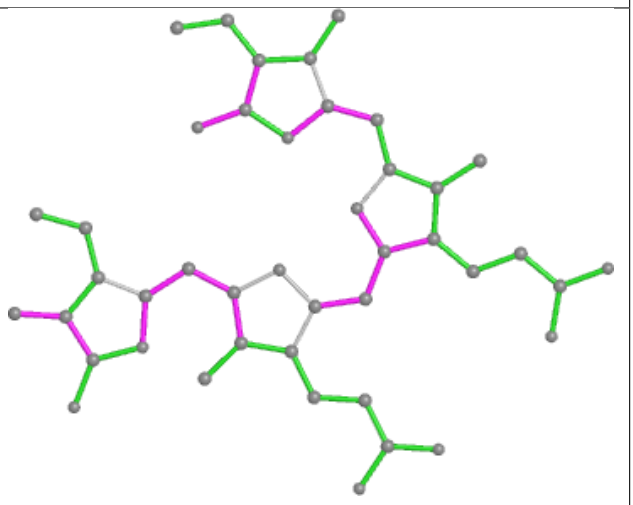

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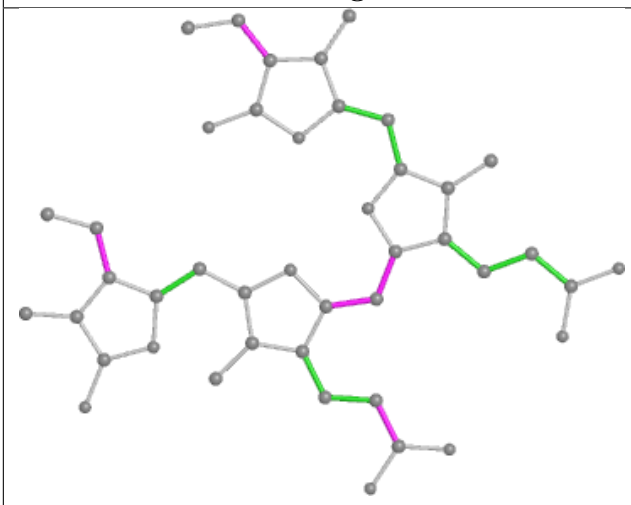

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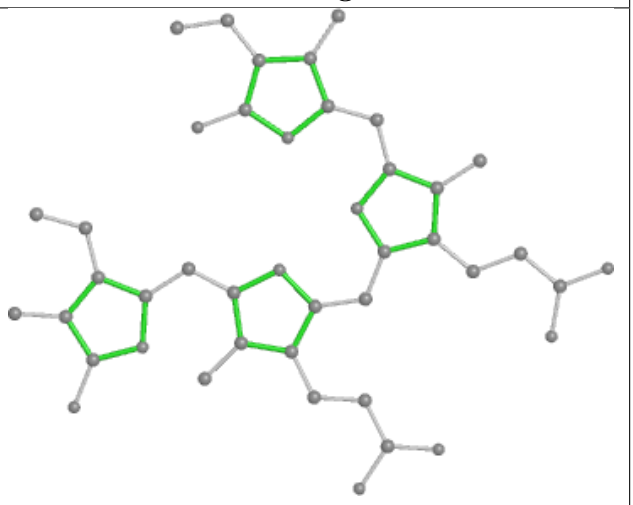

Rings

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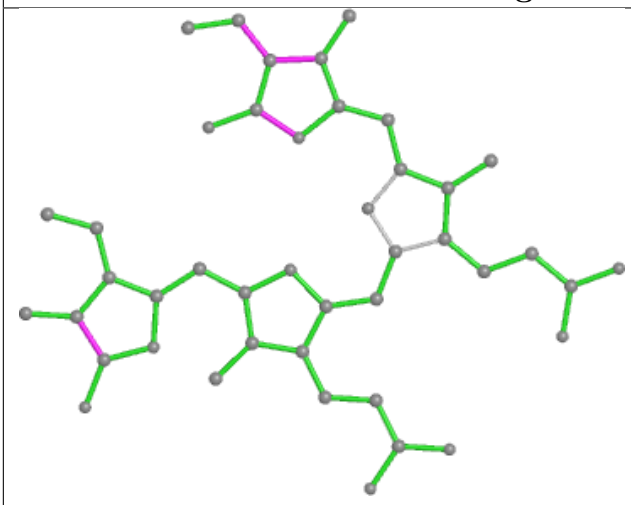

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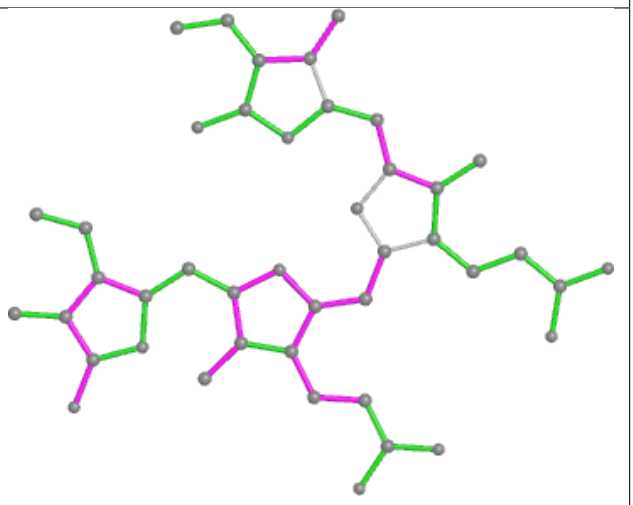

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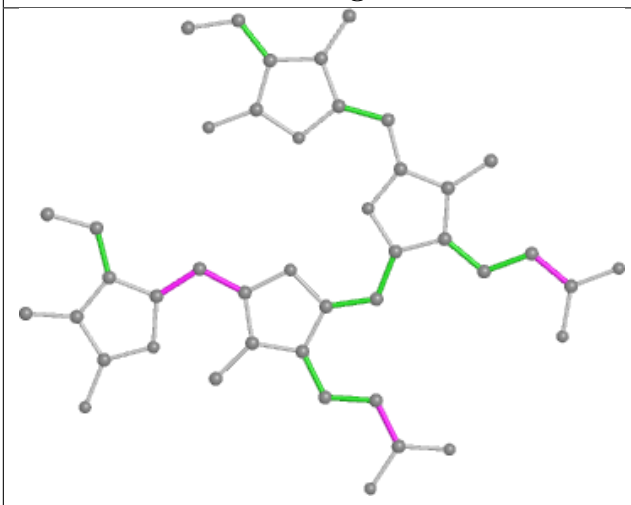

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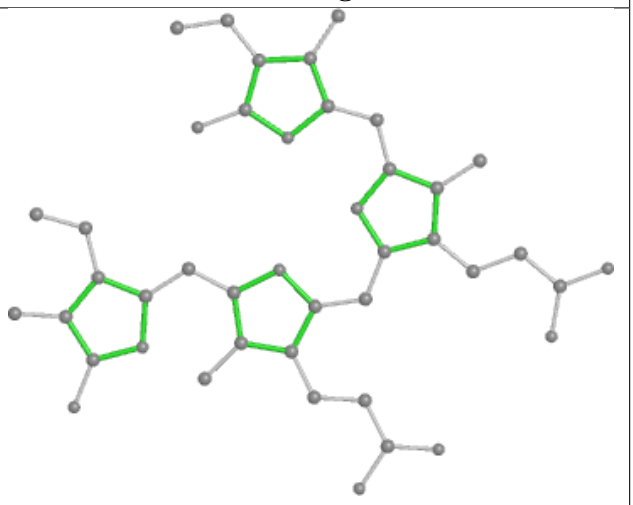

Rings

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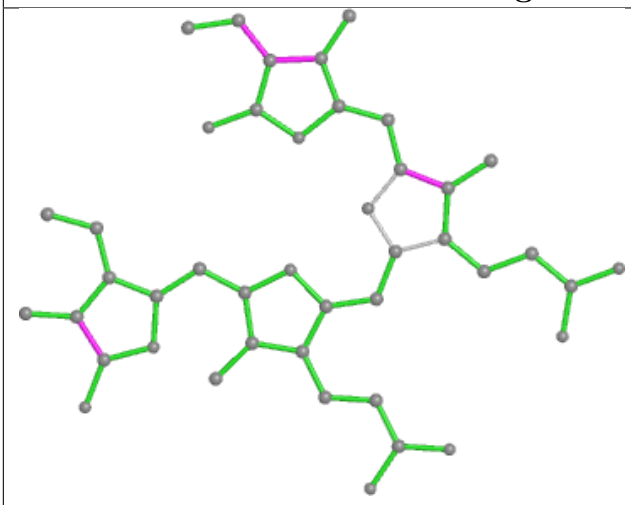

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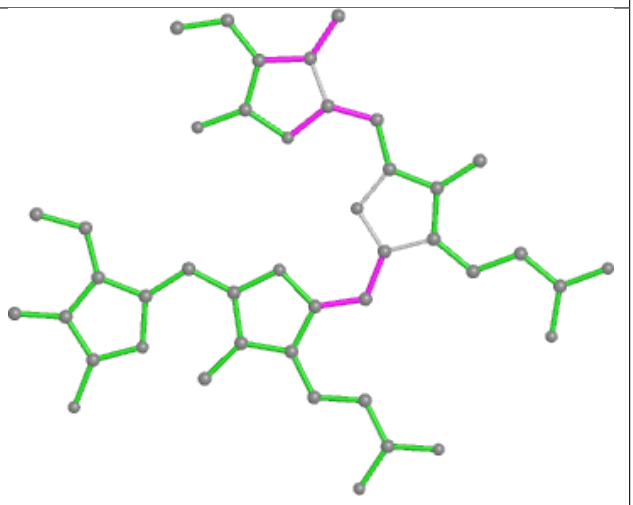

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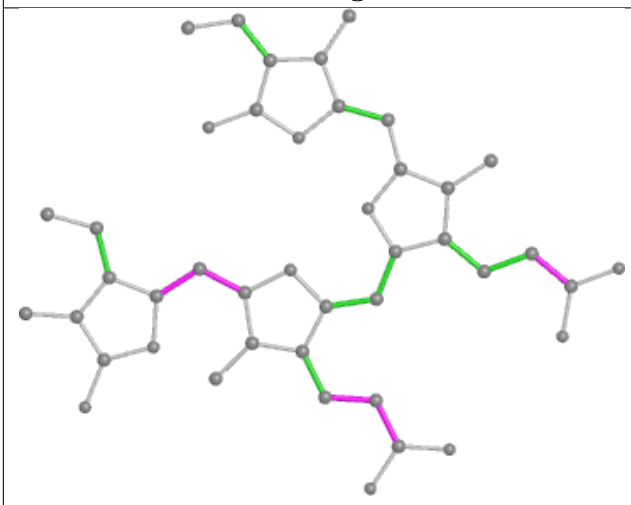

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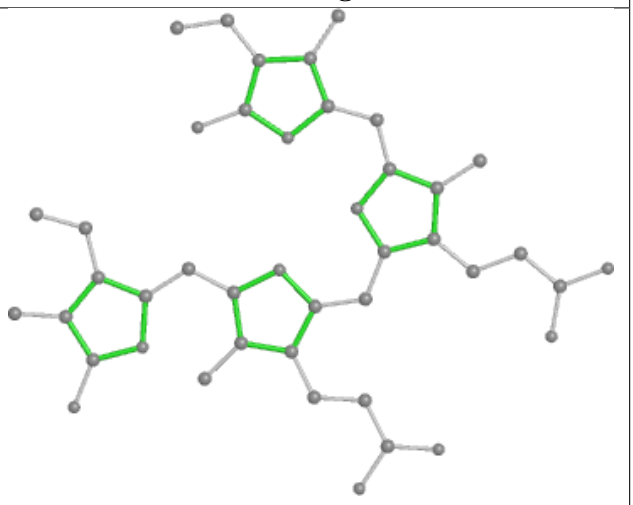

Rings

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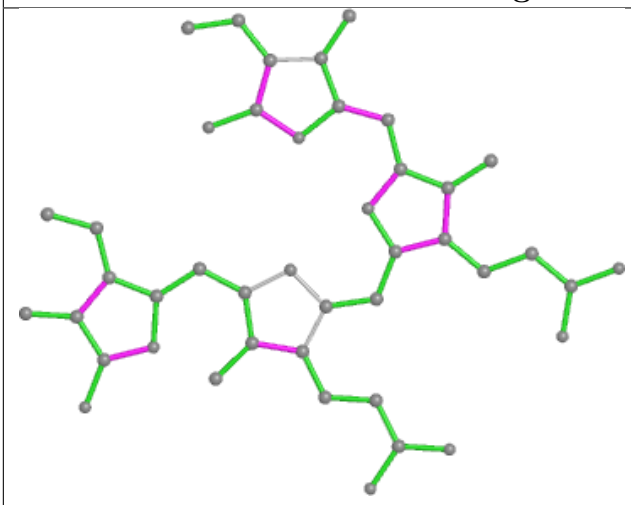

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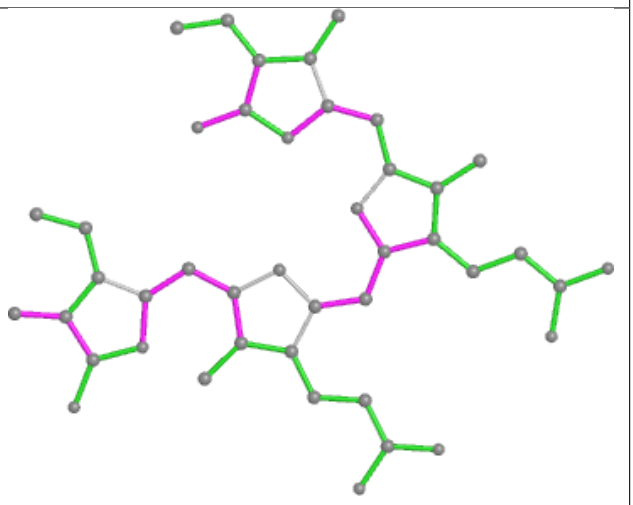

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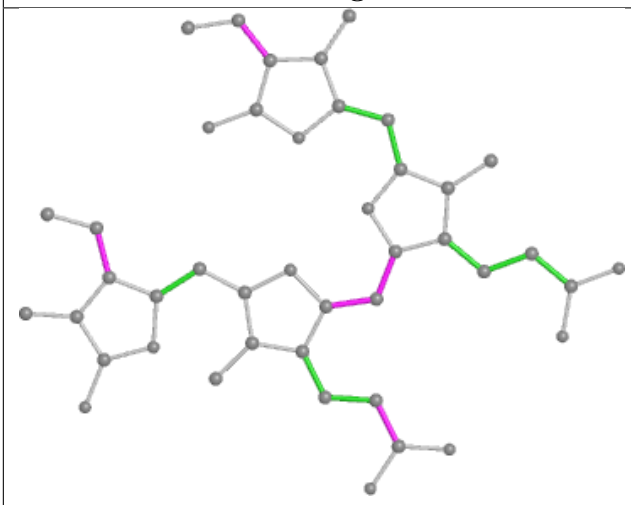

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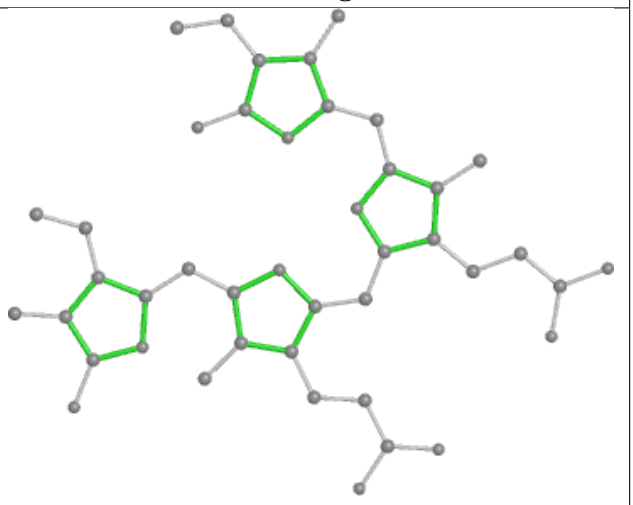
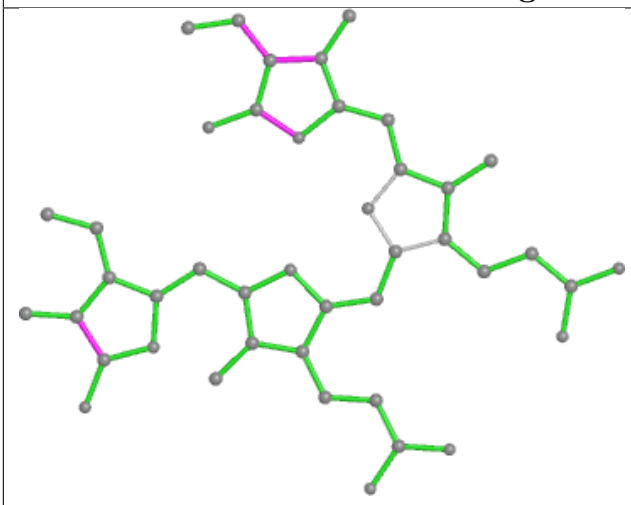


Rings

Ligand PEB p6 201



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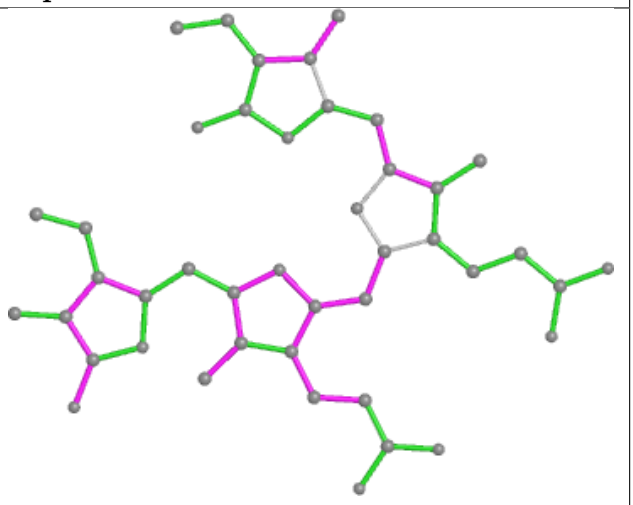

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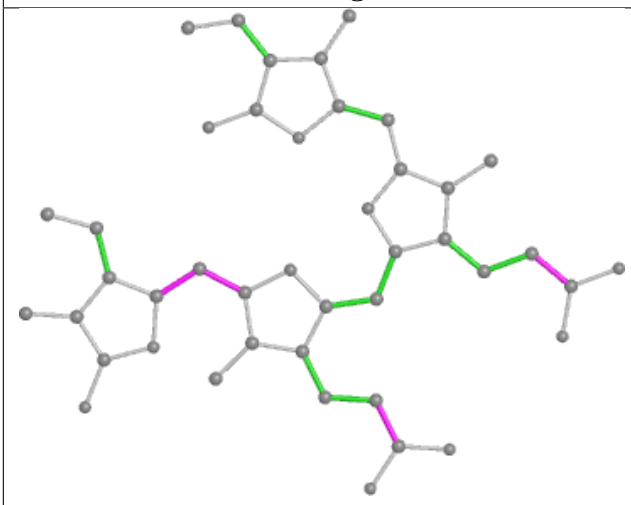

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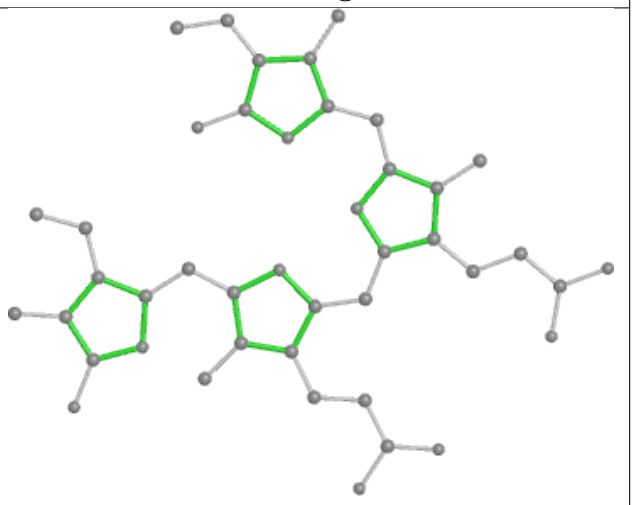
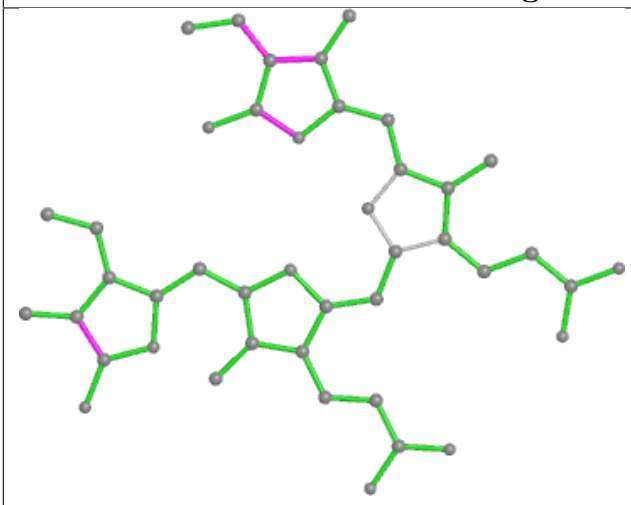


Rings

Ligand PEB s8 201



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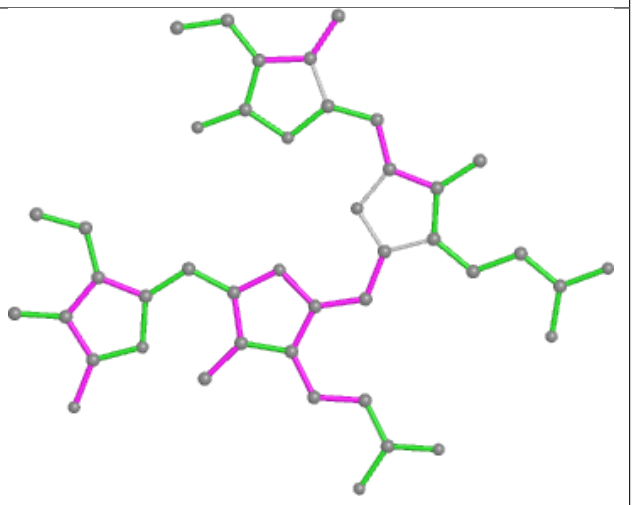

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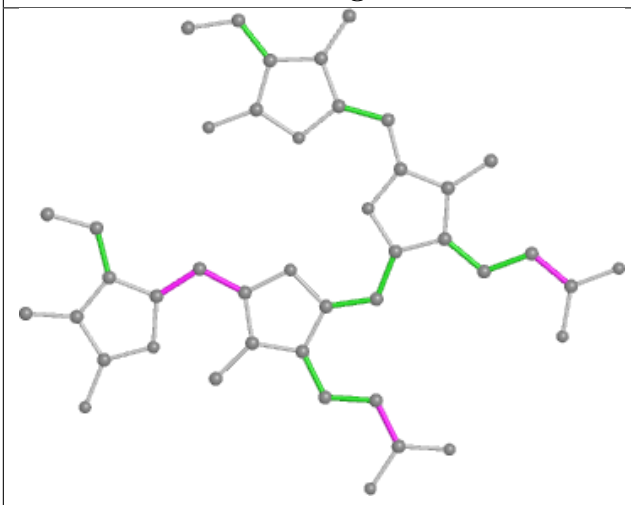

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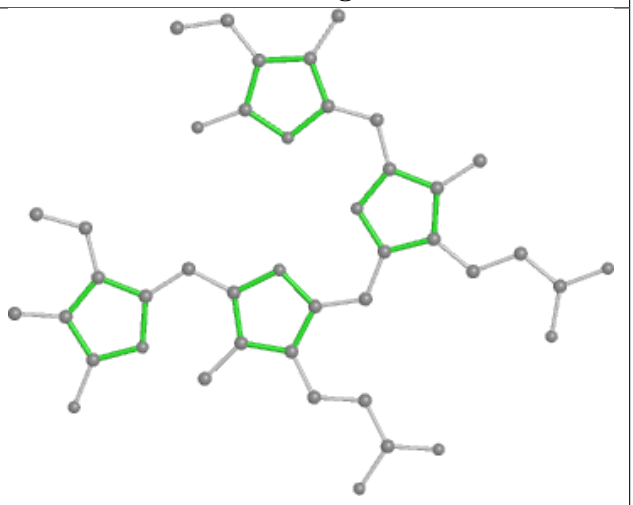
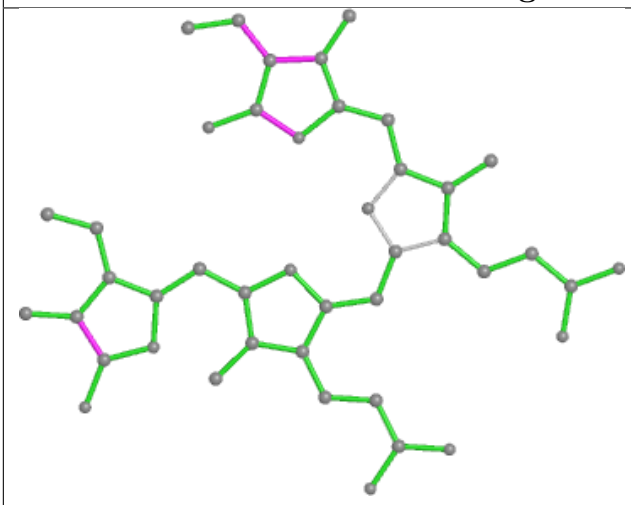


Rings

Ligand PEB h2 201



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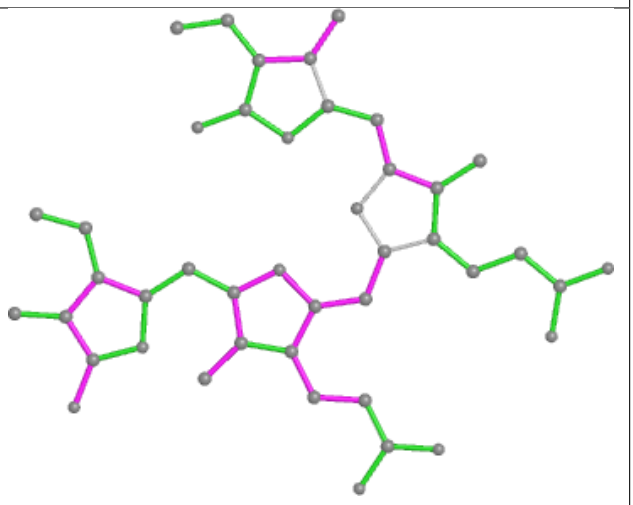

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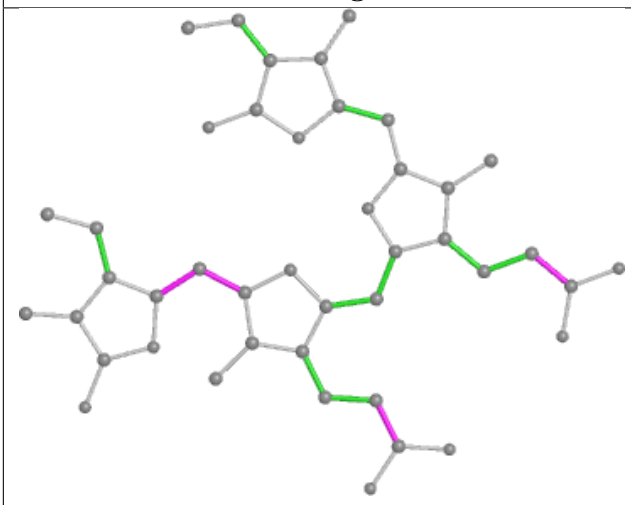

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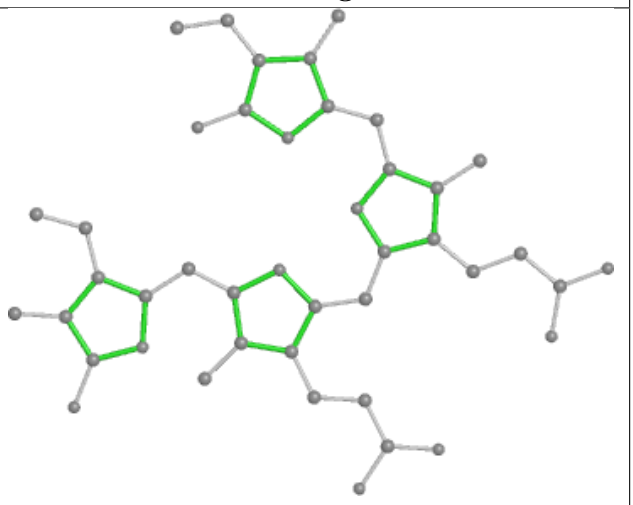

Rings

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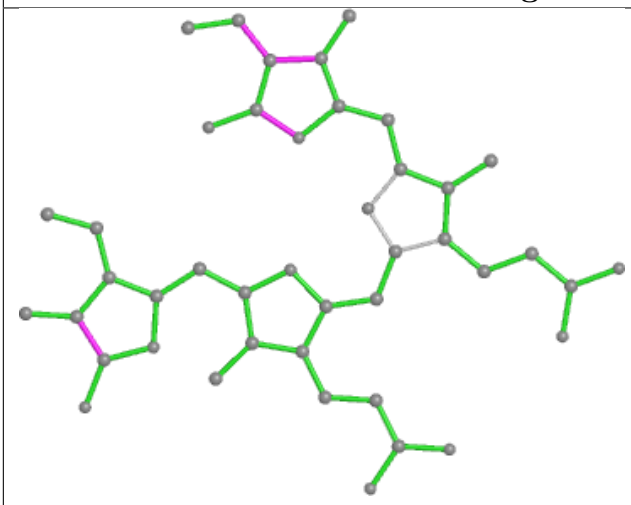

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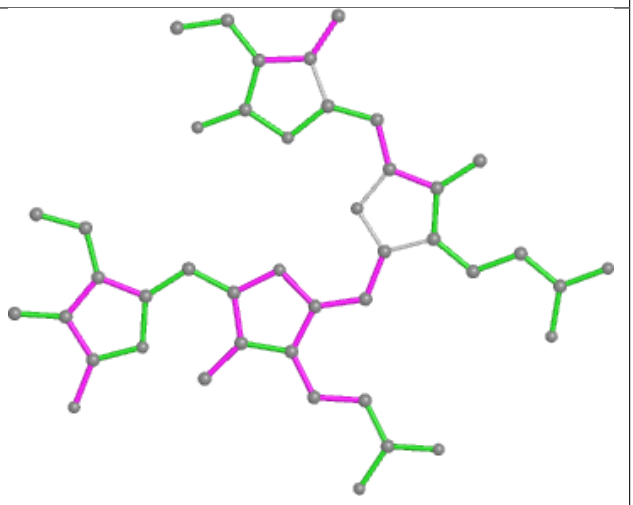

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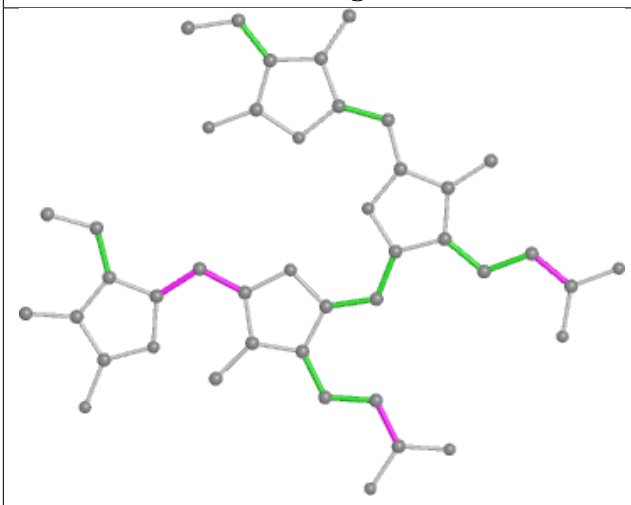

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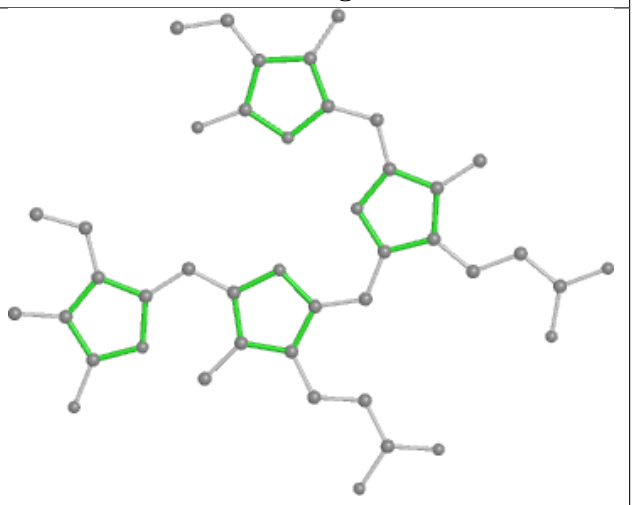

Rings

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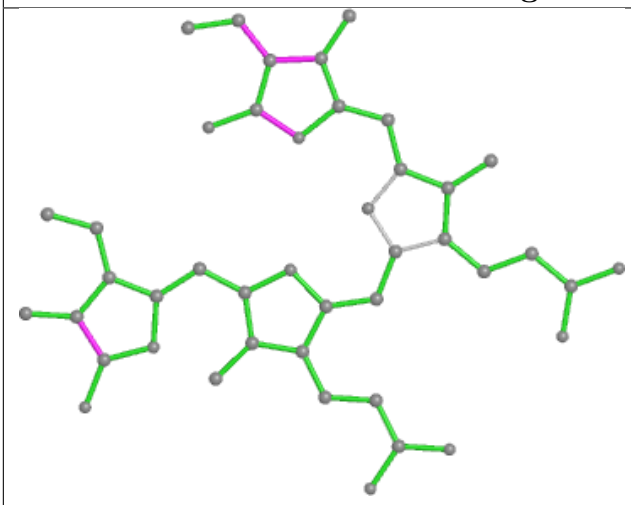

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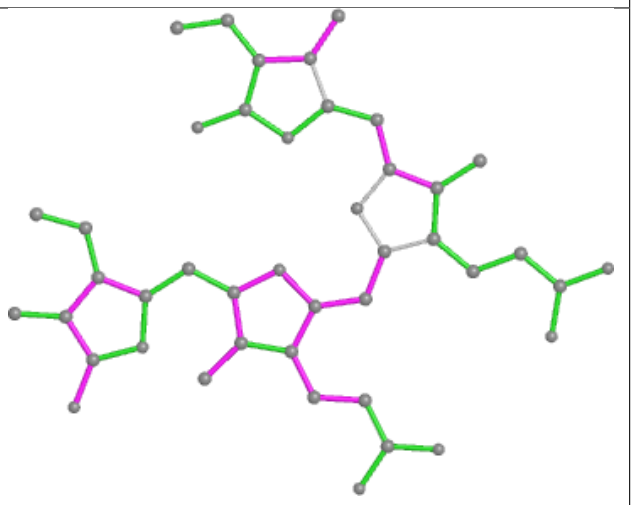
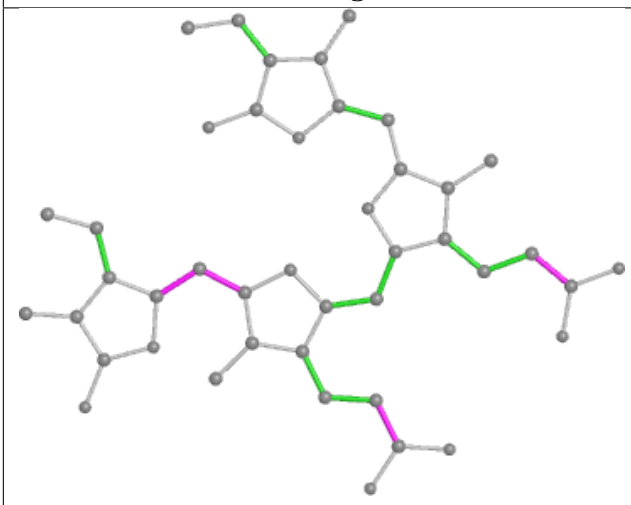
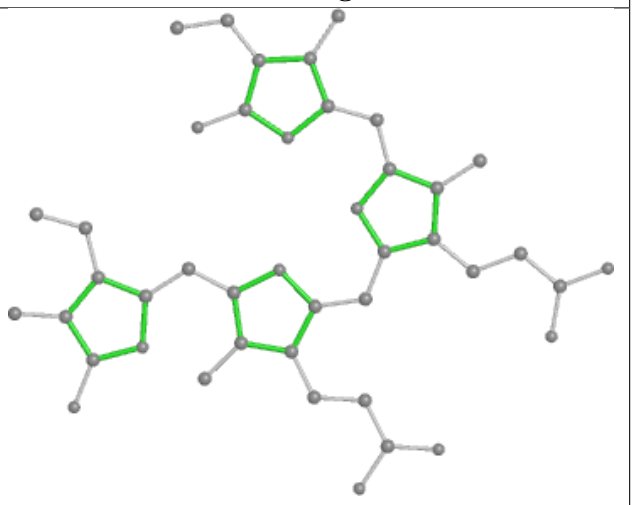


Bond angles

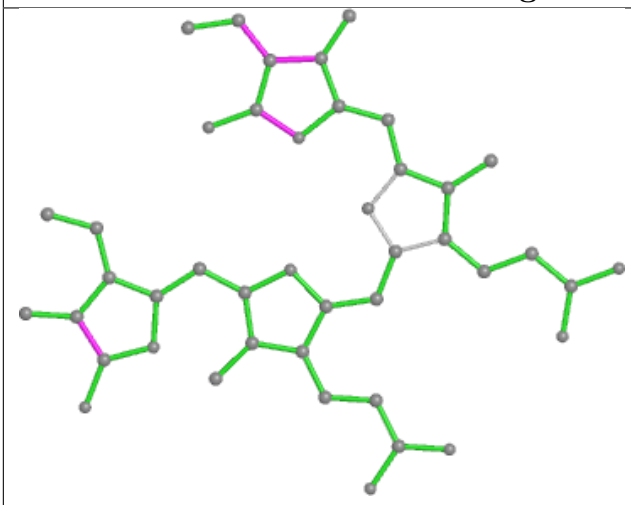


Torsions



Rings

Ligand PEB v7 201



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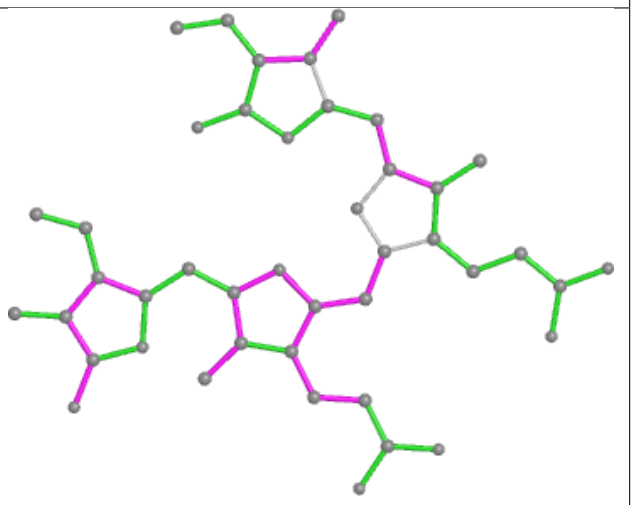

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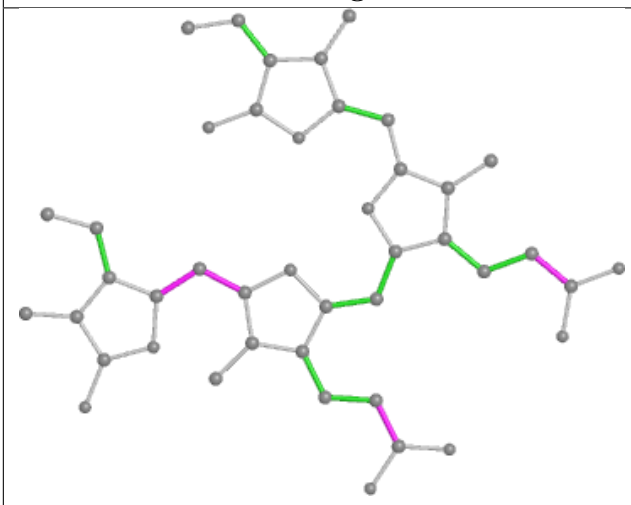

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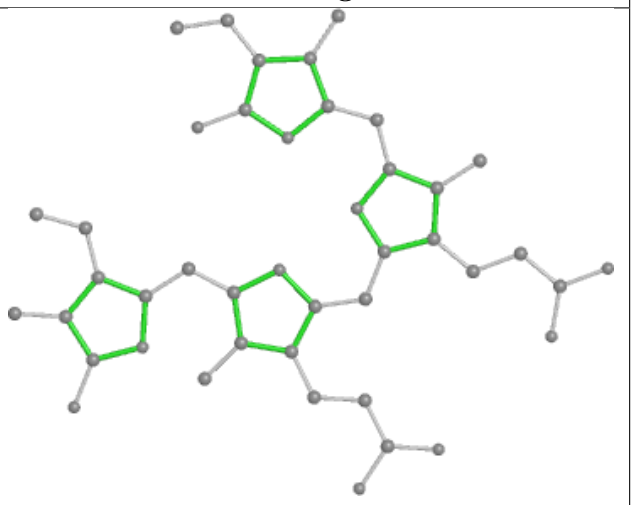
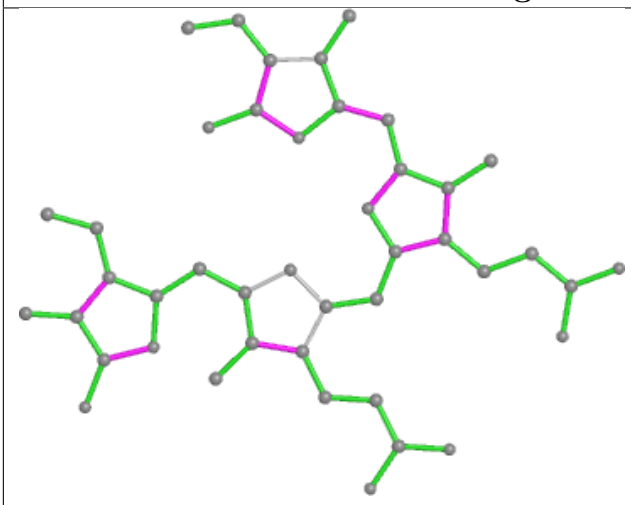


Rings

Ligand PUB B6 203



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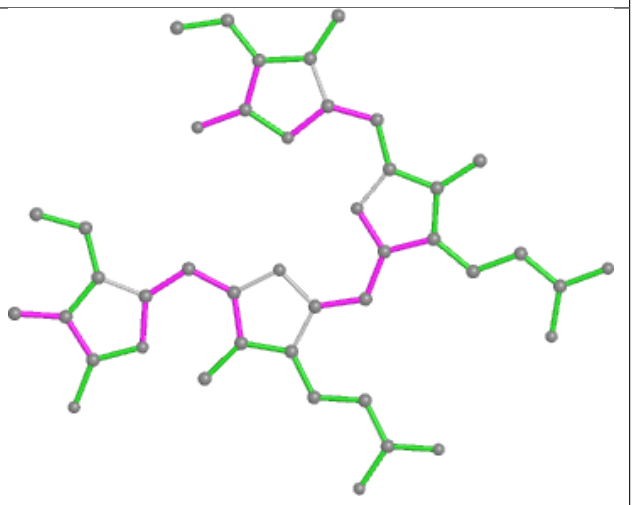

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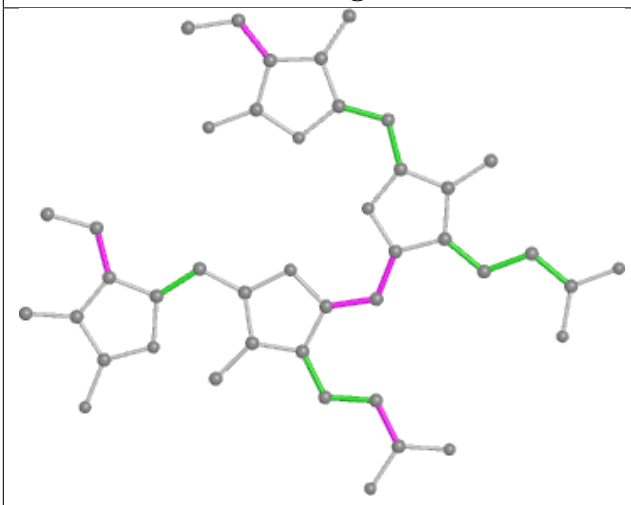

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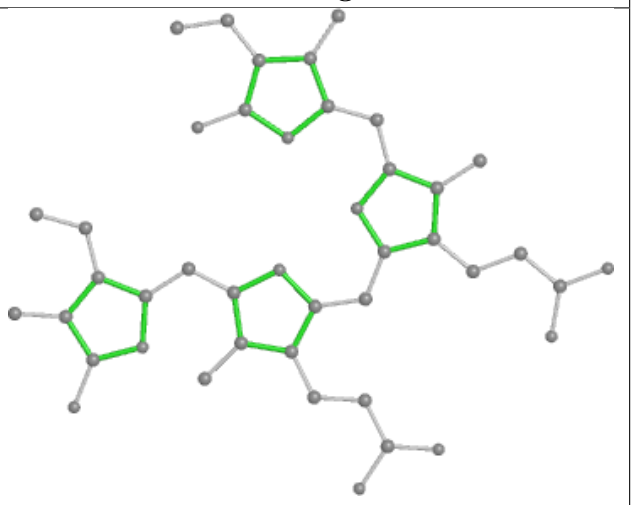
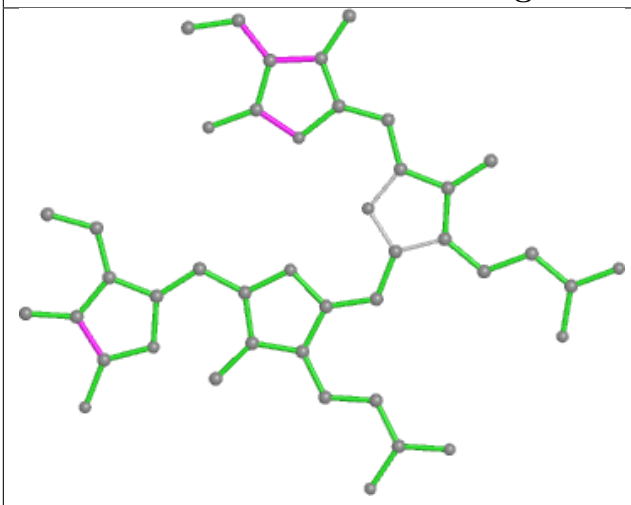


Rings

Ligand PEB H9 201



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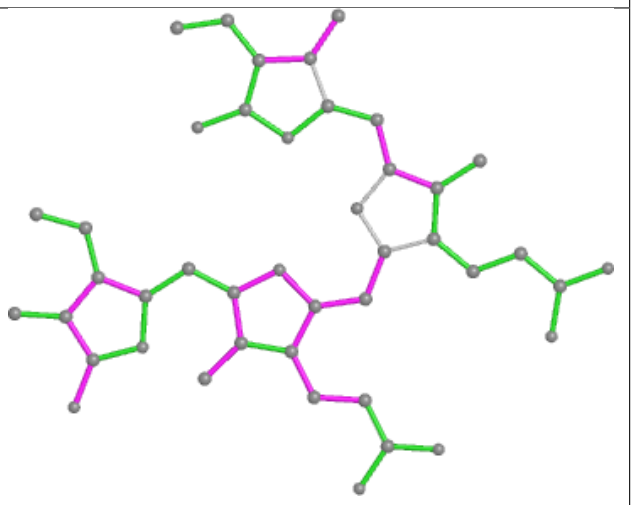

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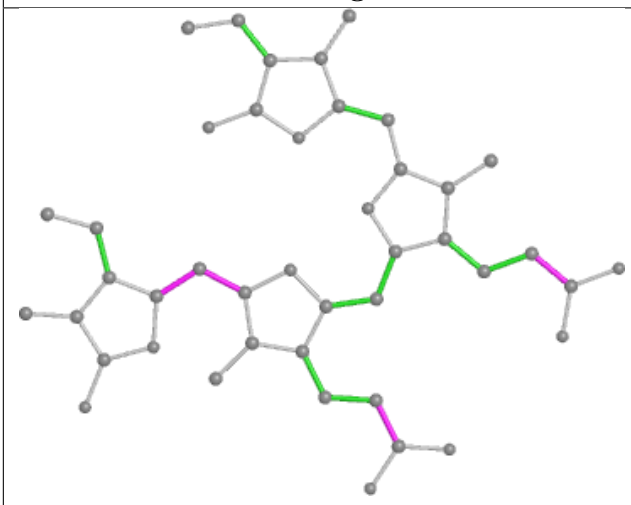

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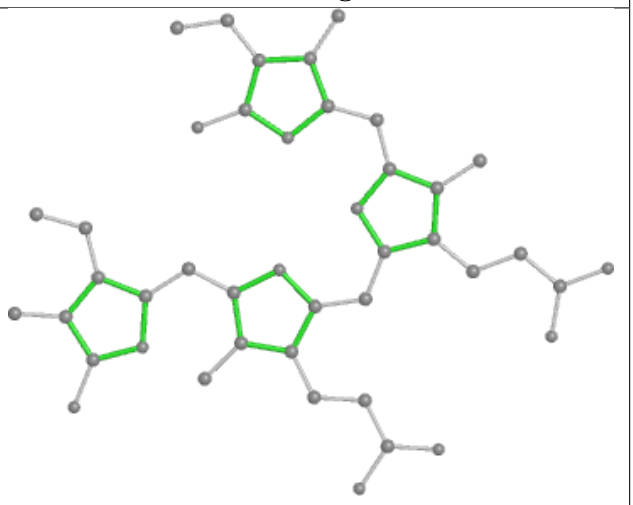

Rings

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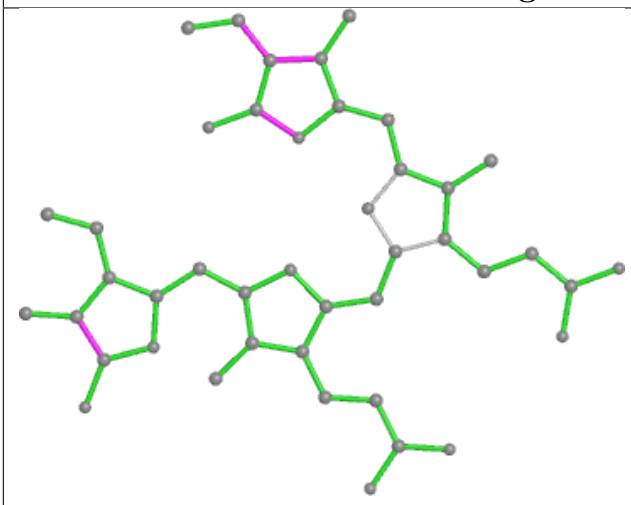

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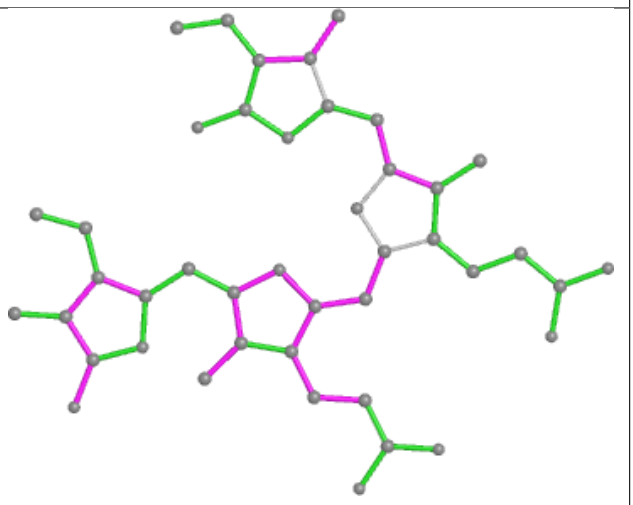

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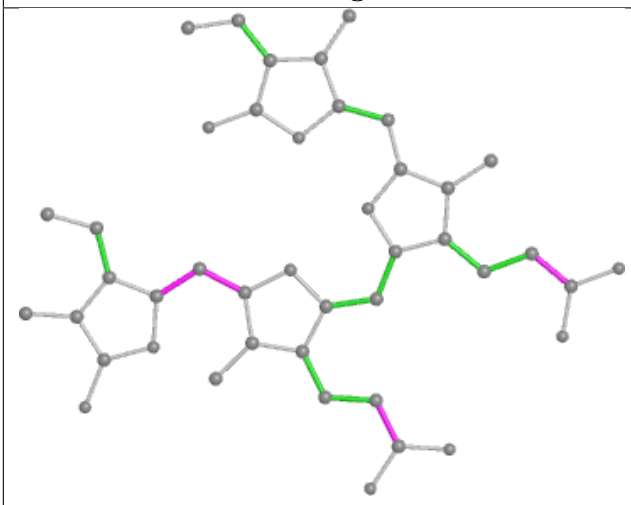

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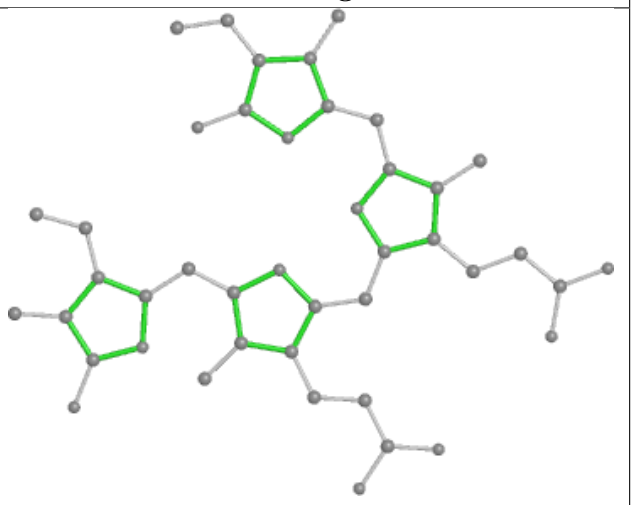

Rings

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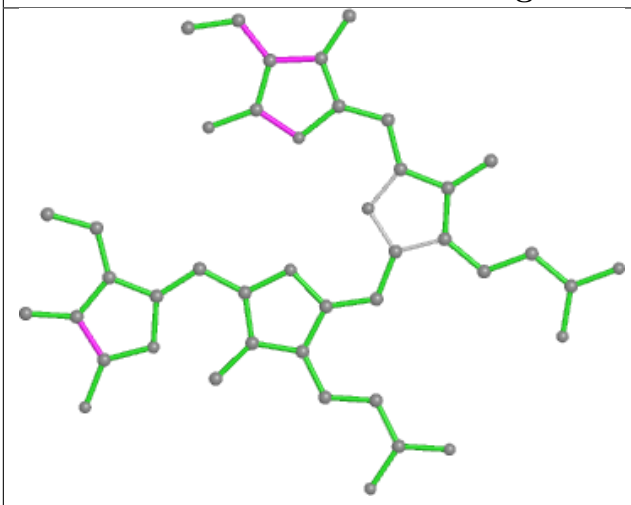

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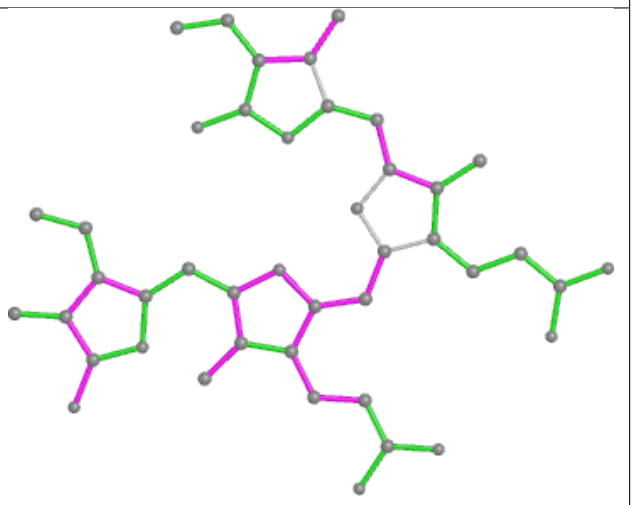

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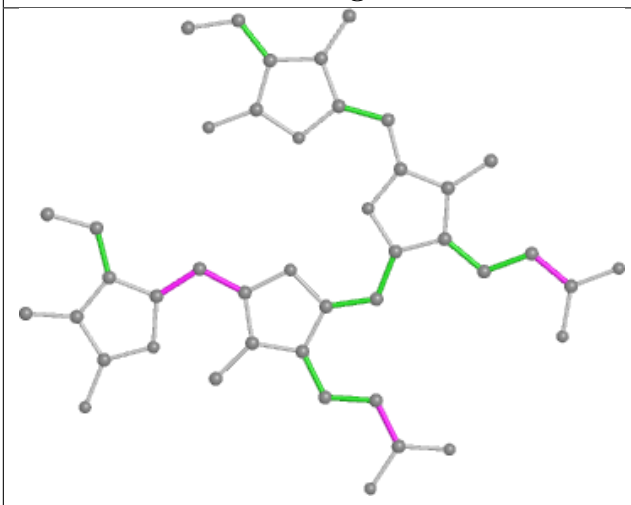

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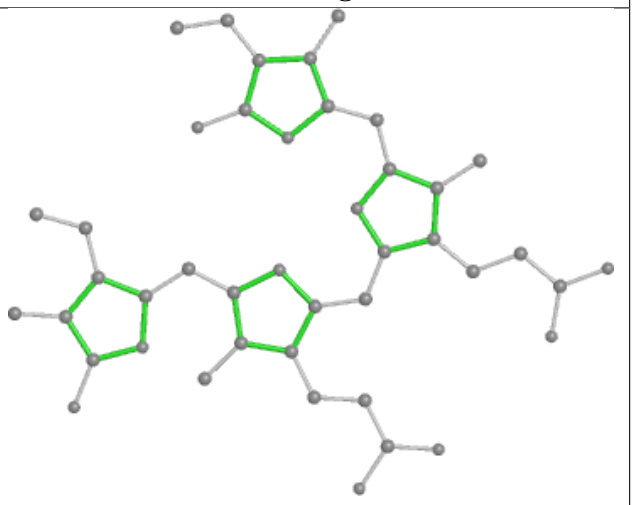
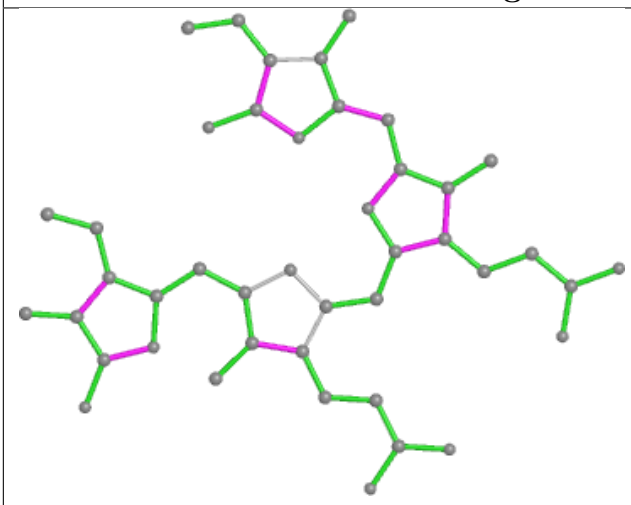


Rings

Ligand PUB kX 1003



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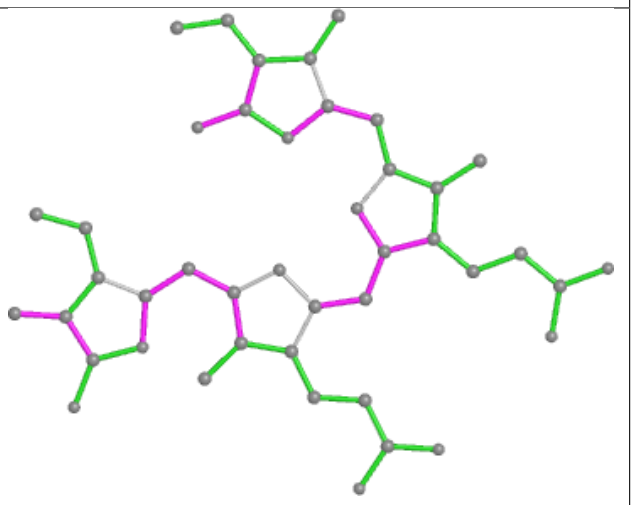

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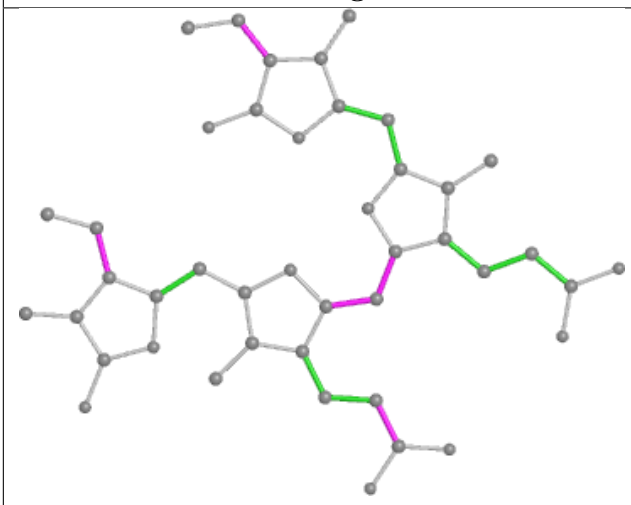

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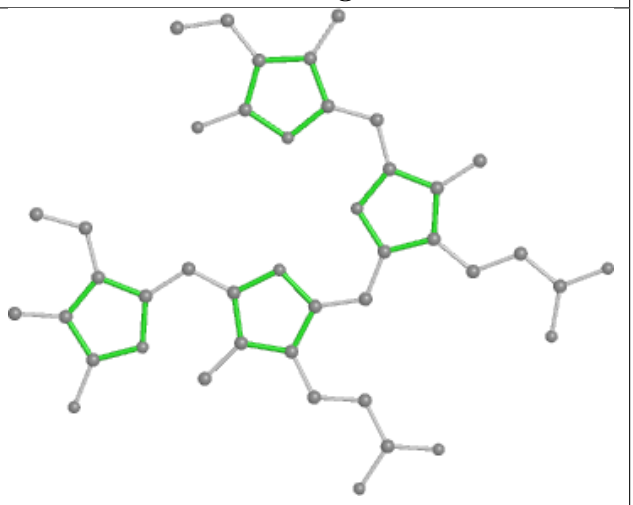

Rings

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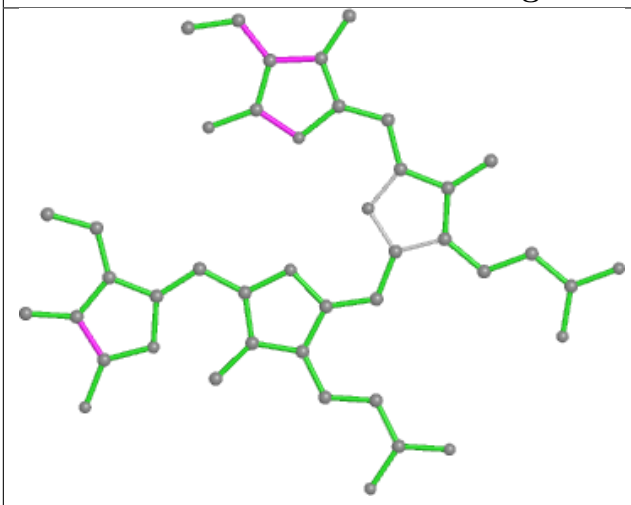

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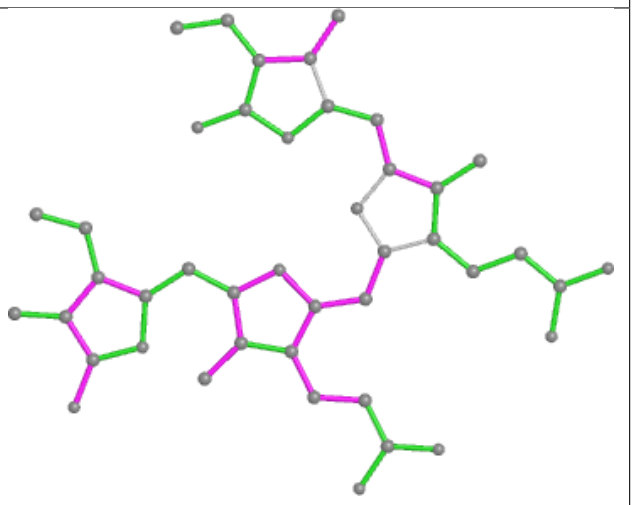

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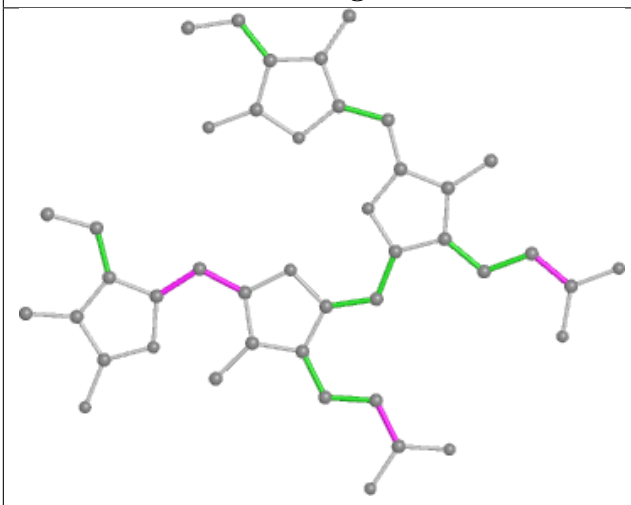

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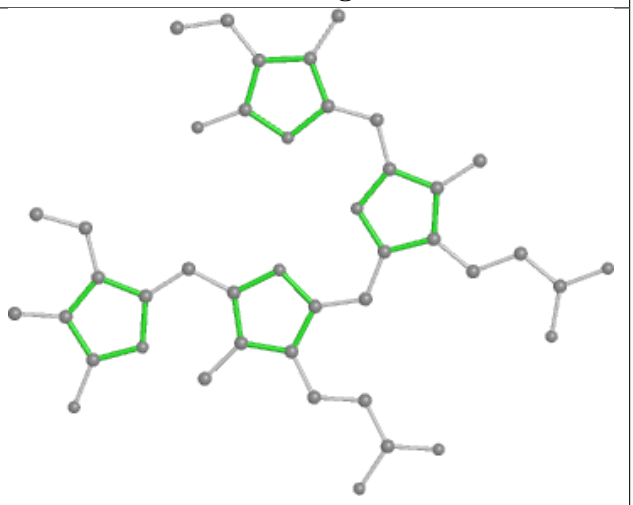
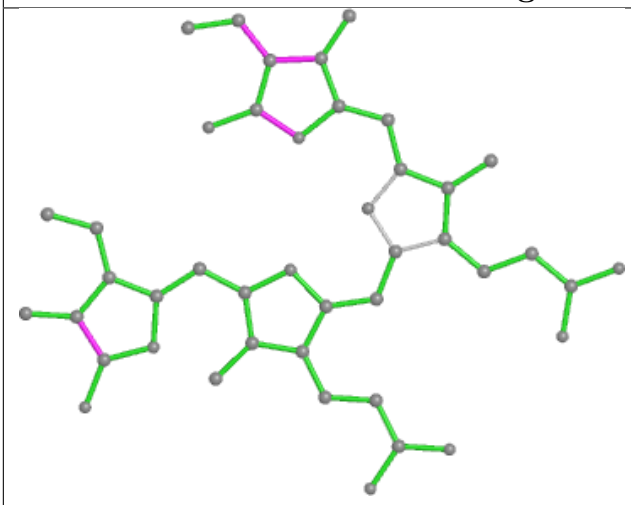


Rings

Ligand PEB Z7 201



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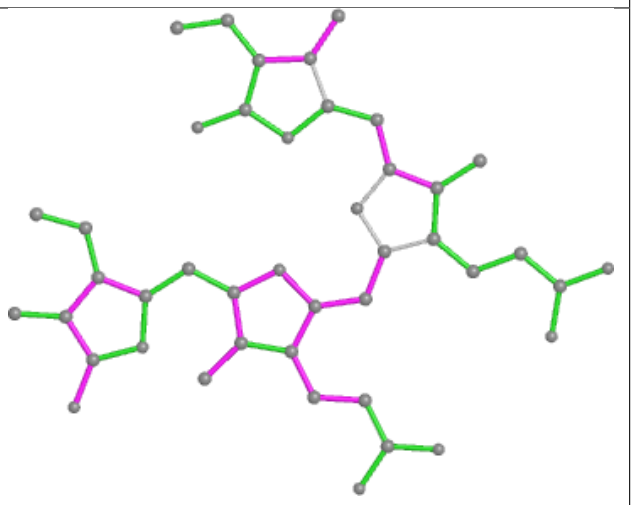
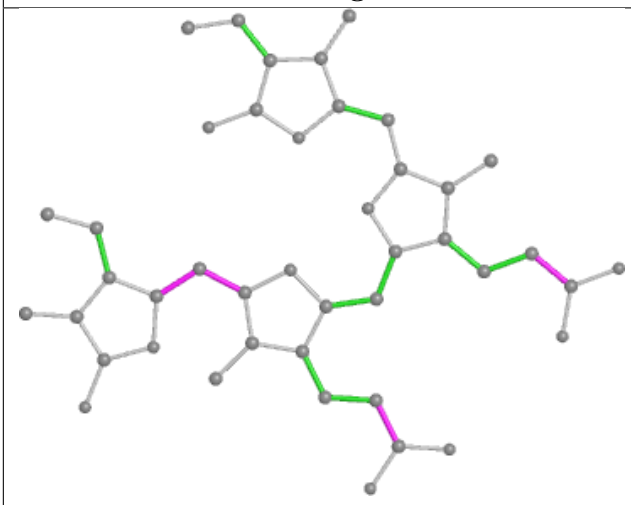


Bond angles



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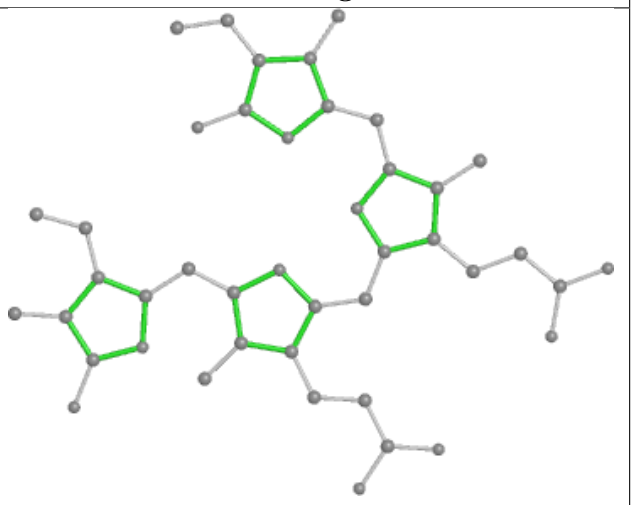
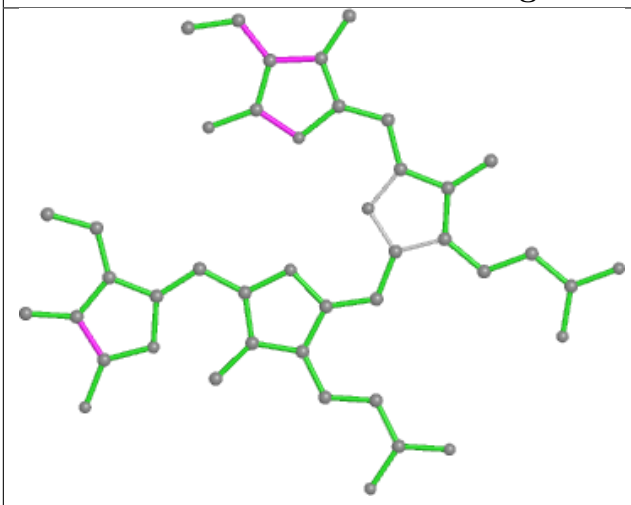


Rings

Ligand PEB x6 201



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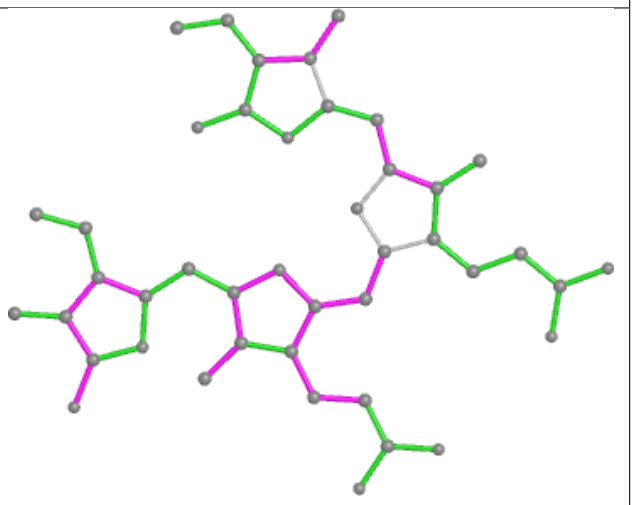

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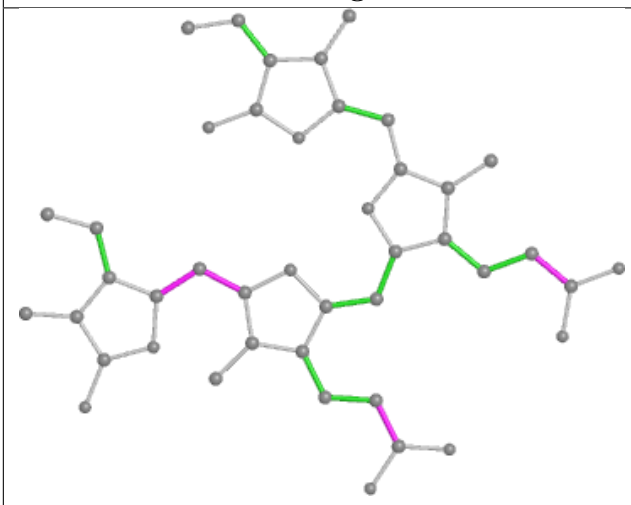

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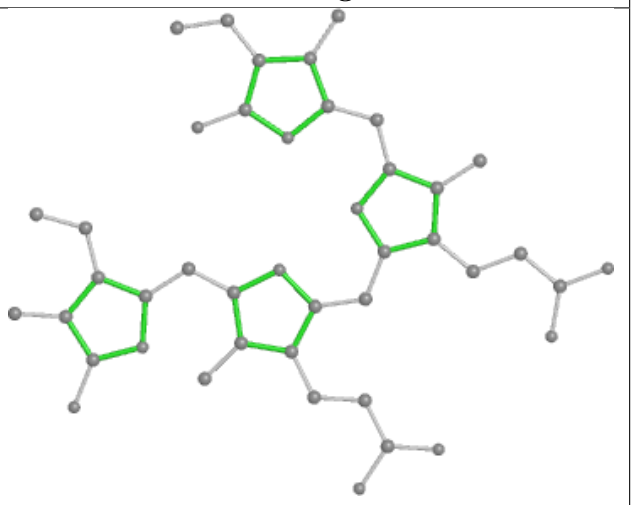
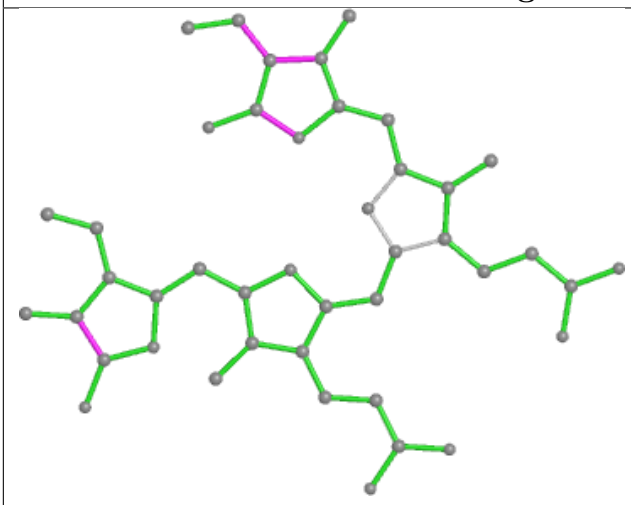


Rings

Ligand PEB aF 201



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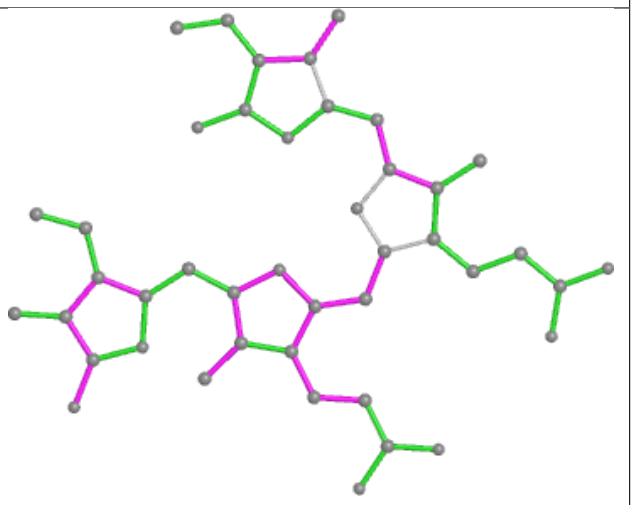

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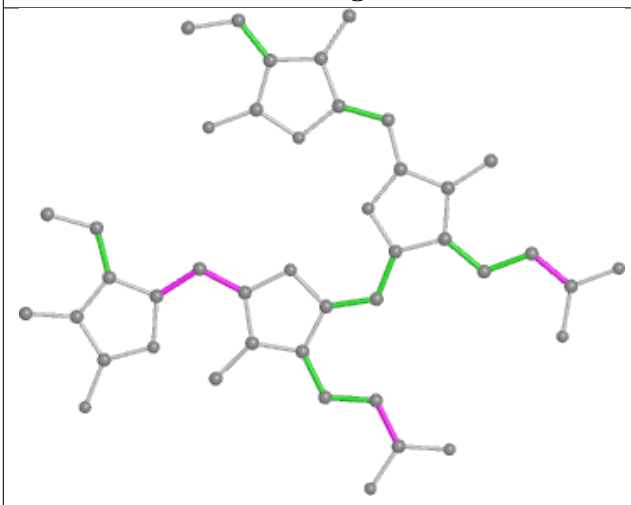

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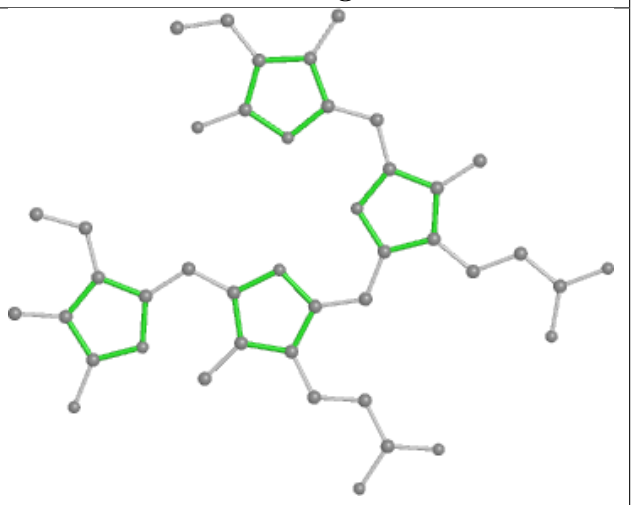

Rings

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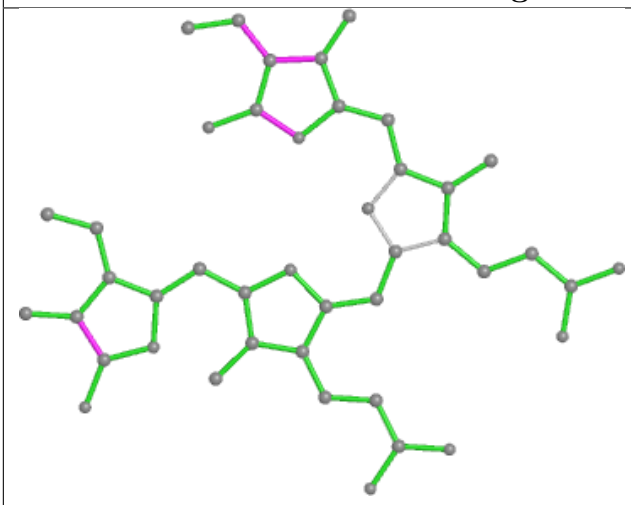

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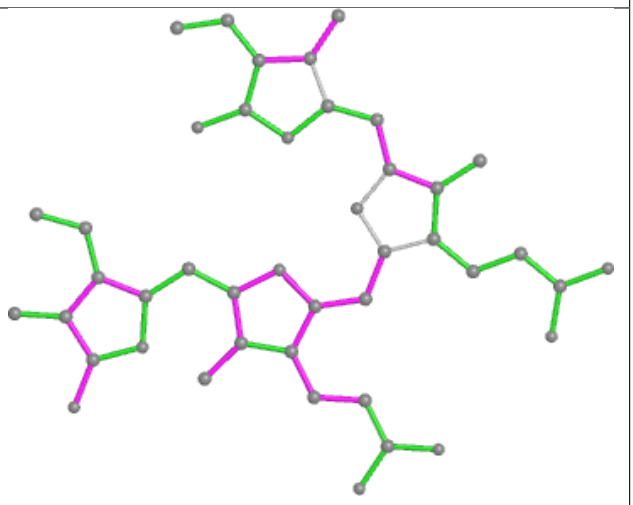

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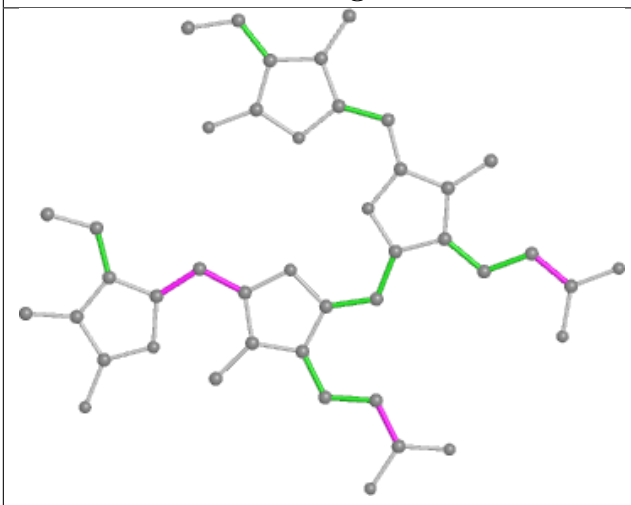

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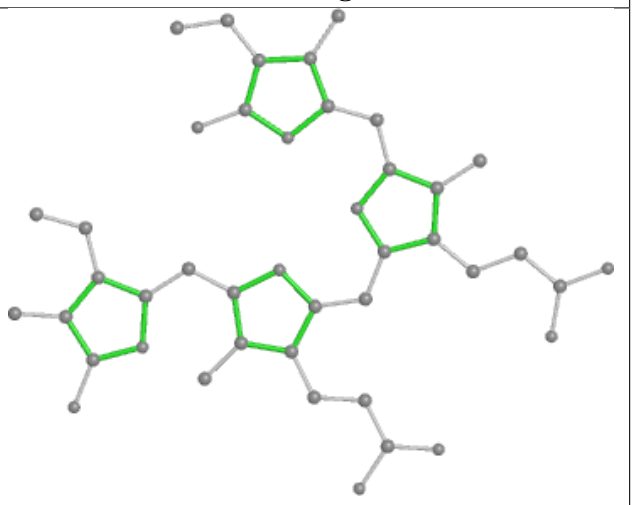
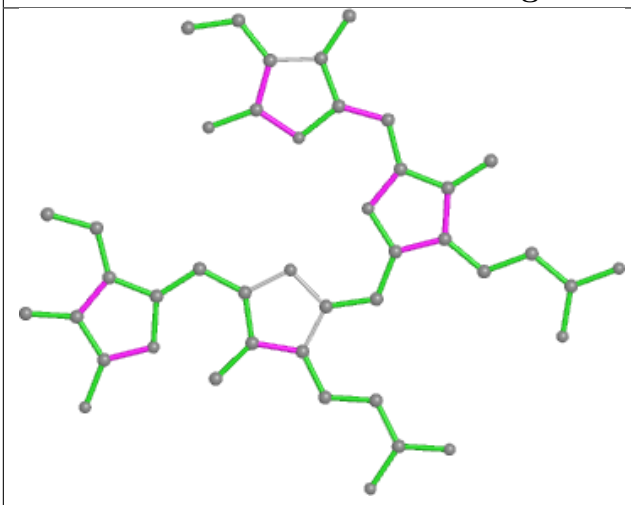


Rings

Ligand PUB f8 203



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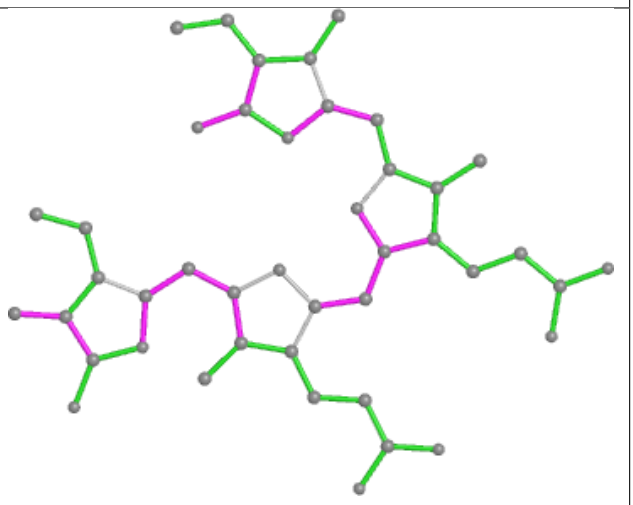

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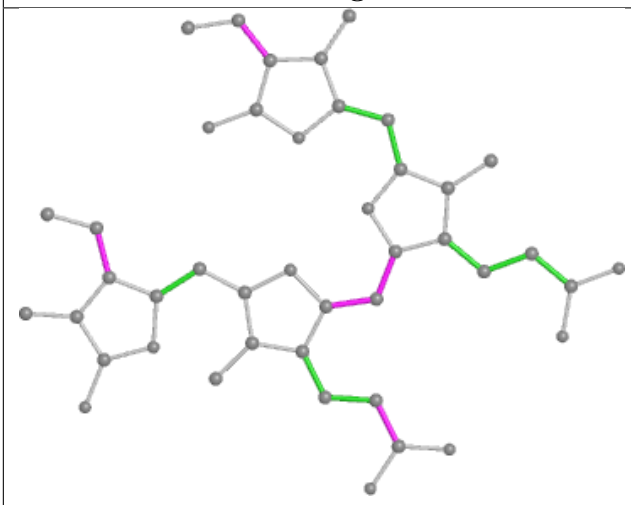

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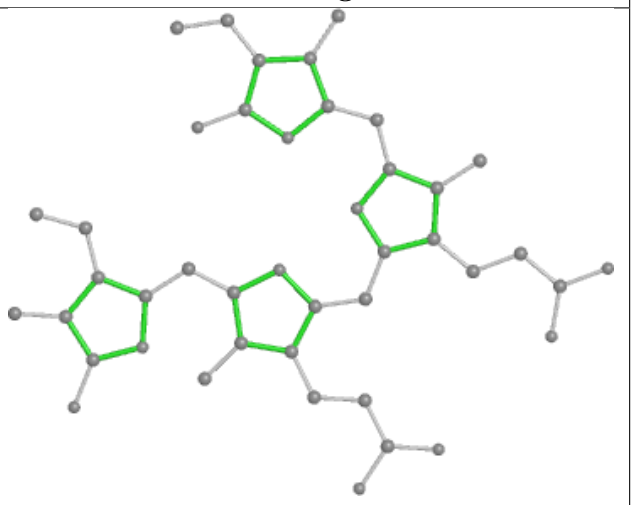
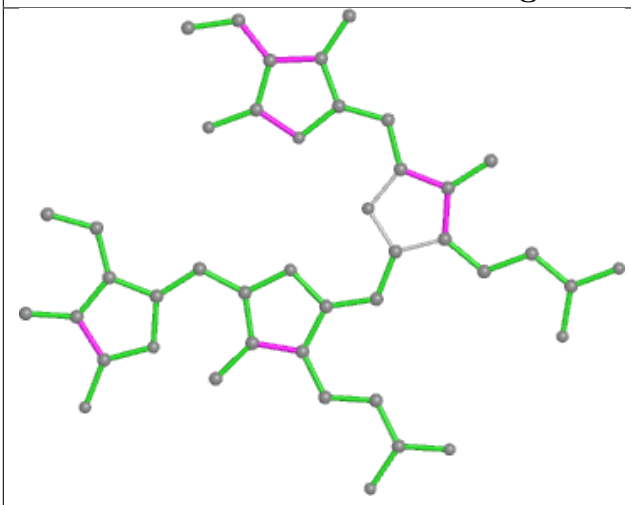


Rings

Ligand PEB cd 202



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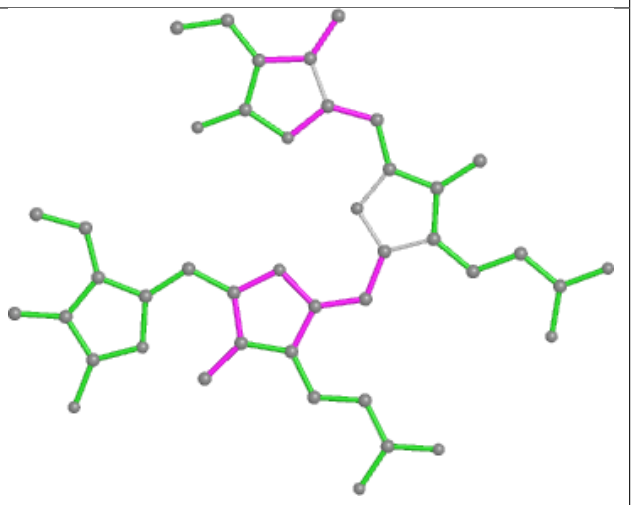
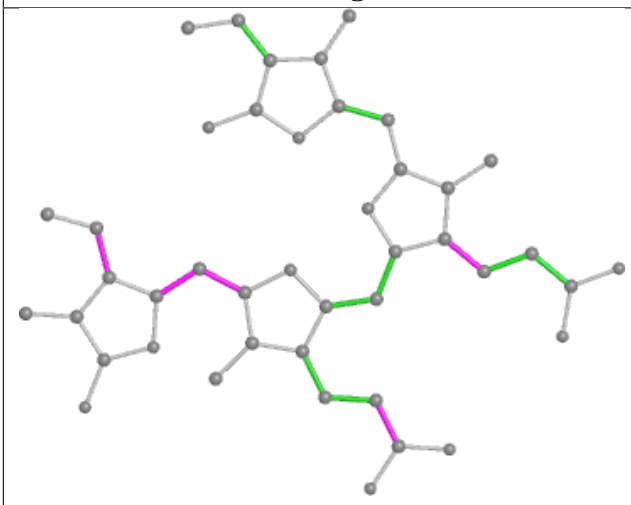
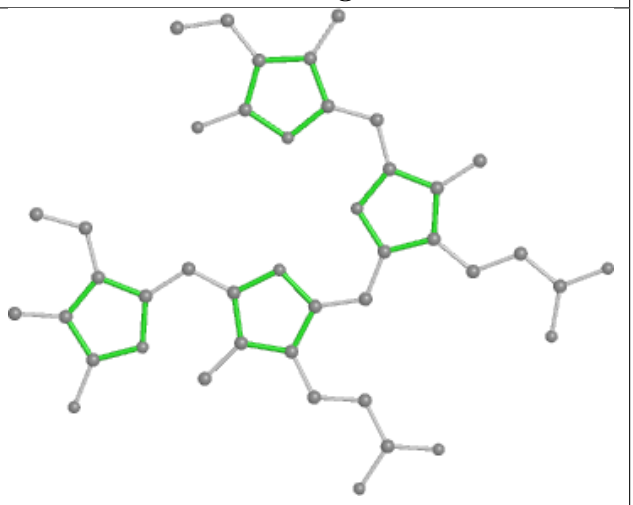


Bond angles

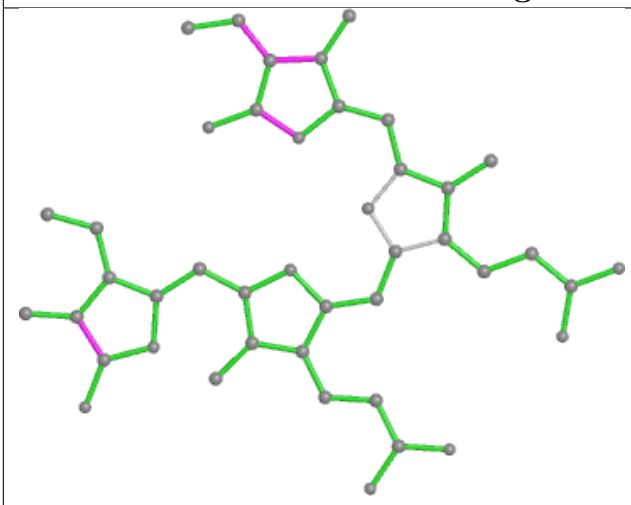


Torsions



Rings

Ligand PEB hD 201



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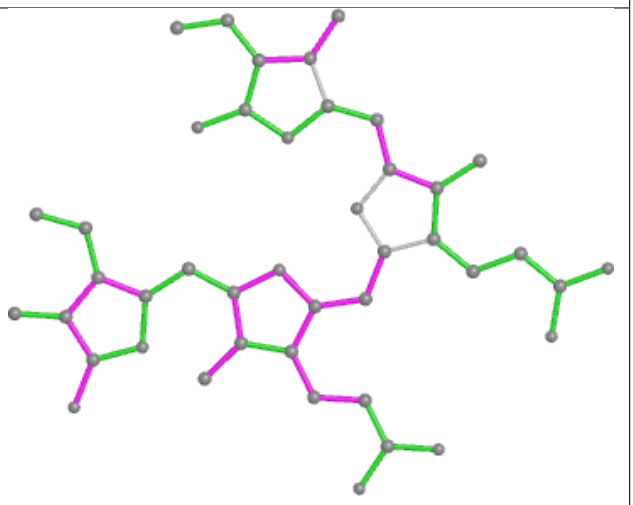
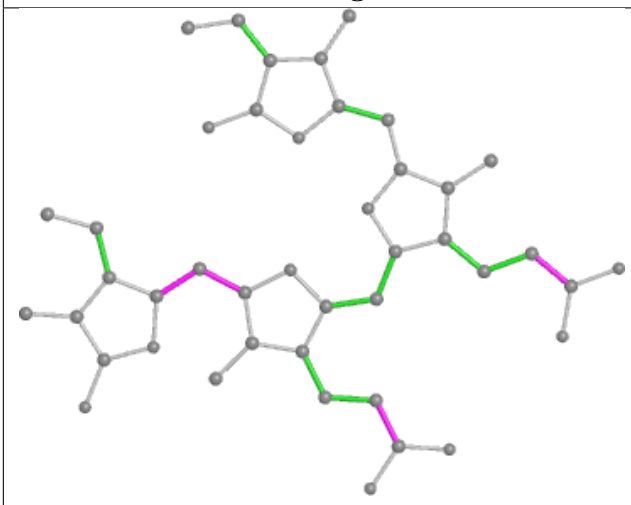


Bond angles



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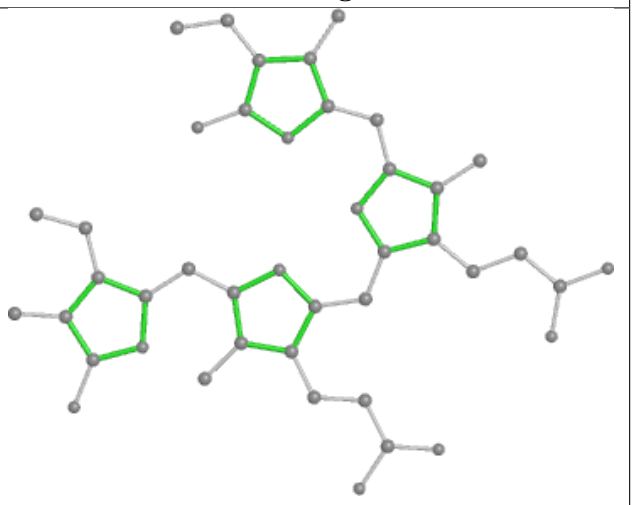
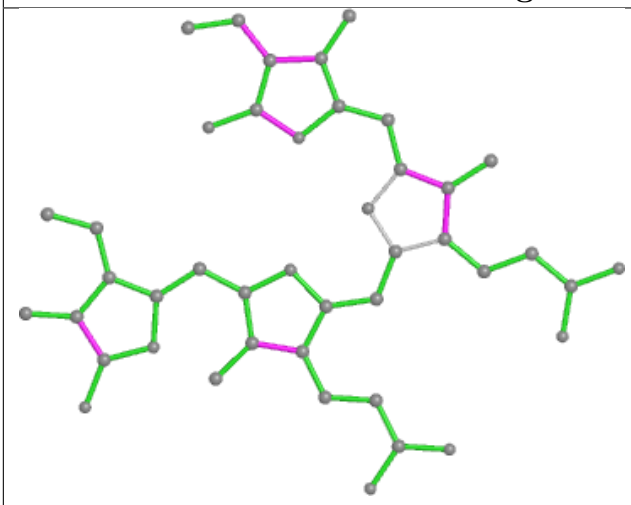


Rings

Ligand PEB eX 201



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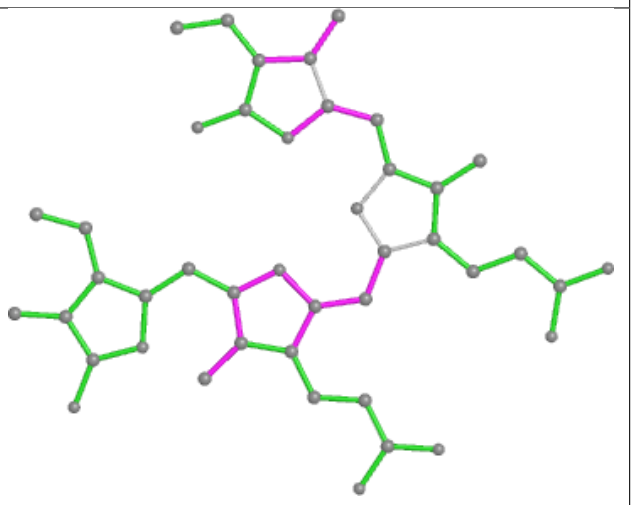

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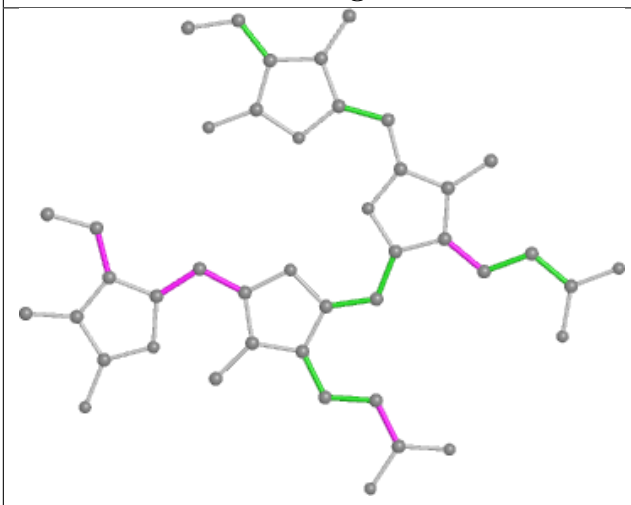

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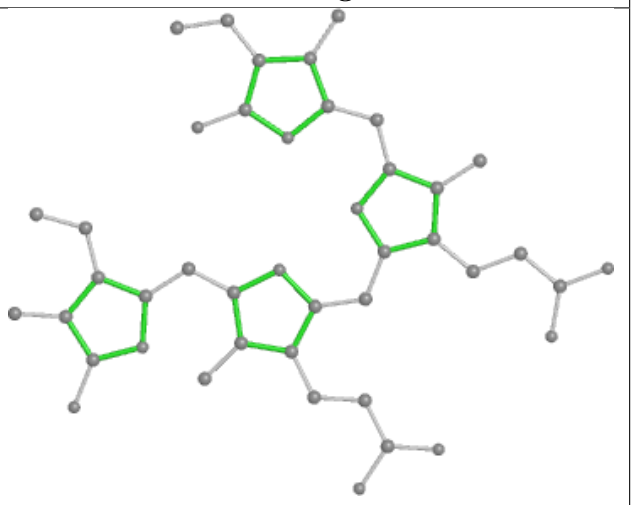
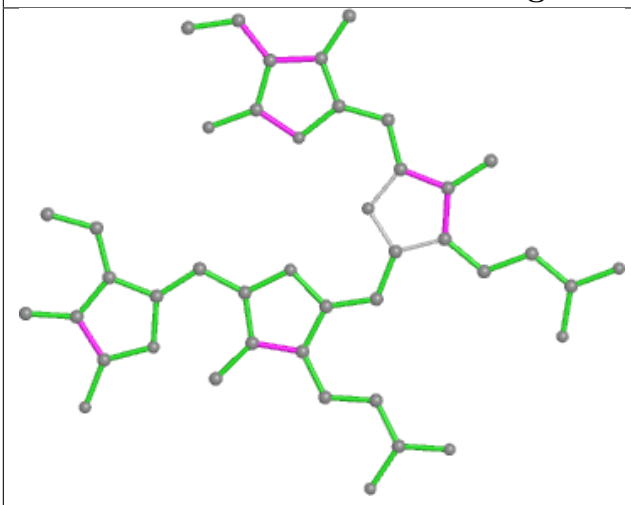


Rings

Ligand PEB fi 202



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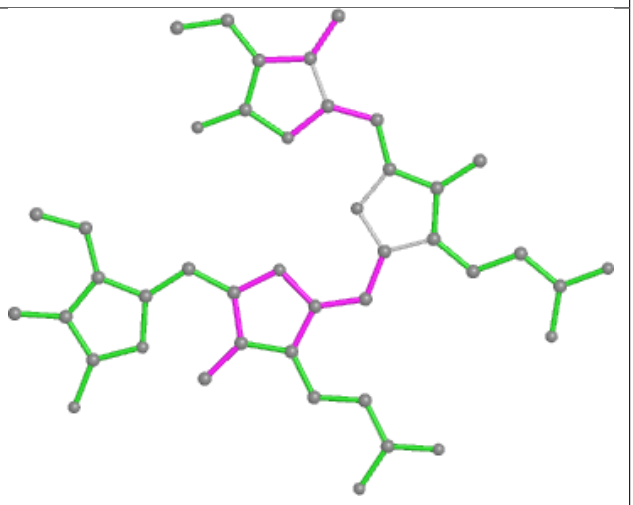

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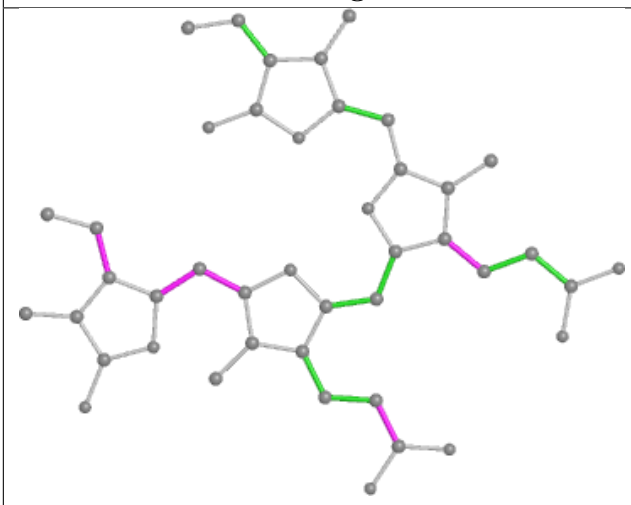

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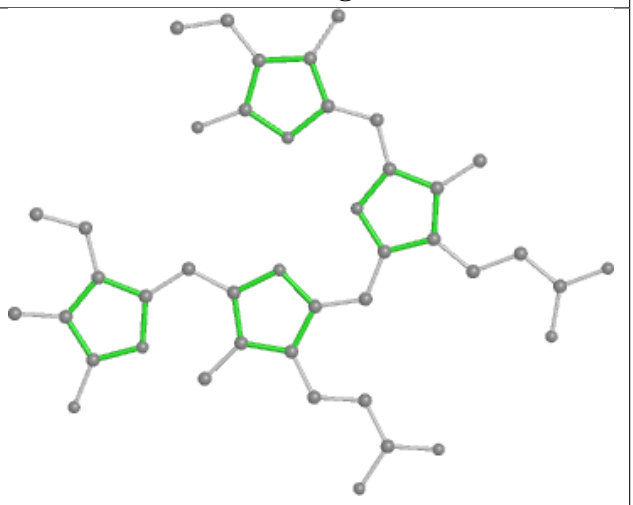
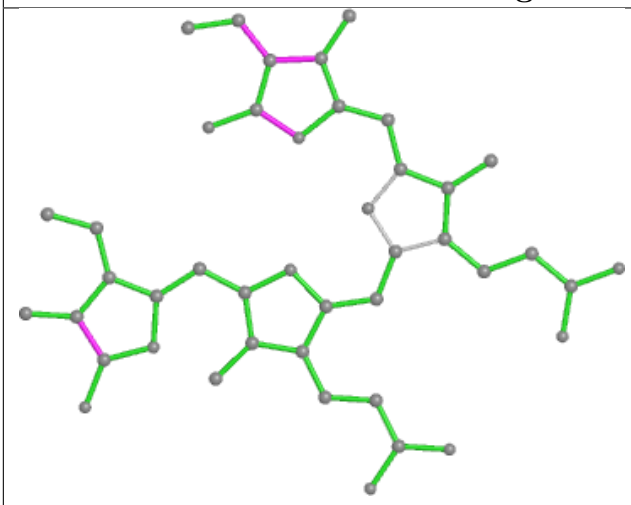


Rings

Ligand PEB C9 201



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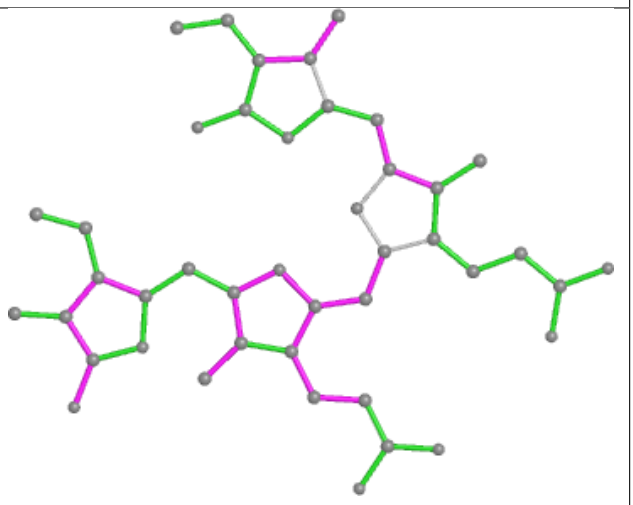
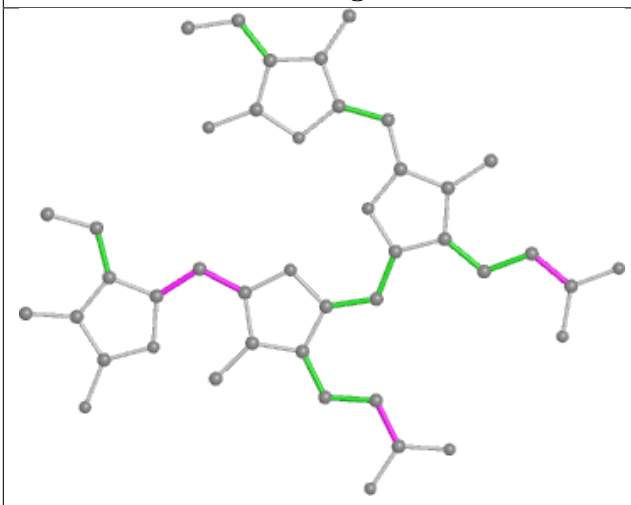


Bond angles



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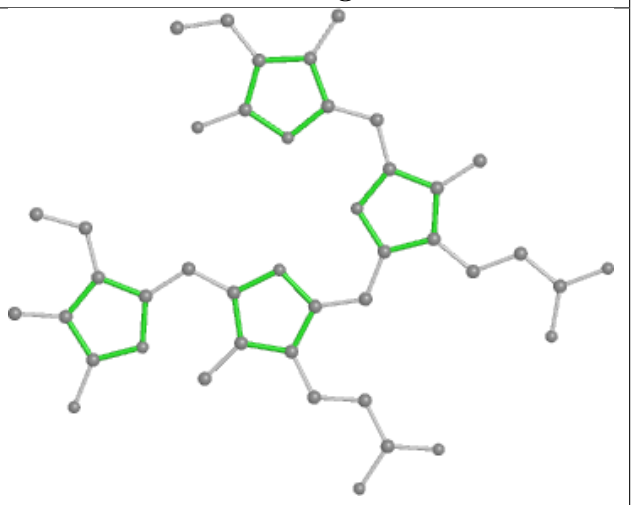
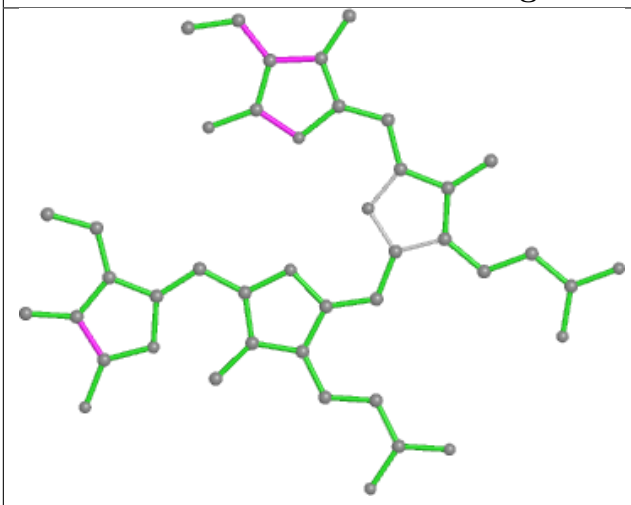


Rings

Ligand PEB ep 201



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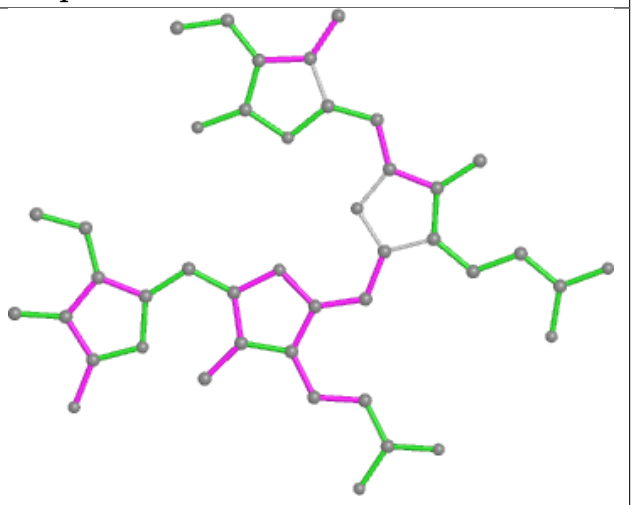

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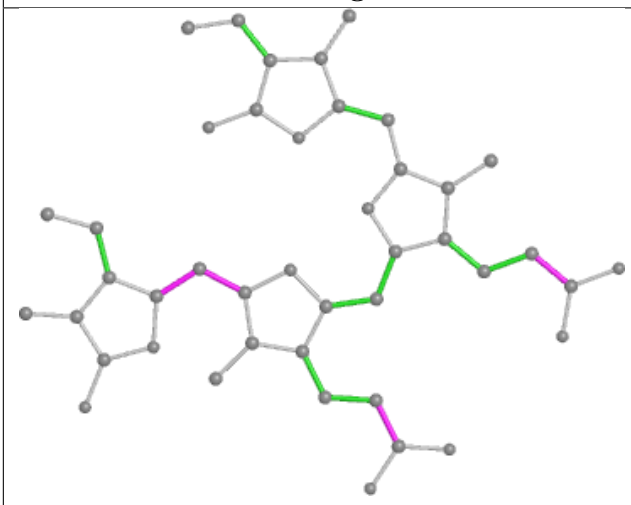

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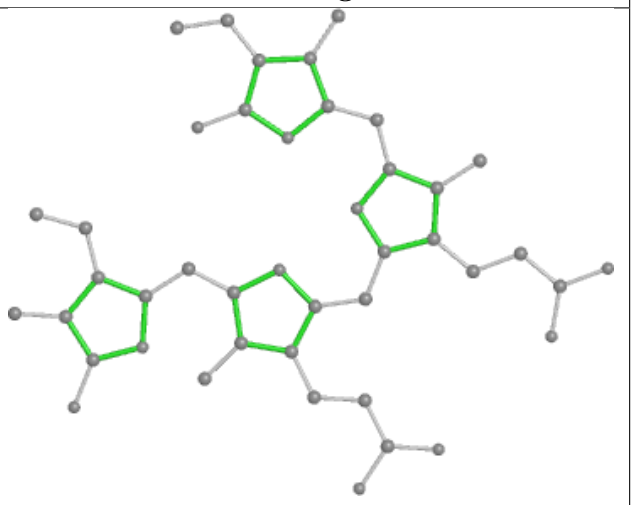

Rings

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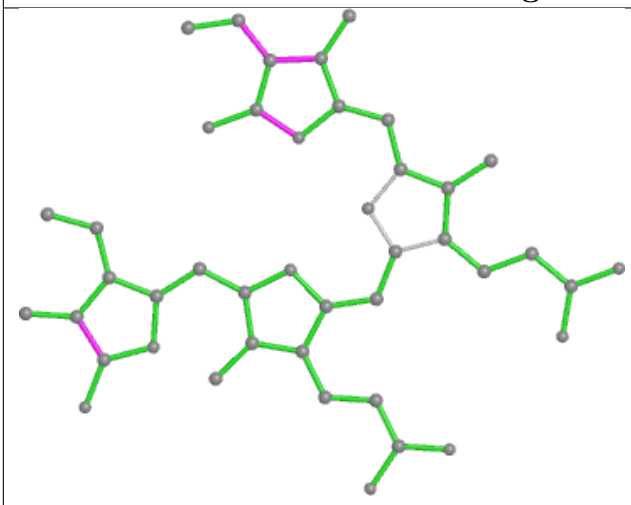

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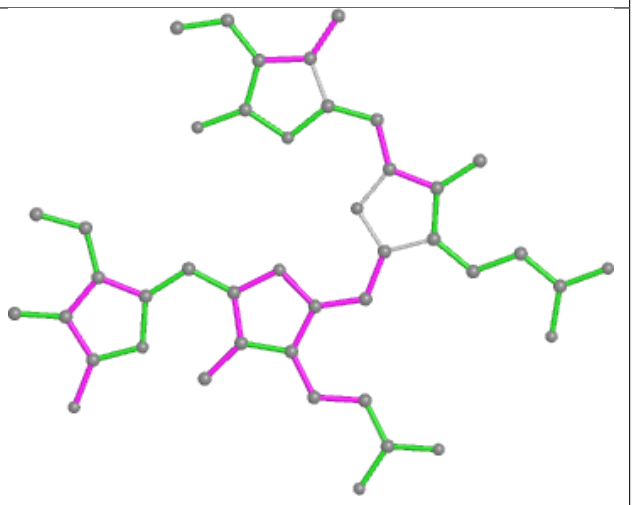

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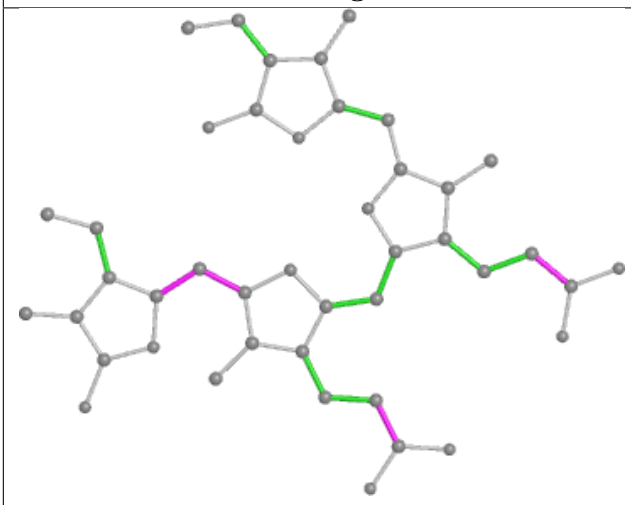

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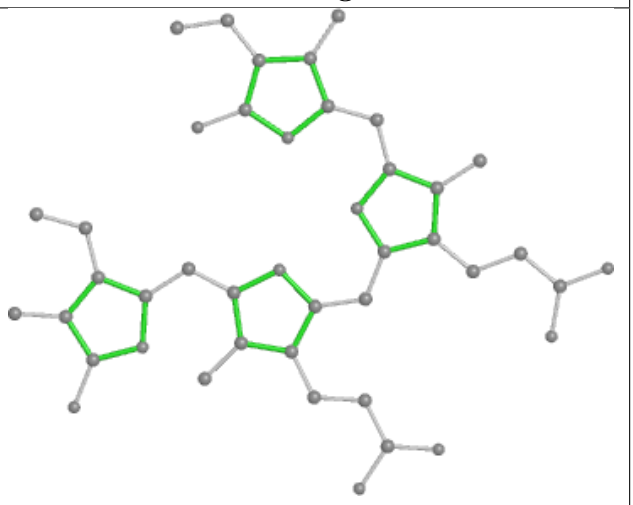
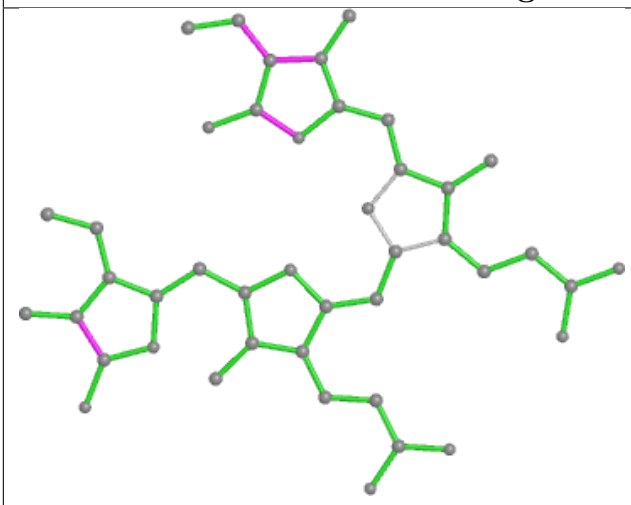


Rings

Ligand PEB dS 201



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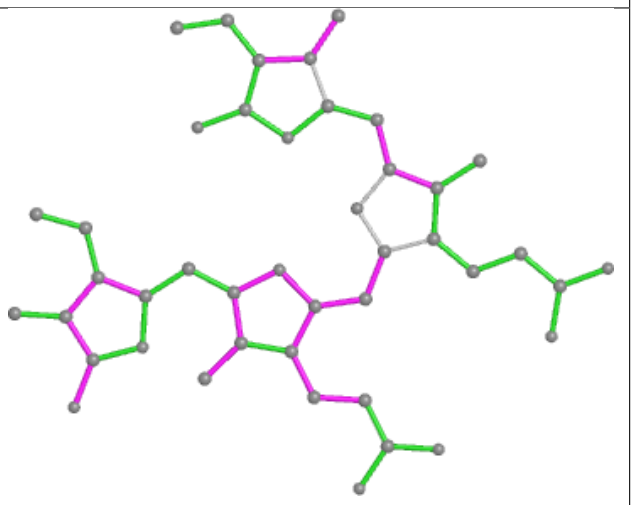
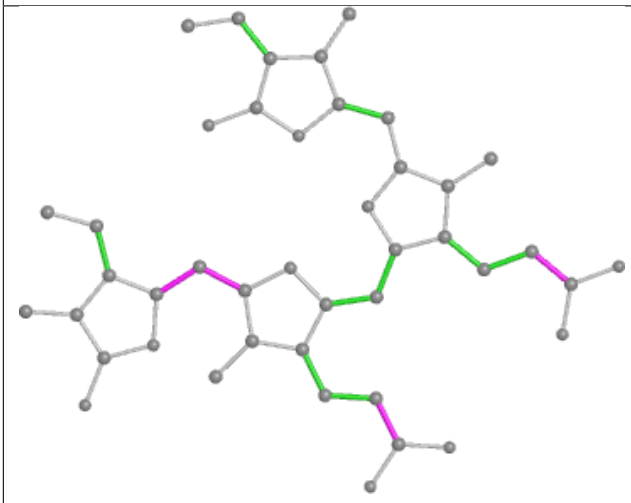


Bond angles



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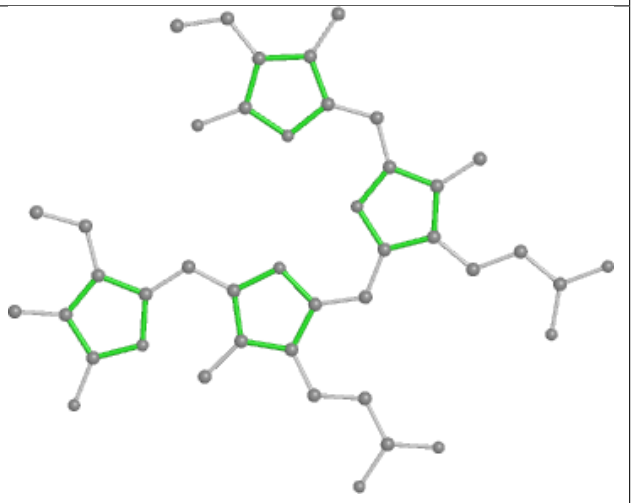
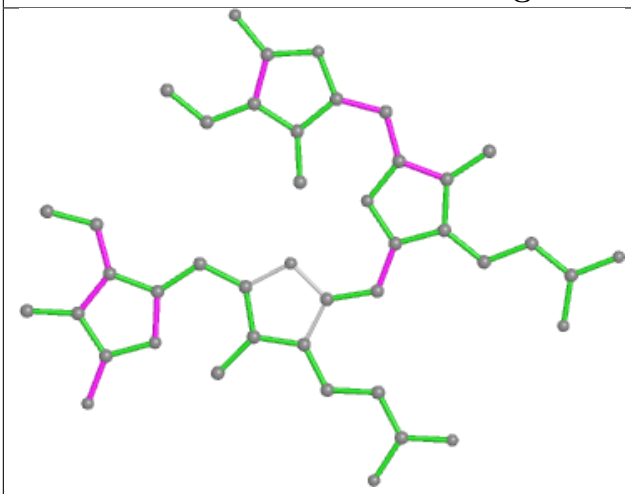


Rings

Ligand PVN bZ 304



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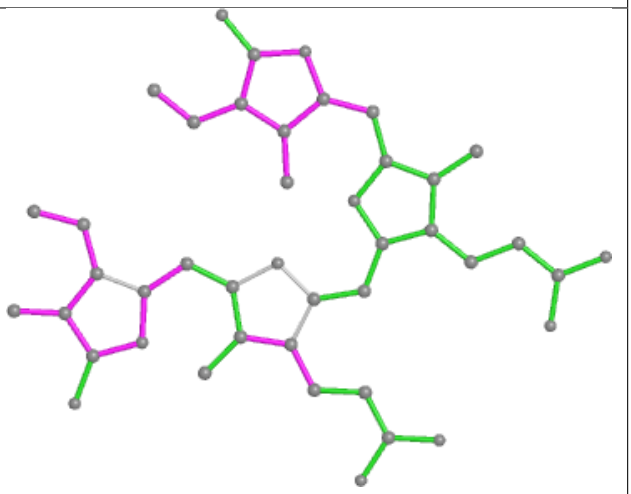

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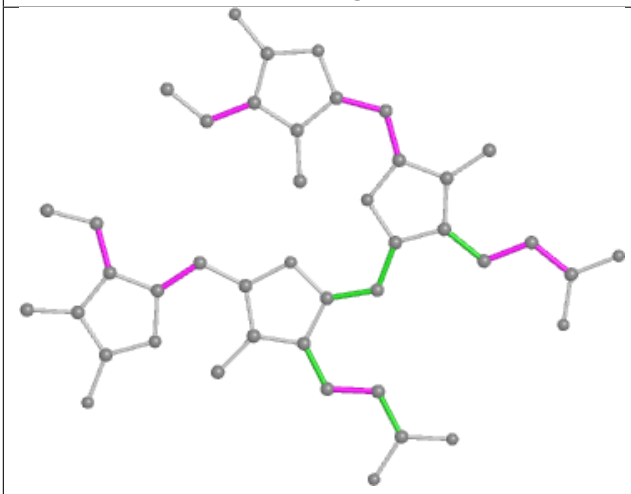

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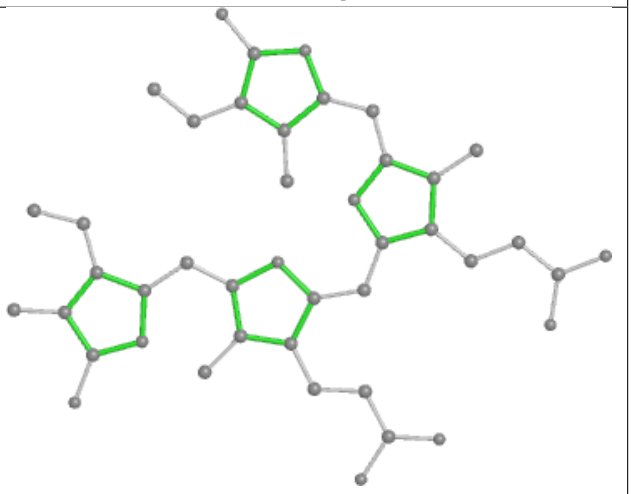

Rings

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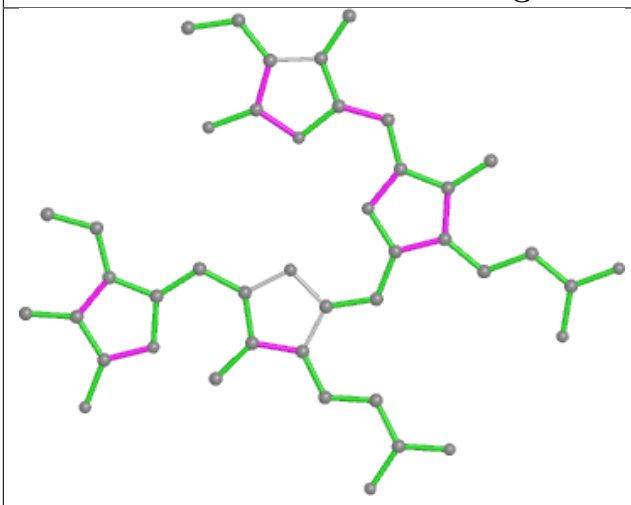

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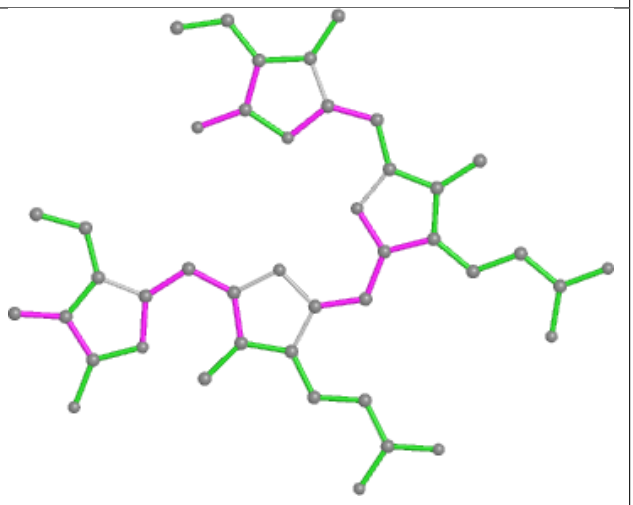

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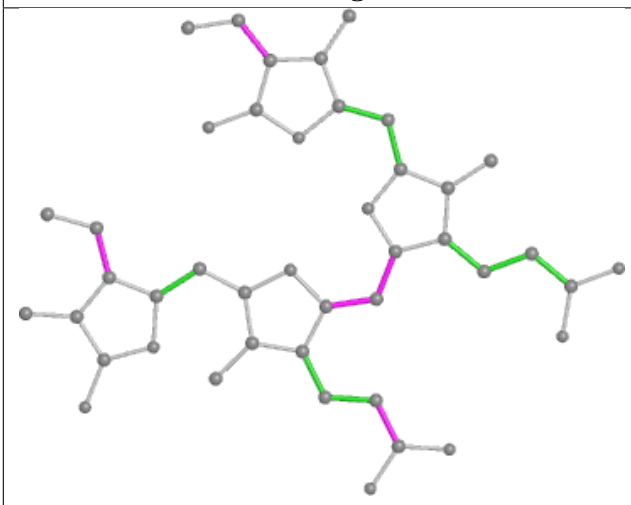

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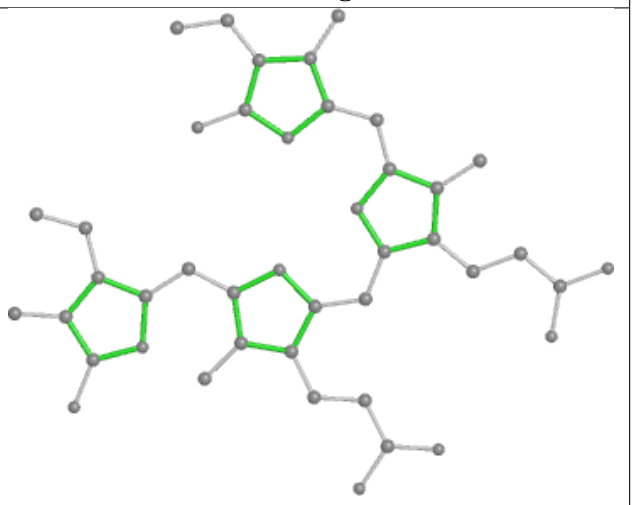
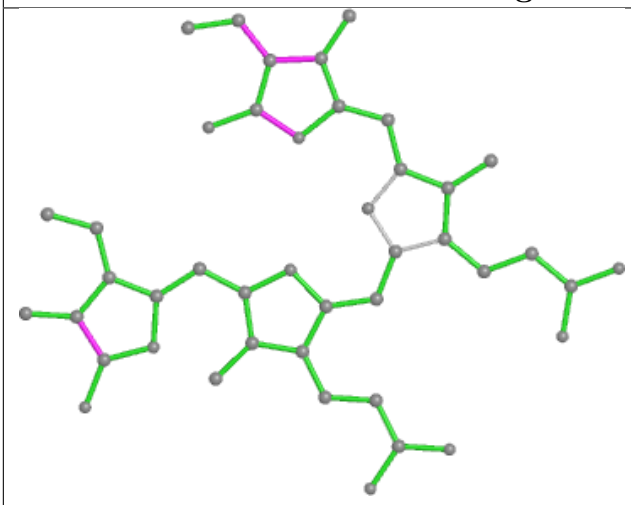


Rings

Ligand PEB V2 201



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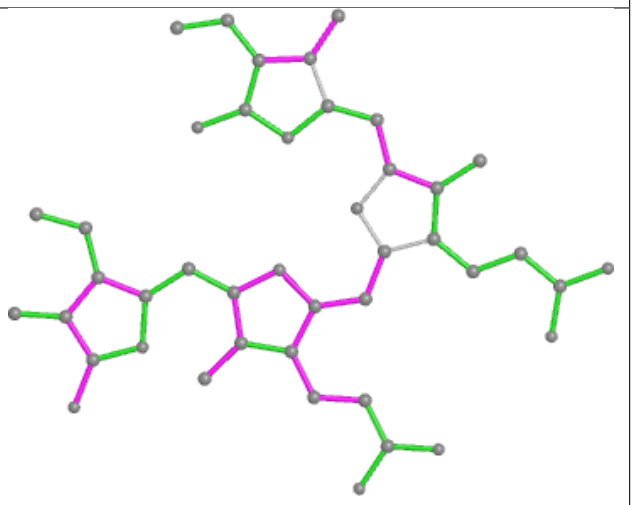

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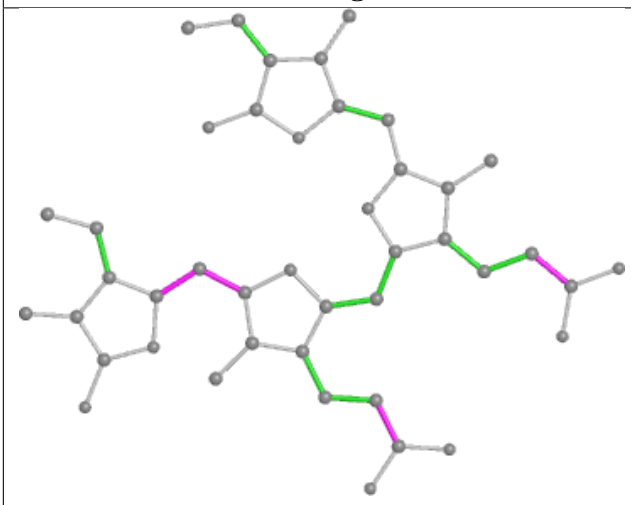

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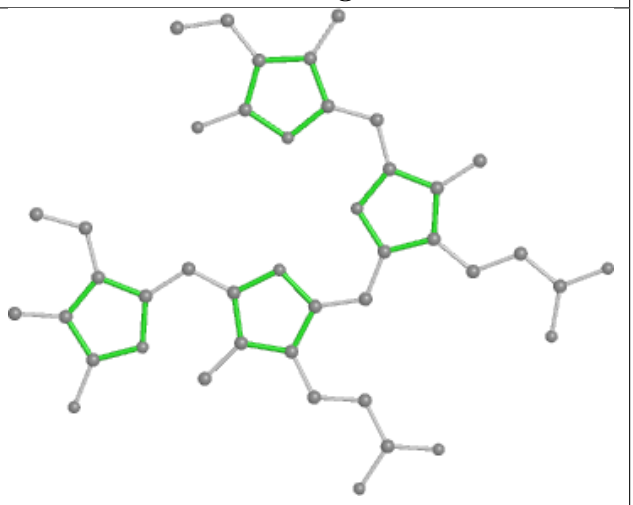

Rings

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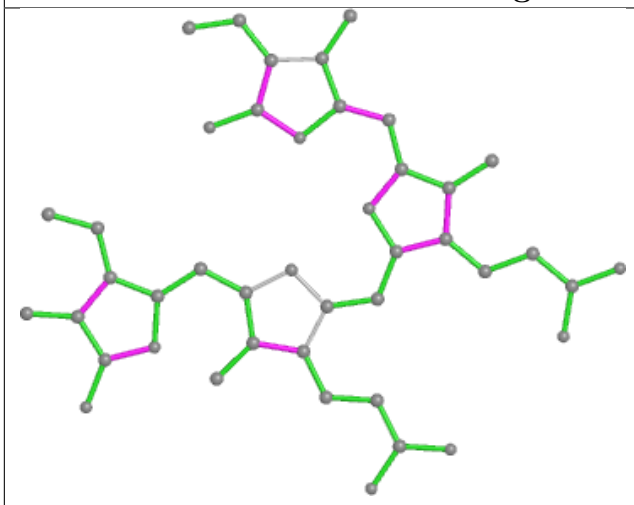

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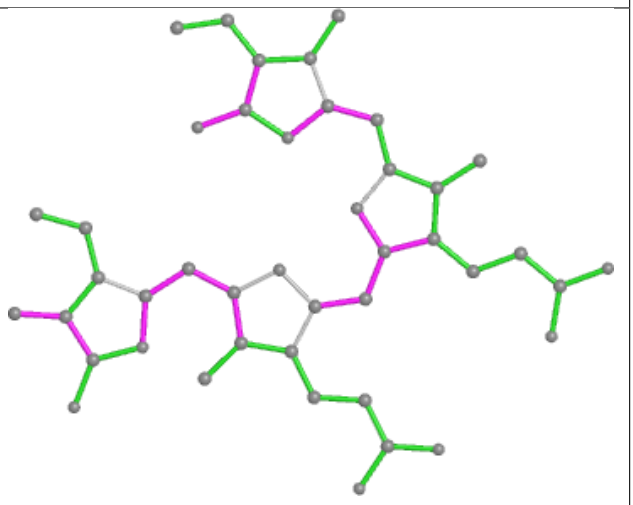

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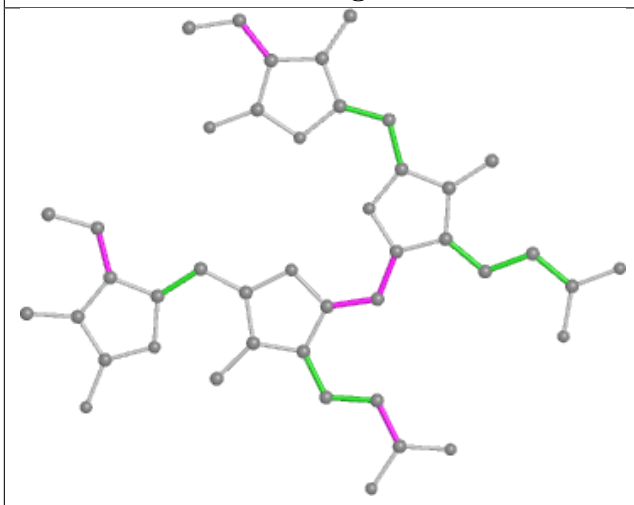

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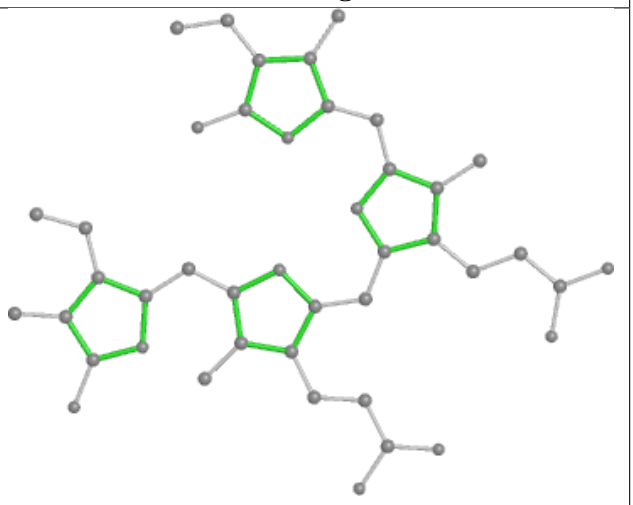
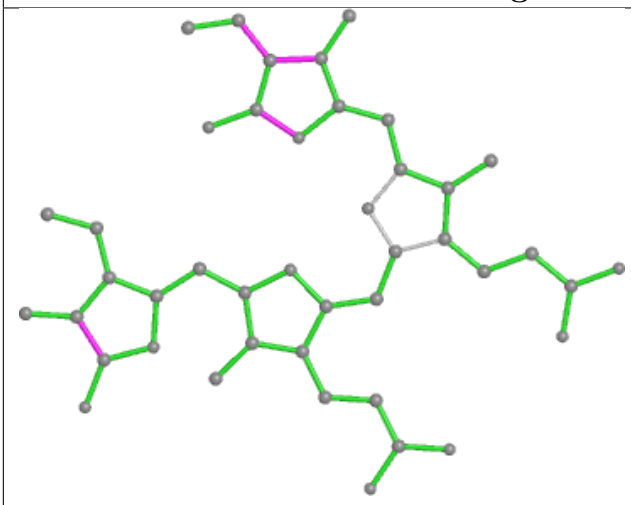


Rings

Ligand PEB o2 1001



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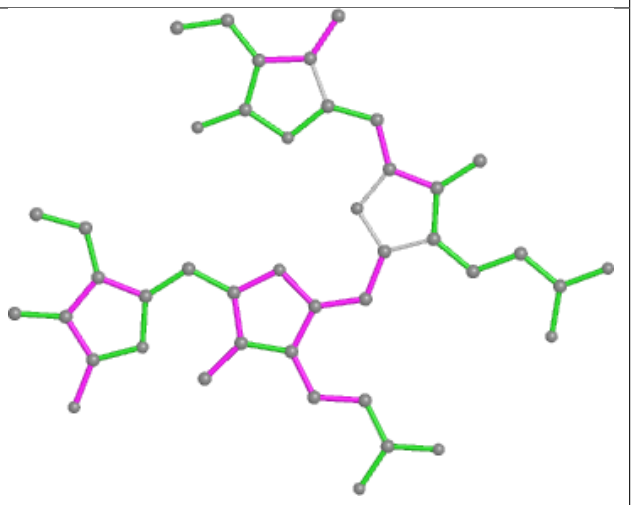
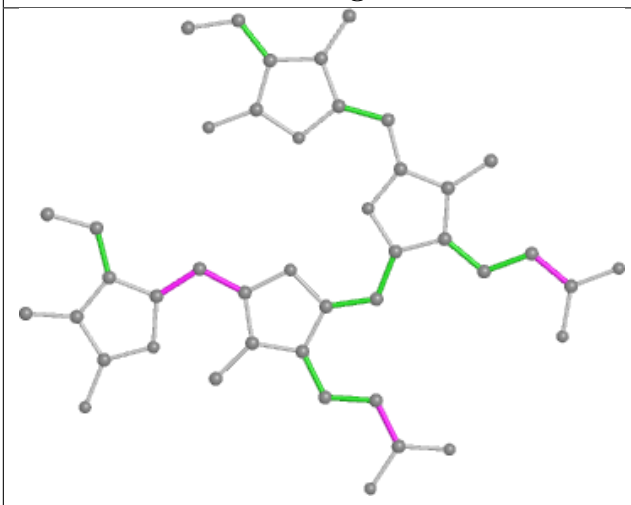


Bond angles



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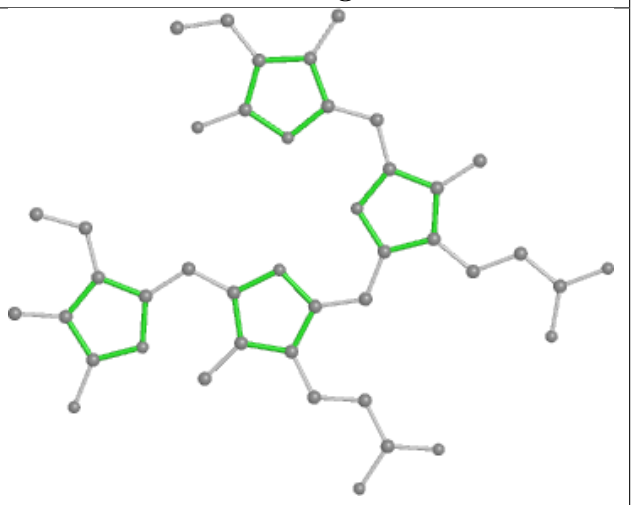
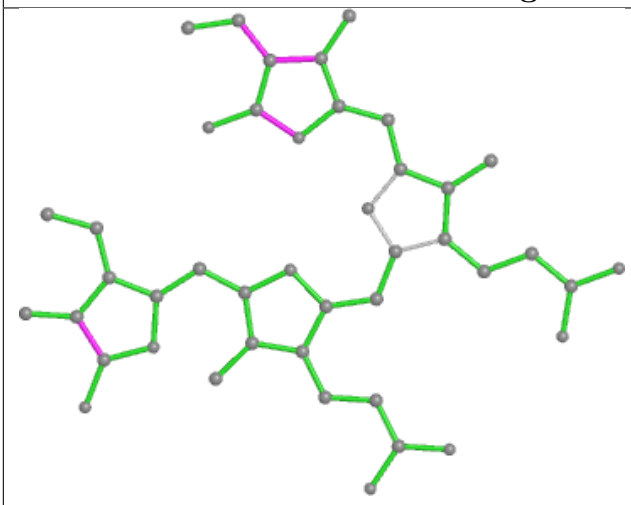


Rings

Ligand PEB a5 201



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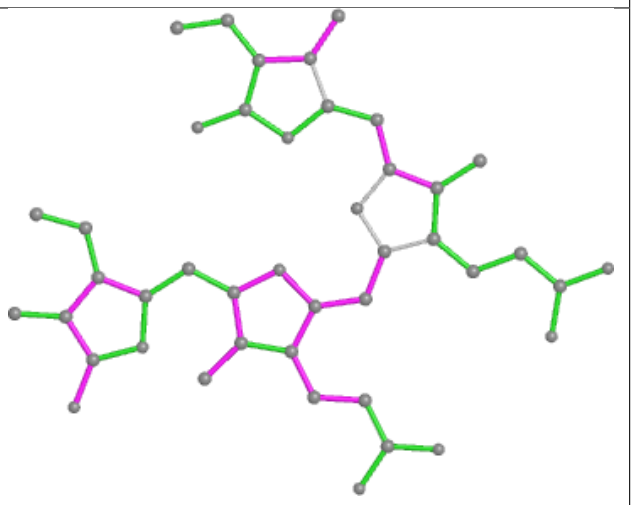
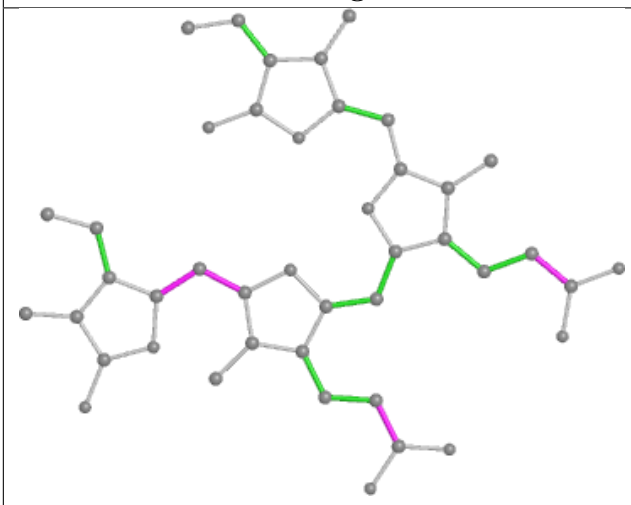


Bond angles



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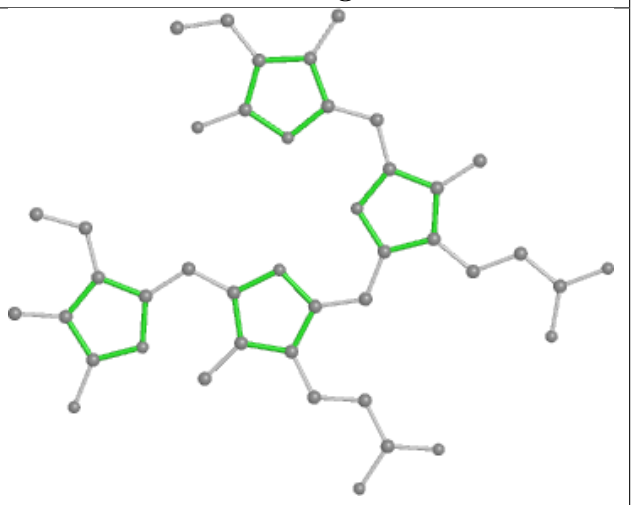
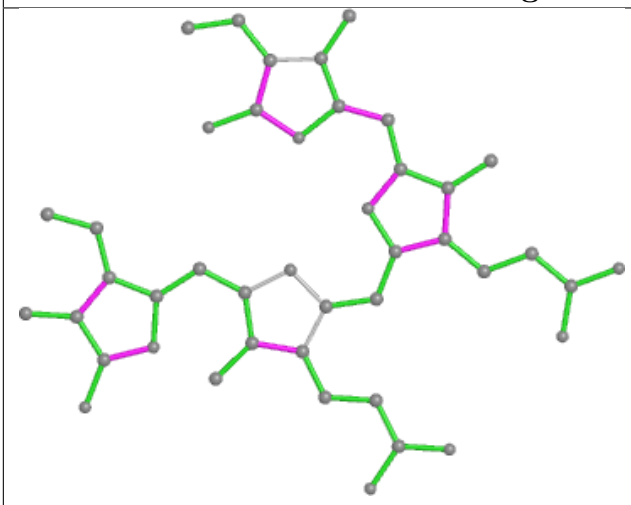
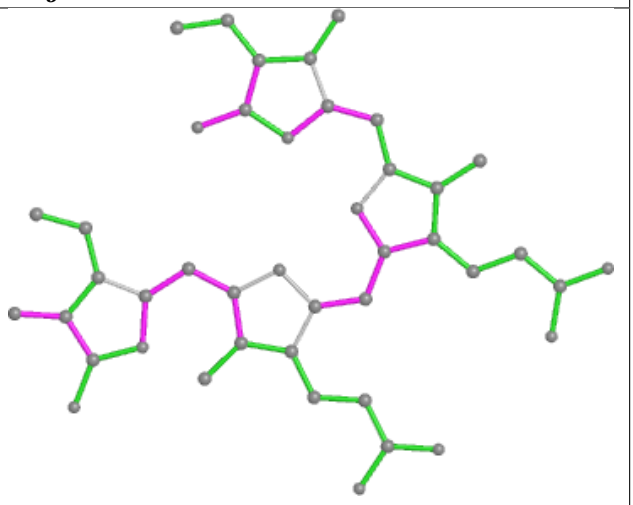


Rings

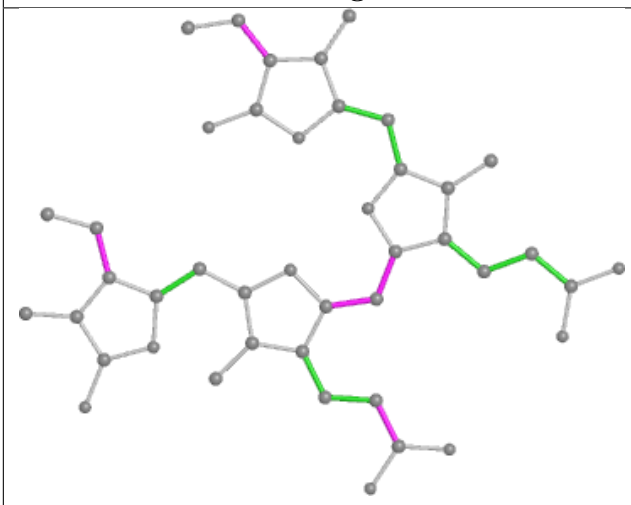
Ligand PUB j3 202



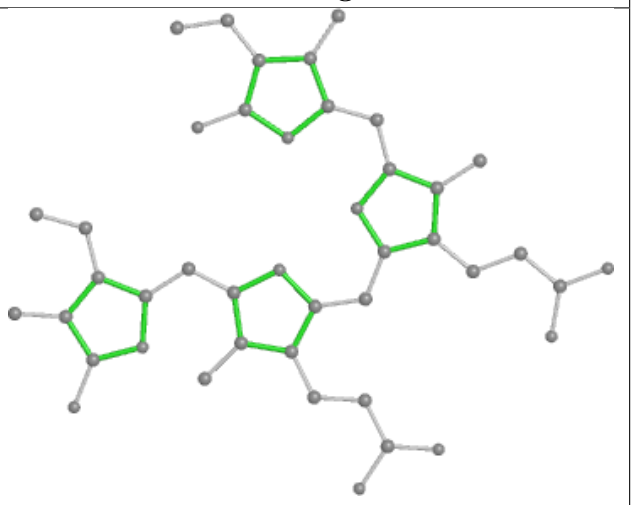
Bond lengths



Bond angles

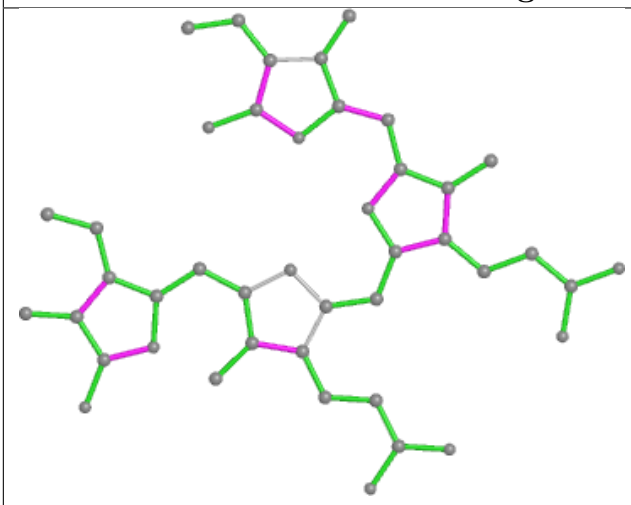


Torsions



Rings

Ligand PUB gy 306



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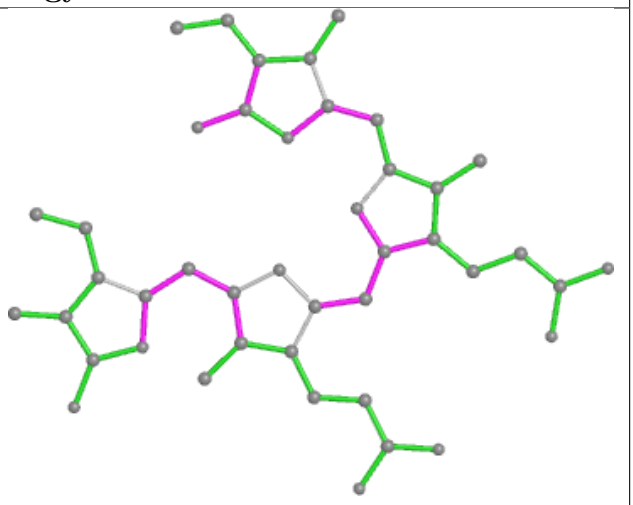

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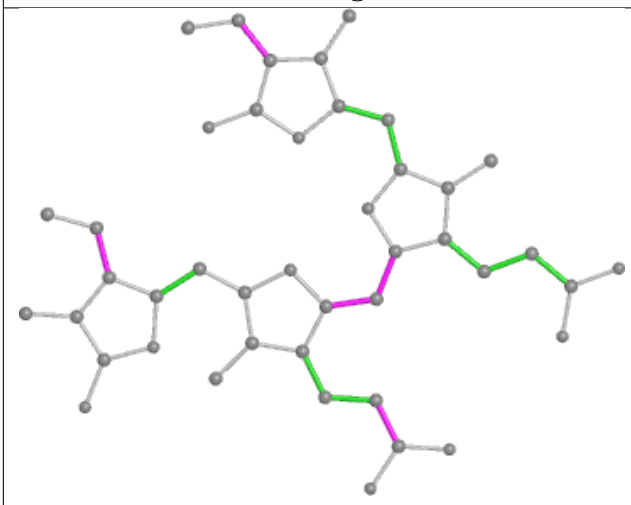

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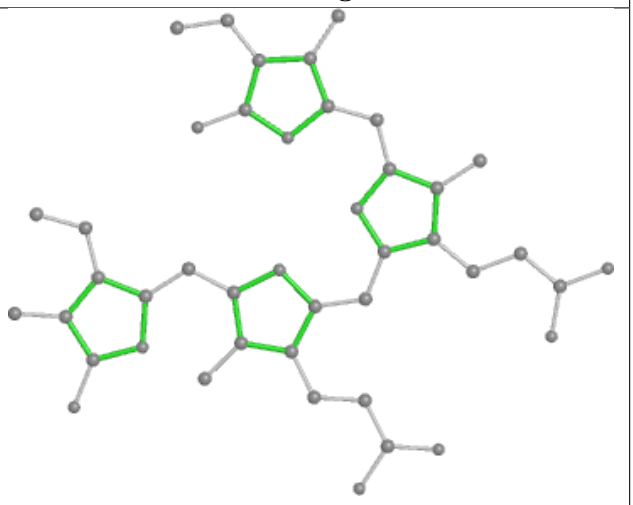
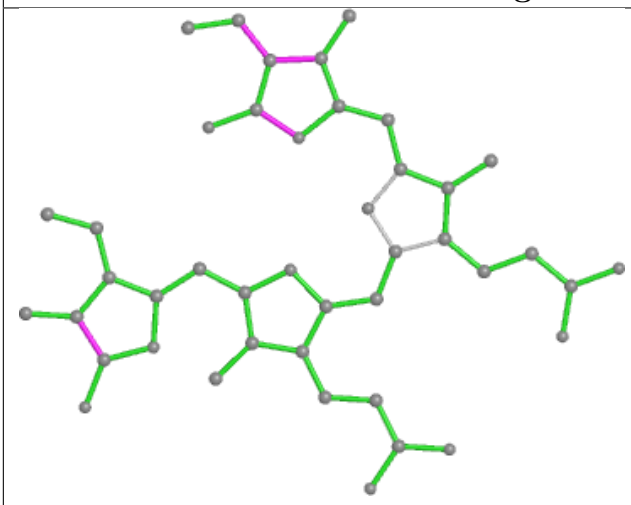


Rings

Ligand PEB dD 202



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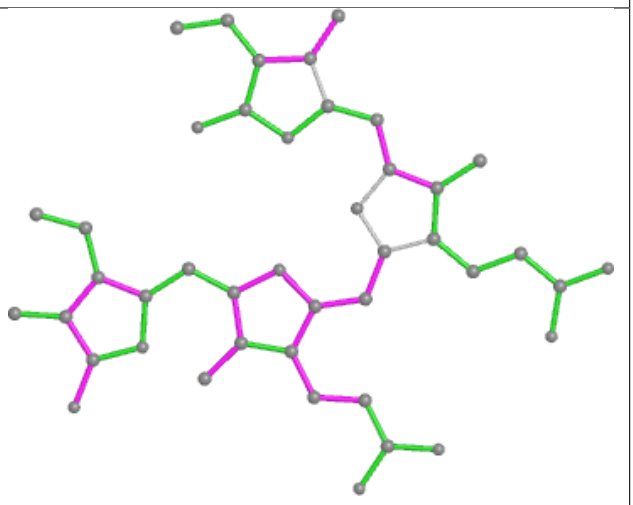

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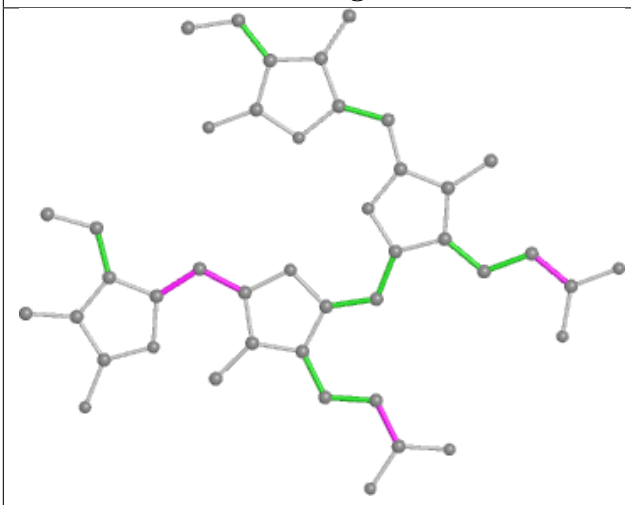

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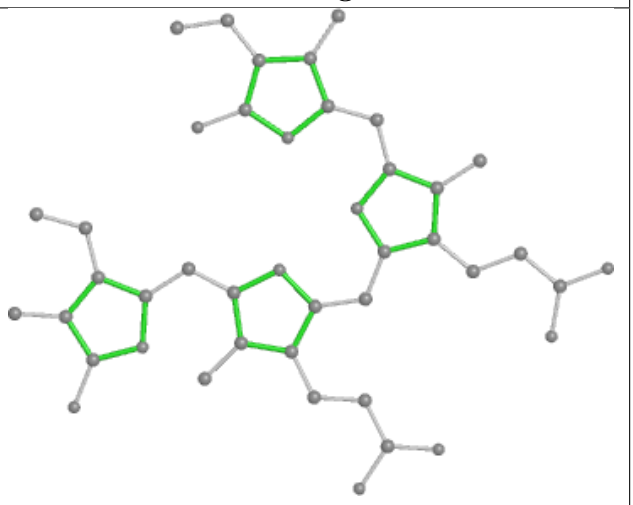
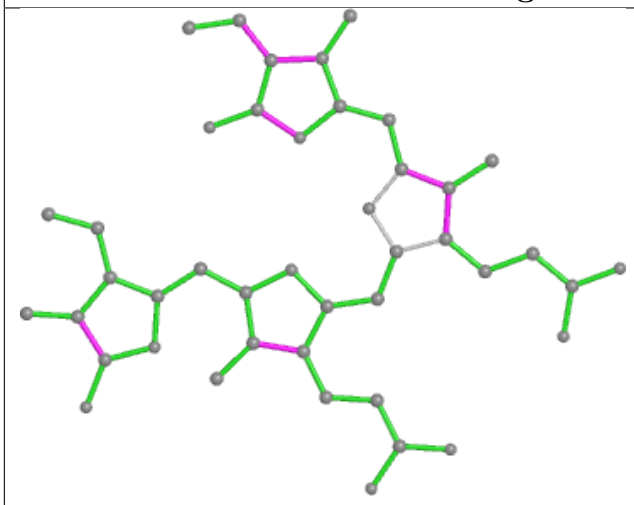


Rings

Ligand PEB B5 202



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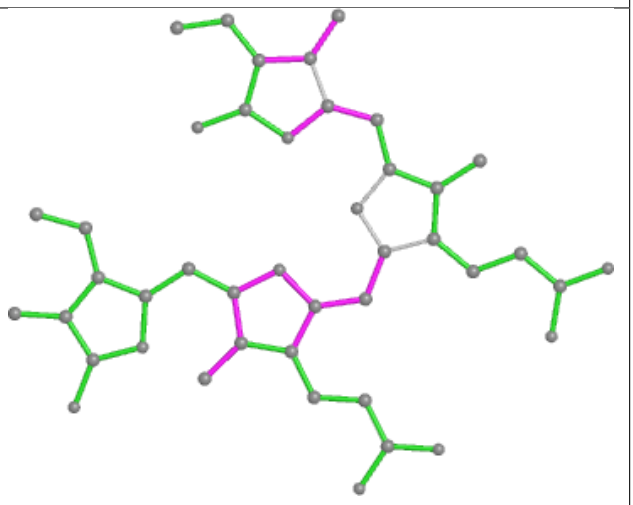

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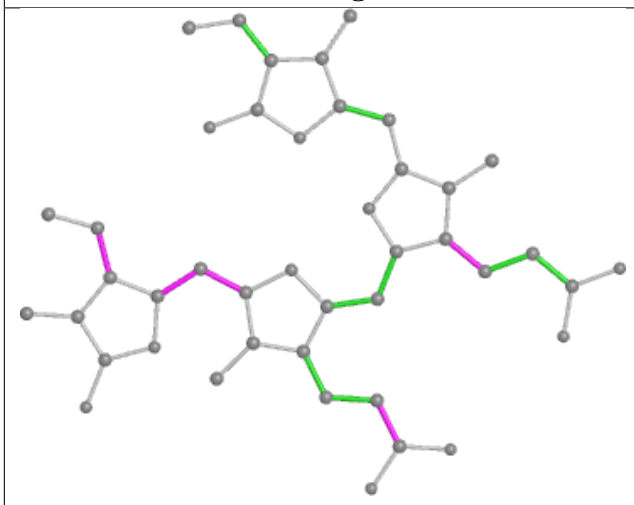

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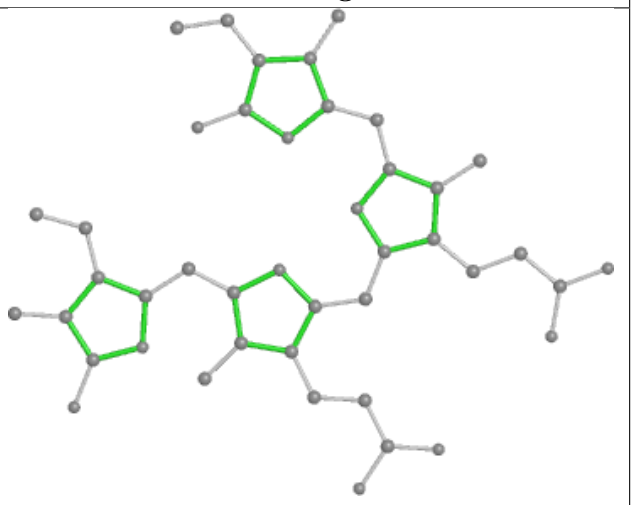
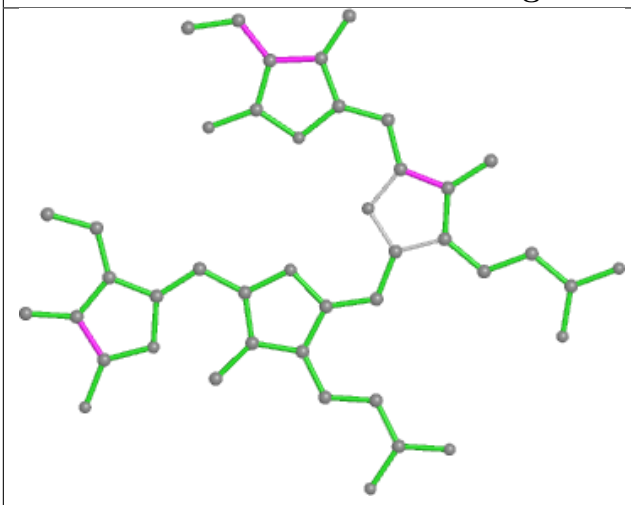


Rings

Ligand PEB ct 202



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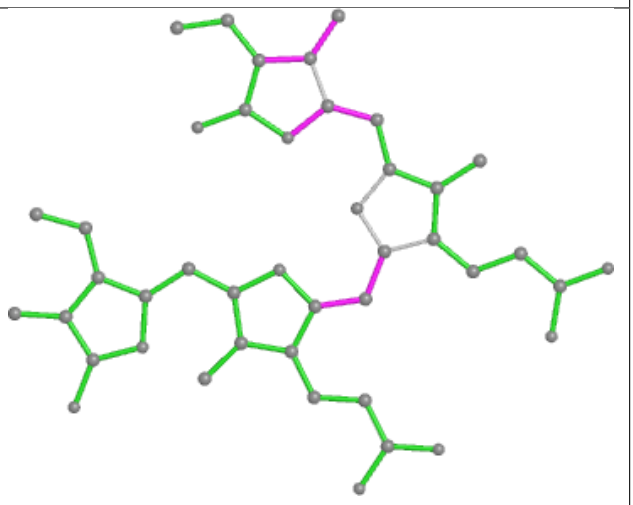

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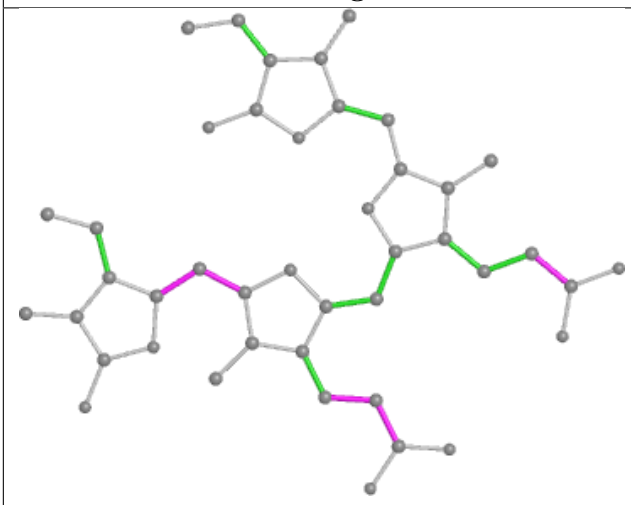

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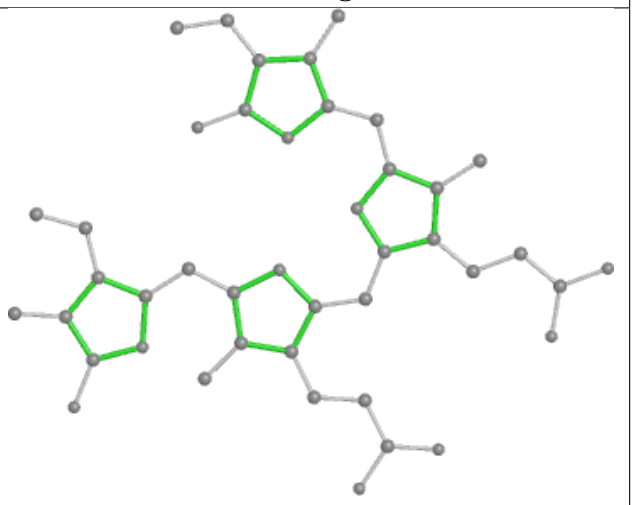

Rings

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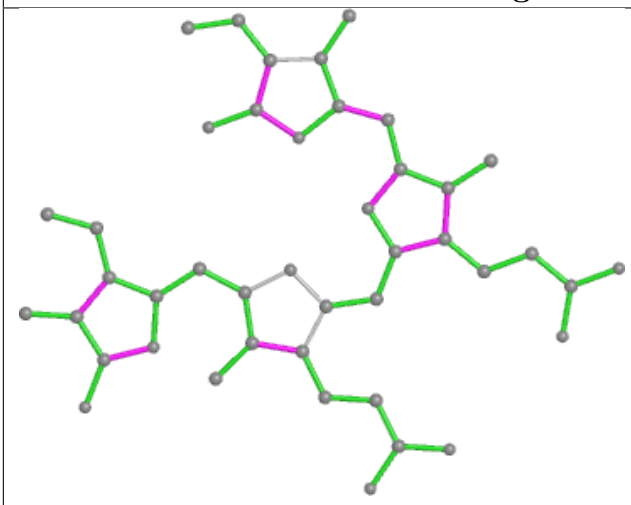

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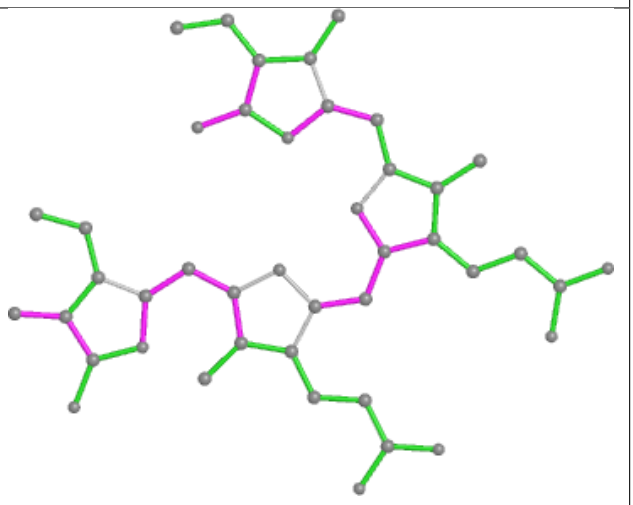

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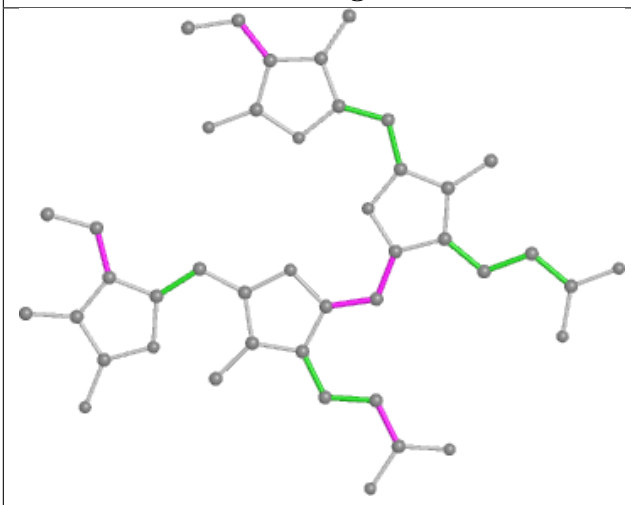

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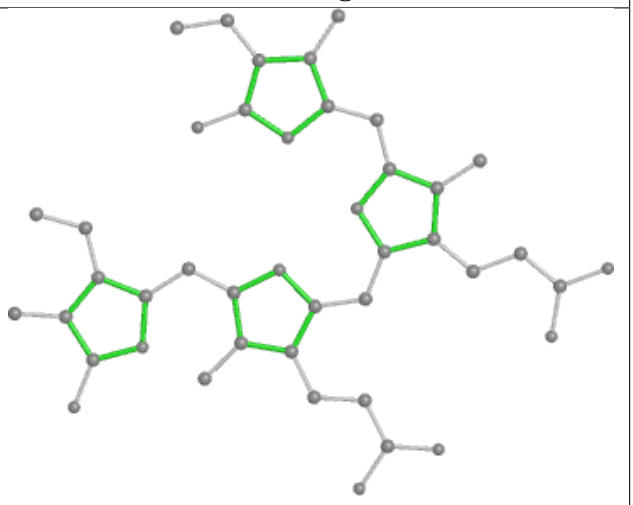
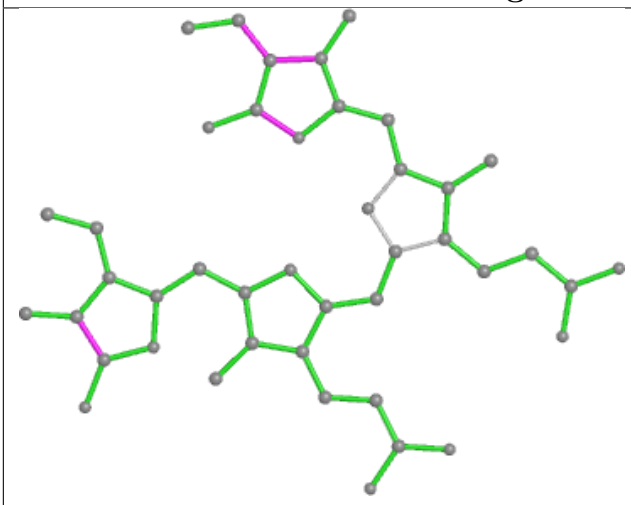


Rings

Ligand PEB C3 1001



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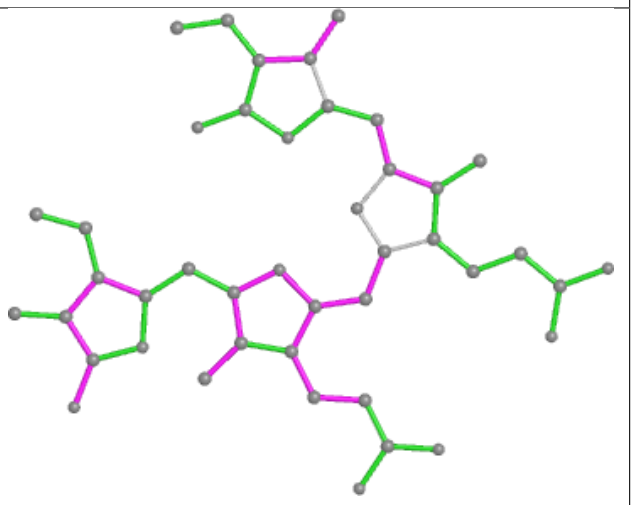

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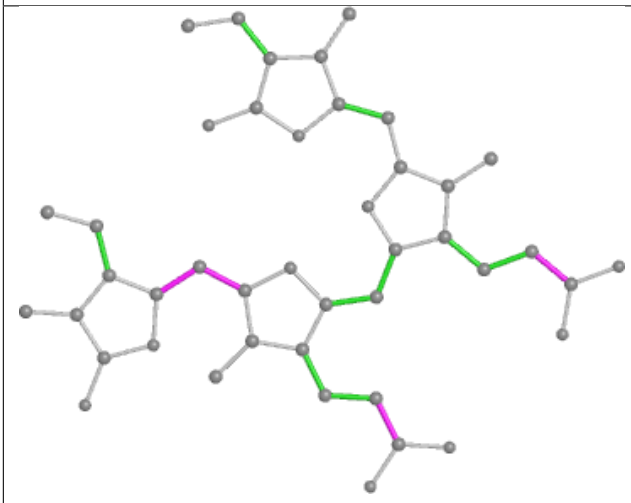

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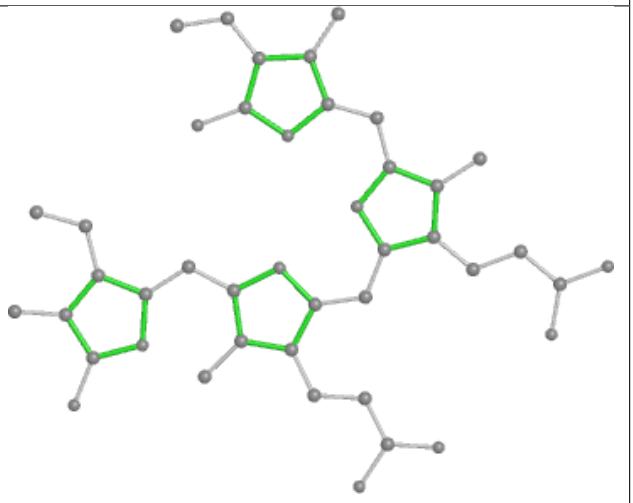
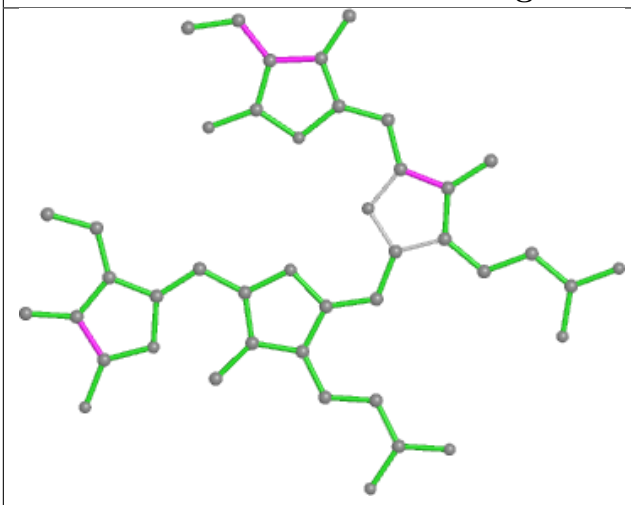


Rings

Ligand PEB C5 202



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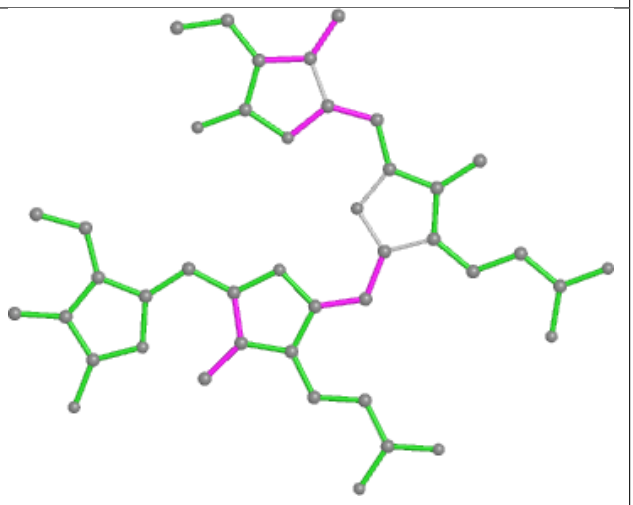

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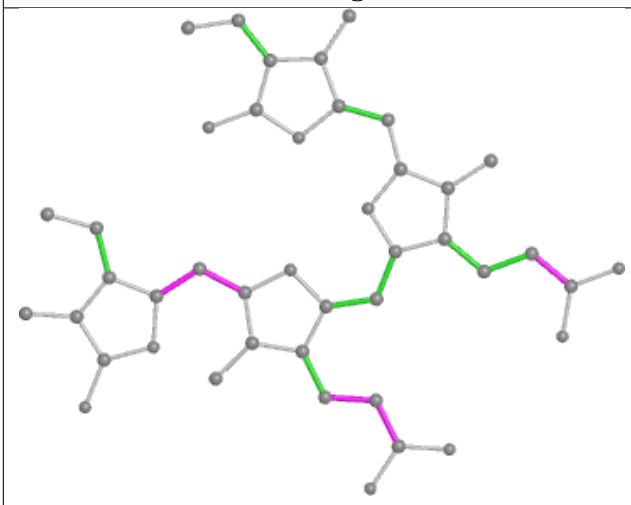

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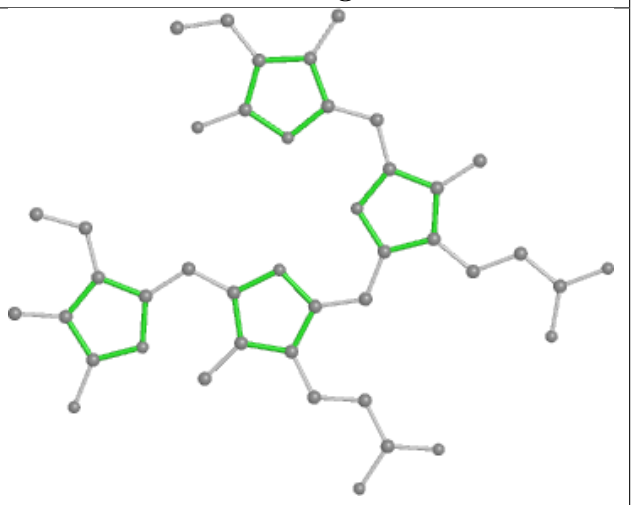
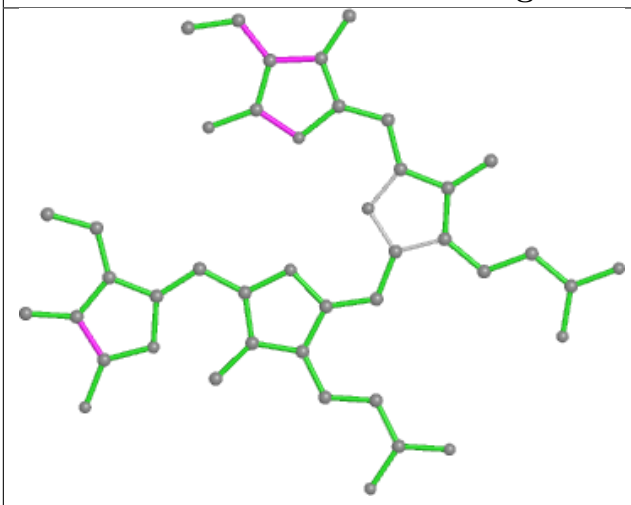


Rings

Ligand PEB P7 201



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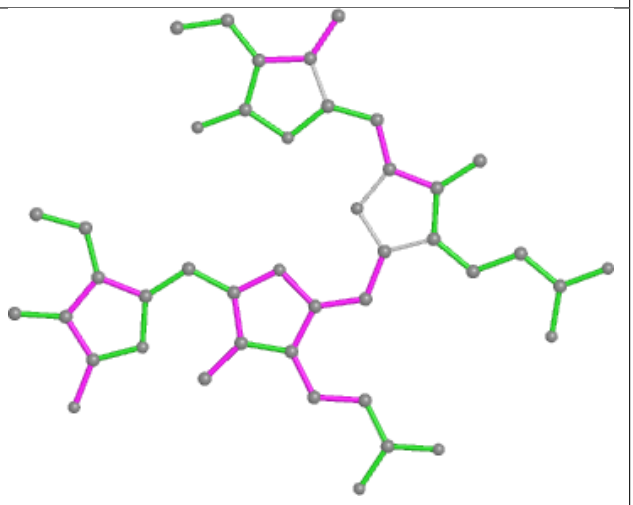

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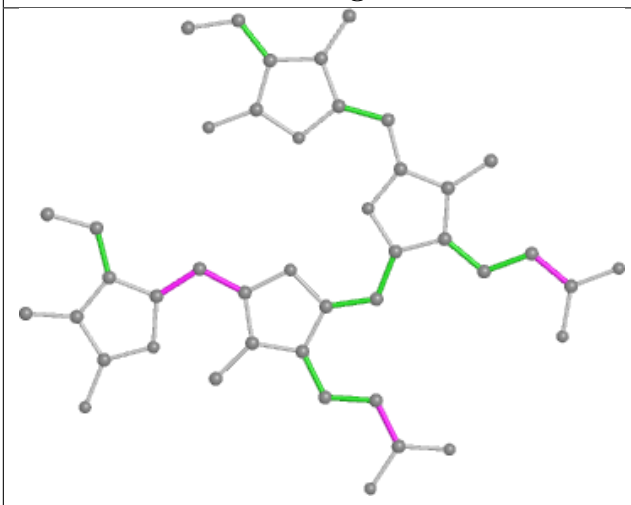

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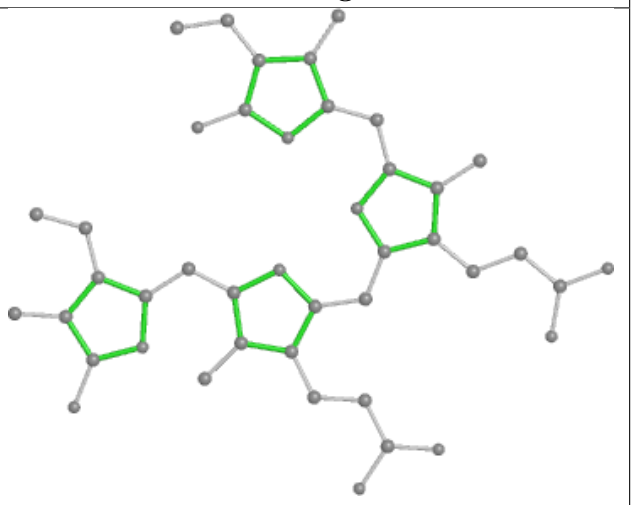
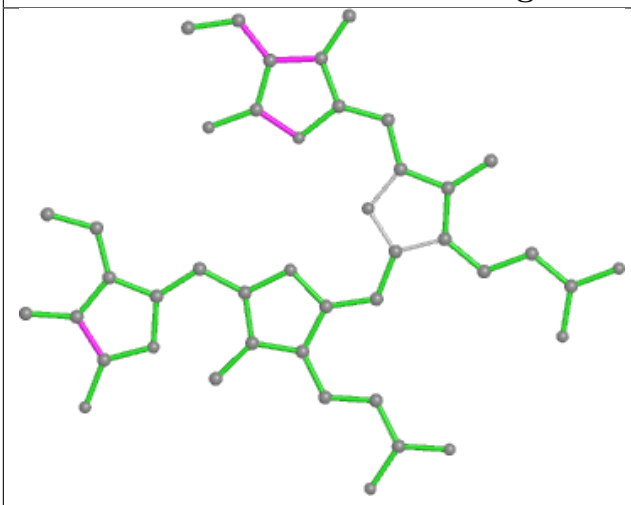


Rings

Ligand PEB aP 201



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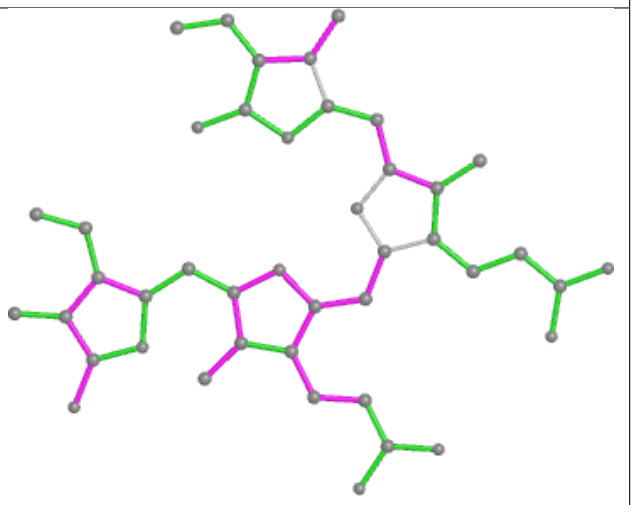

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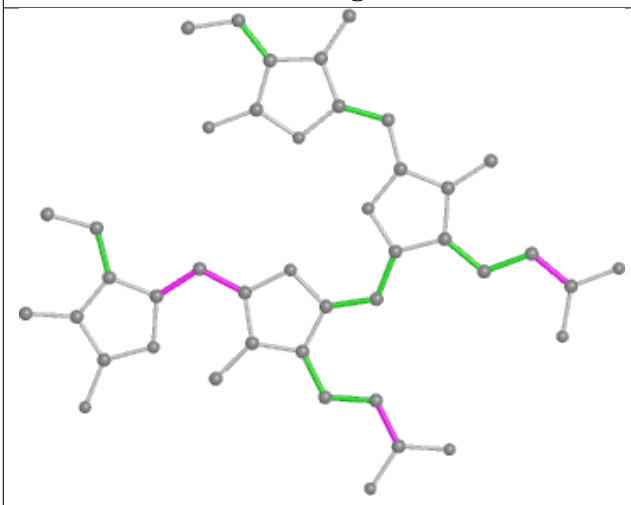

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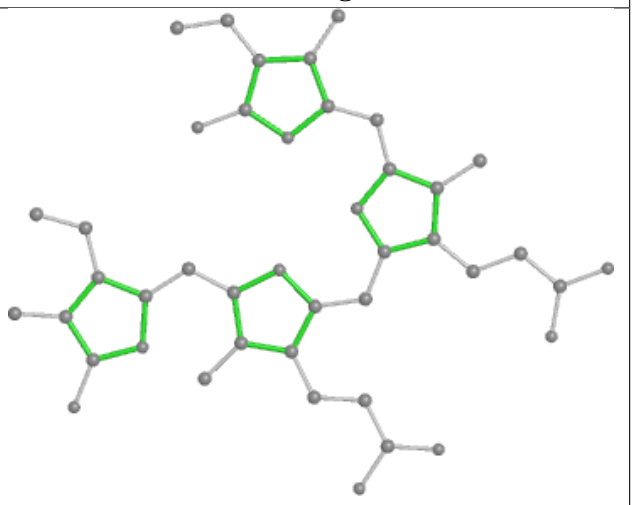
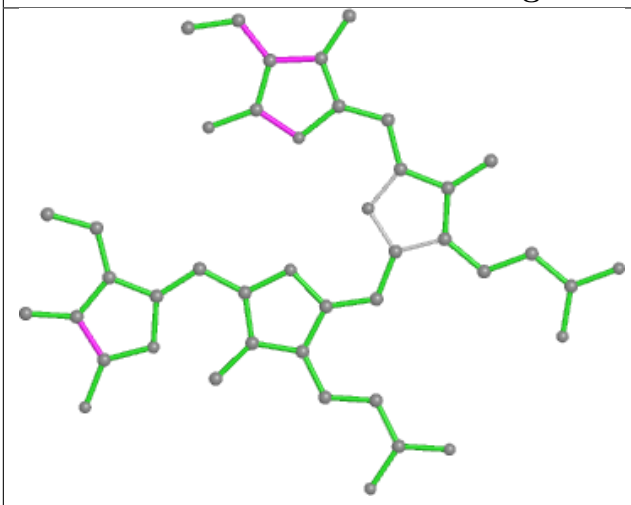


Rings

Ligand PEB ct 201



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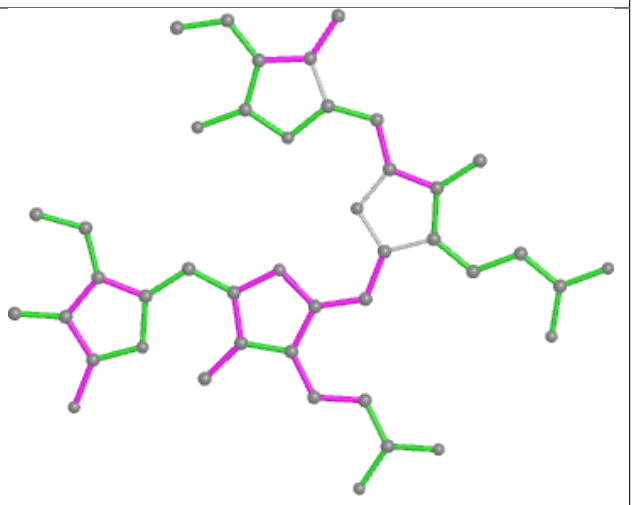

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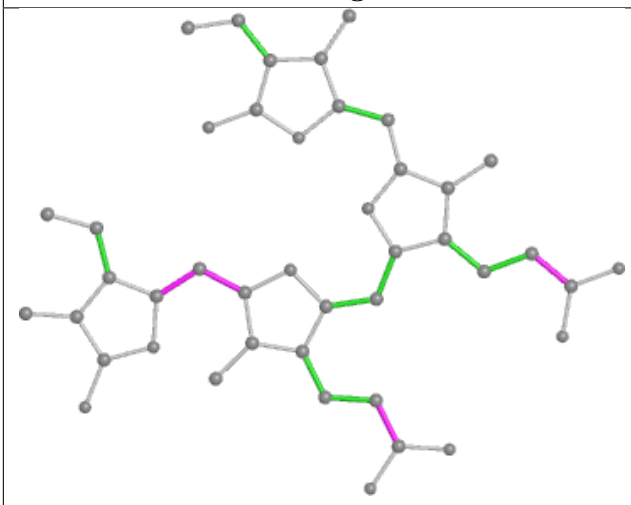

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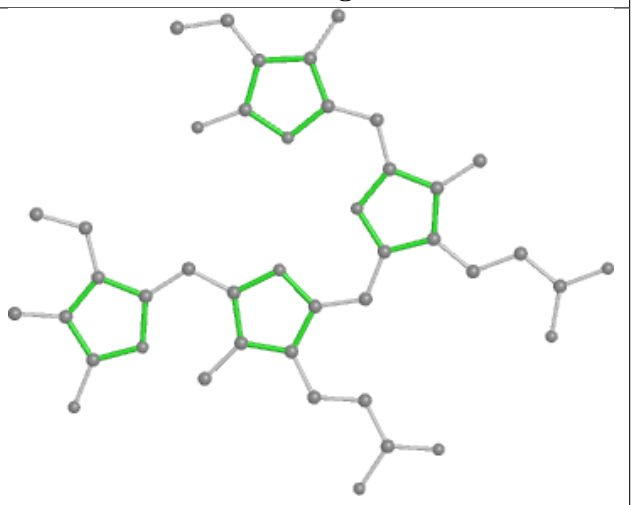
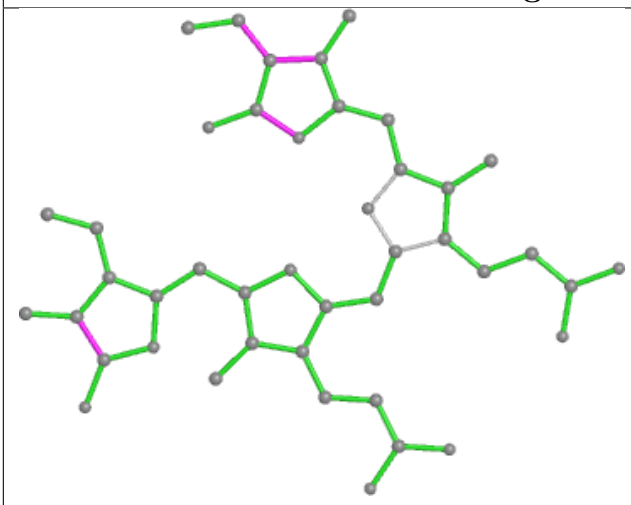


Rings

Ligand PEB l8 201



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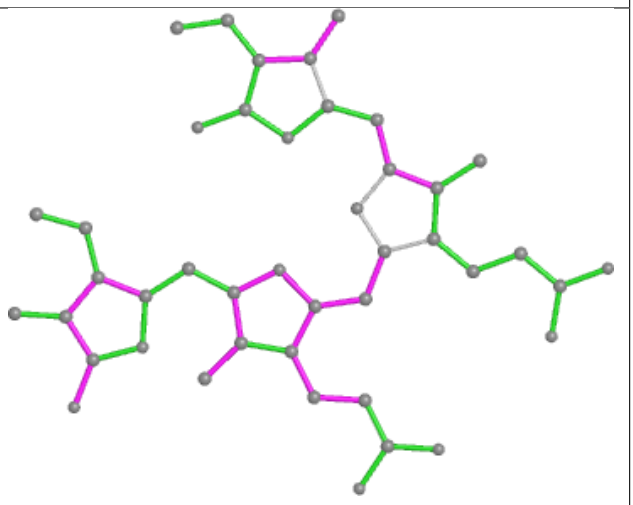

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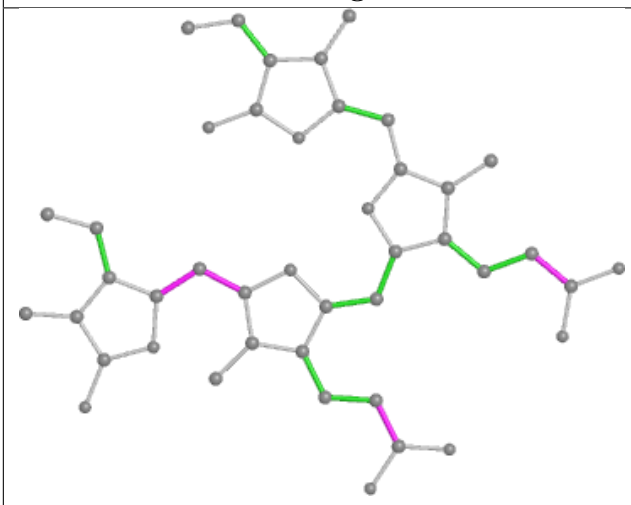

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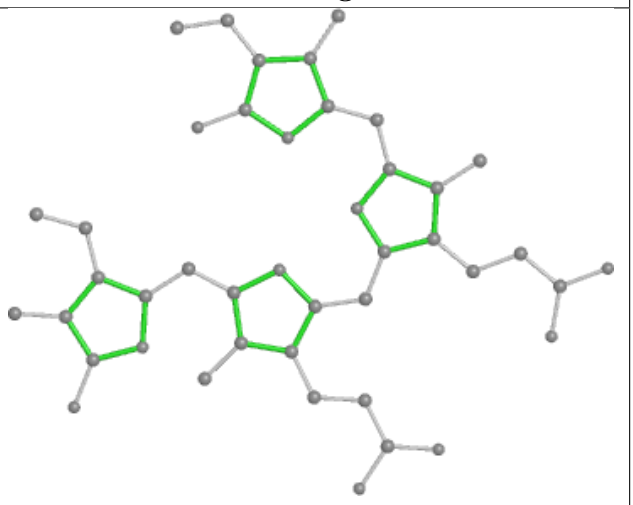
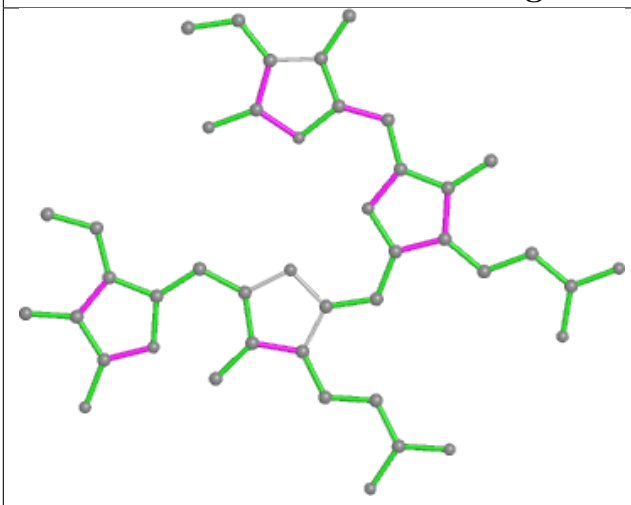


Rings

Ligand PUB ff 203



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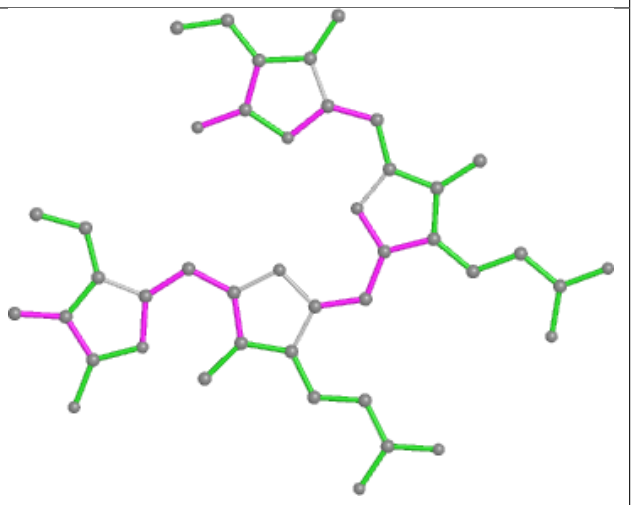
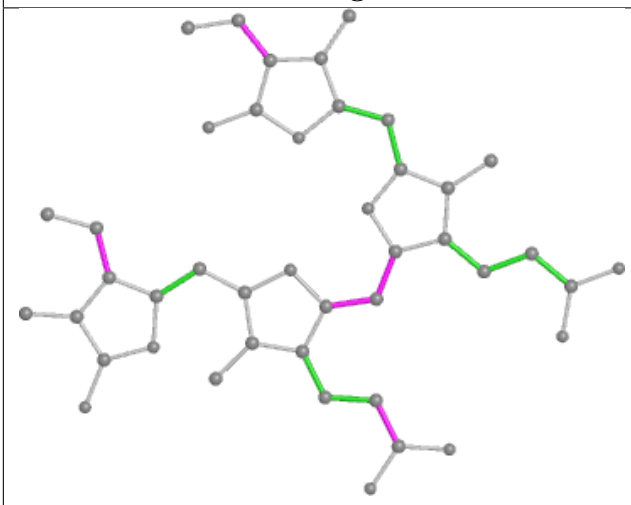


Bond angles



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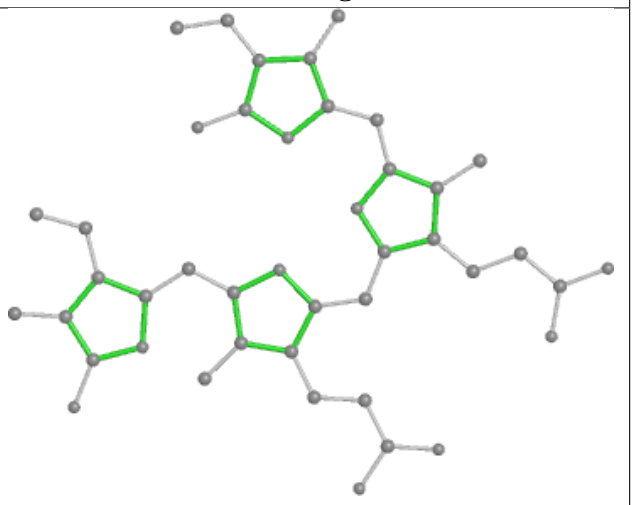
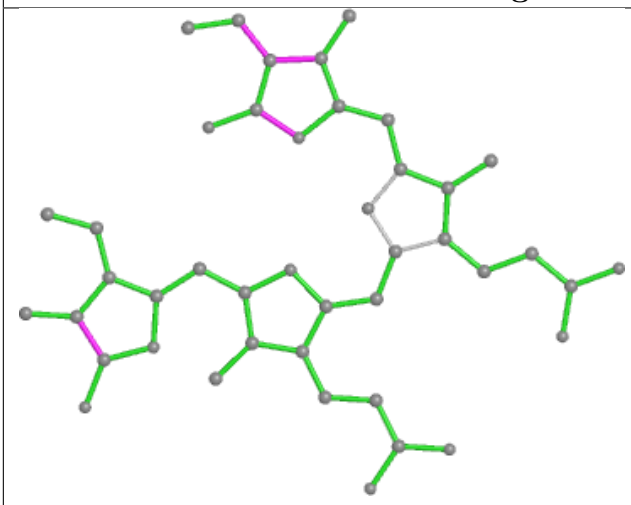
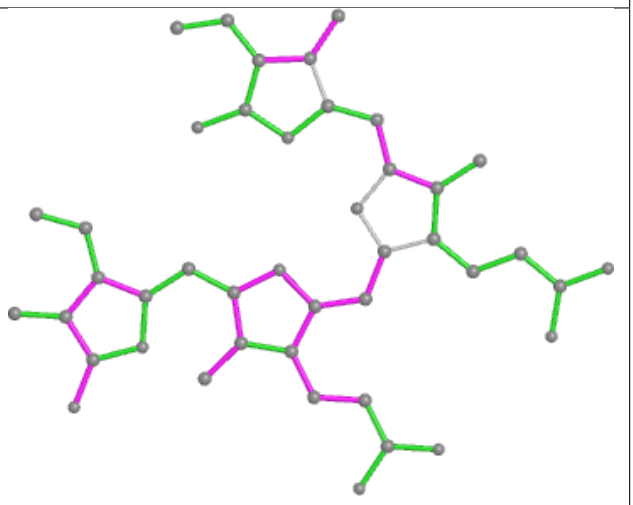


Rings

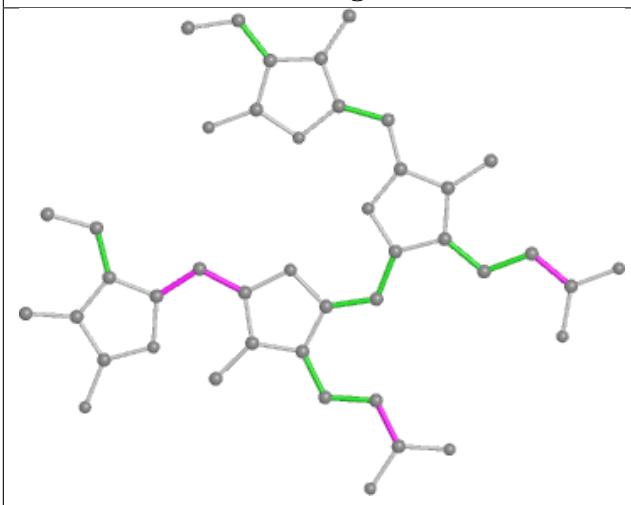
Ligand PEB cW 201



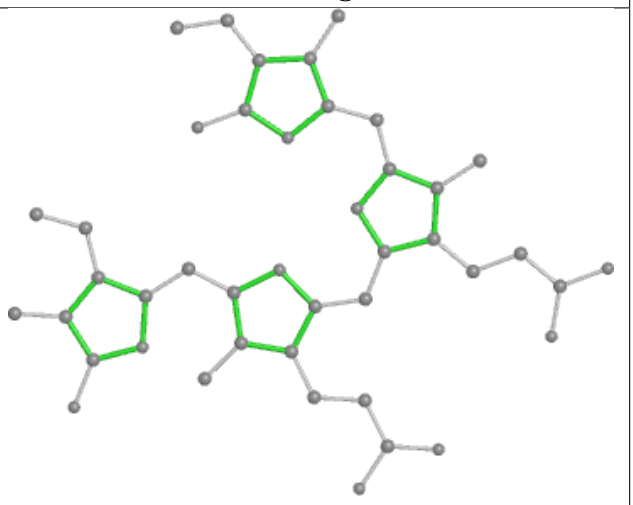
Bond lengths



Bond angles

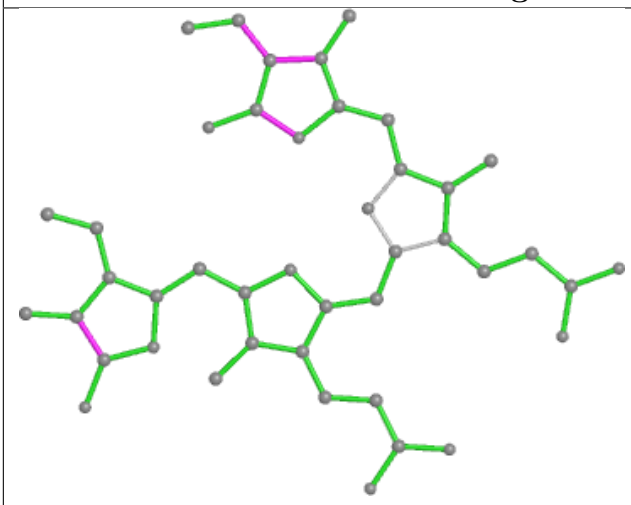


Torsions



Rings

Ligand PEB iB 1001



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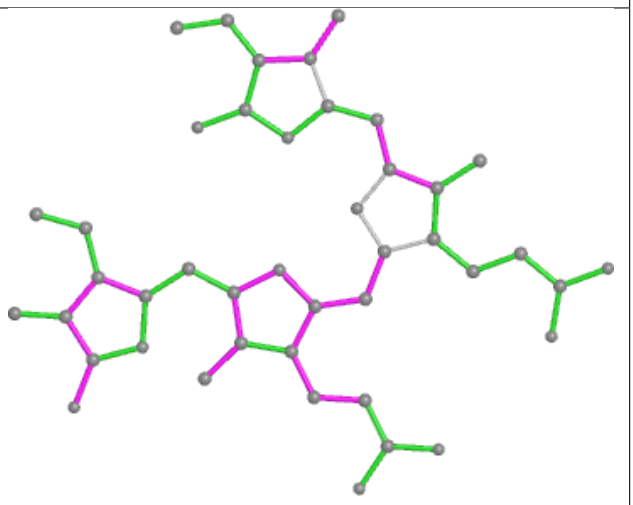

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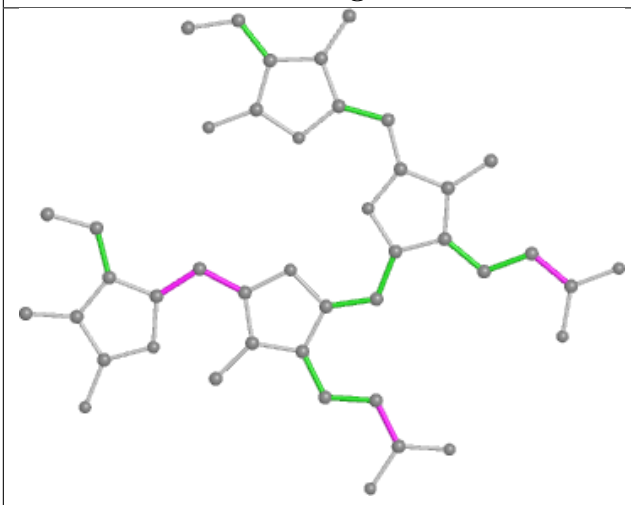

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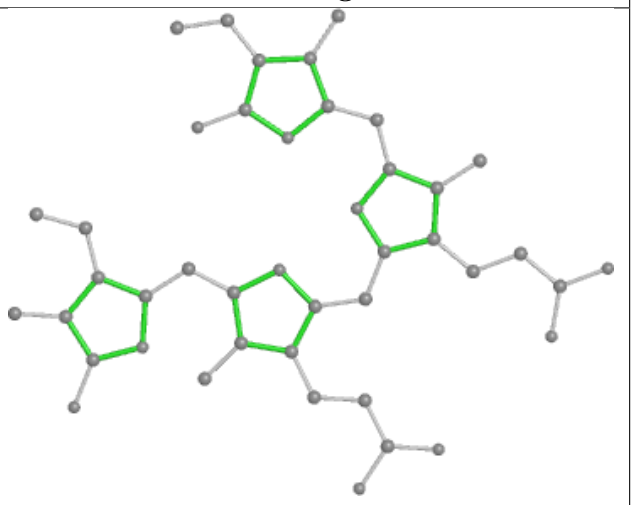
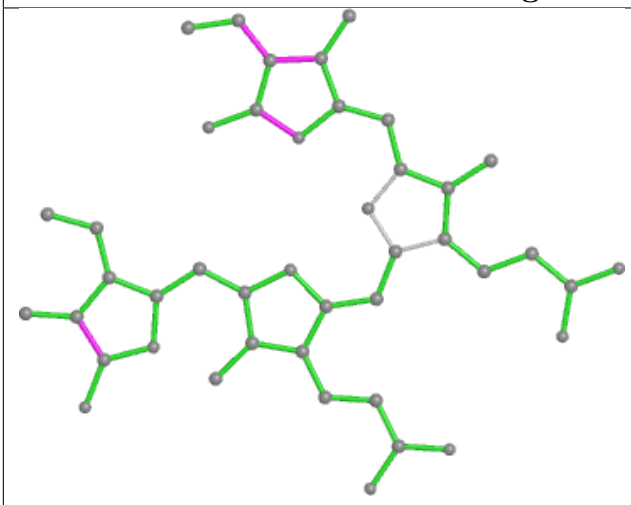


Rings

Ligand PEB gs 201



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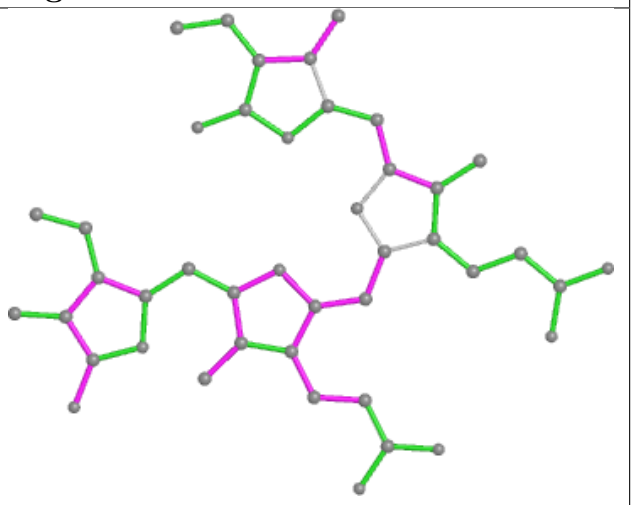

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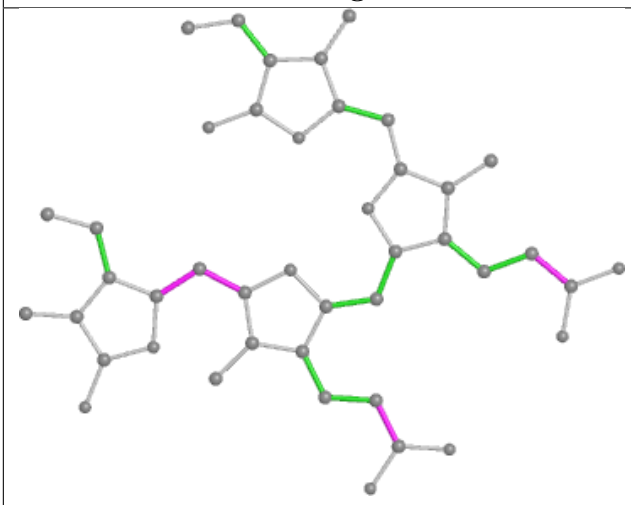

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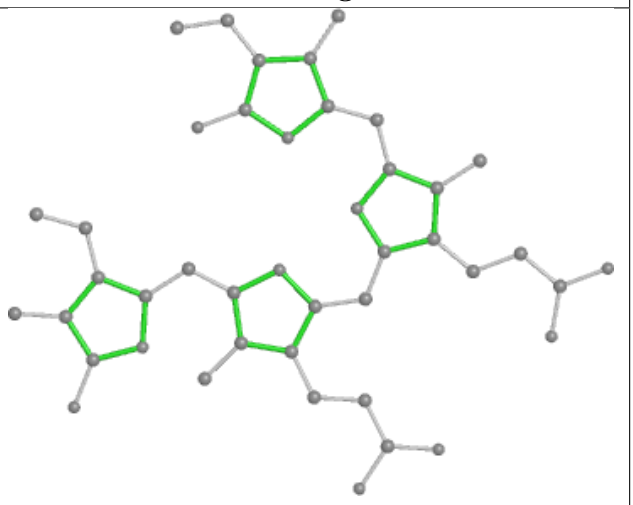
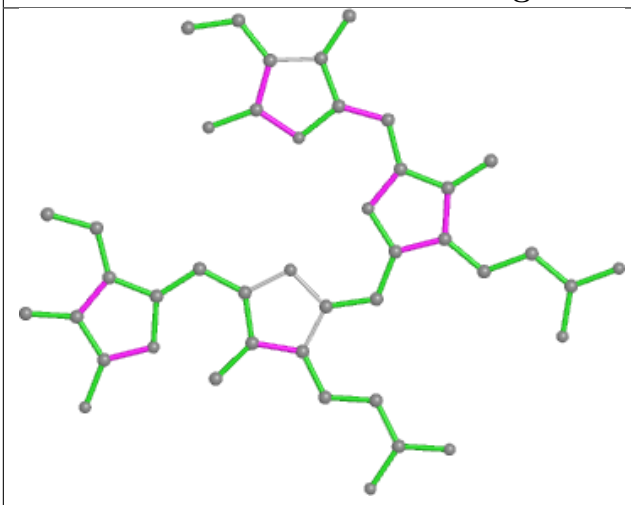


Rings

Ligand PUB D2 305



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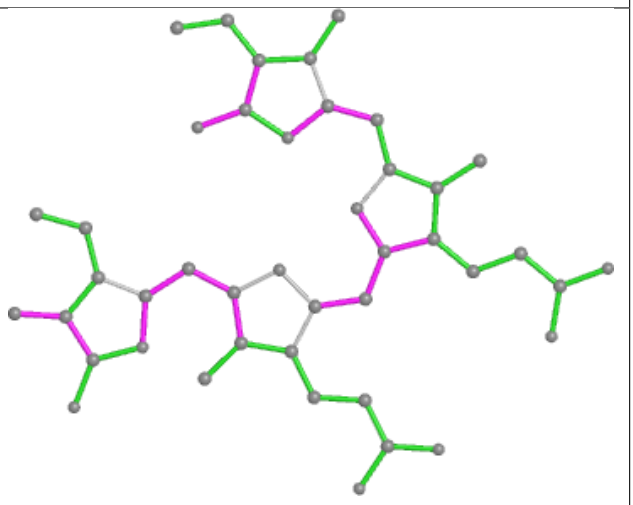

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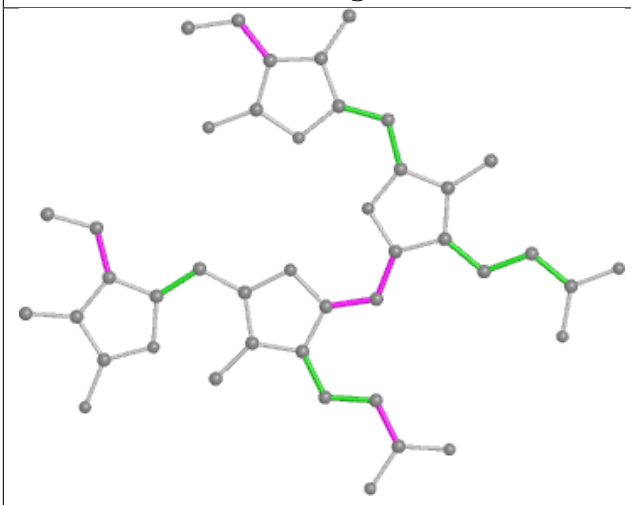

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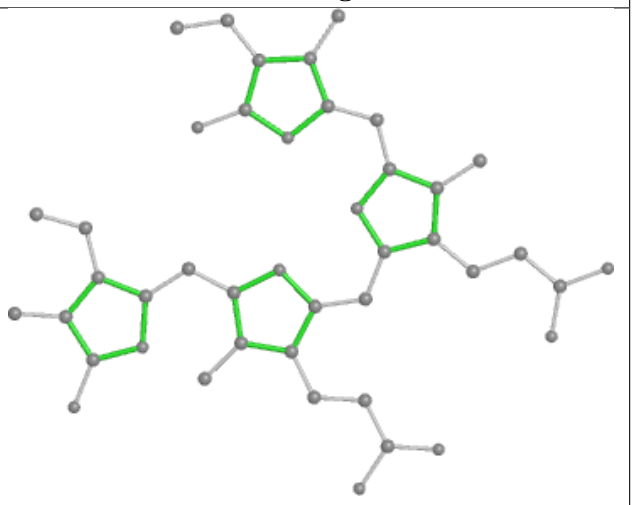
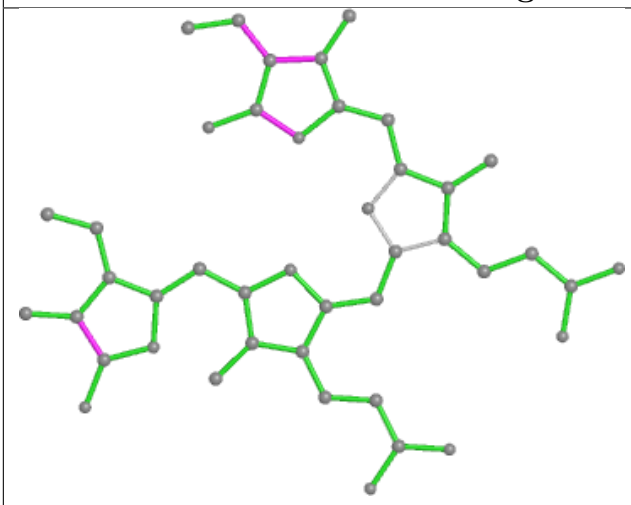


Rings

Ligand PEB E3 201



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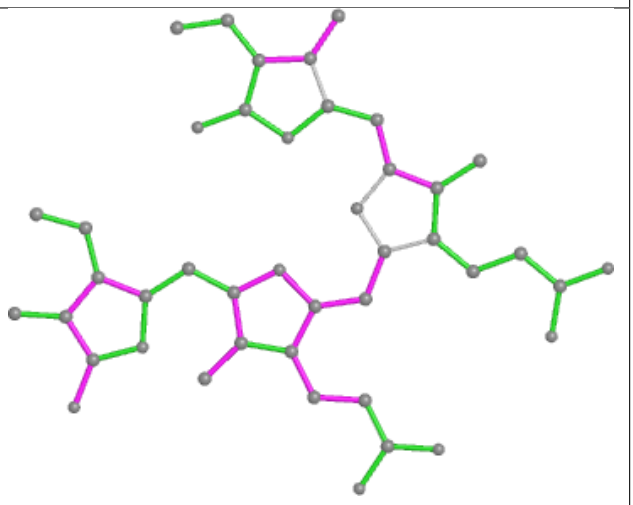
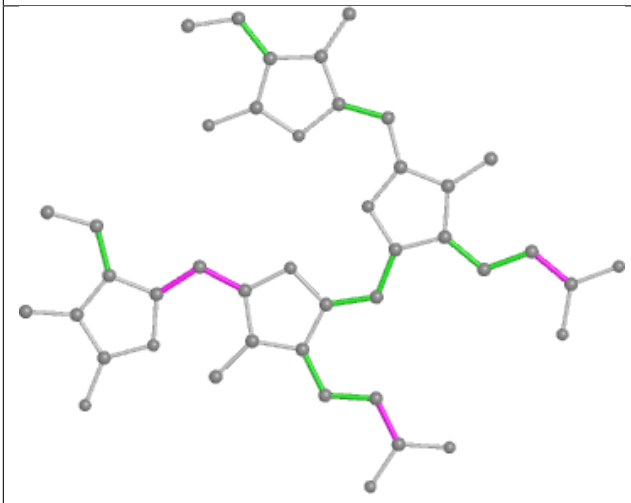


Bond angles



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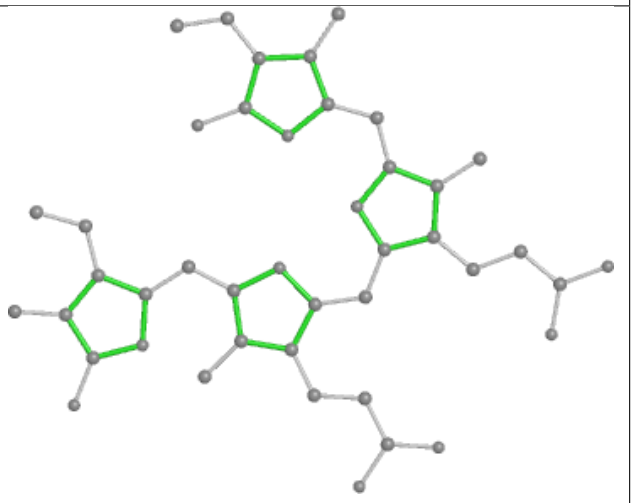
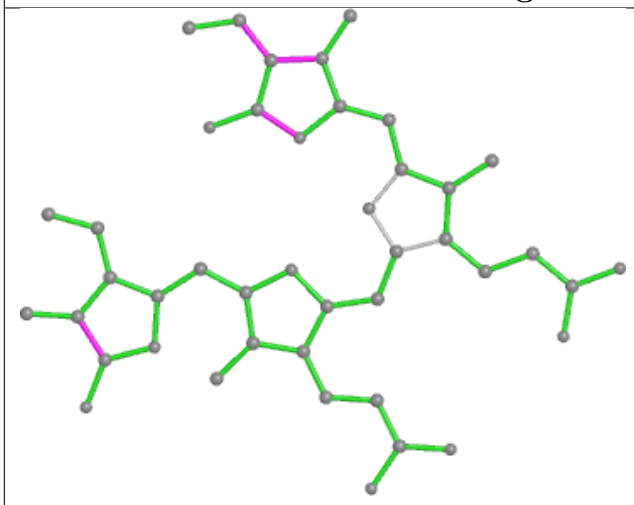


Rings

Ligand PEB la 1002



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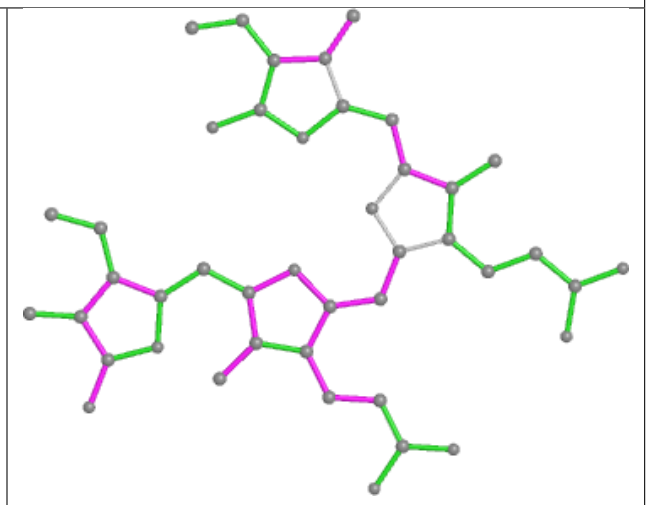
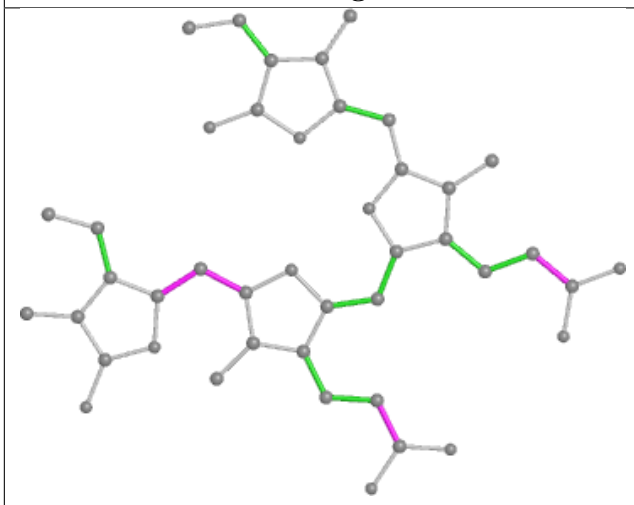


Bond angles



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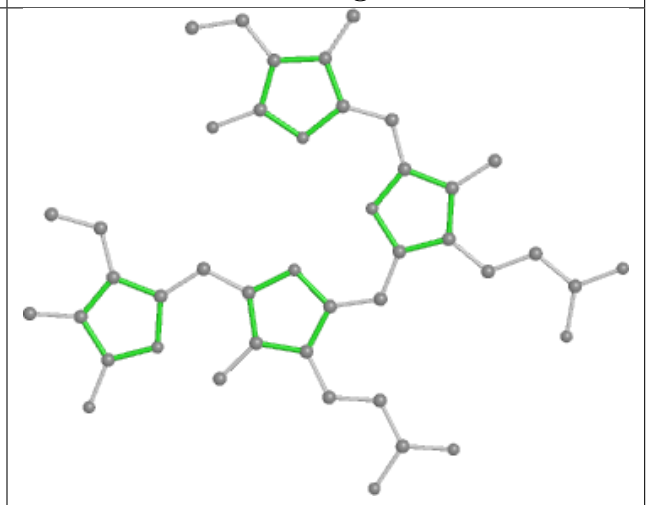
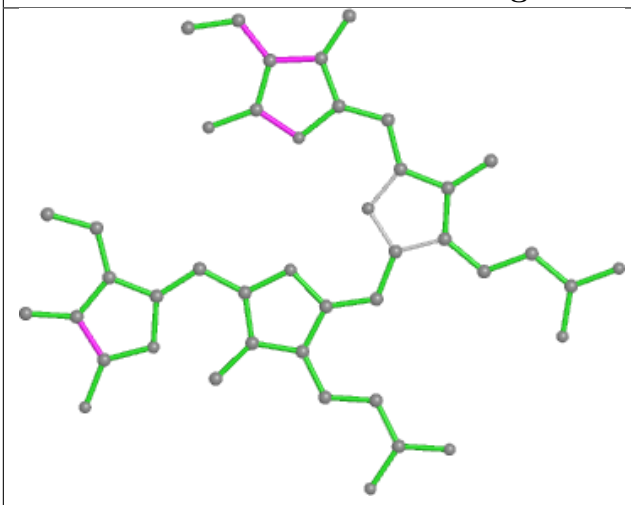


Rings

Ligand PEB W5 301



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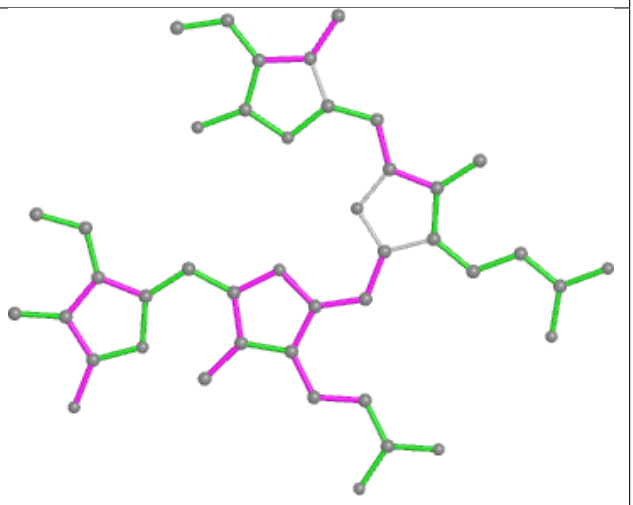
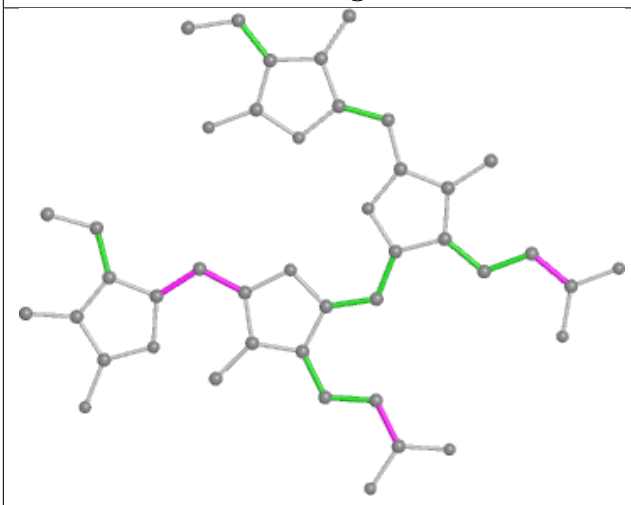


Bond angles



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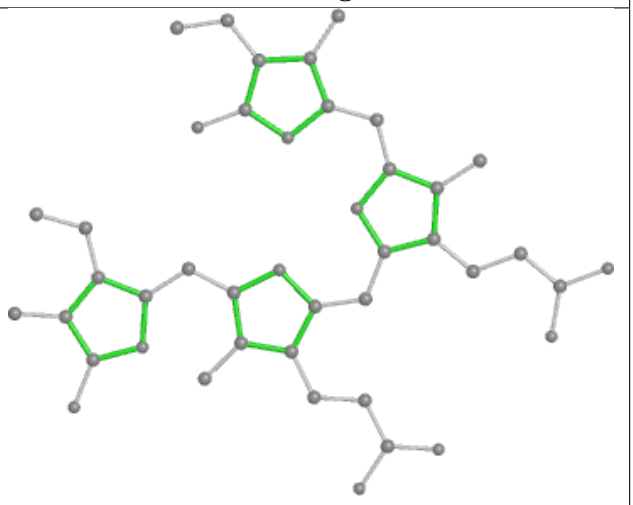
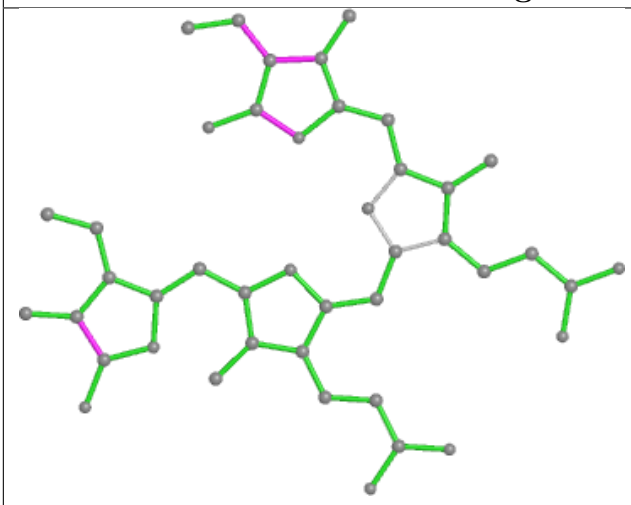


Rings

Ligand PEB bC 201



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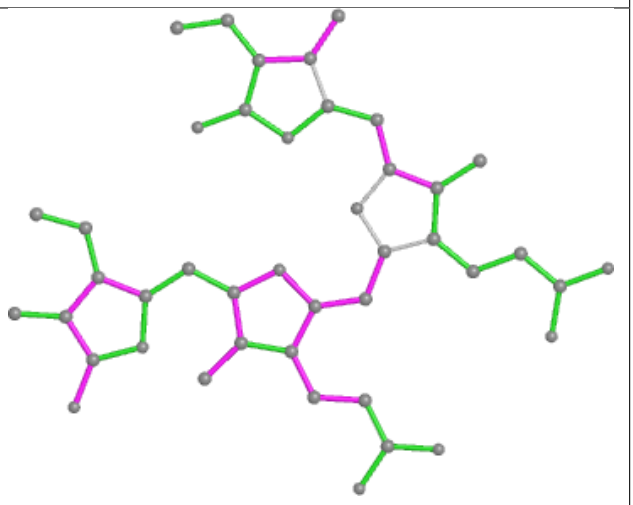
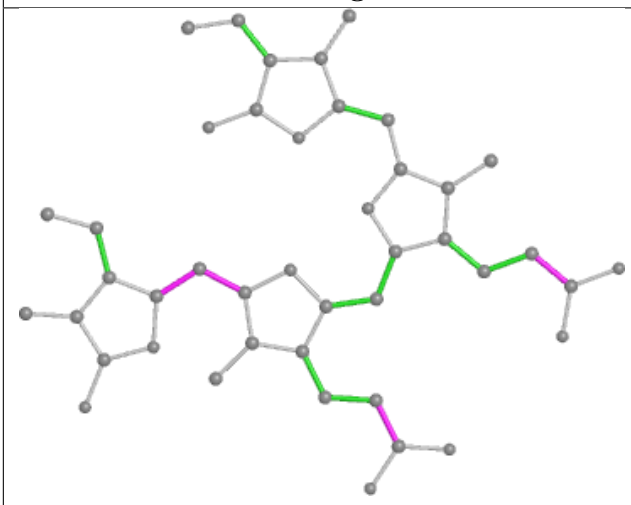


Bond angles



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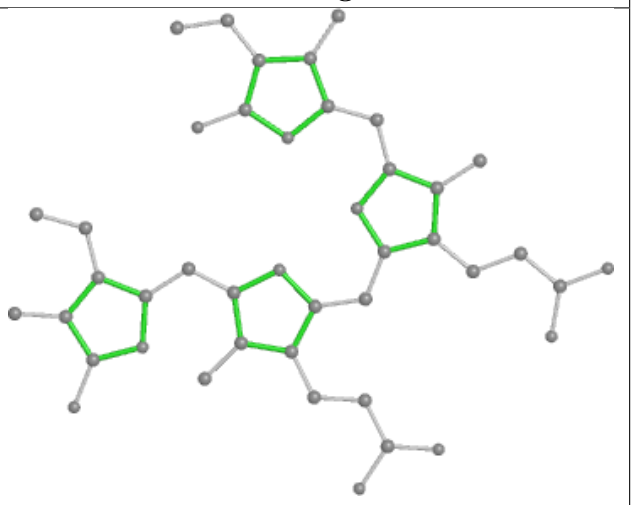
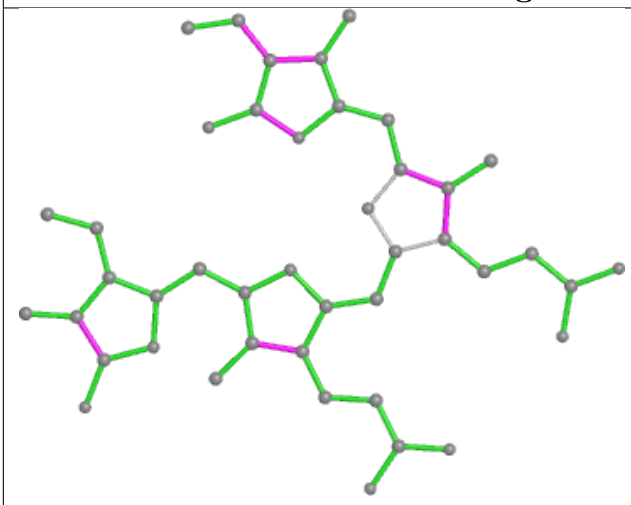


Rings

Ligand PEB V5 202



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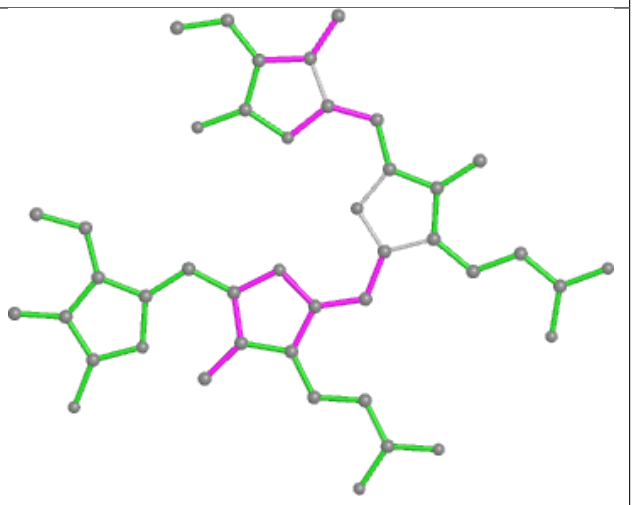
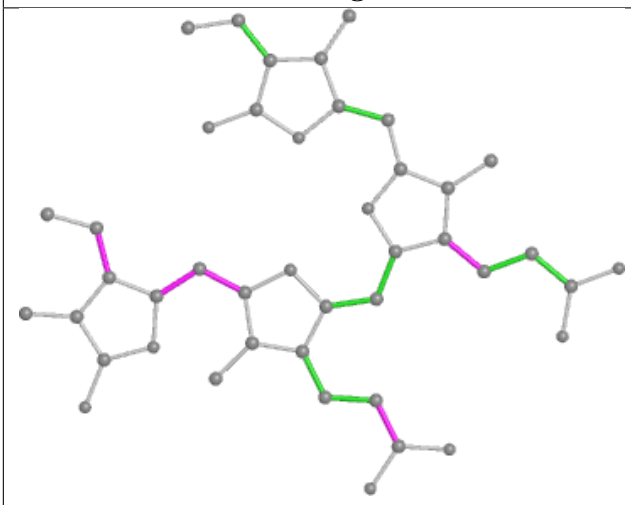


Bond angles



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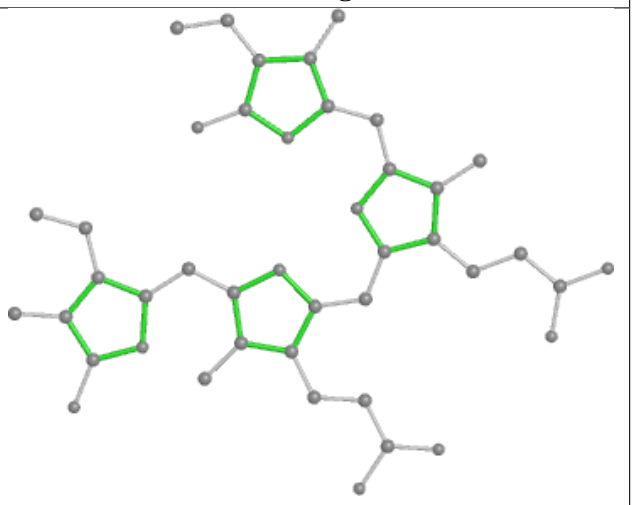
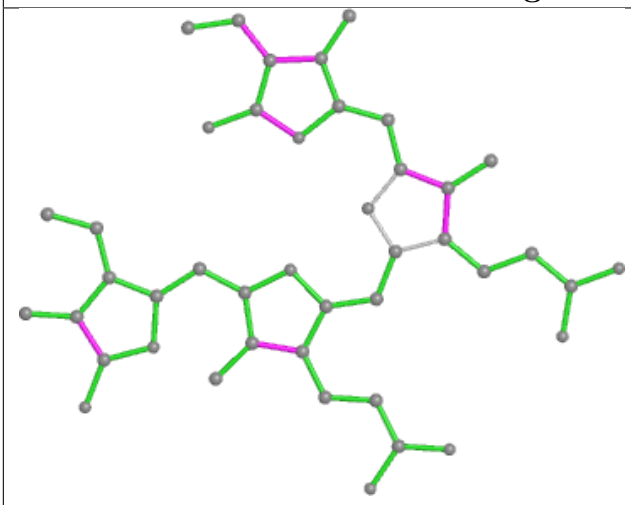


Rings

Ligand PEB l4 202



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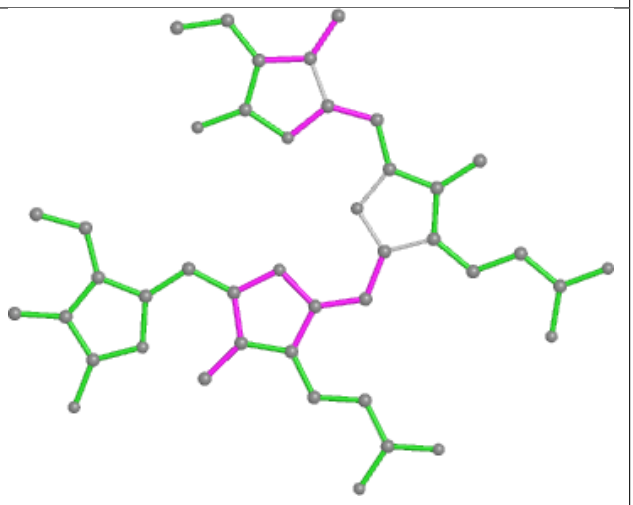

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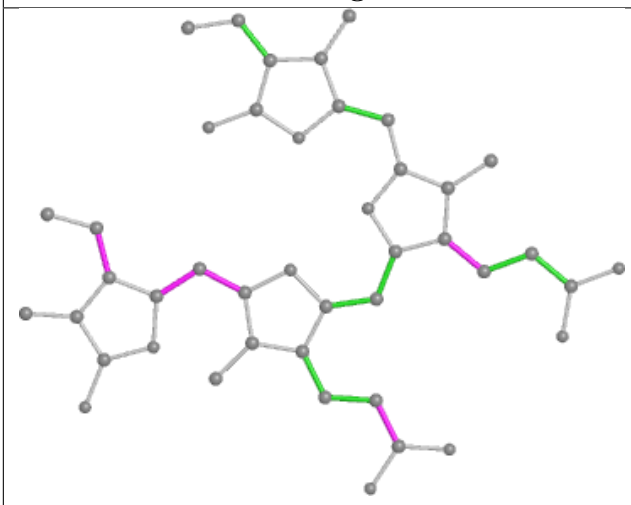

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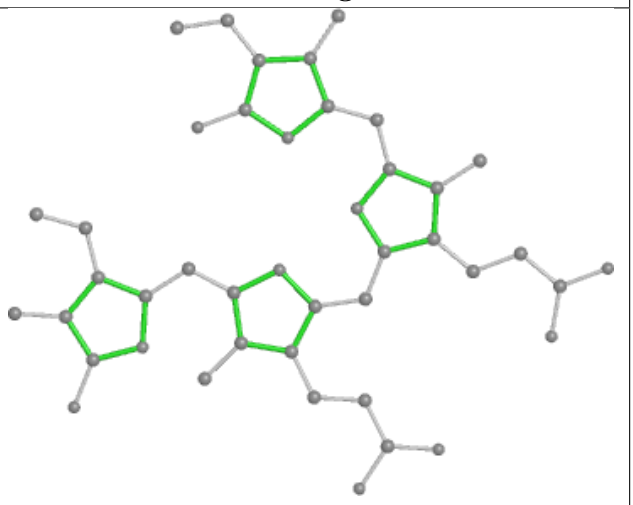
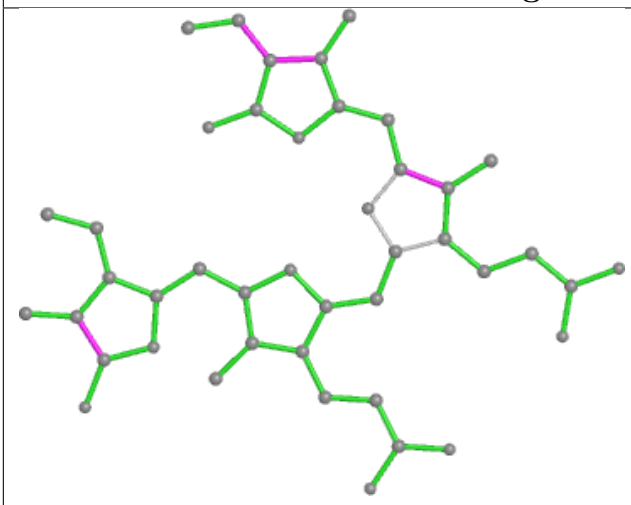


Rings

Ligand PEB lu 202



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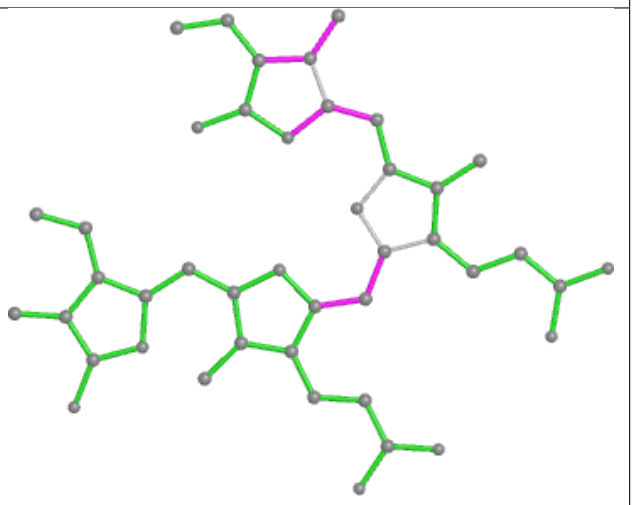
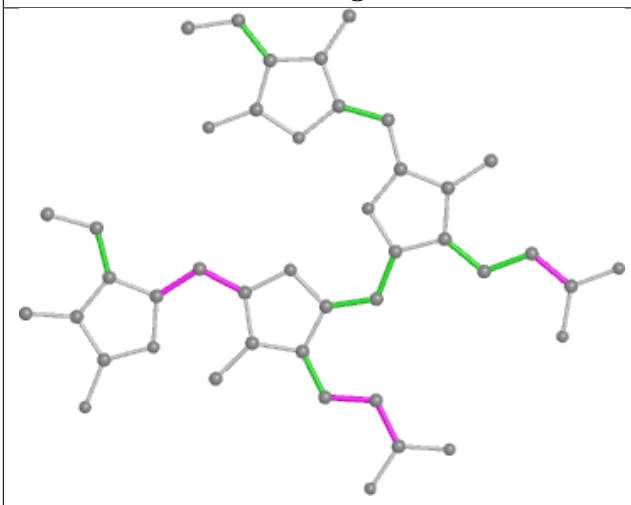


Bond angles



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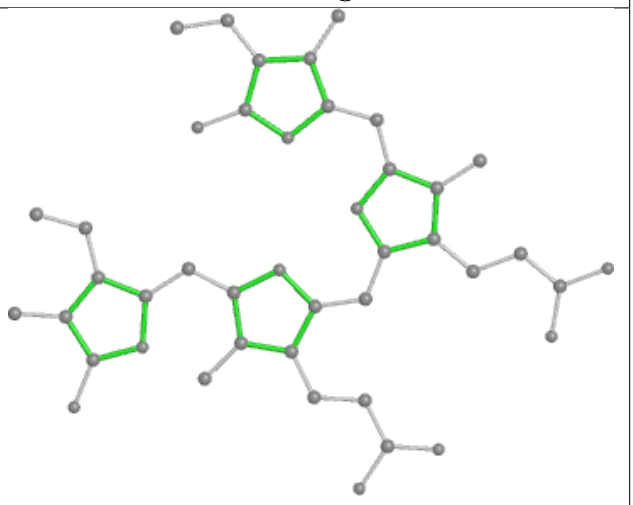
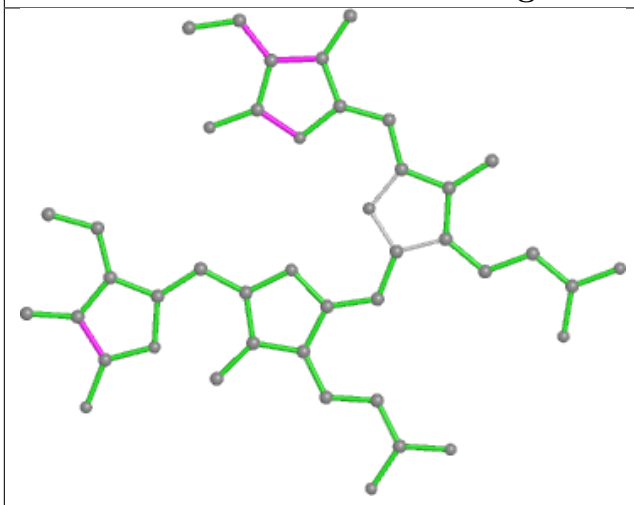


Rings

Ligand PEB bZ 303



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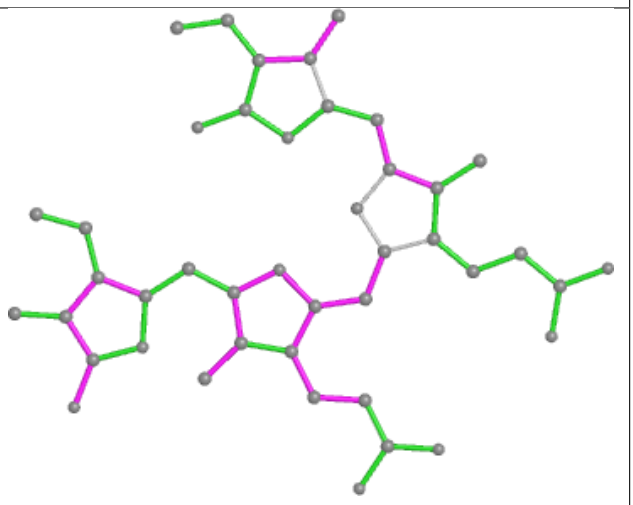
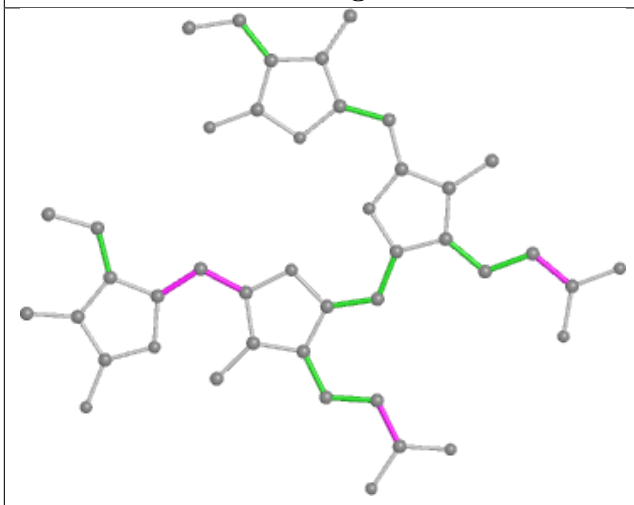


Bond angles



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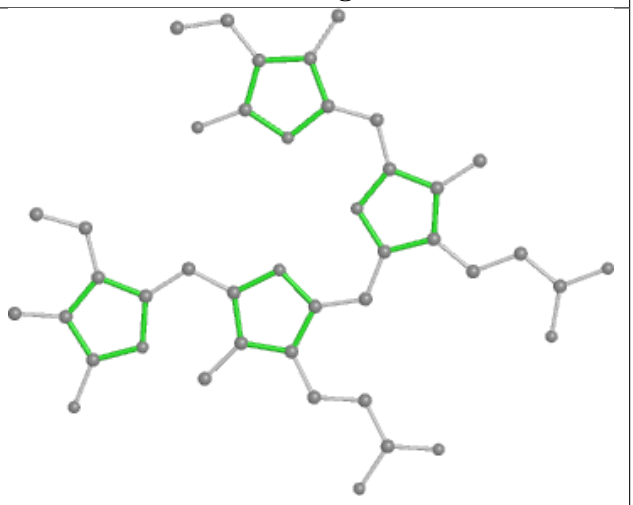
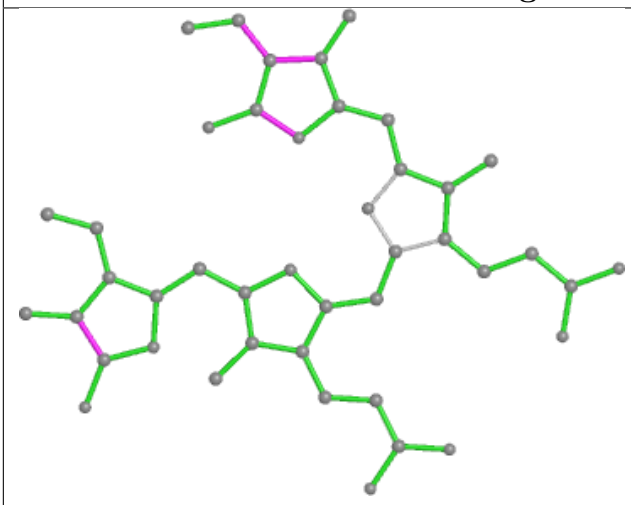


Rings

Ligand PEB y6 203



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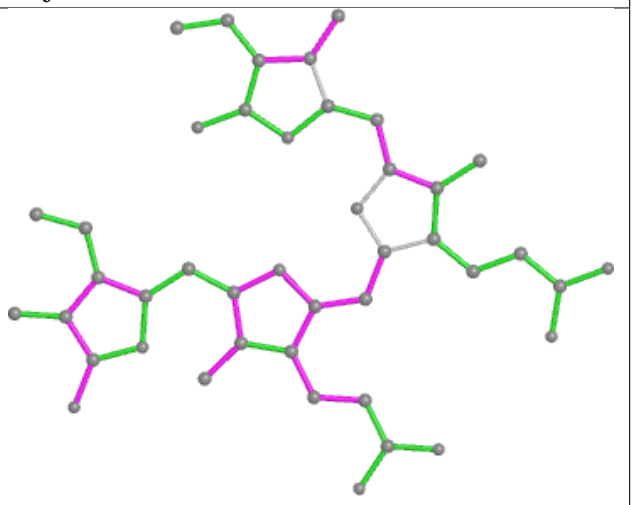
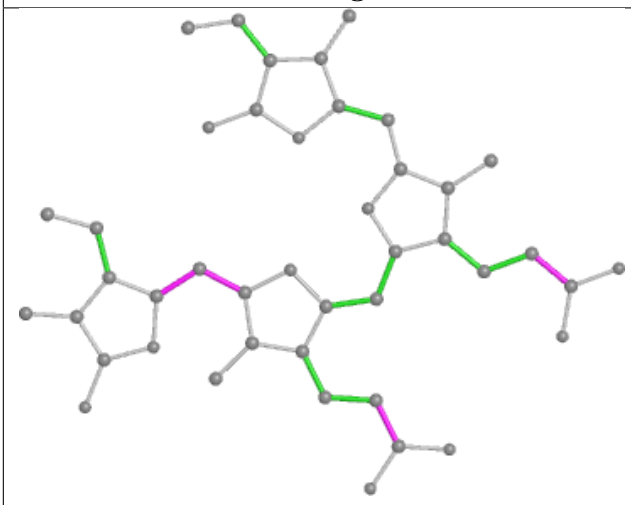


Bond angles



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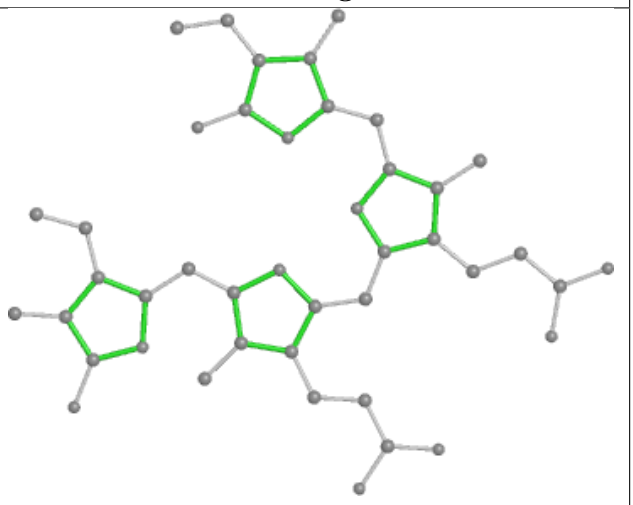
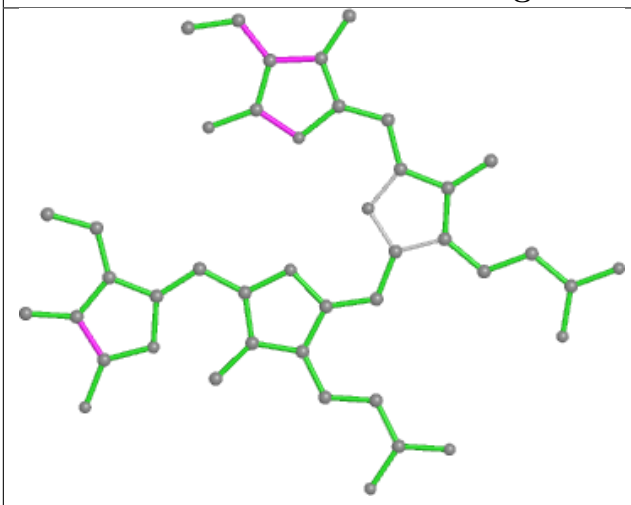


Rings

Ligand PEB hK 201



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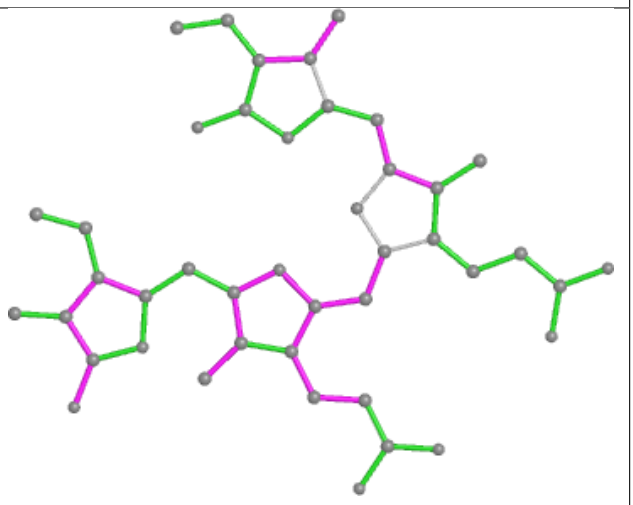
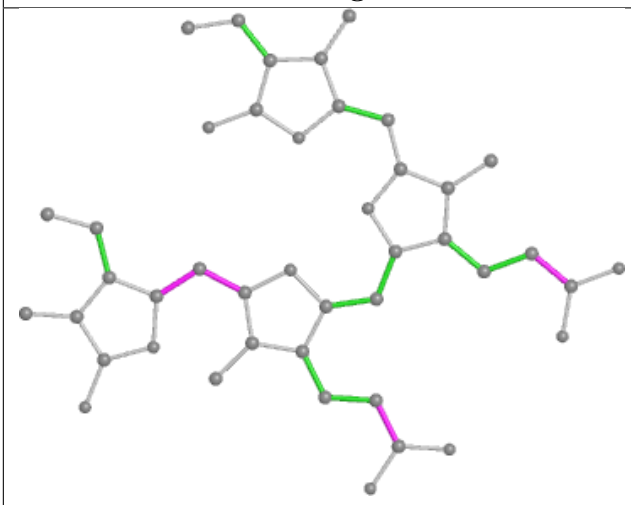
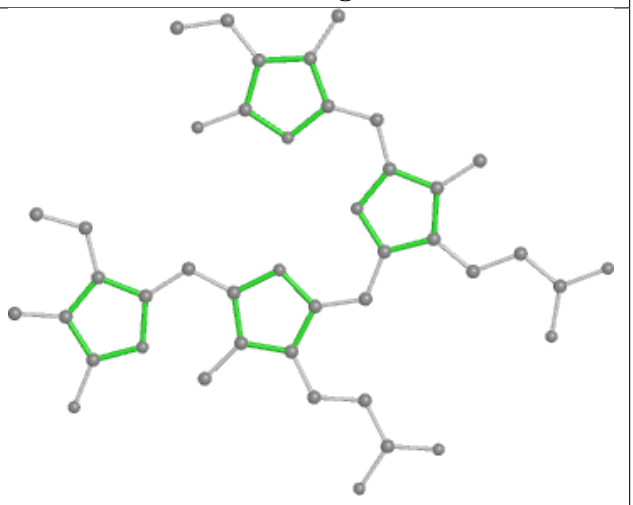


Bond angles

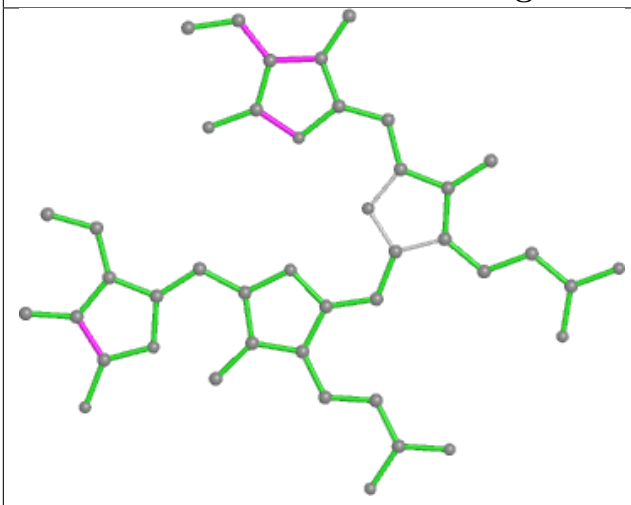


Torsions



Rings

Ligand PEB dP 201



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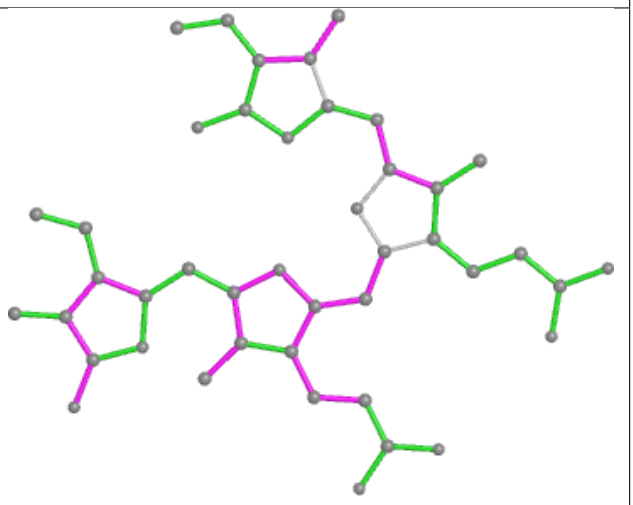

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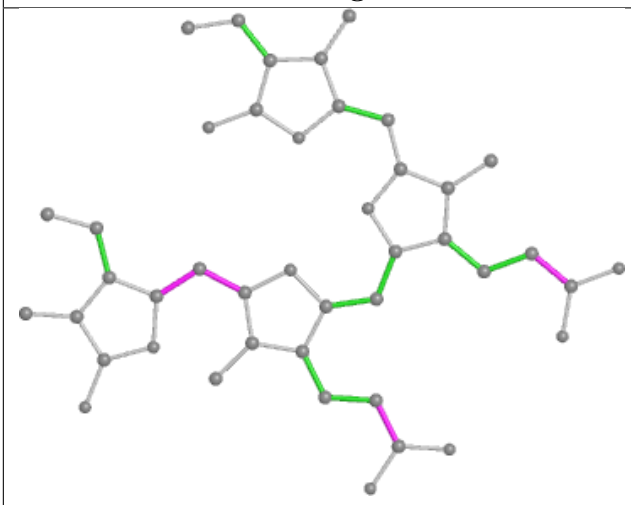

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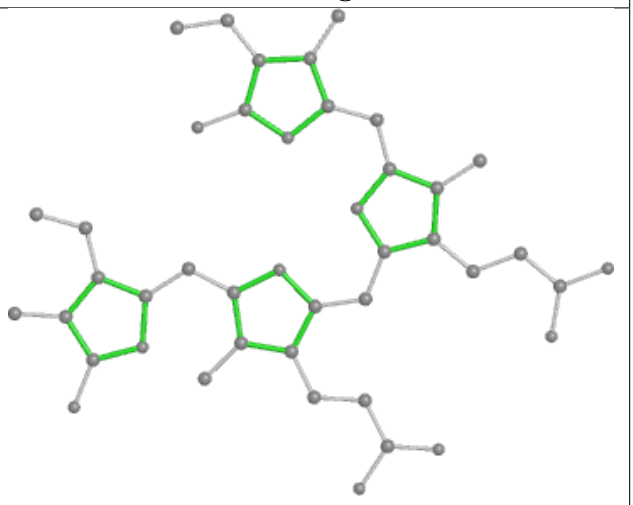
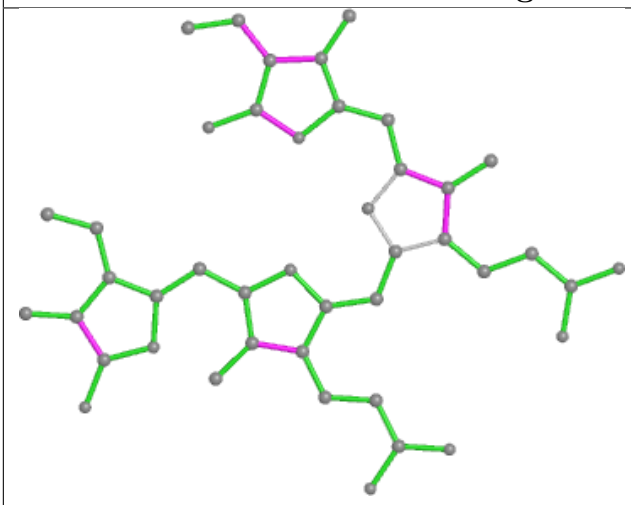


Rings

Ligand PEB P5 201



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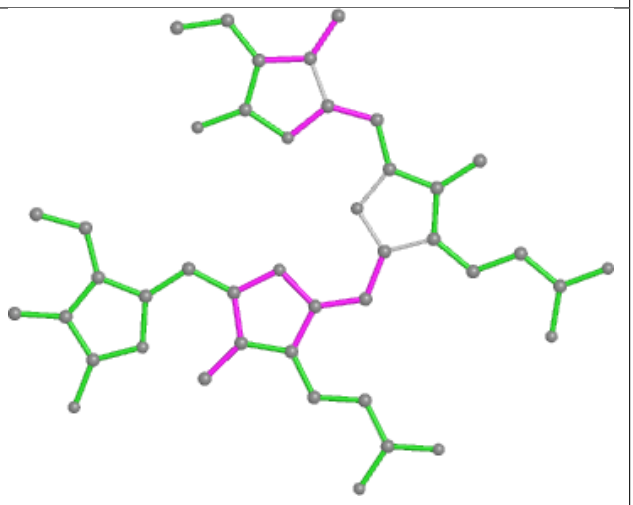

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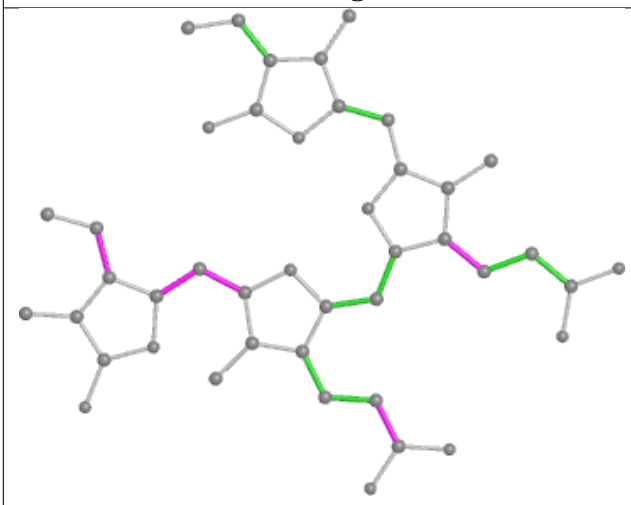

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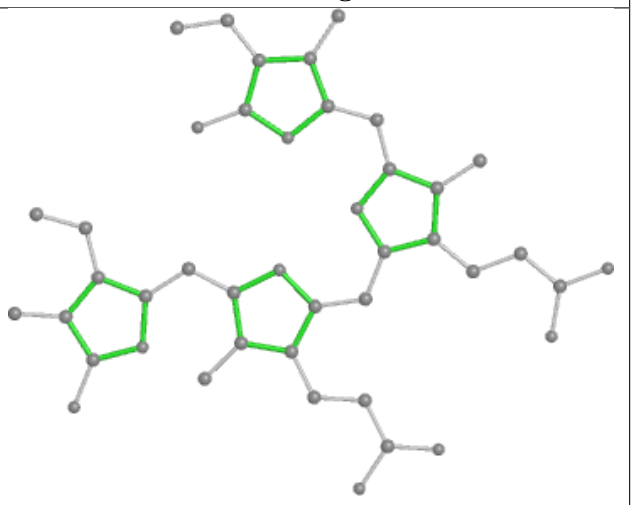

Rings

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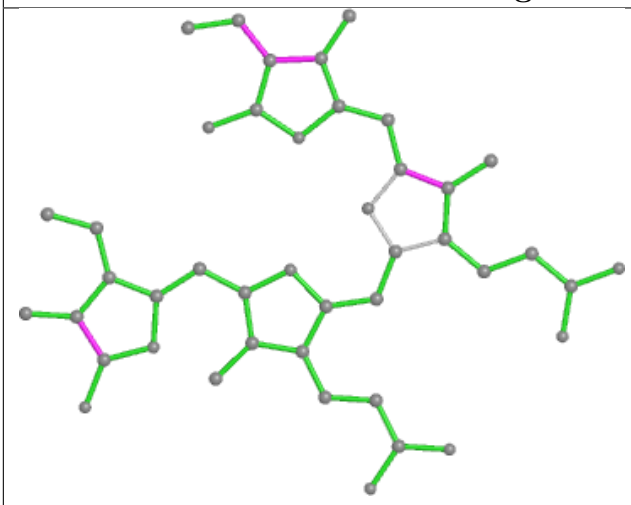

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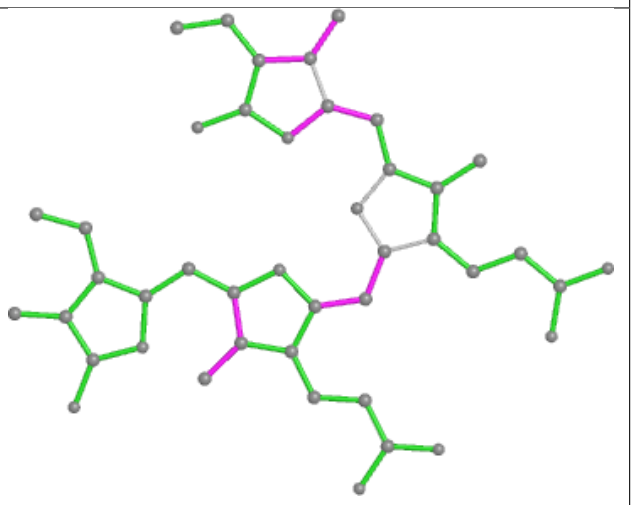

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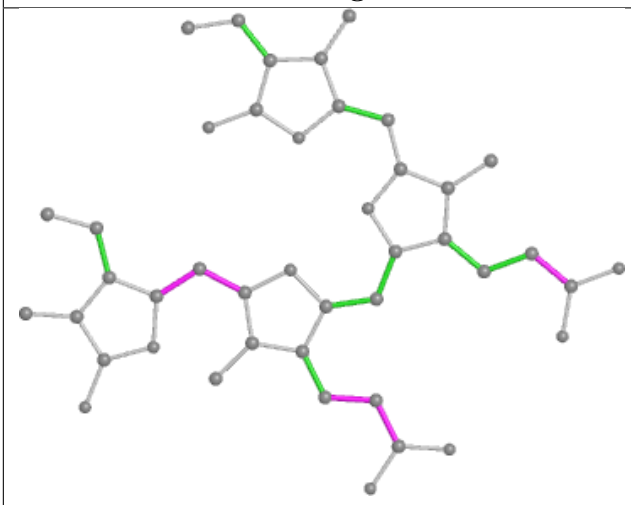

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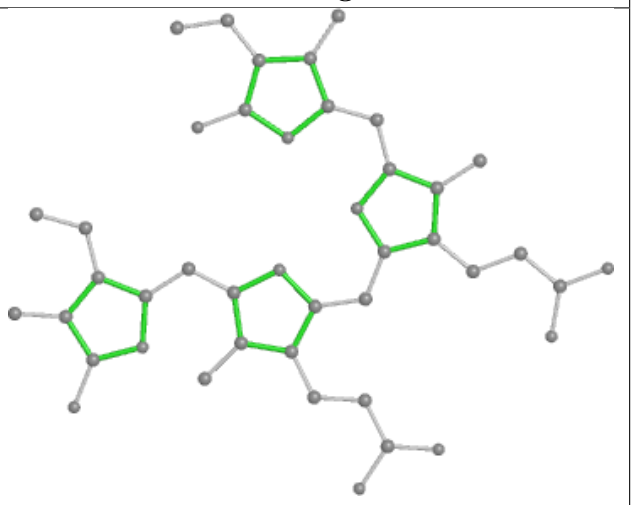
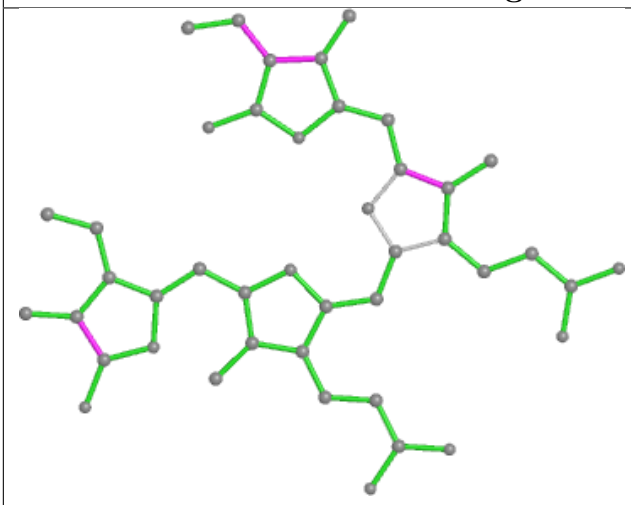


Rings

Ligand PEB bY 1002



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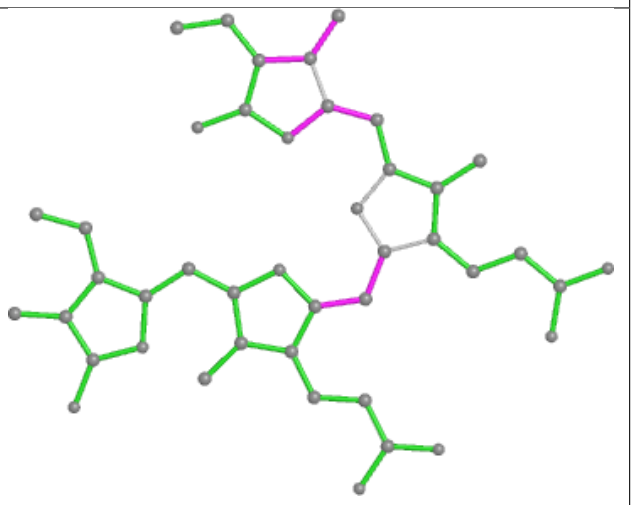

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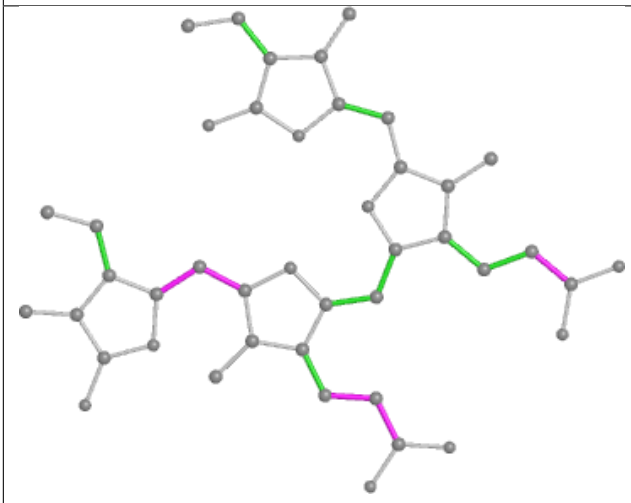

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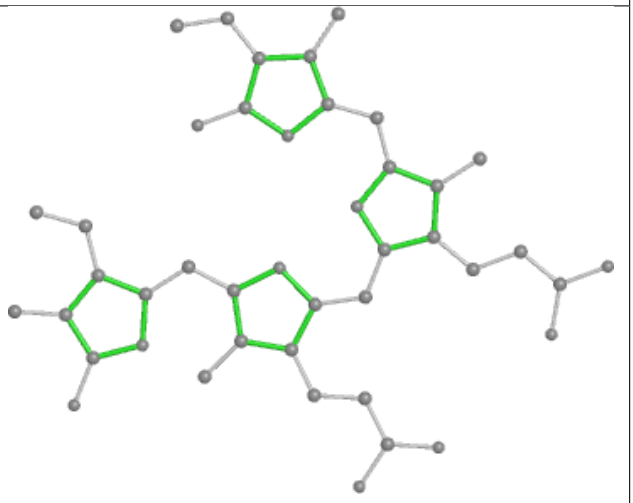

Rings

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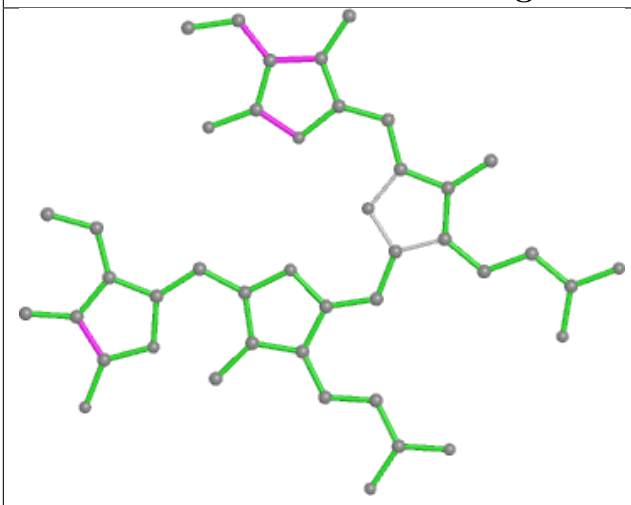

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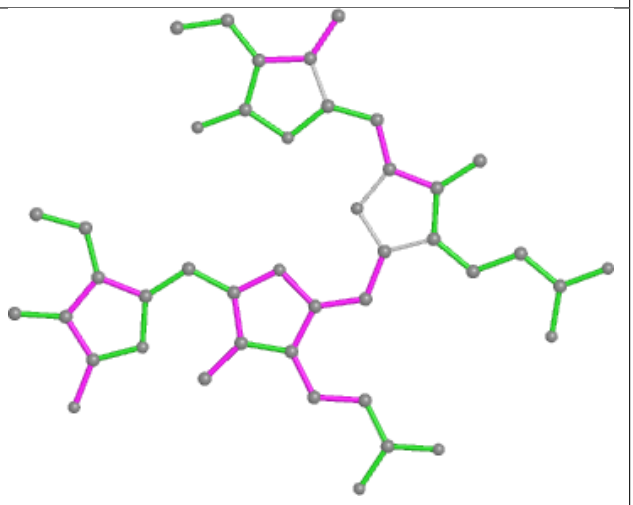

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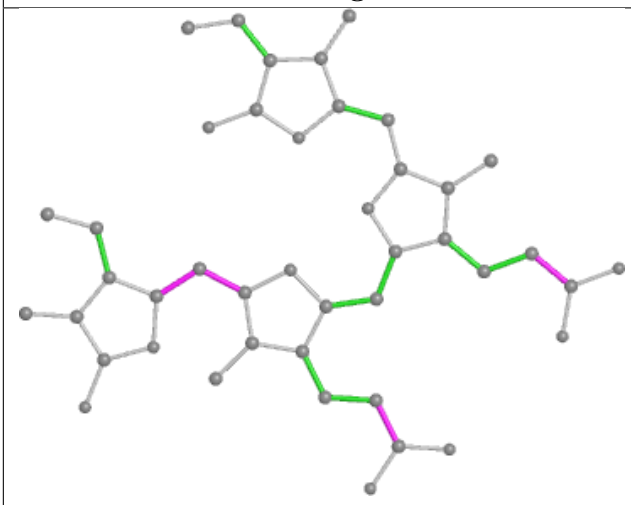

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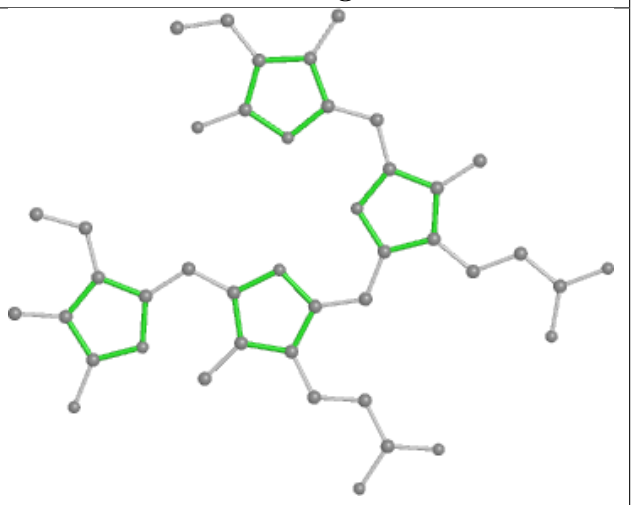

Rings

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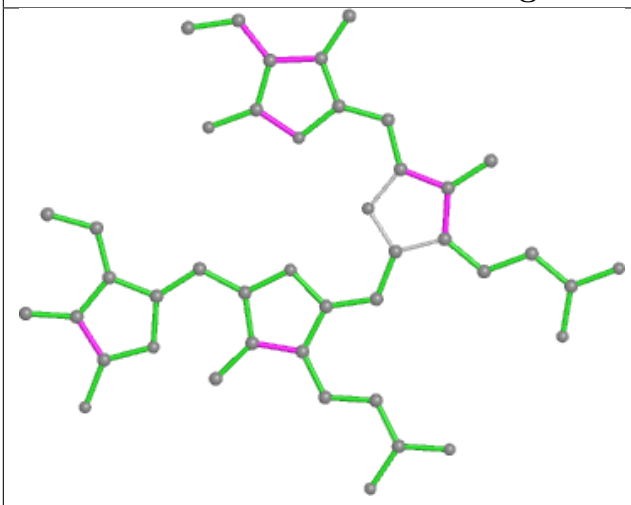

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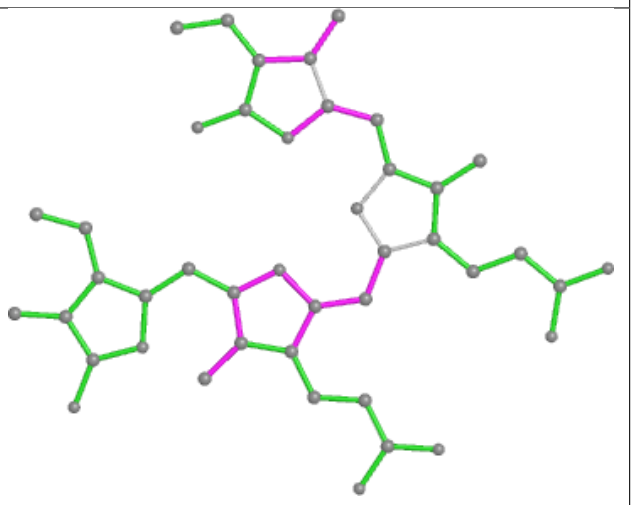

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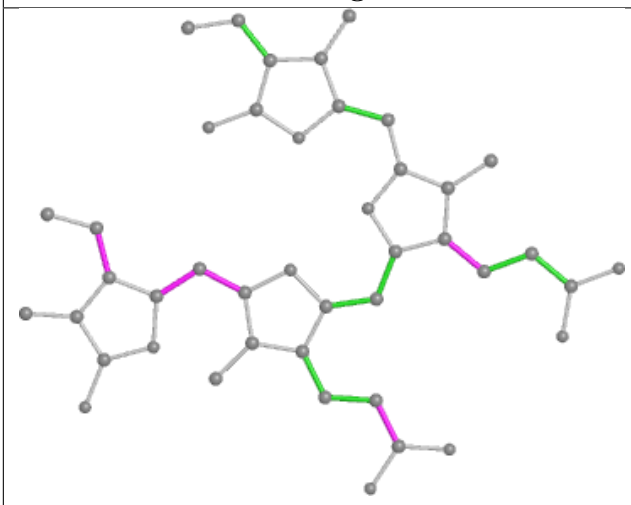

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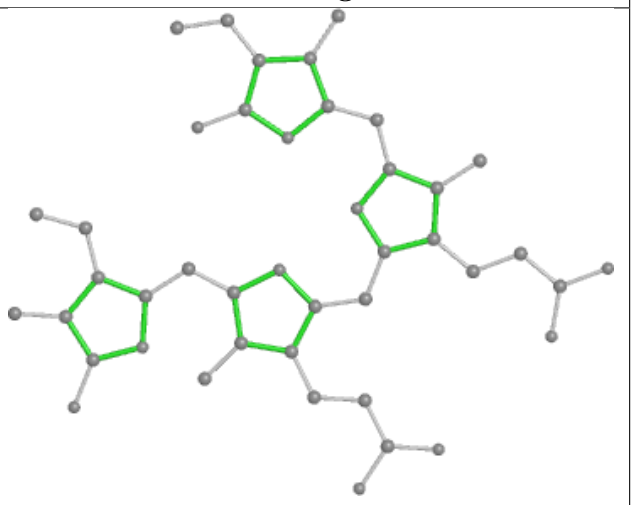

Rings

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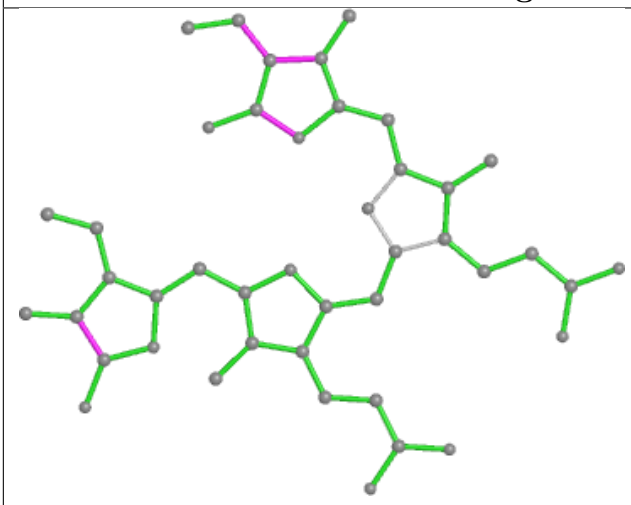

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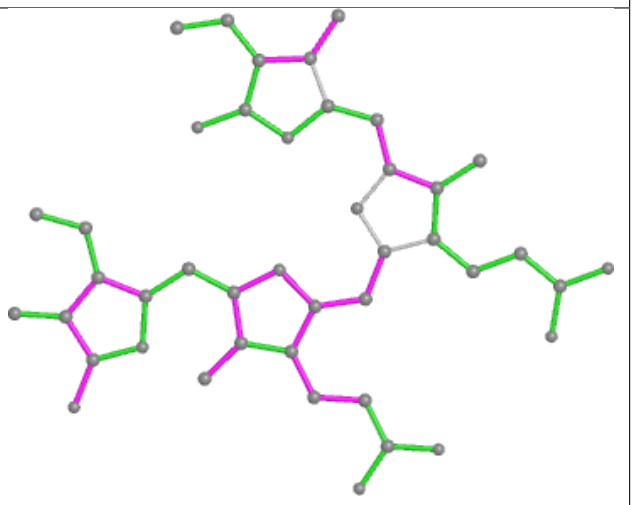

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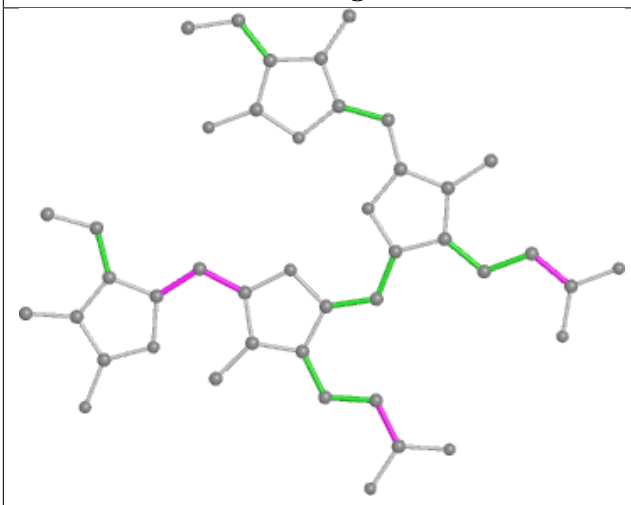

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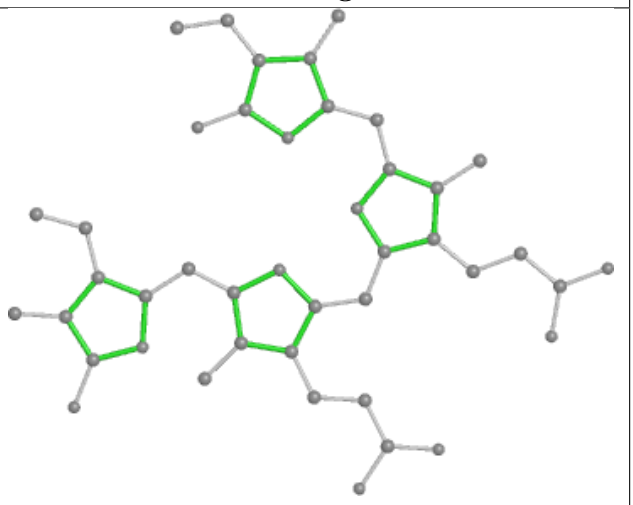
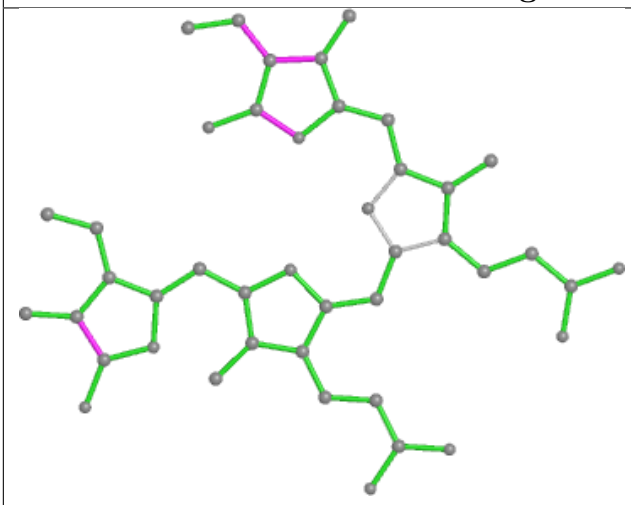


Rings

Ligand PEB k8 202



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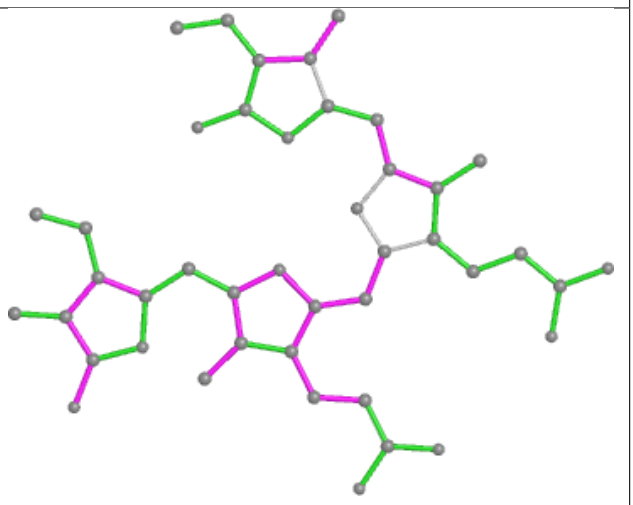

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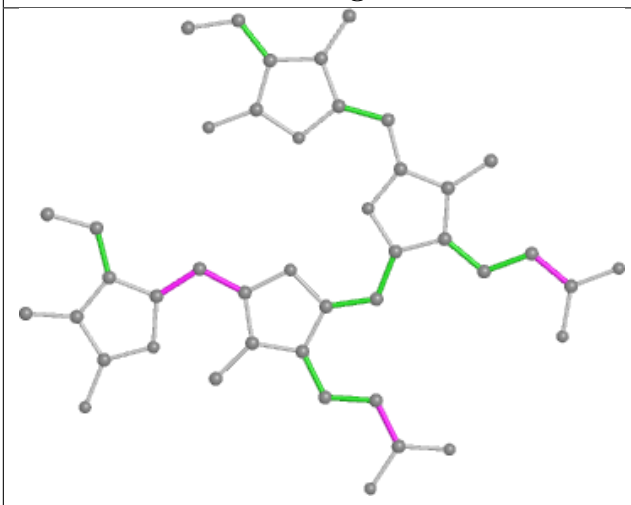

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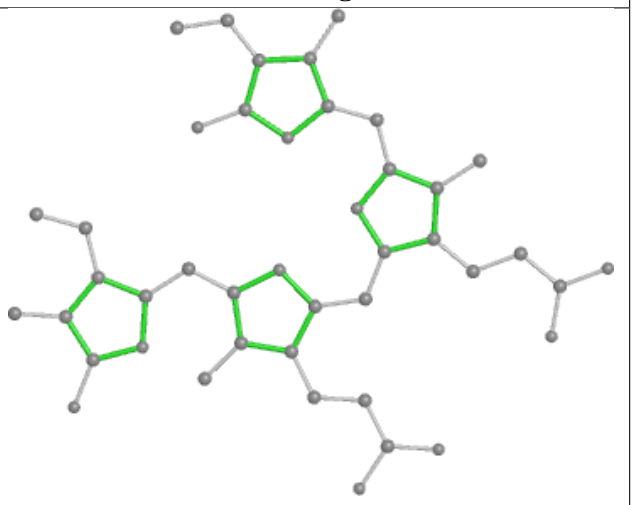

Rings

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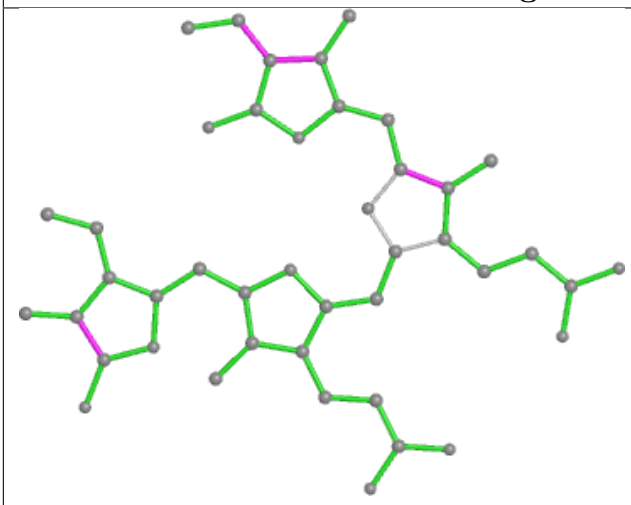

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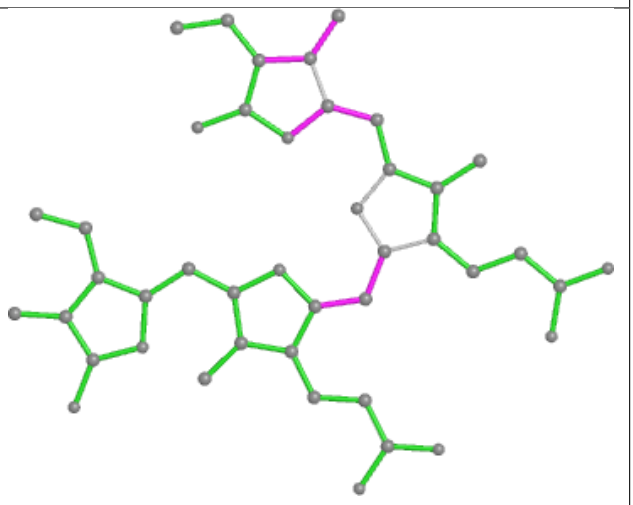

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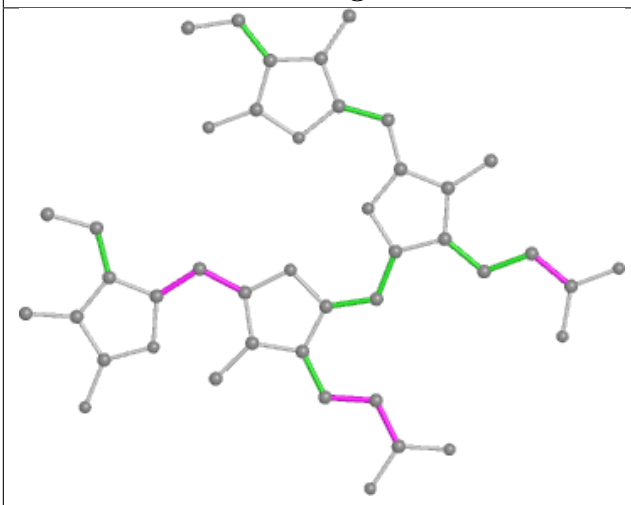

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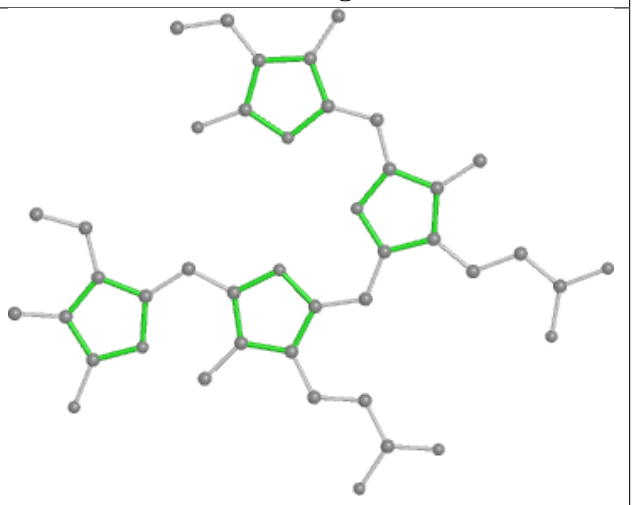
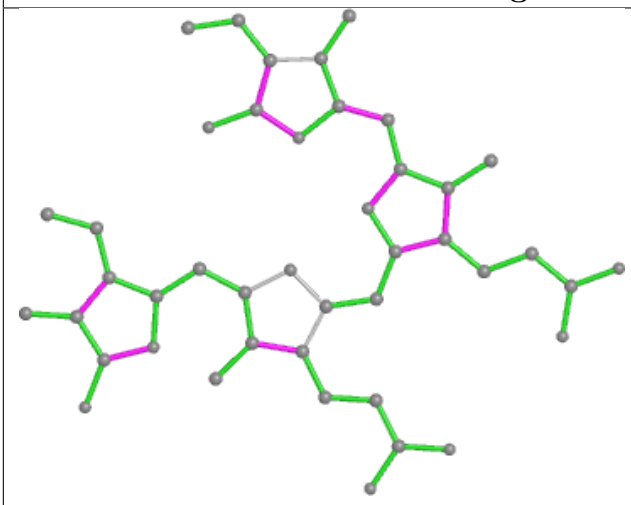


Rings

Ligand PUB iE 1003



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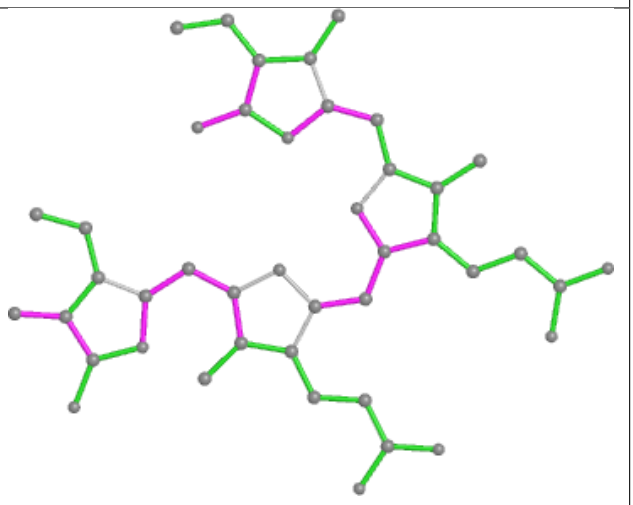

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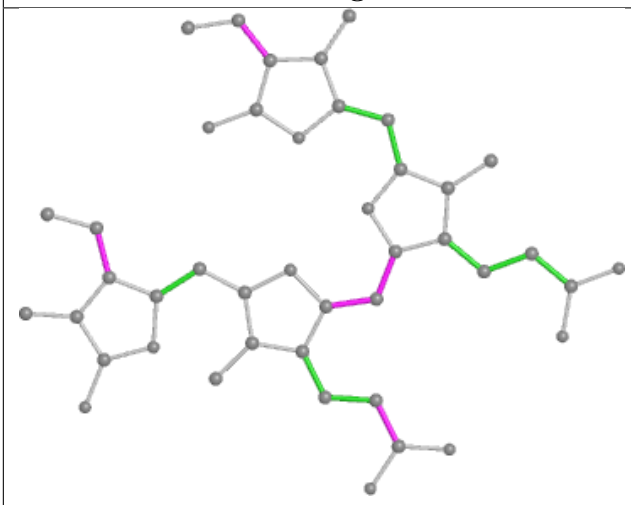

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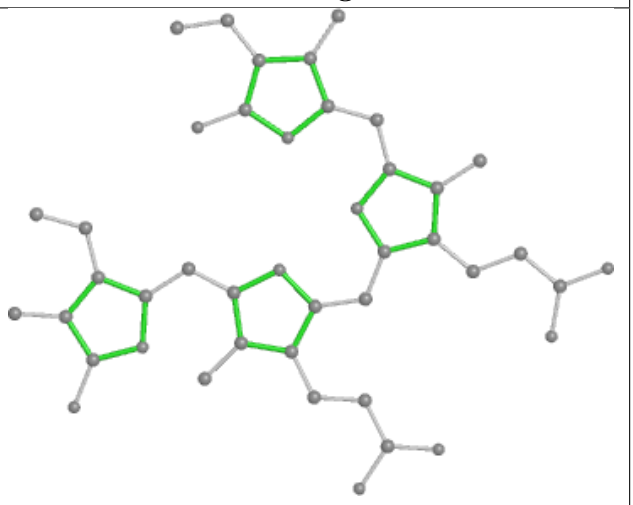
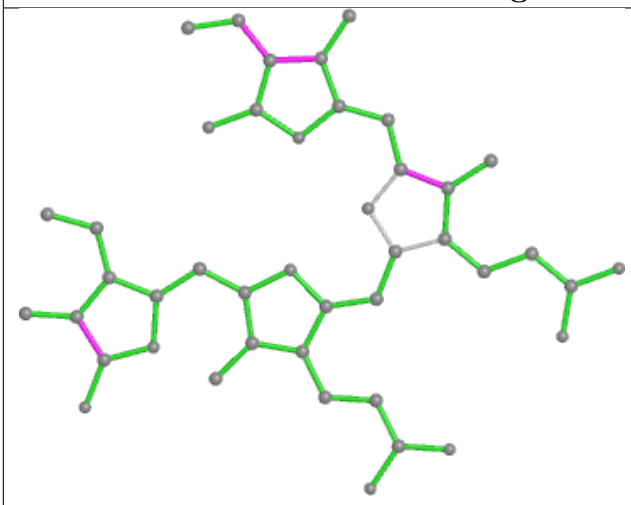


Rings

Ligand PEB k7 1002



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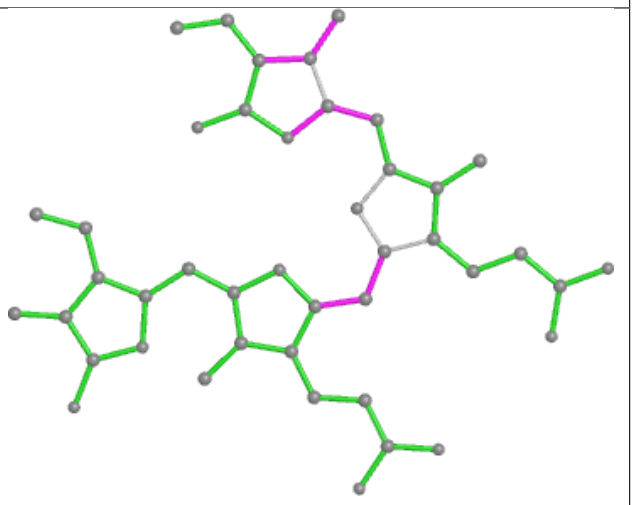

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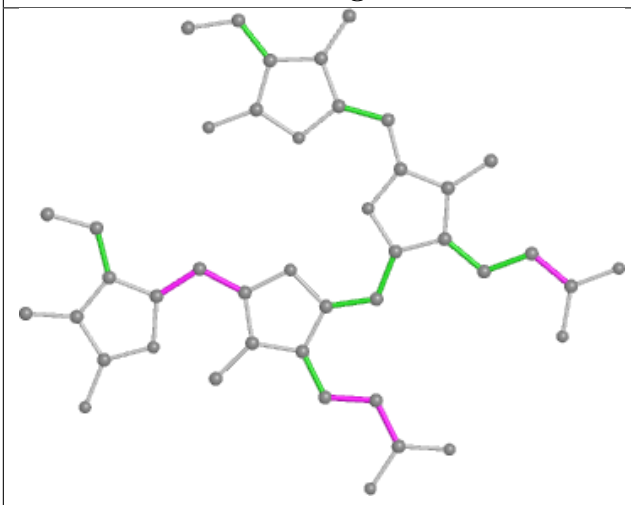

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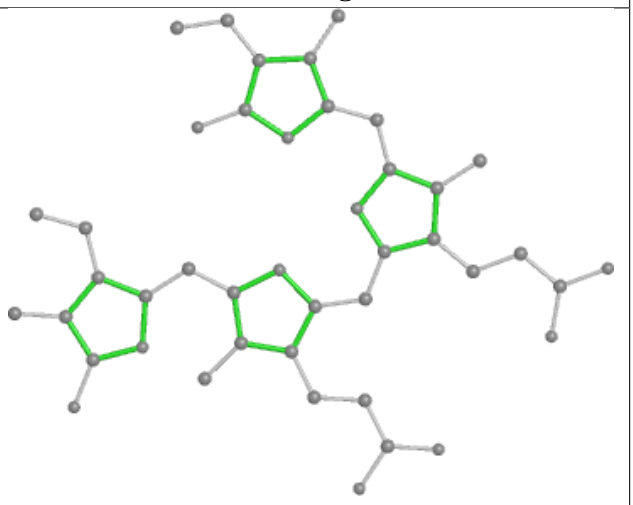
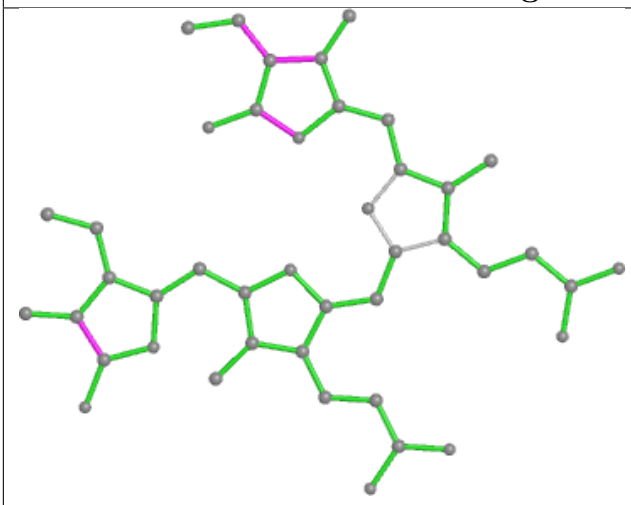


Rings

Ligand PEB ee 201



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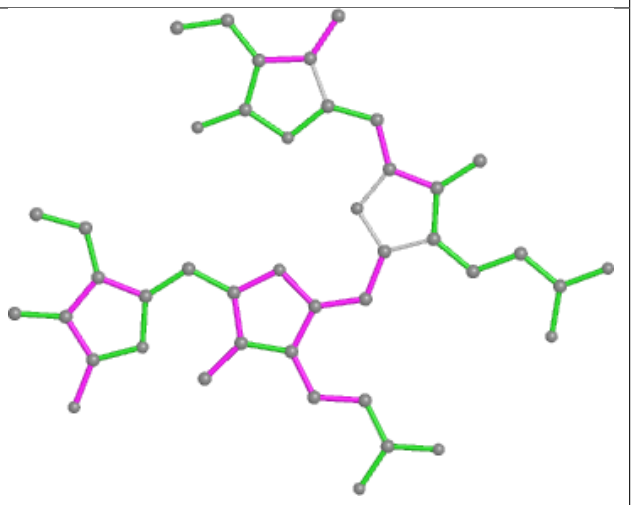

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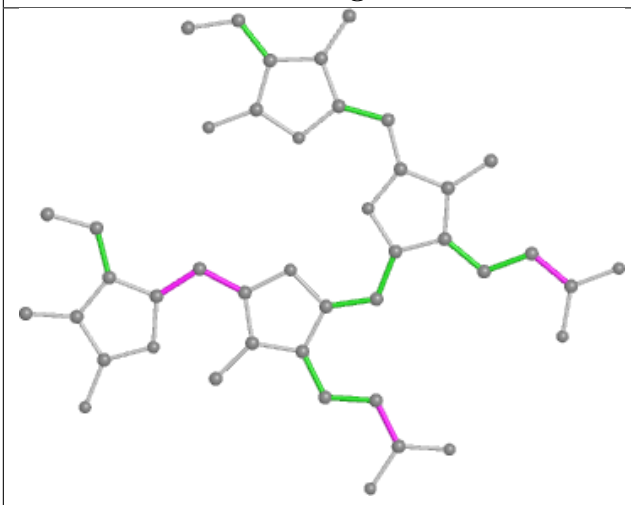

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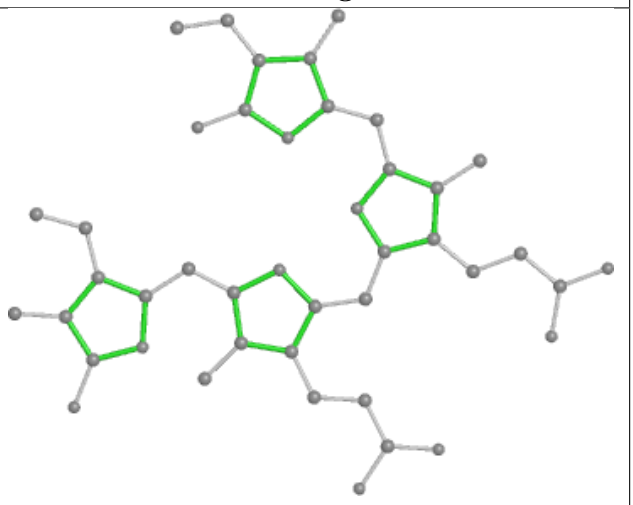
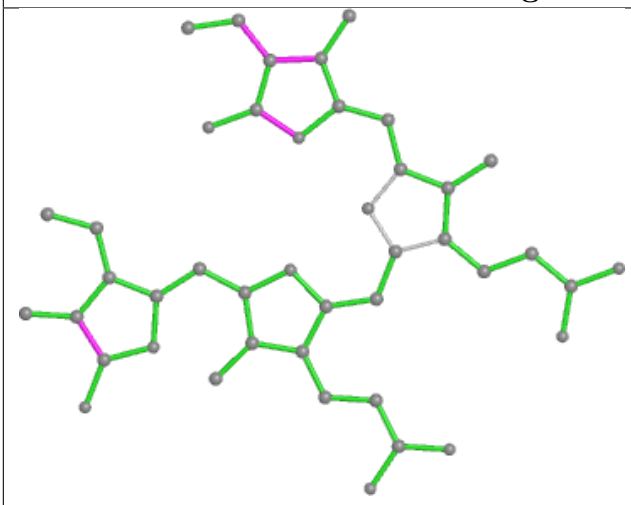


Rings

Ligand PEB t9 201



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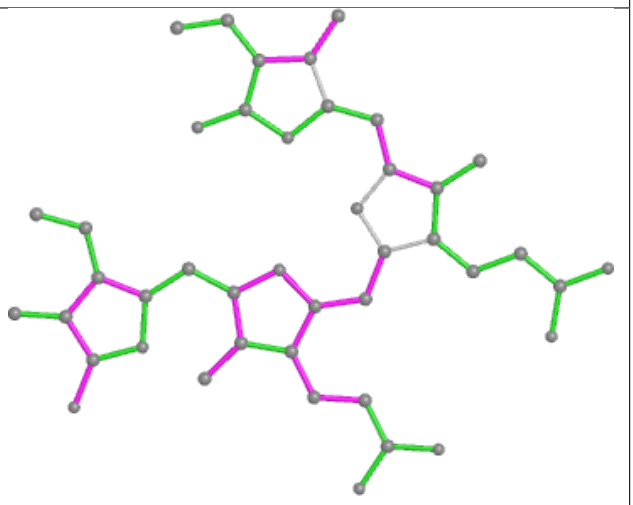
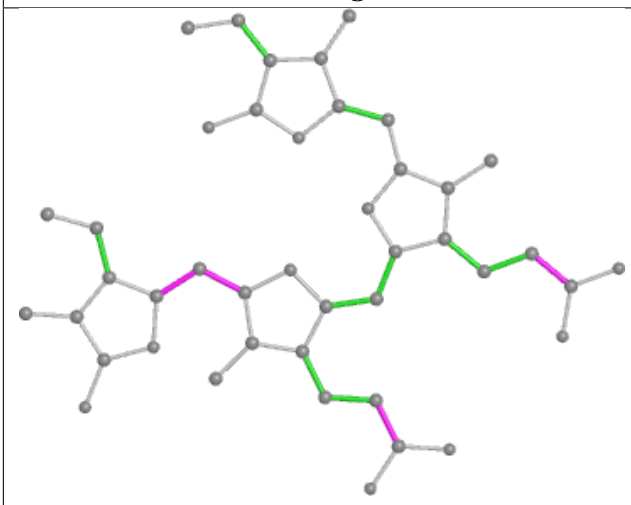
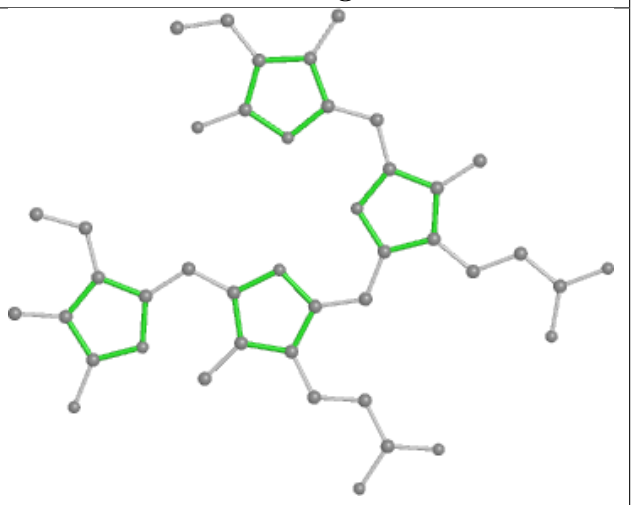


Bond angles

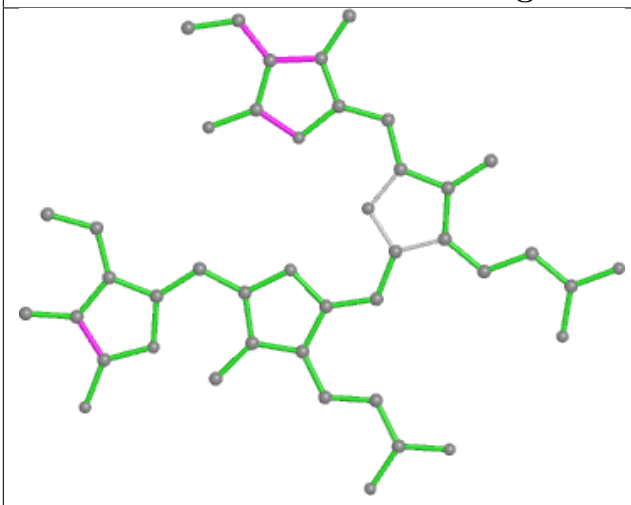


Torsions



Rings

Ligand PEB T9 201



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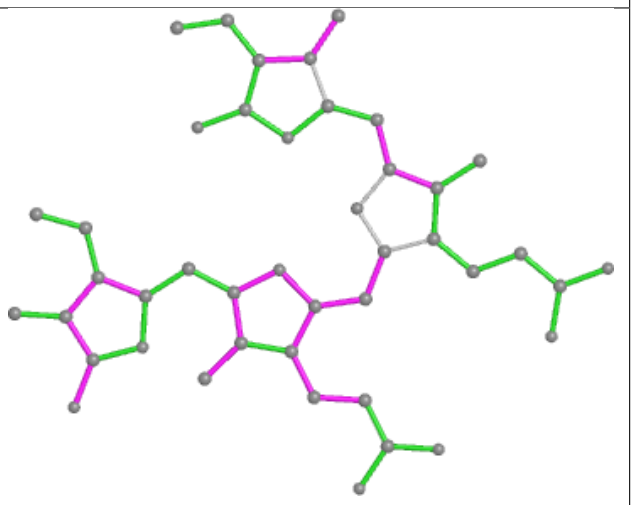

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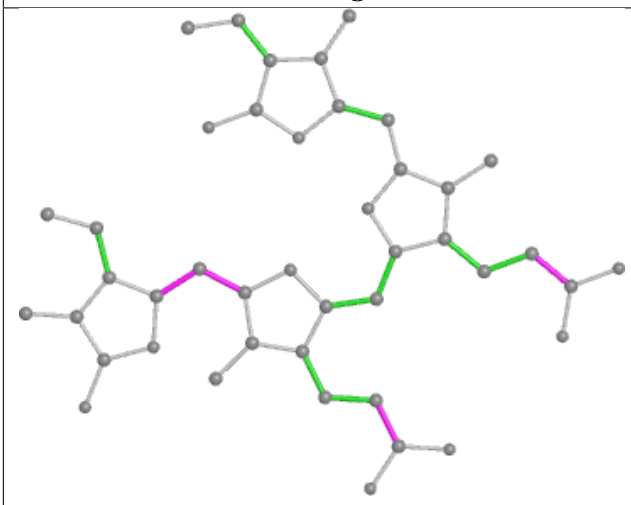

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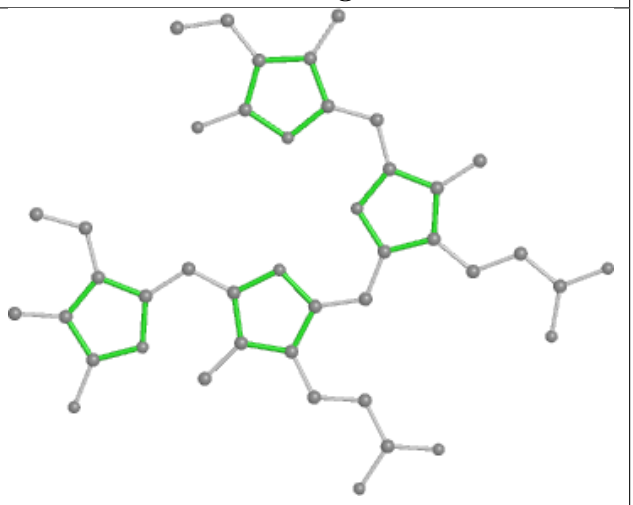
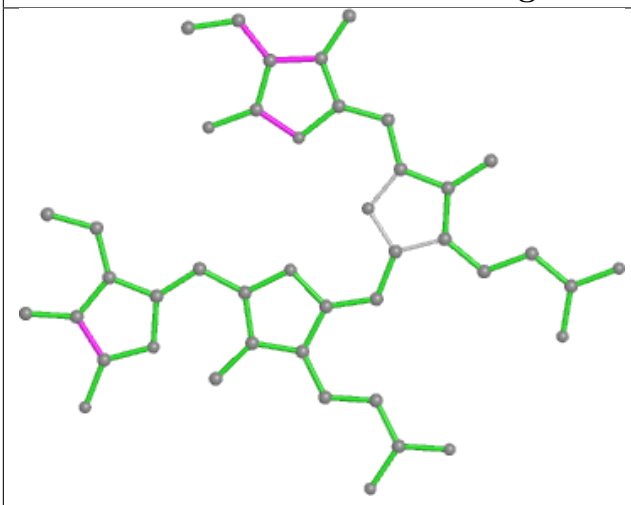


Rings

Ligand PEB eF 201



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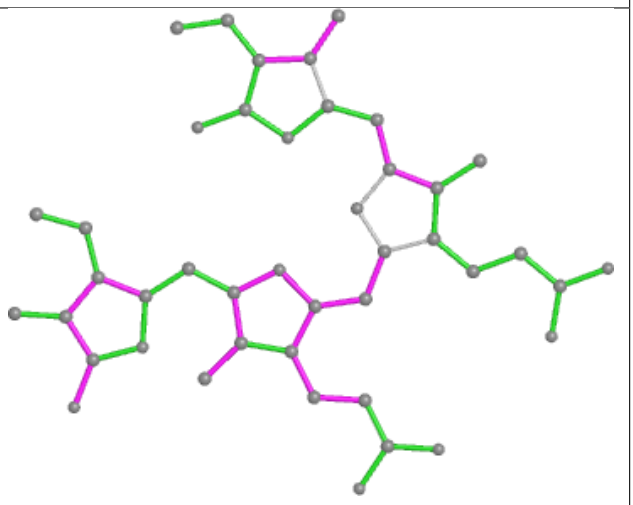

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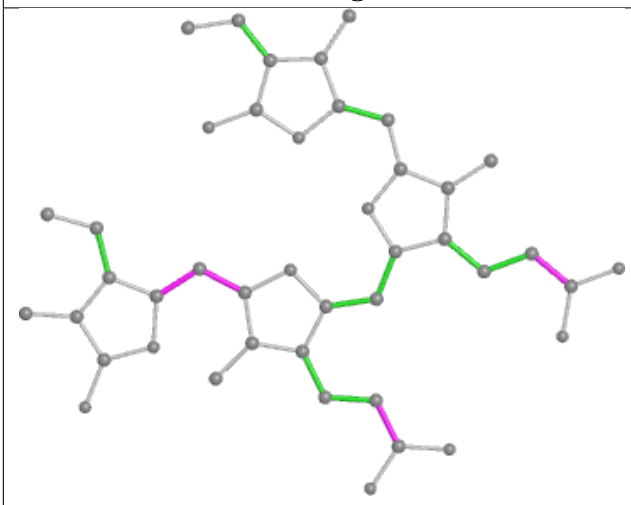

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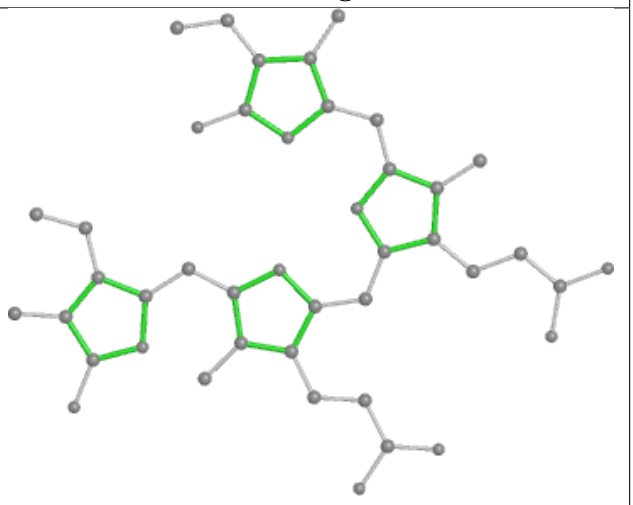
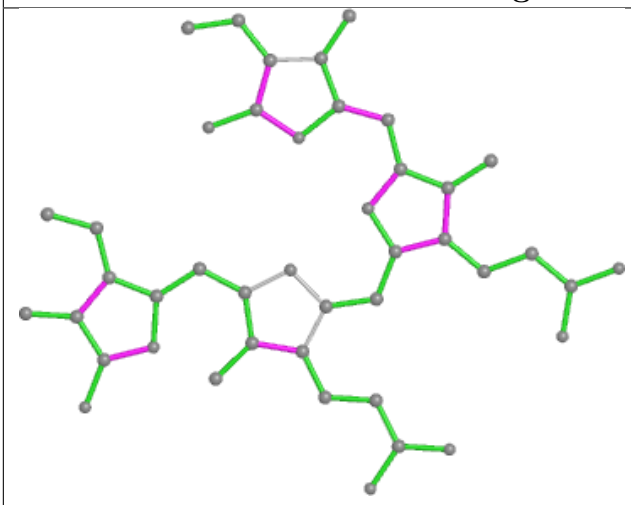


Rings

Ligand PUB H3 203



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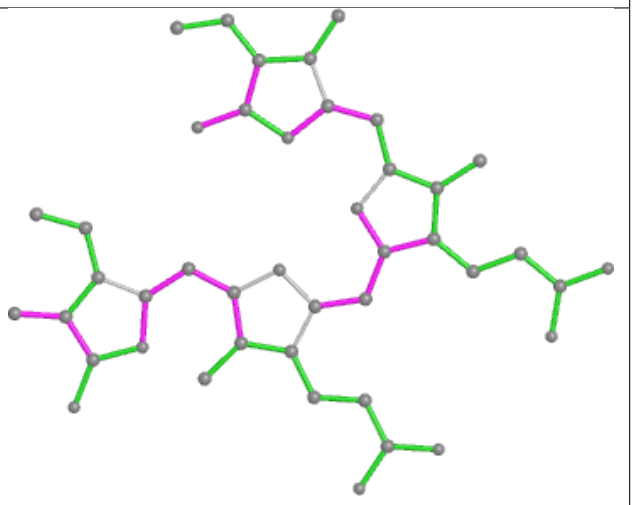

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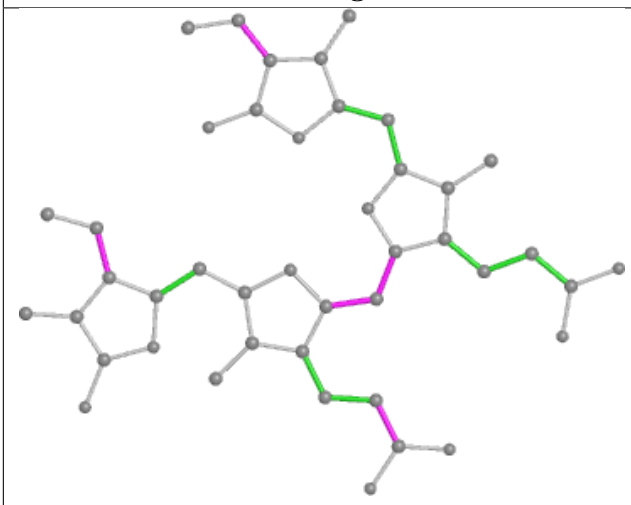

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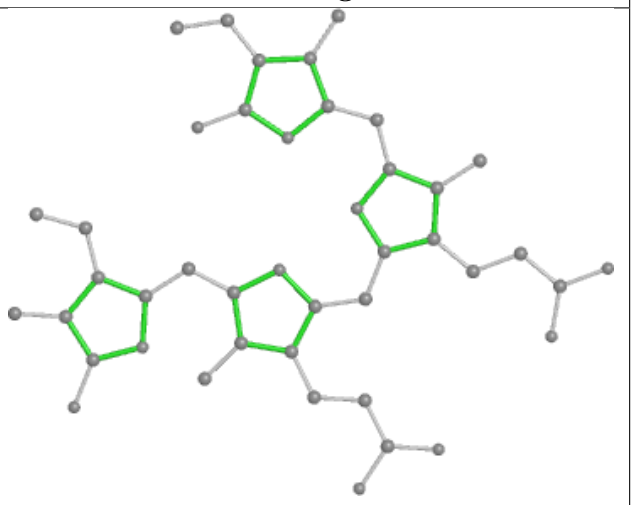
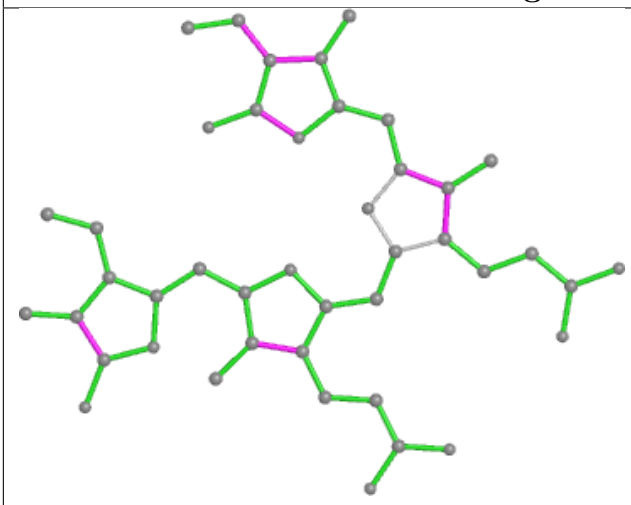


Rings

Ligand PEB af 202



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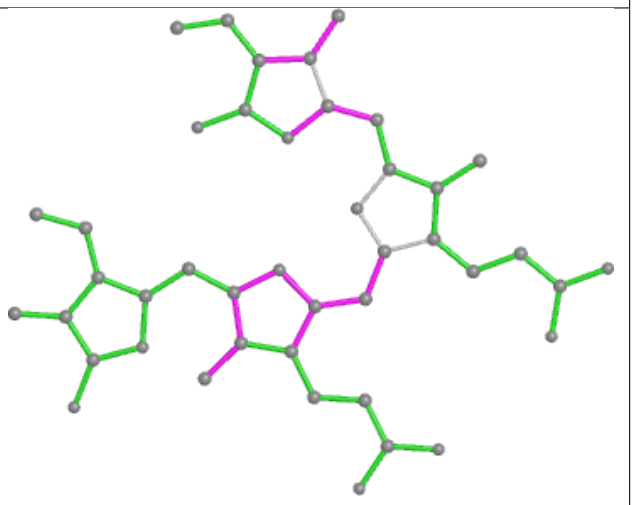

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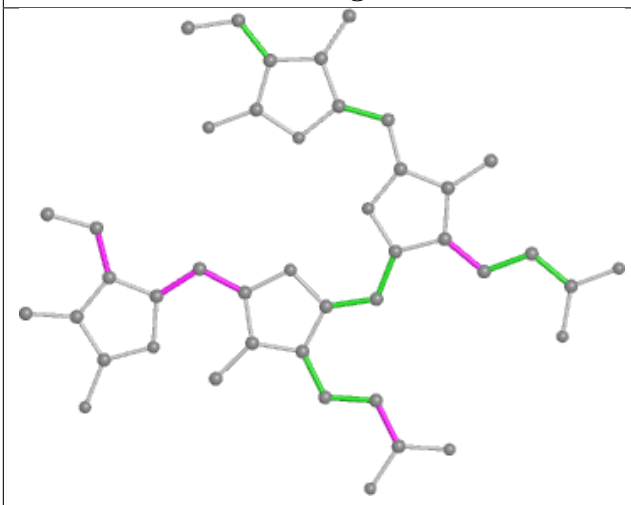

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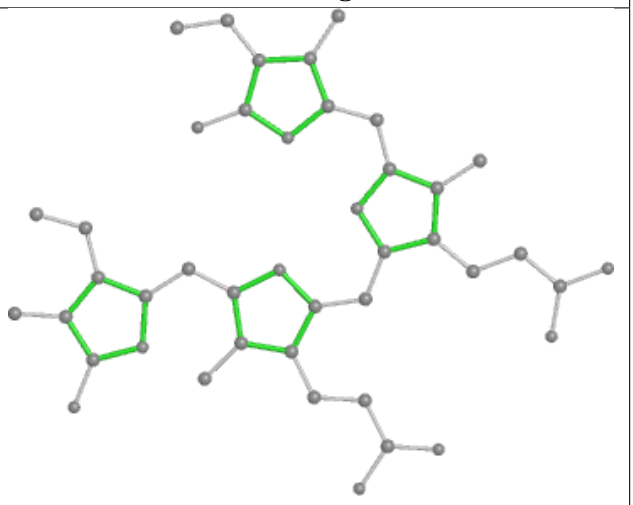
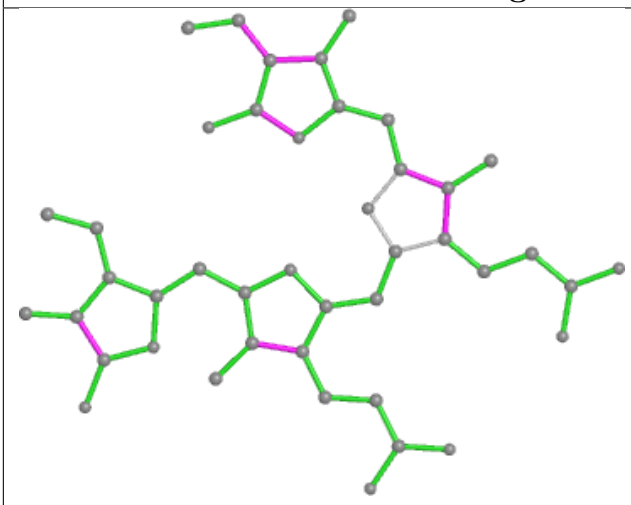


Rings

Ligand PEB kS 1002



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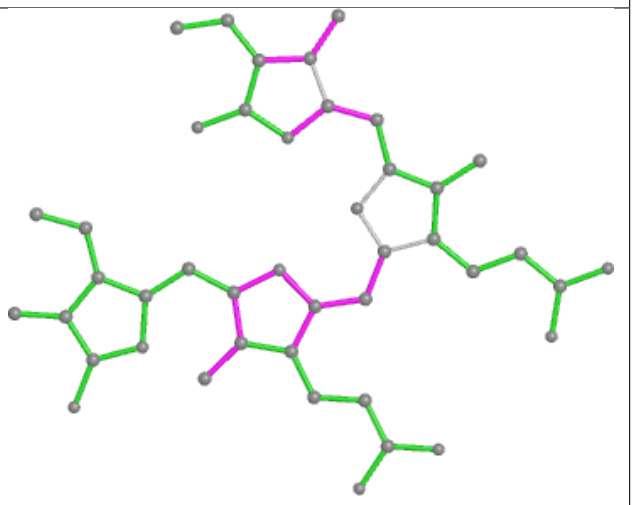

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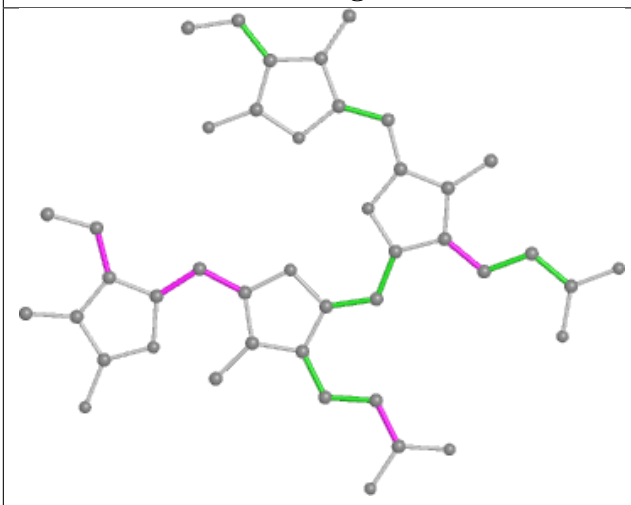

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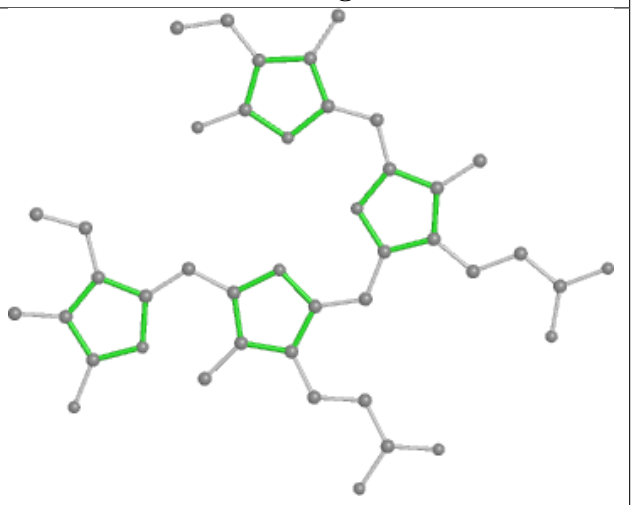
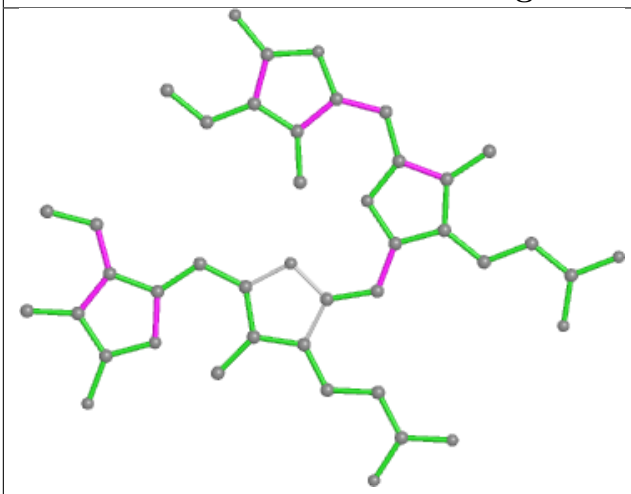


Rings

Ligand PVN eZ 402



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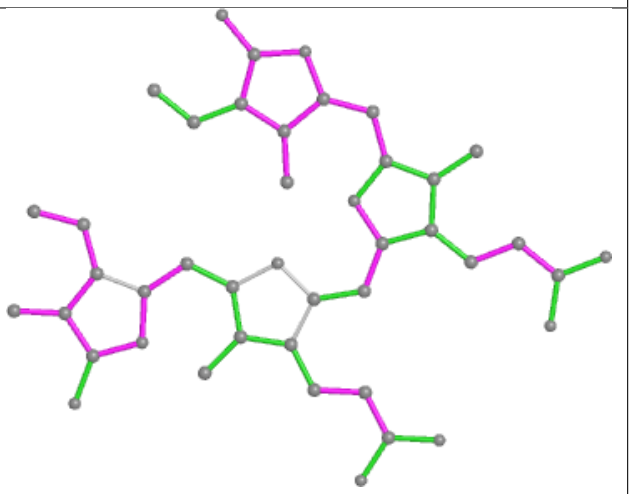

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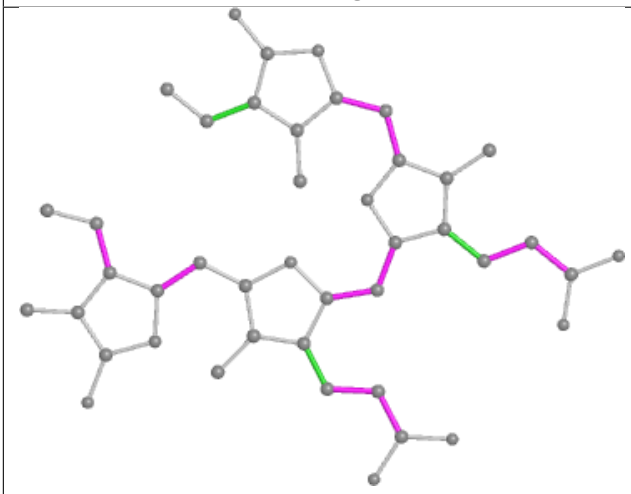

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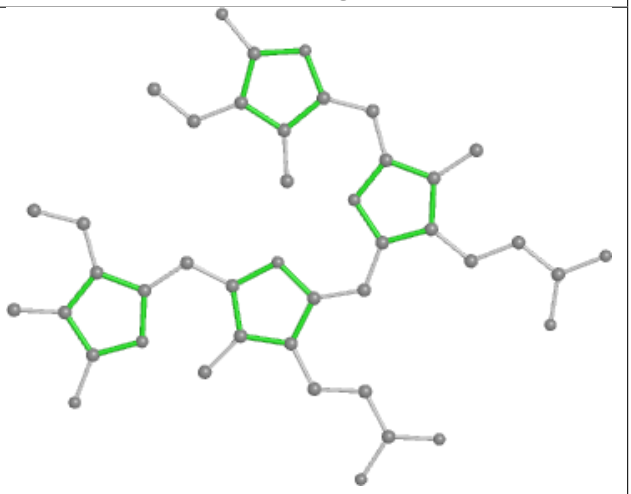
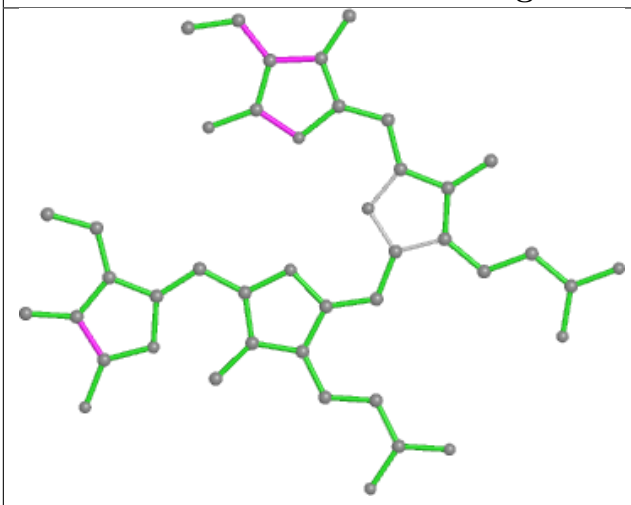


Rings

Ligand PEB cU 202



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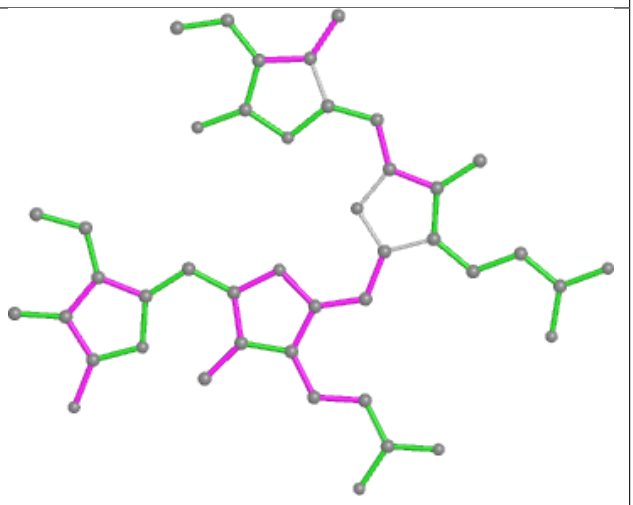

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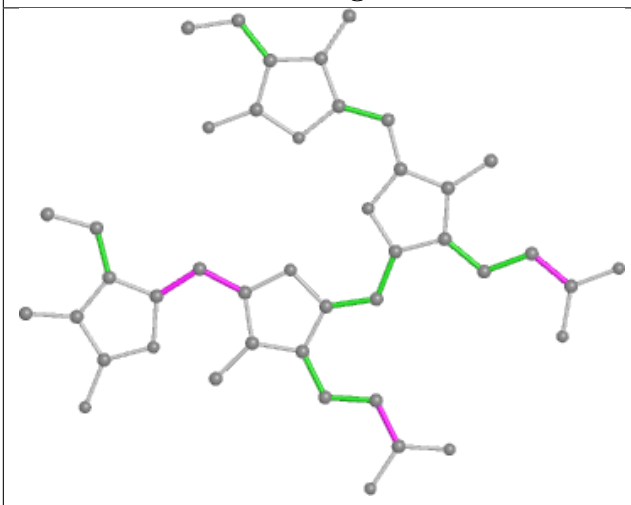

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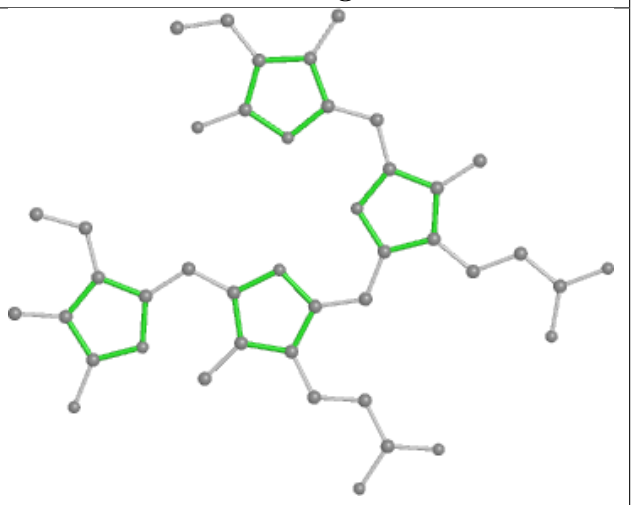
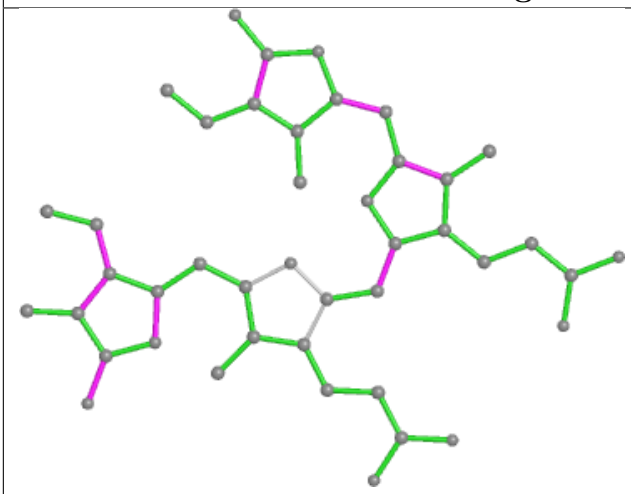


Rings

Ligand PVN Z5 304



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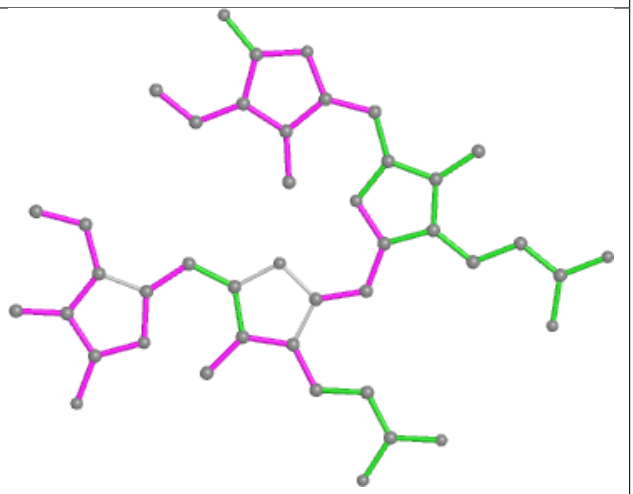

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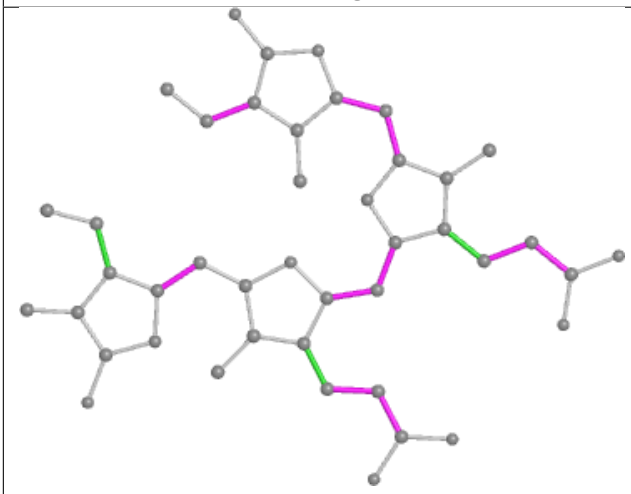

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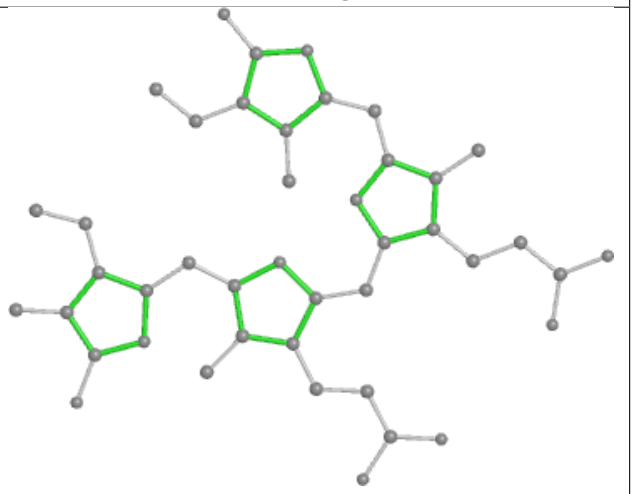

Rings

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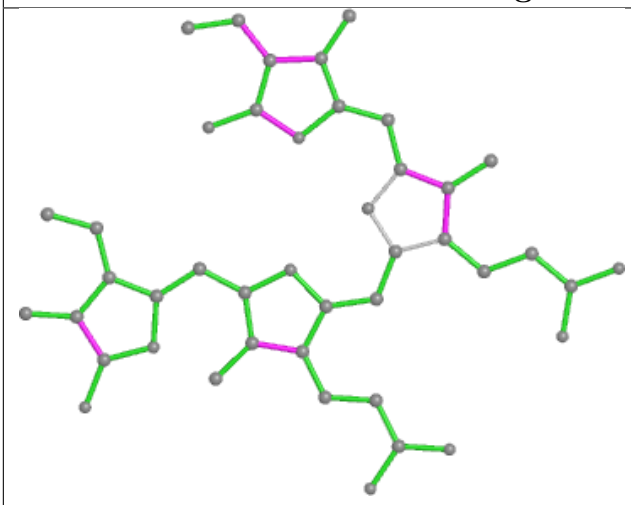

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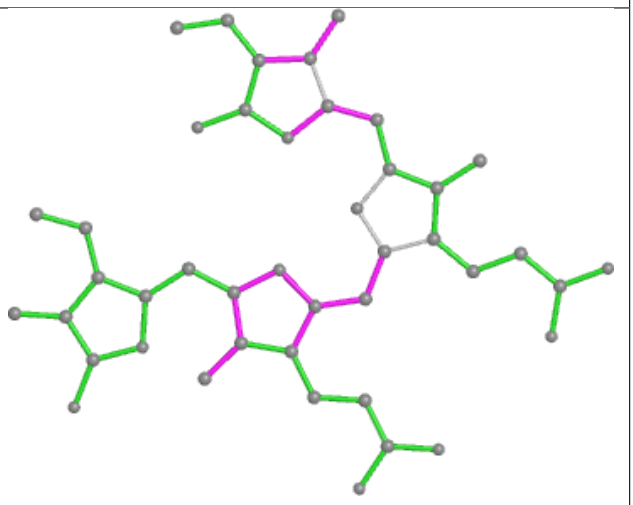

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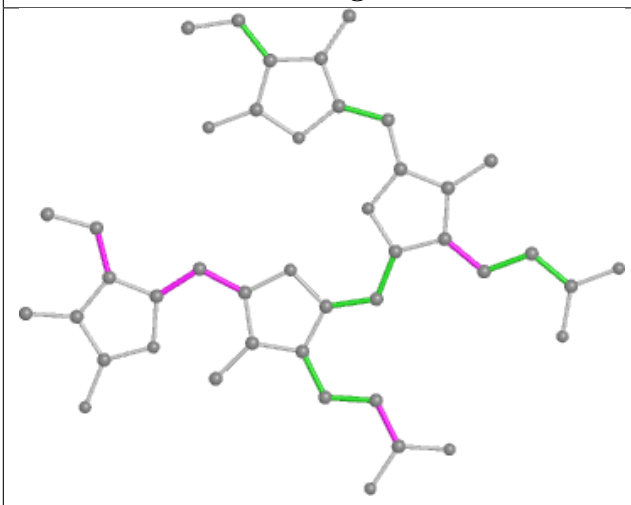

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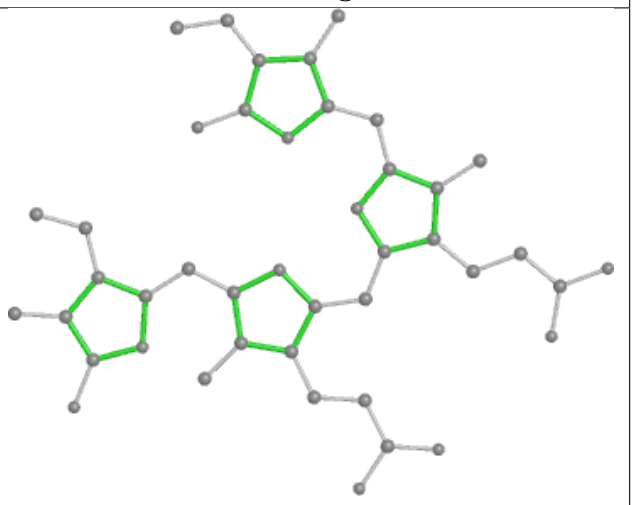
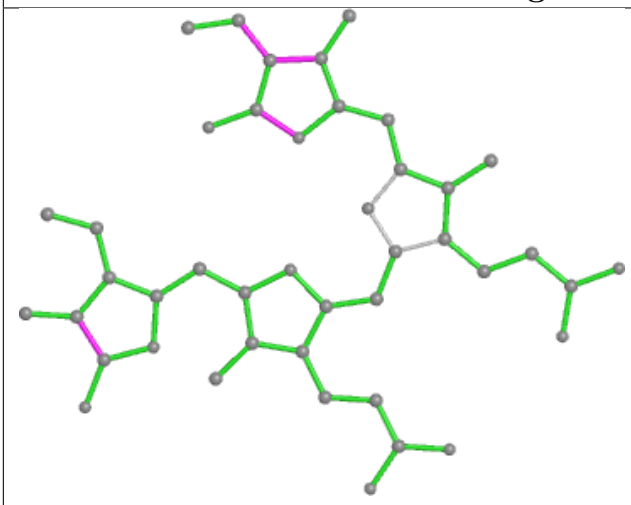


Rings

Ligand PEB ll 201



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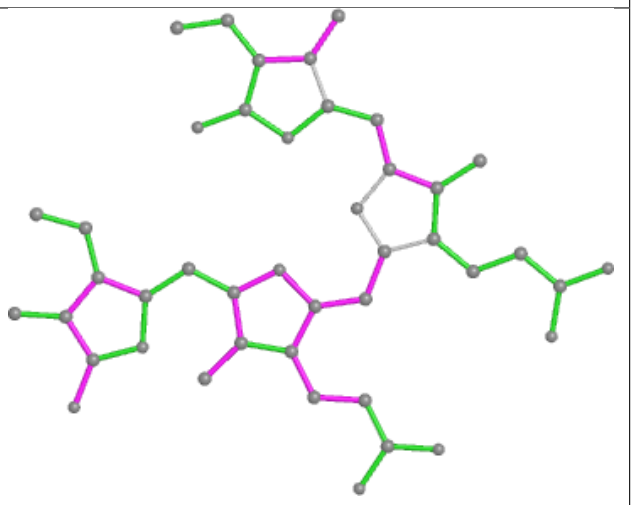

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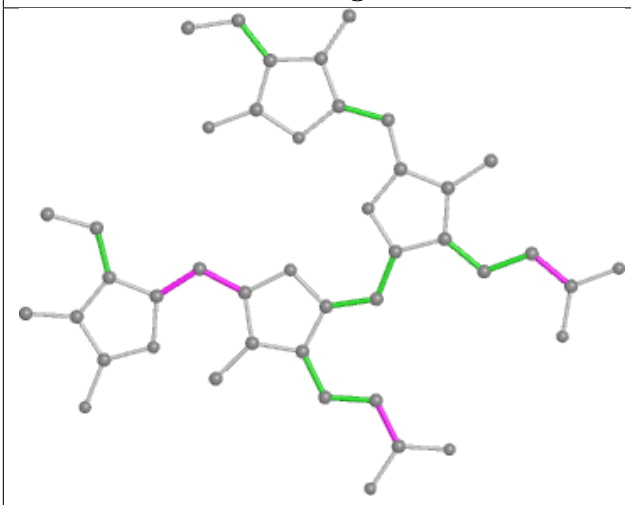

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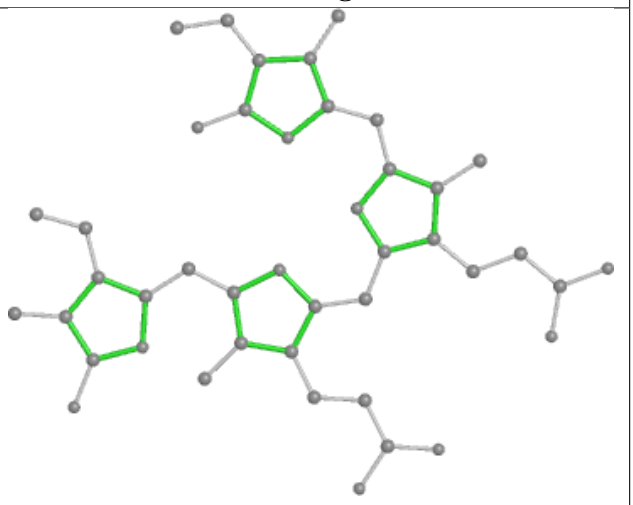
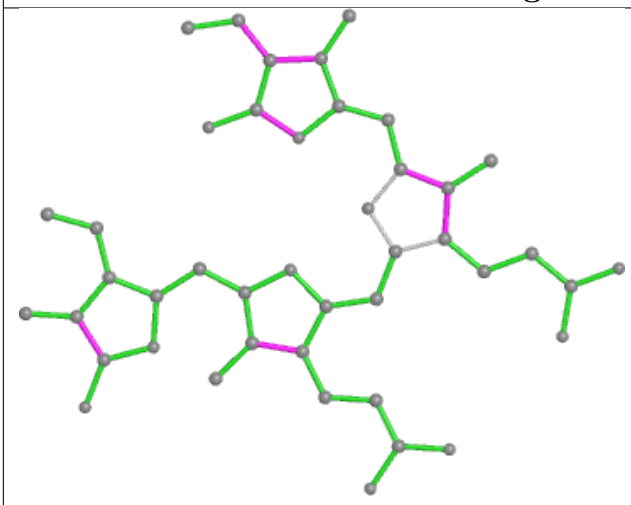


Rings

Ligand PEB j2 202



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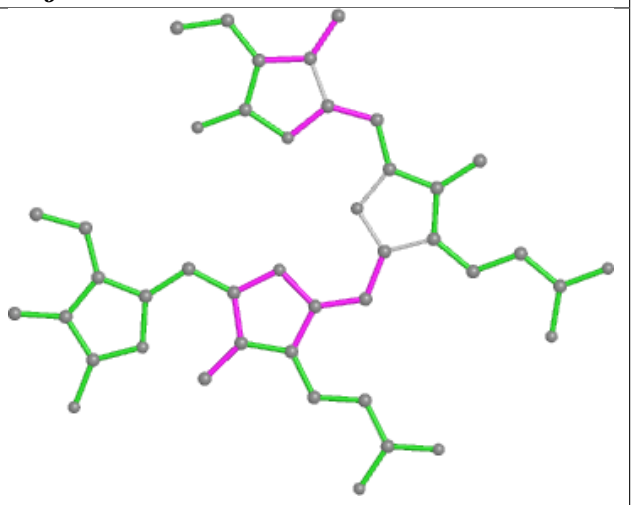

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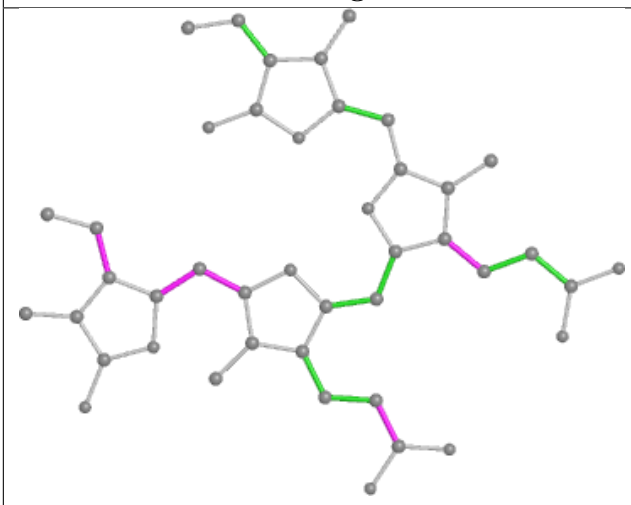

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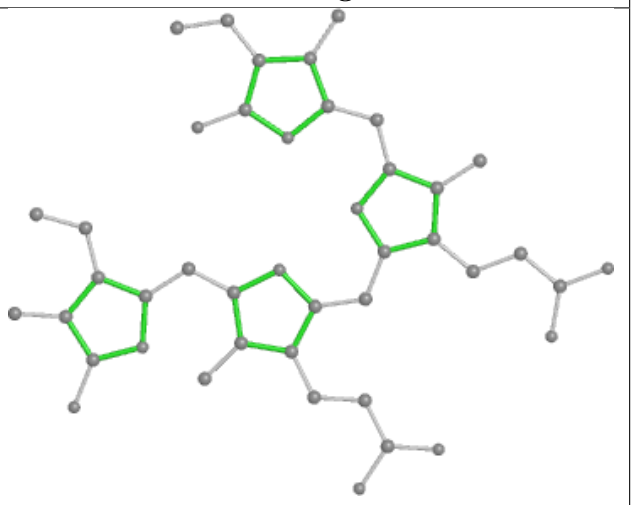
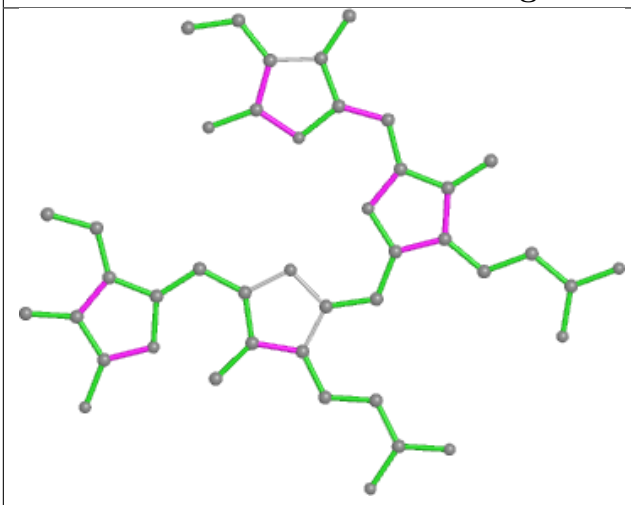


Rings

Ligand PUB t6 203



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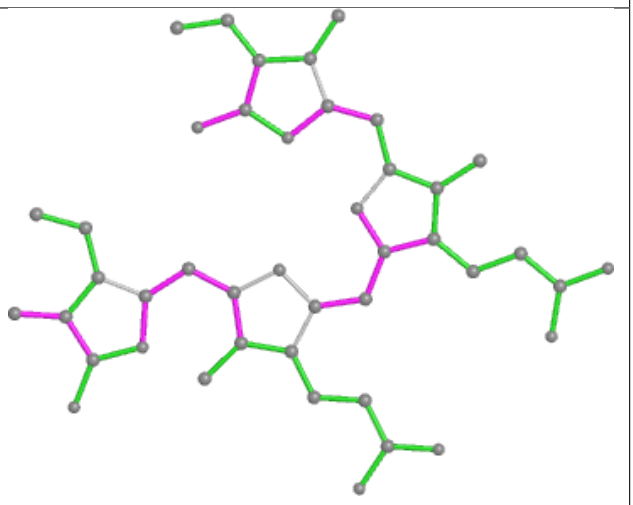

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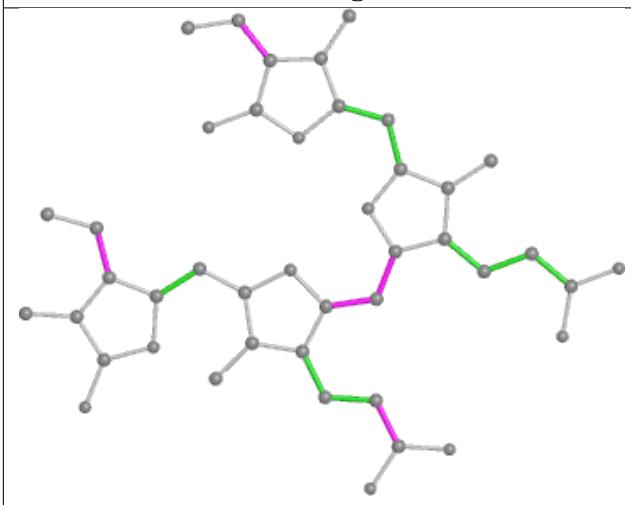

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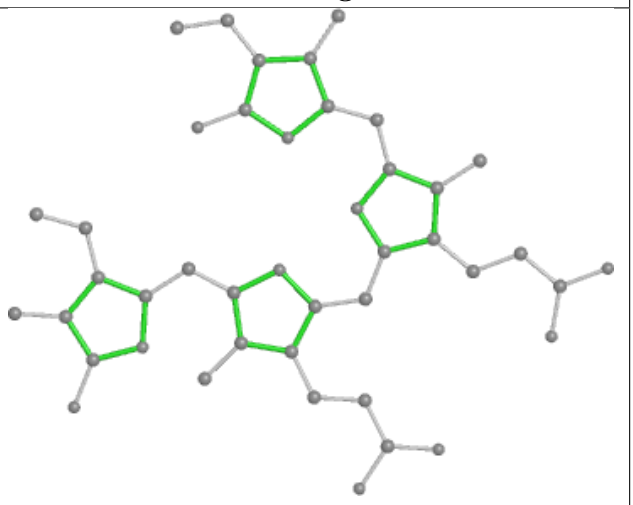
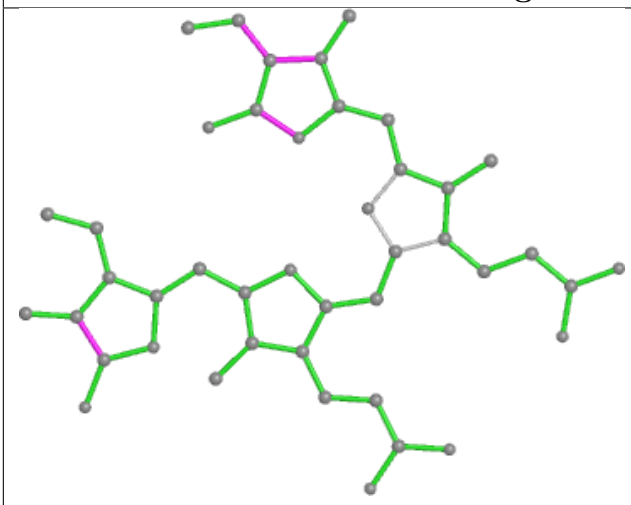


Rings

Ligand PEB dC 201



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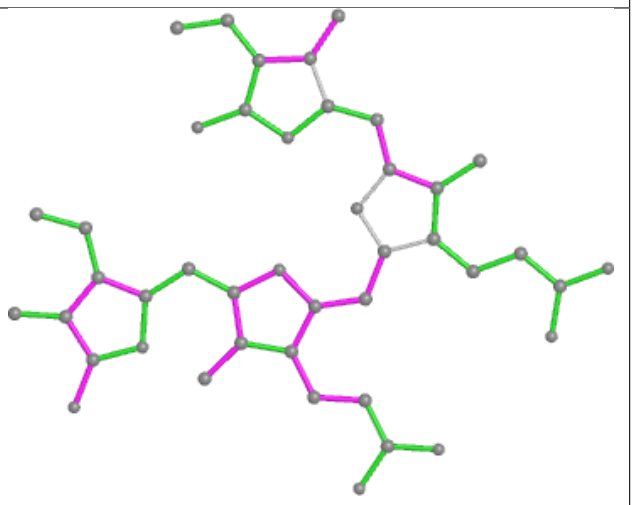
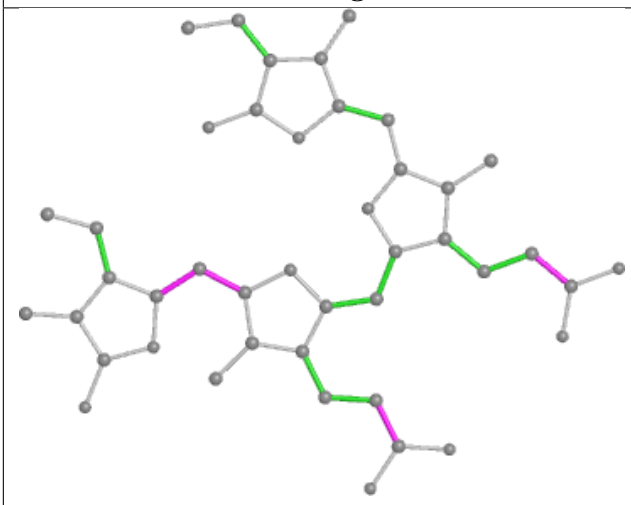


Bond angles



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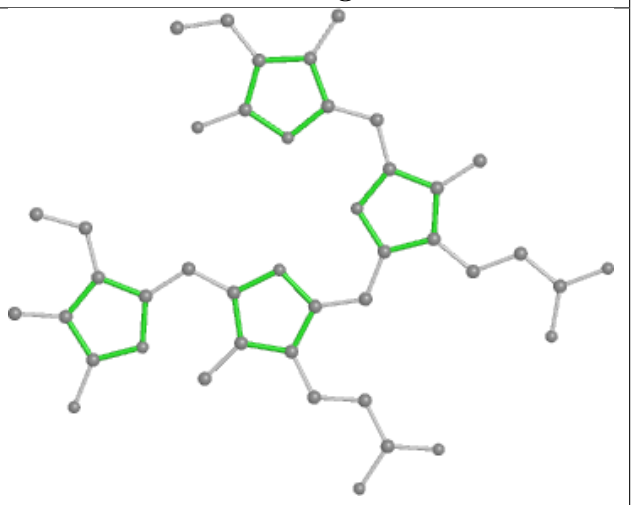
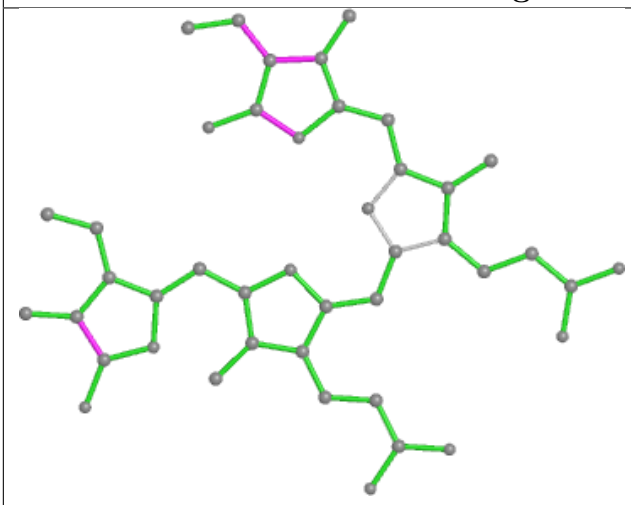
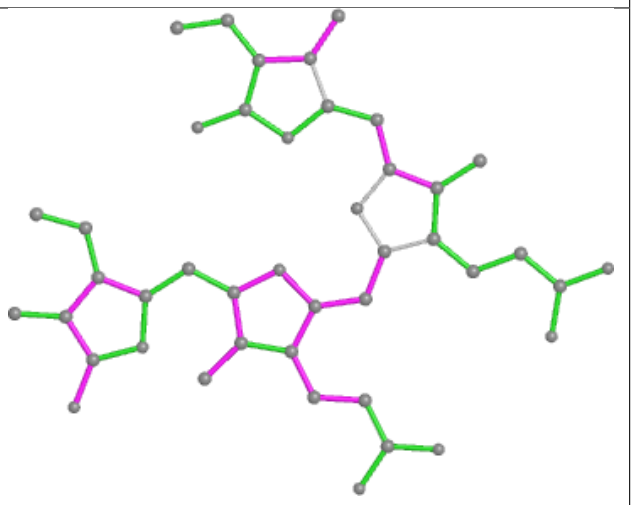


Rings

Ligand PEB cM 201



Bond lengths



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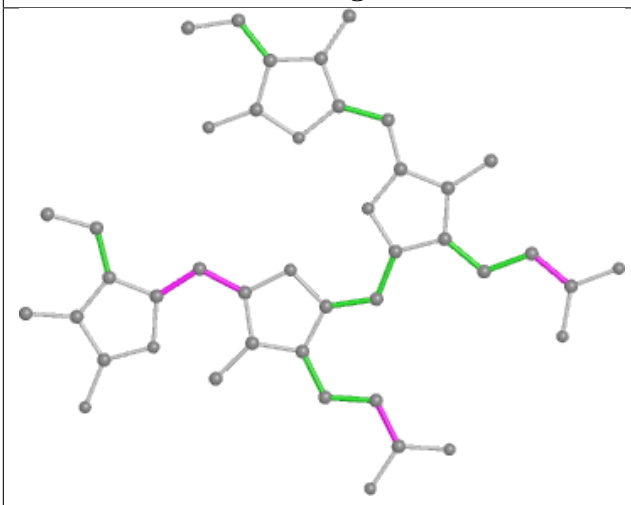
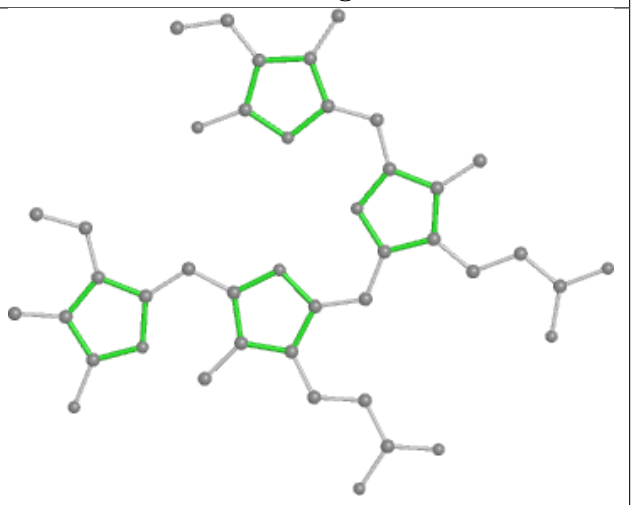
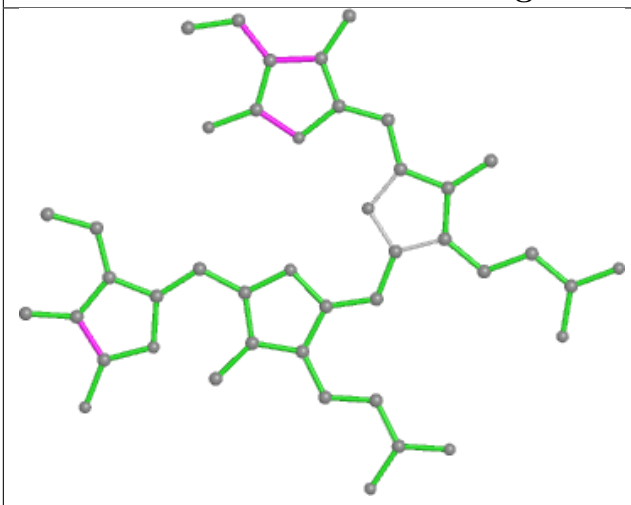


Torsions



Rings

Ligand PEB dP 202



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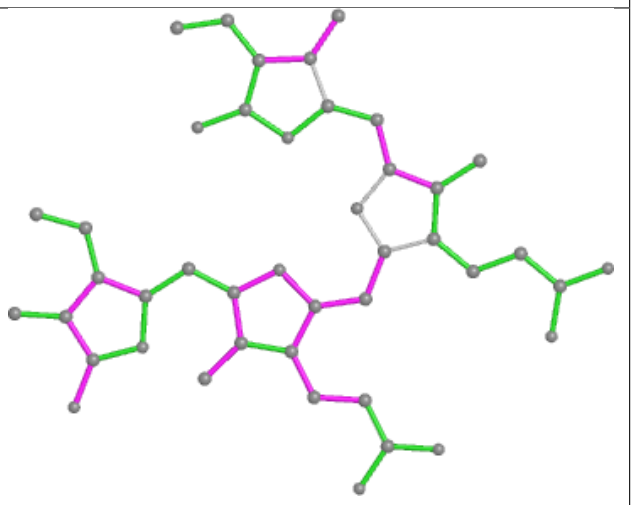

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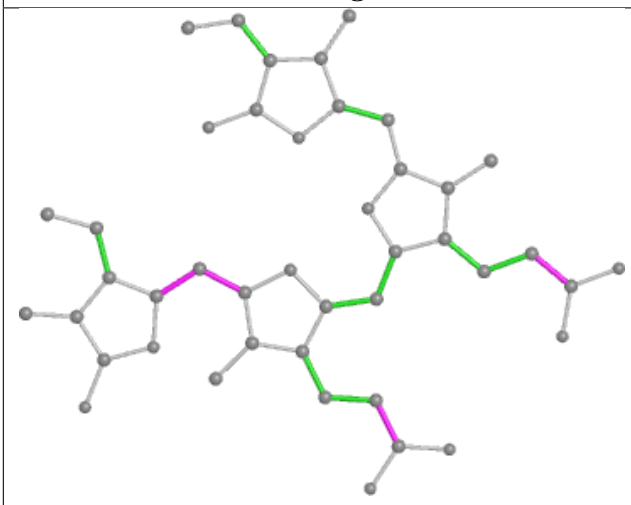

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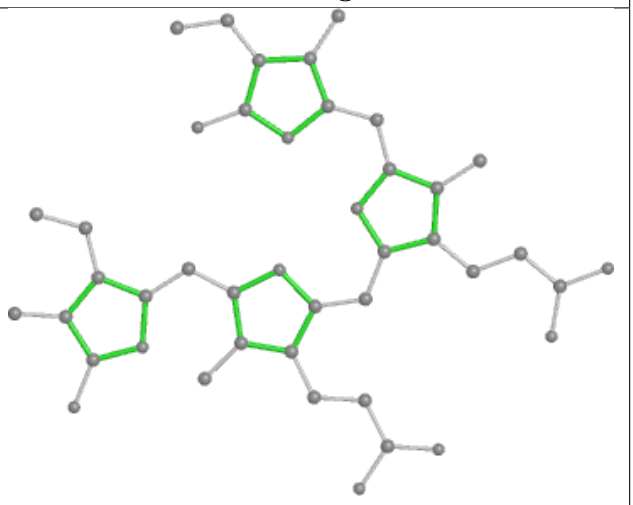
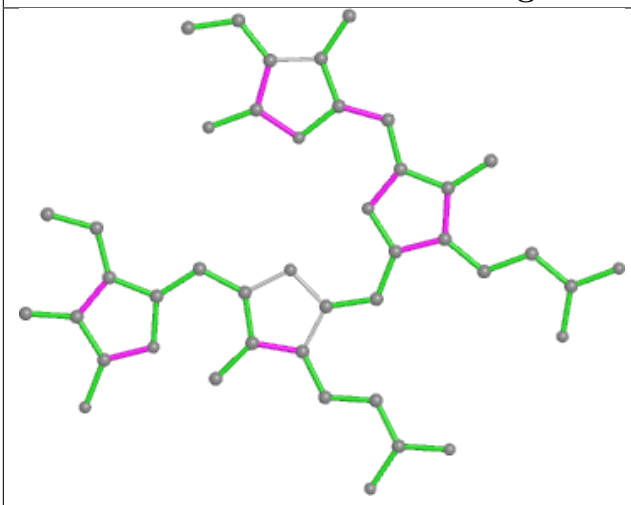


Rings

Ligand PUB J7 202



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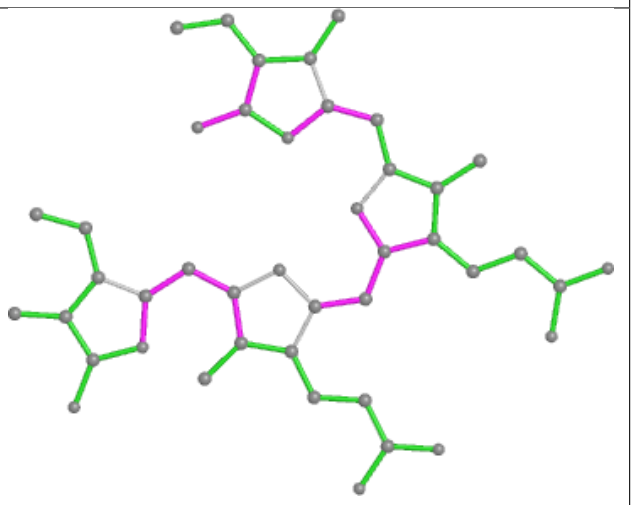

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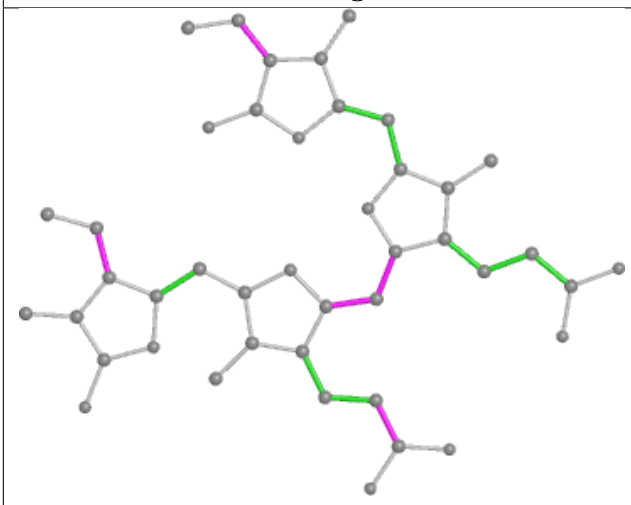

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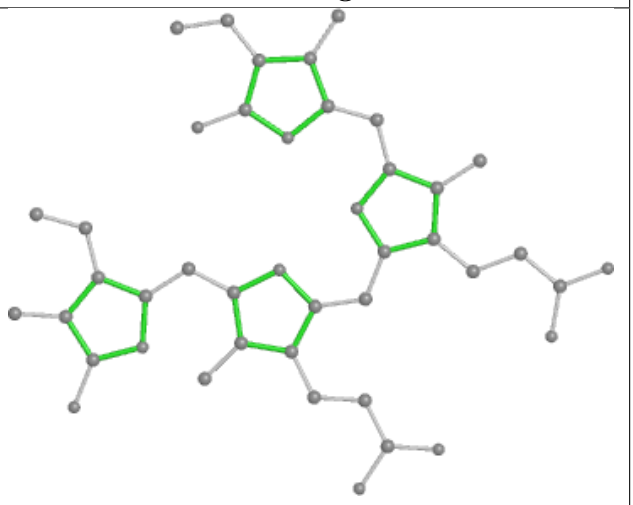

Rings

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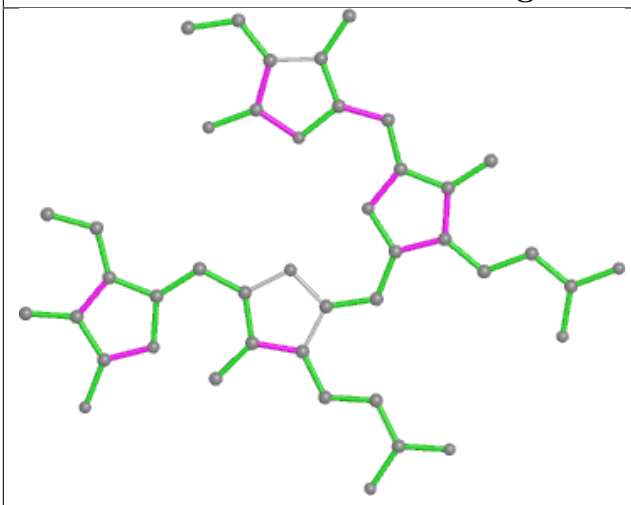

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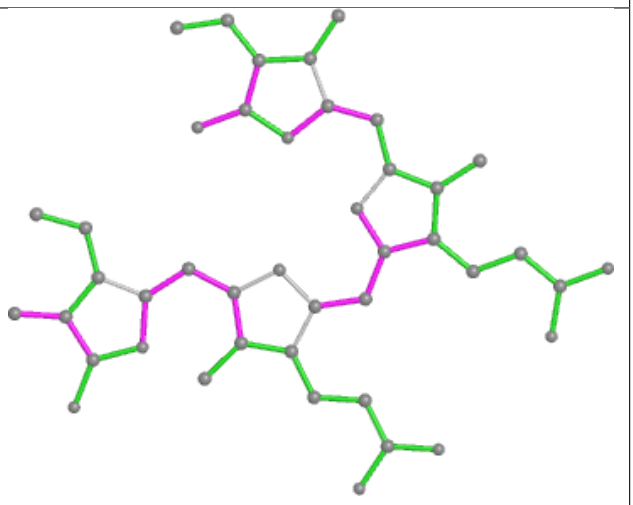

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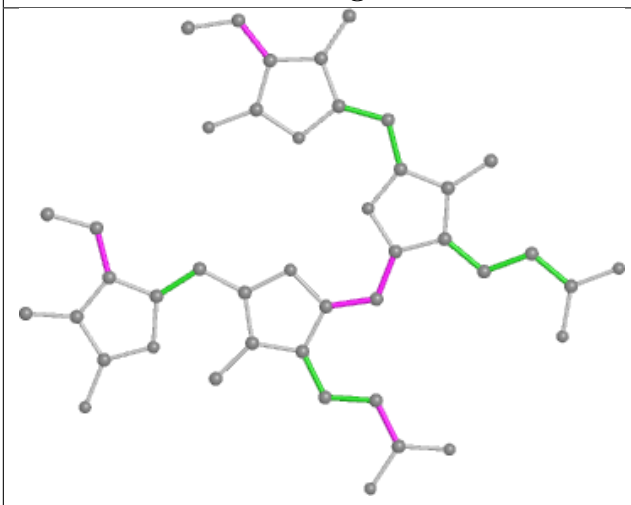

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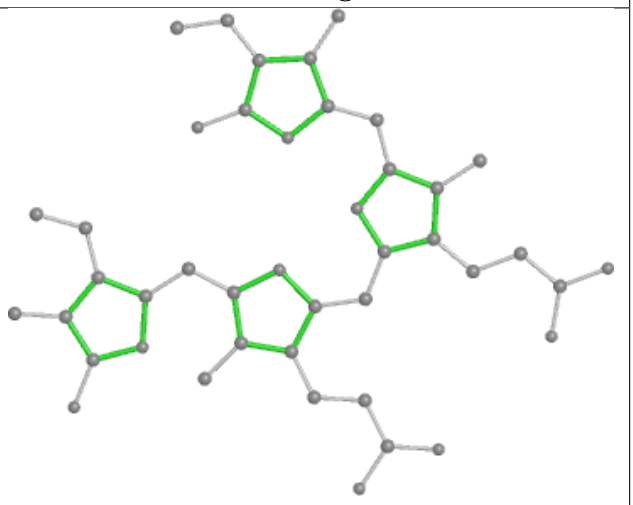

Rings

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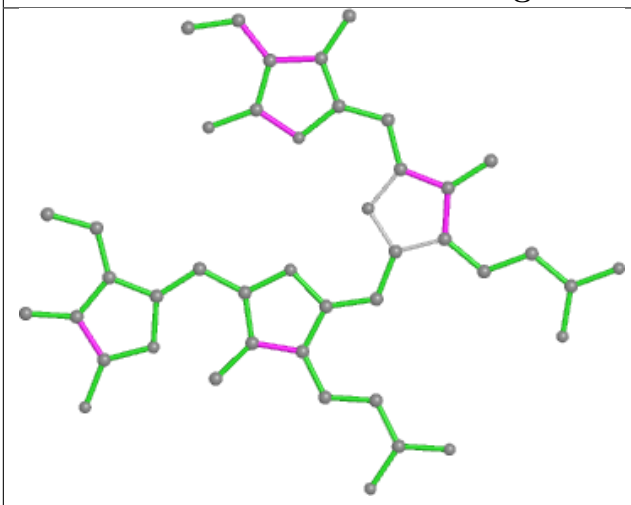

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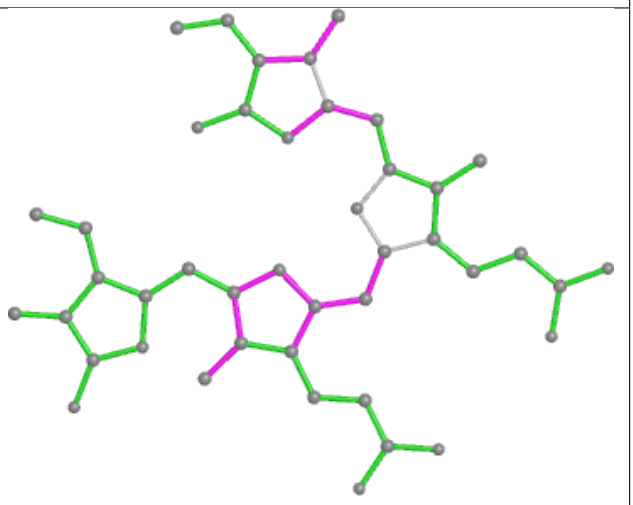

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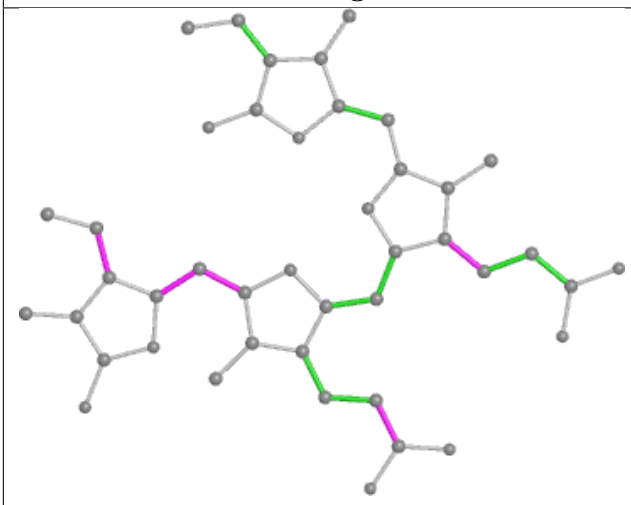

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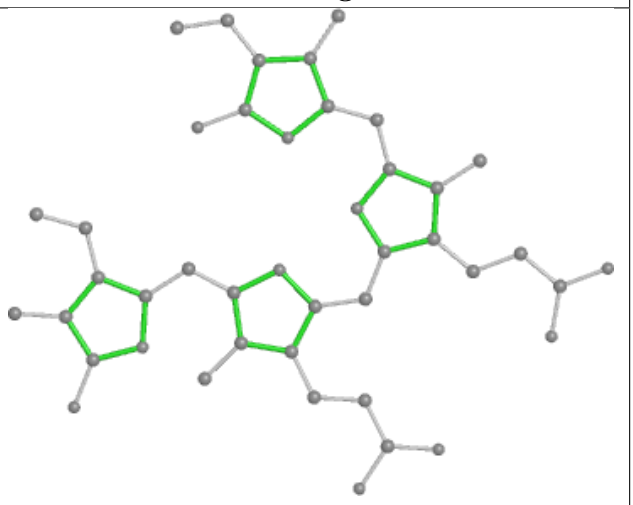

Rings

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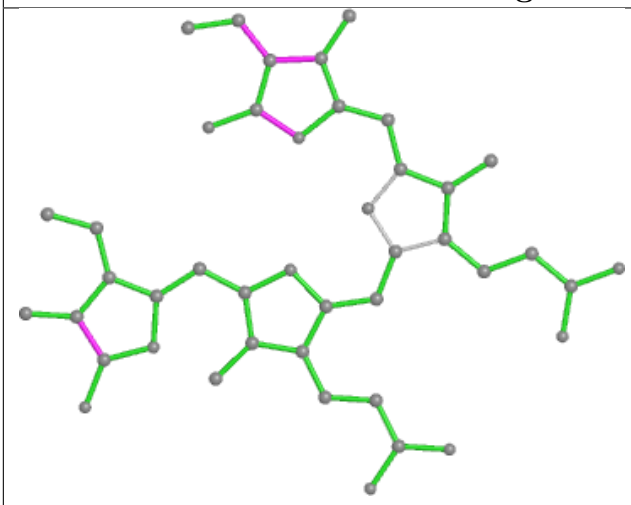

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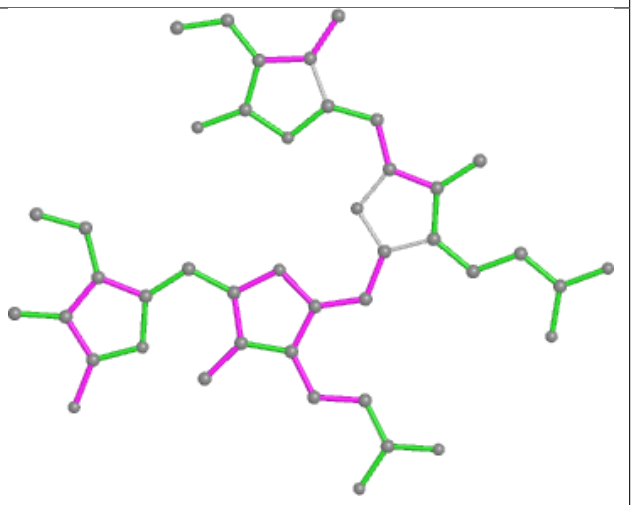

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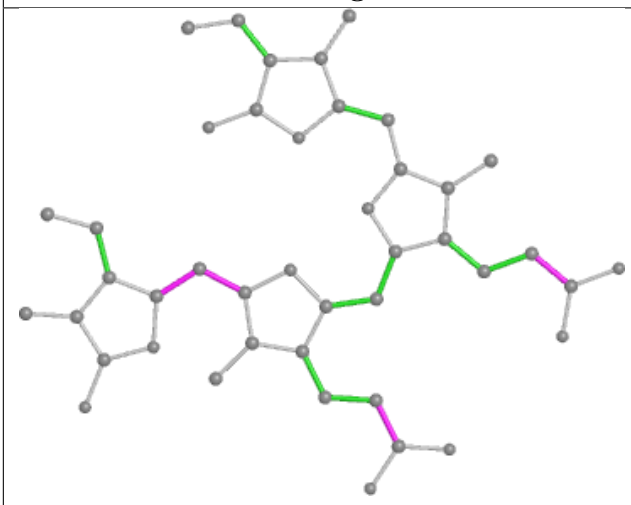

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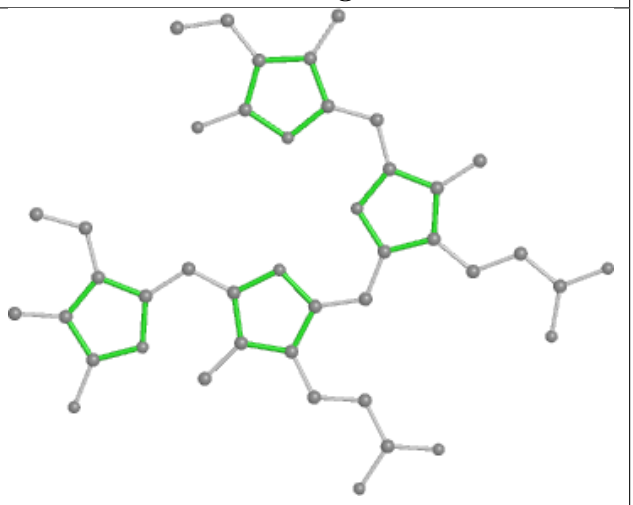

Rings

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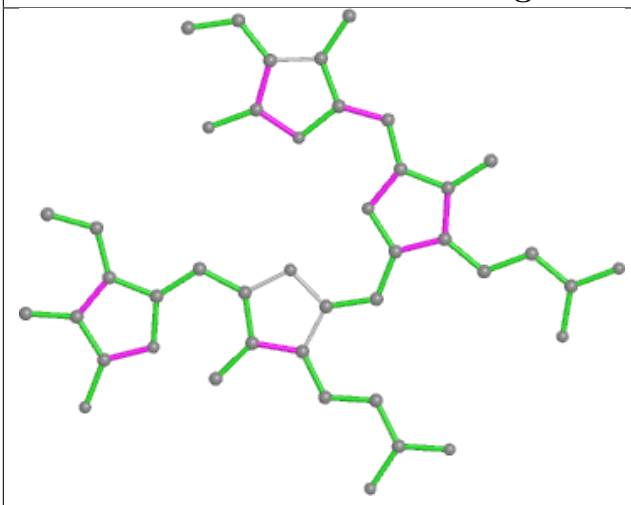

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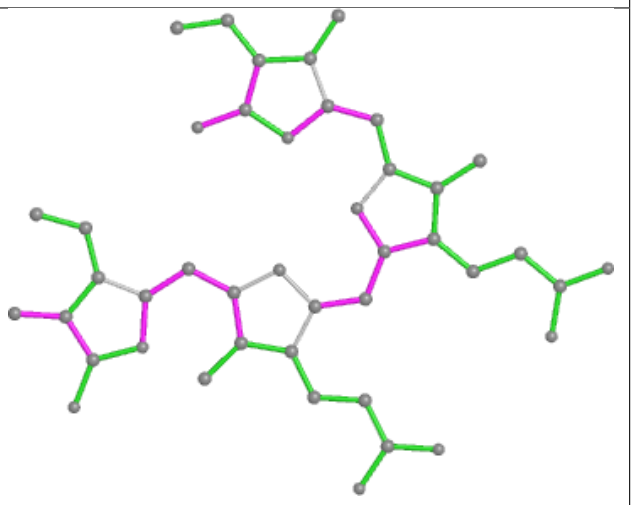

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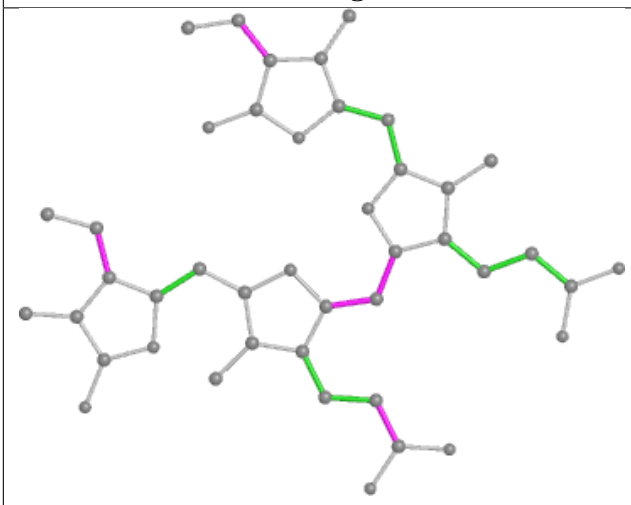

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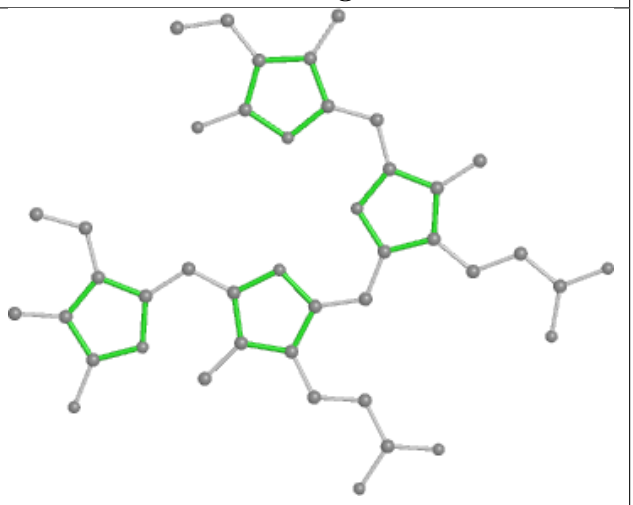

Rings

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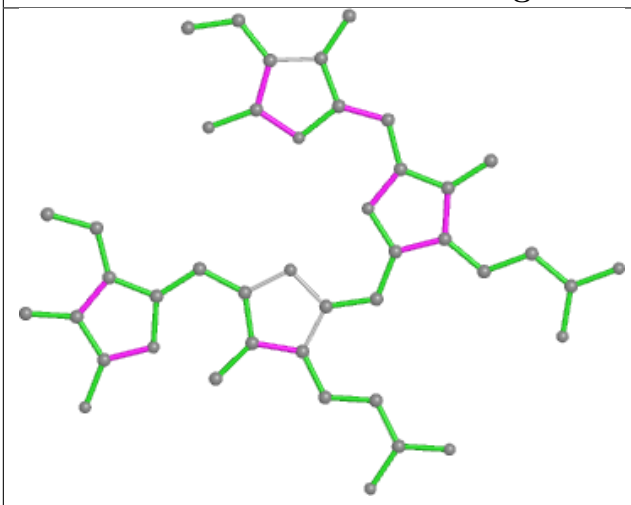

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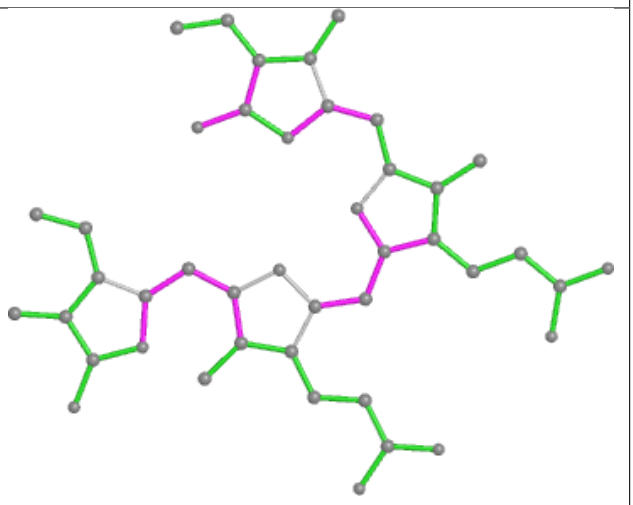

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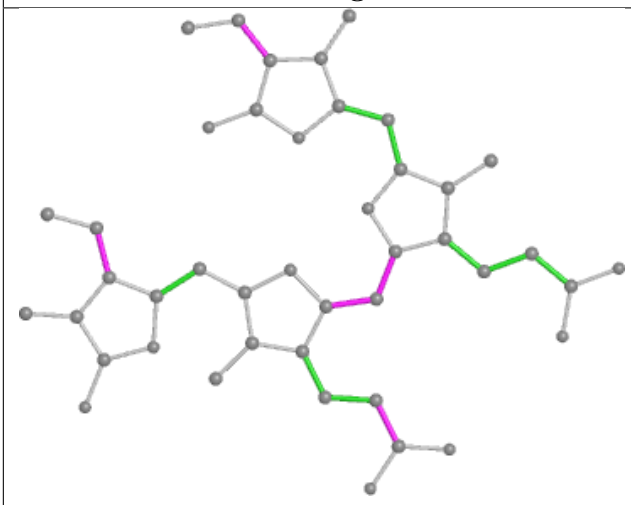

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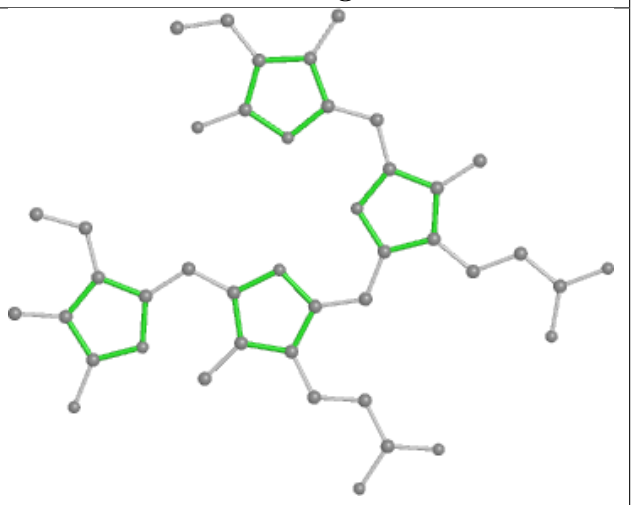

Rings

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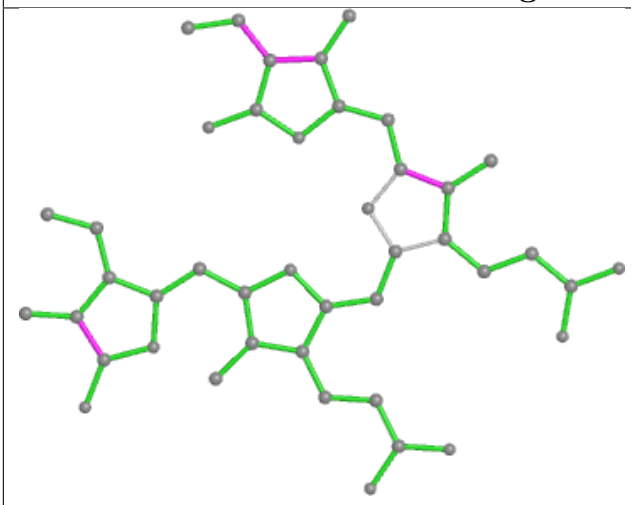

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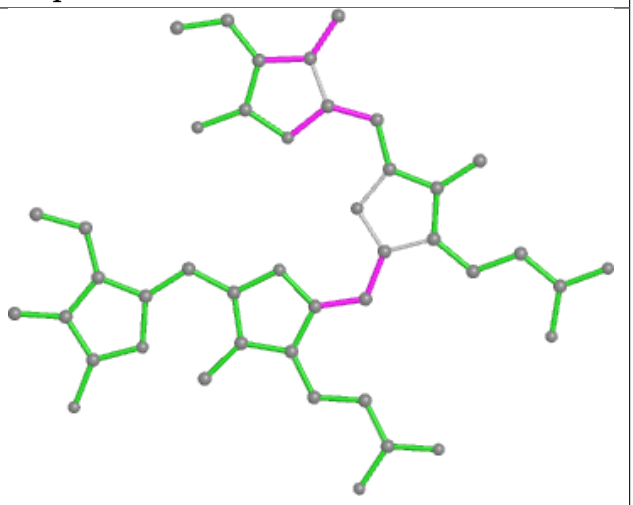

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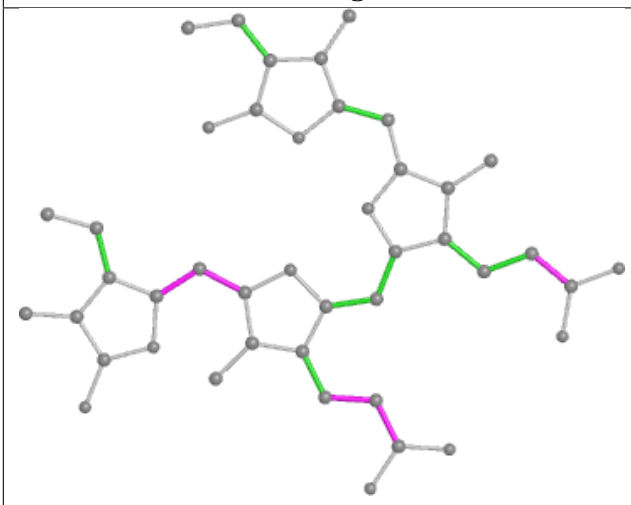

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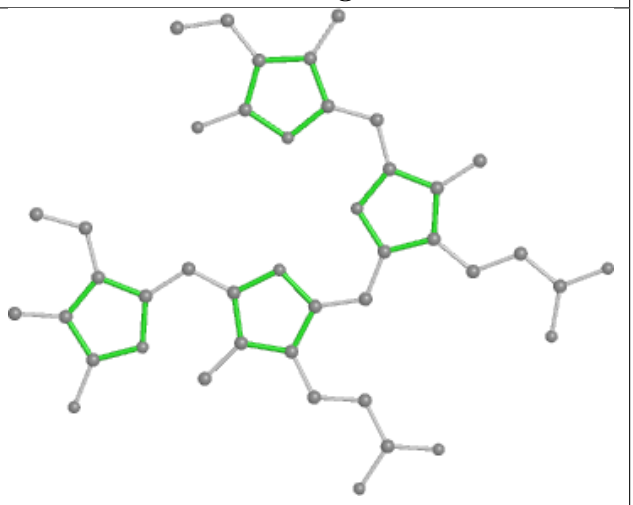

Rings

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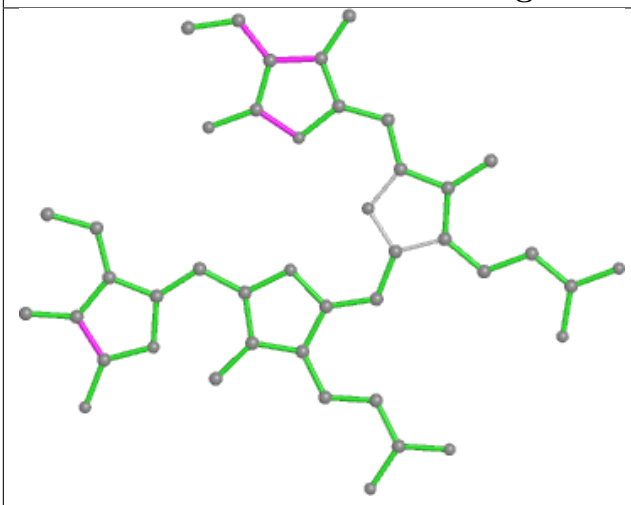

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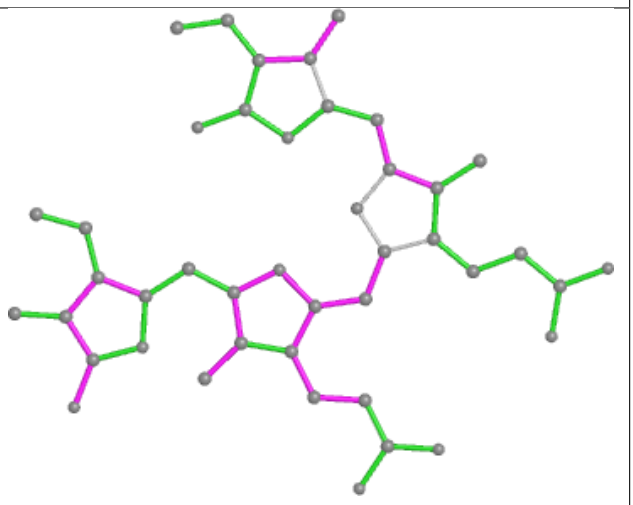

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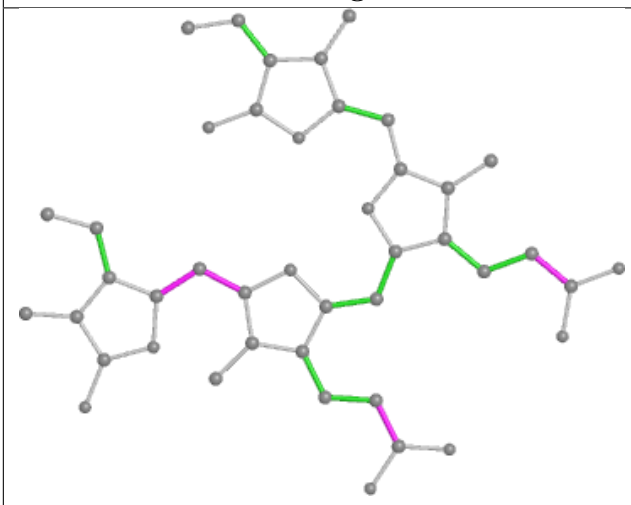

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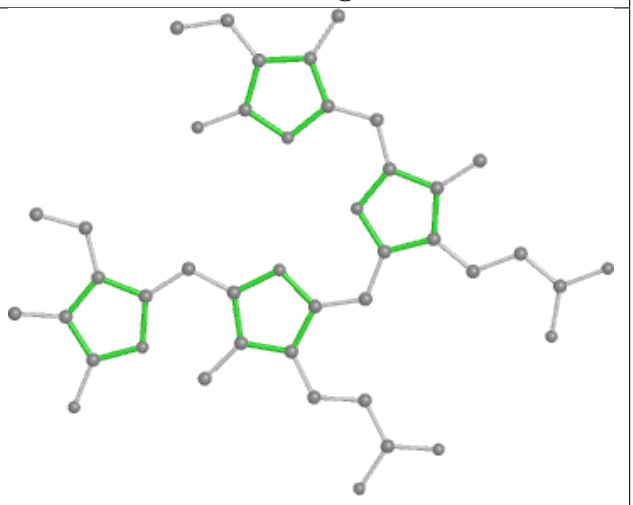

Rings

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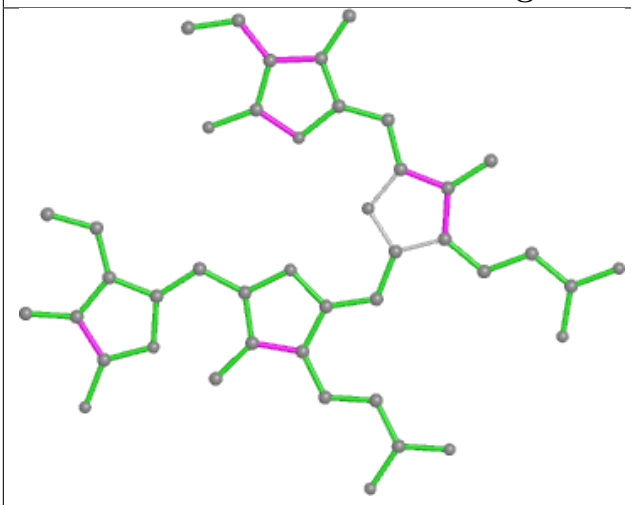

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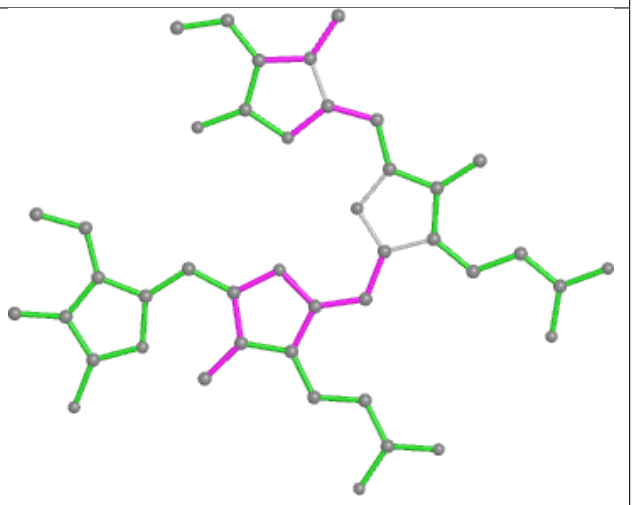

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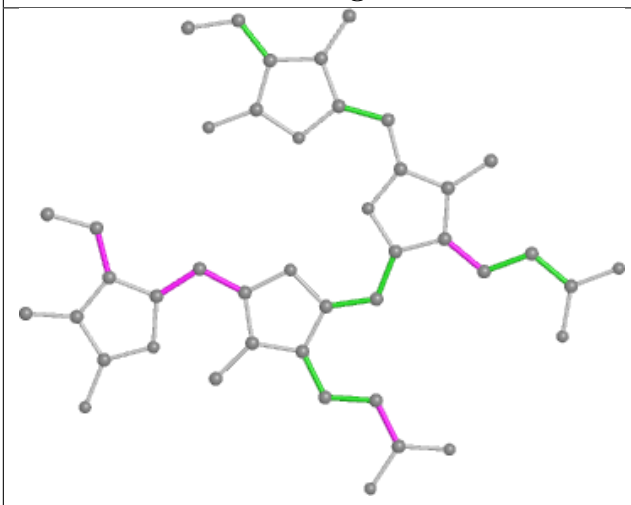

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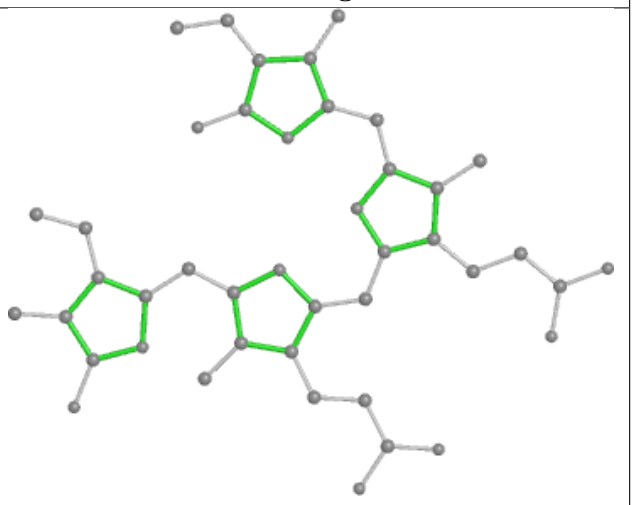
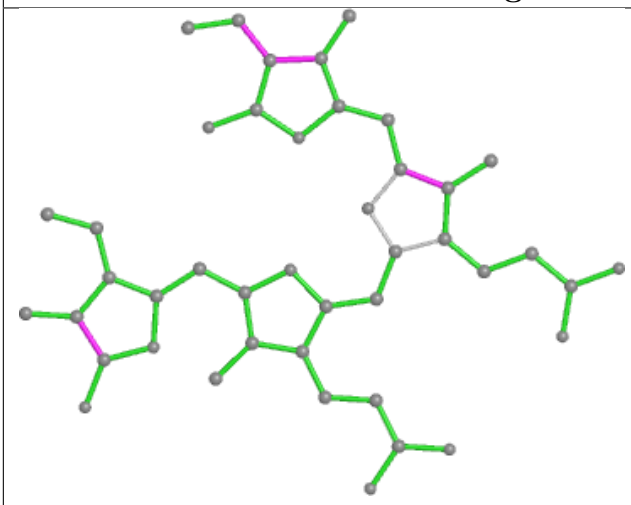


Rings

Ligand PEB m5 1002



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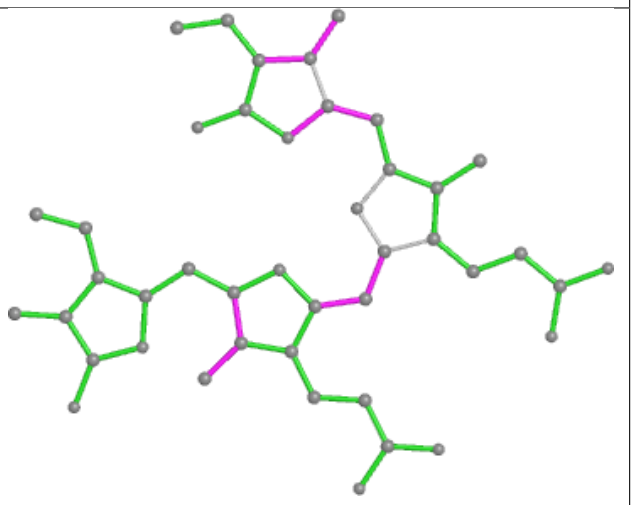

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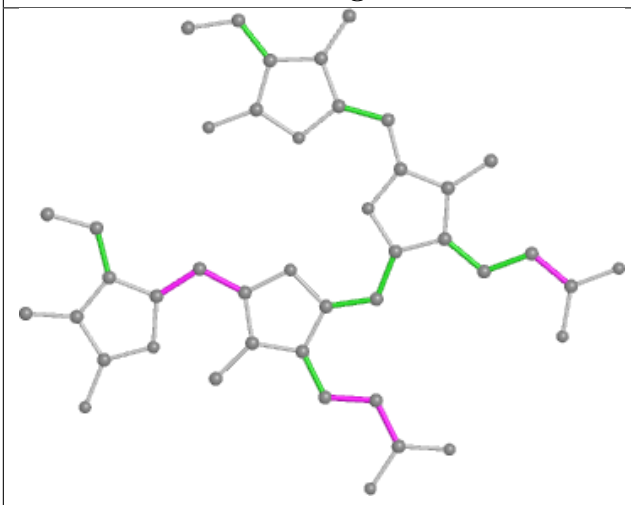

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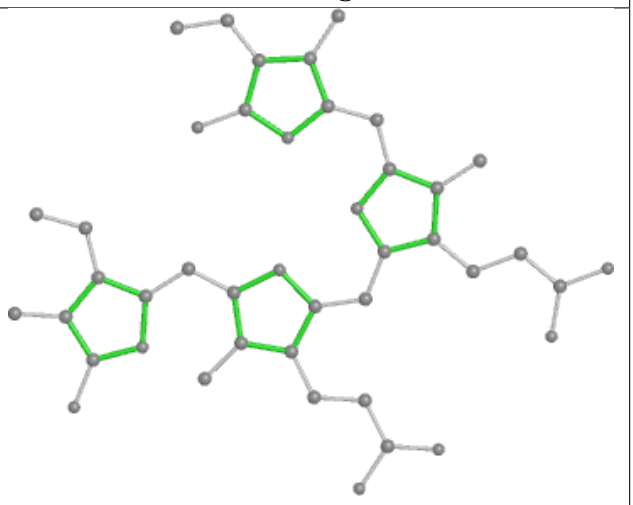

Rings

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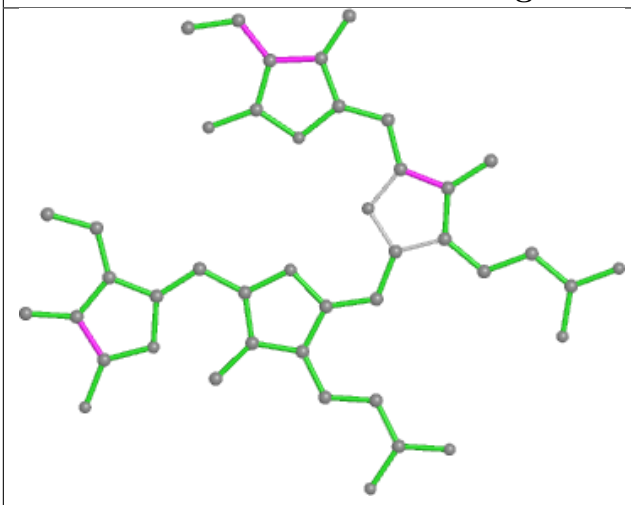

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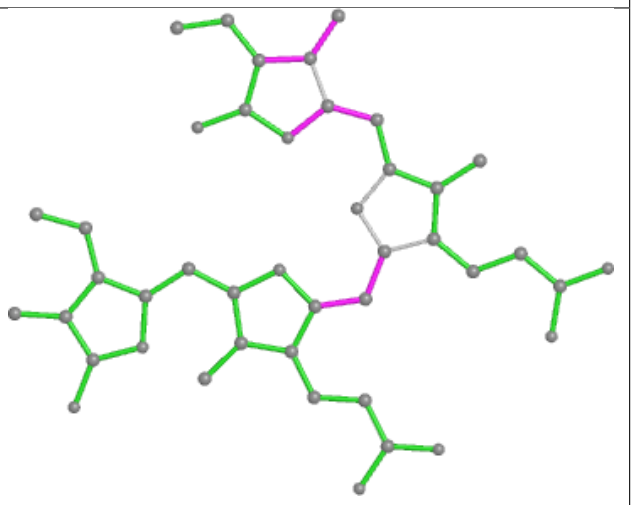

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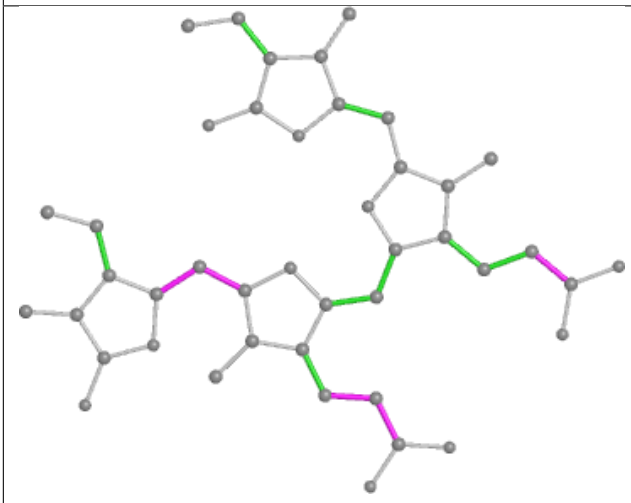

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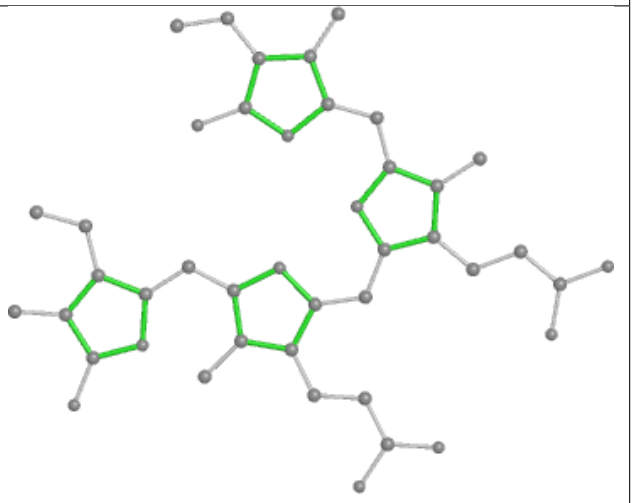
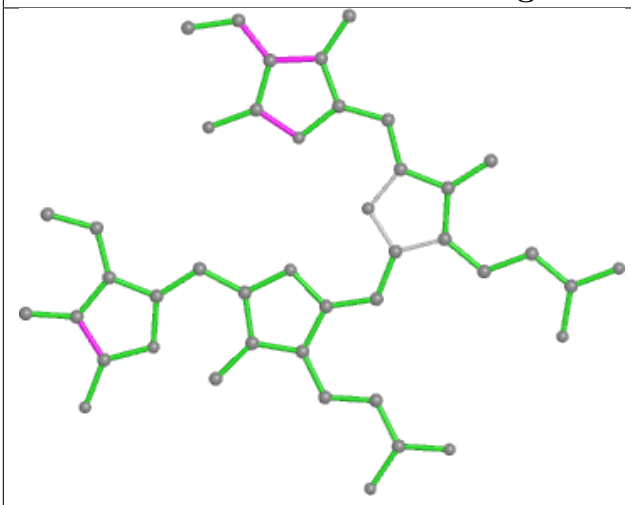


Rings

Ligand PEB F4 201



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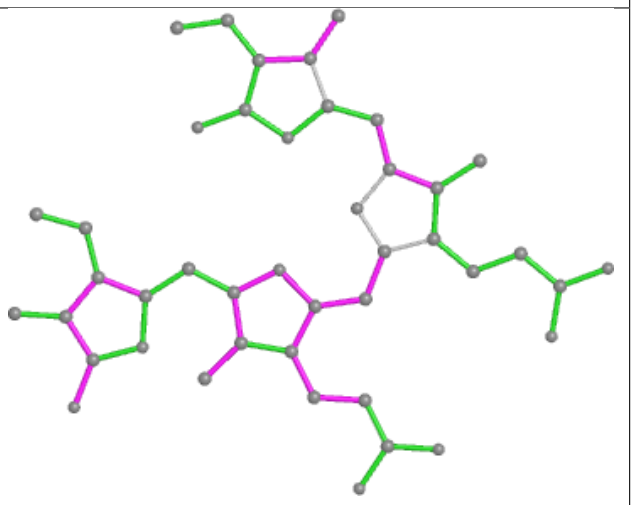
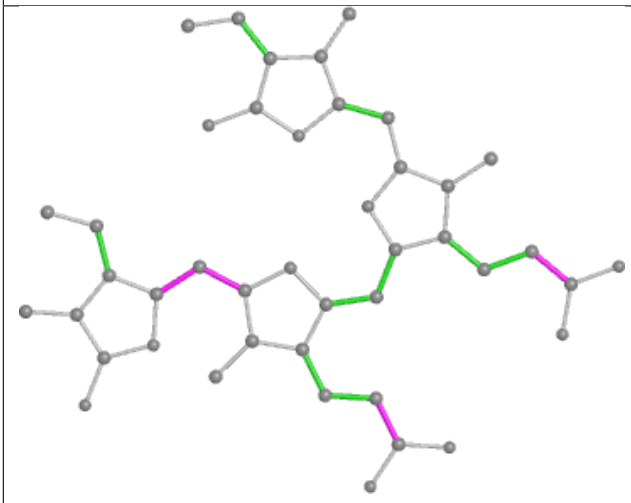
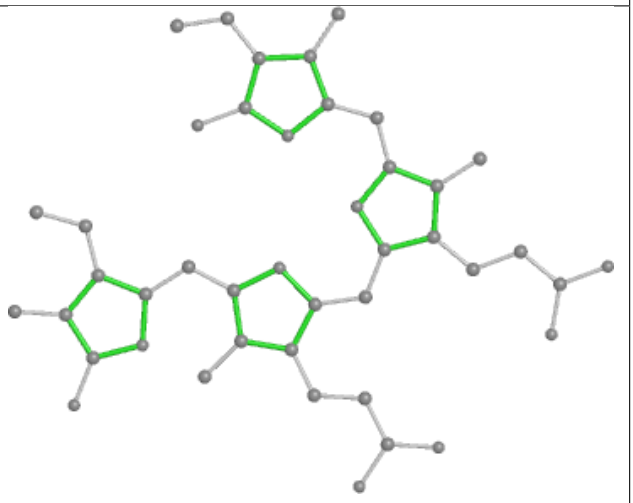


Bond angles

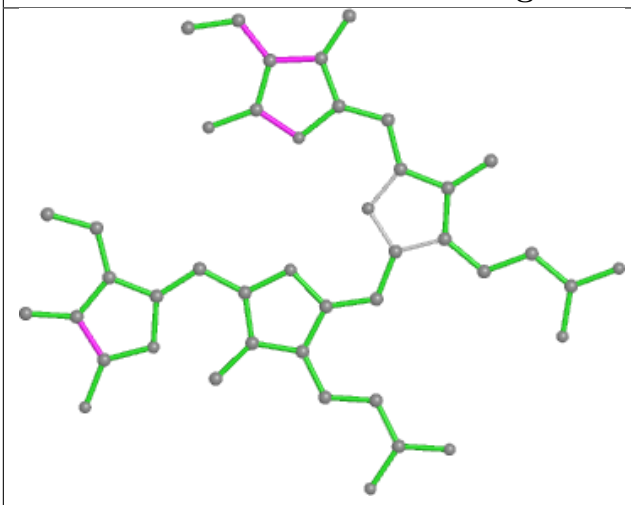


Torsions



Rings

Ligand PEB T3 201



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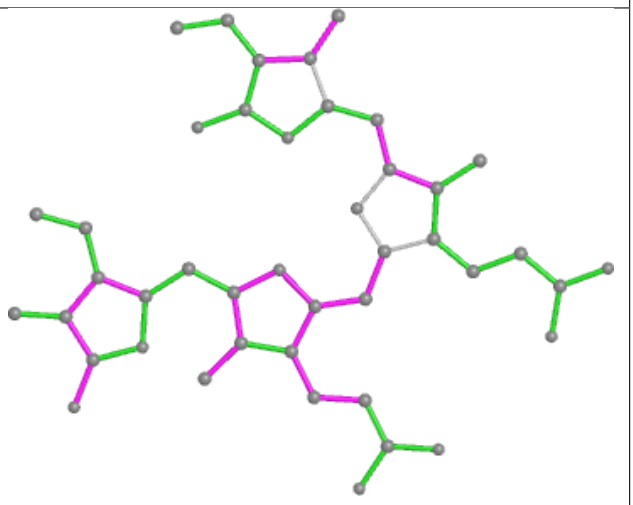

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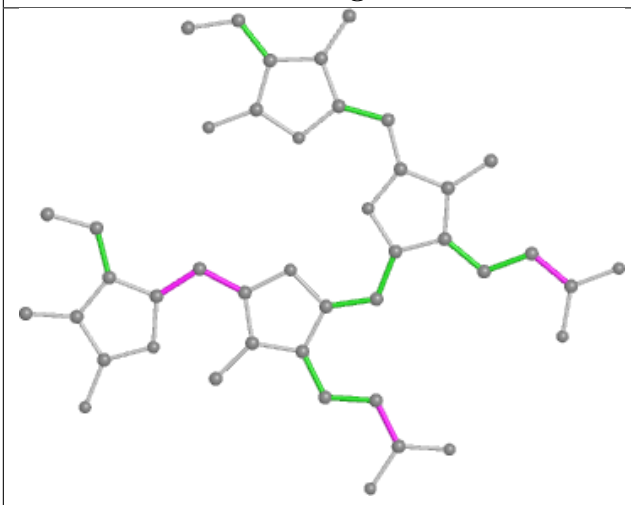

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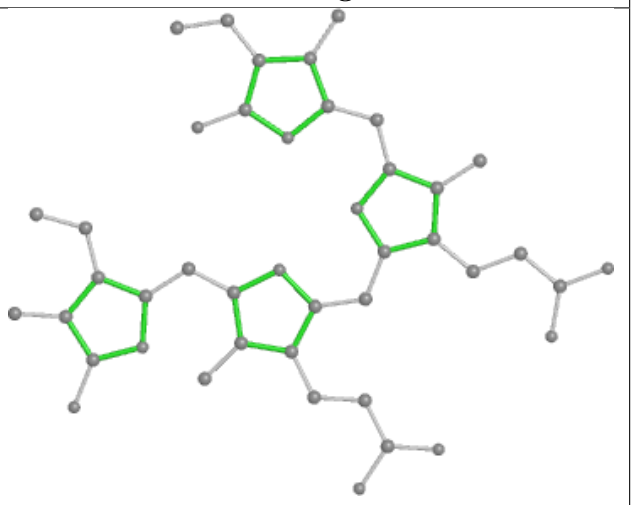
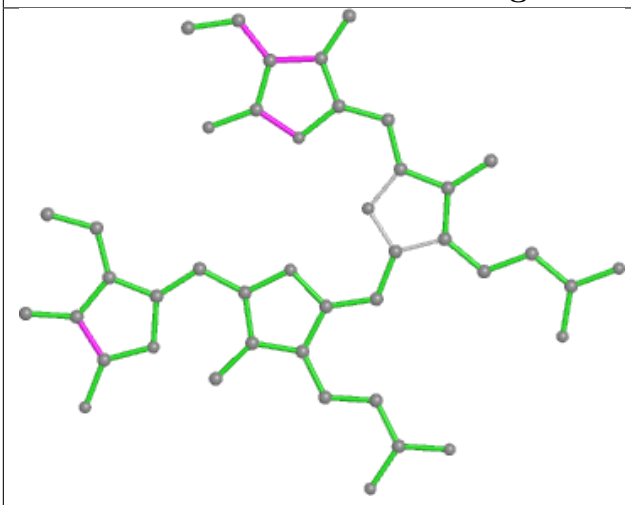


Rings

Ligand PEB jO 1001



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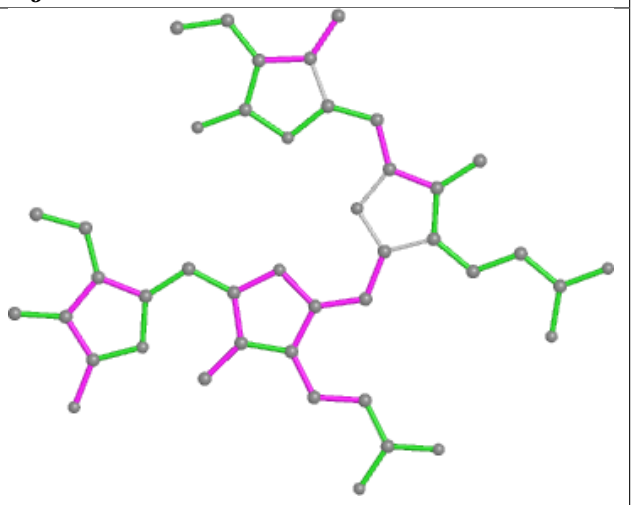

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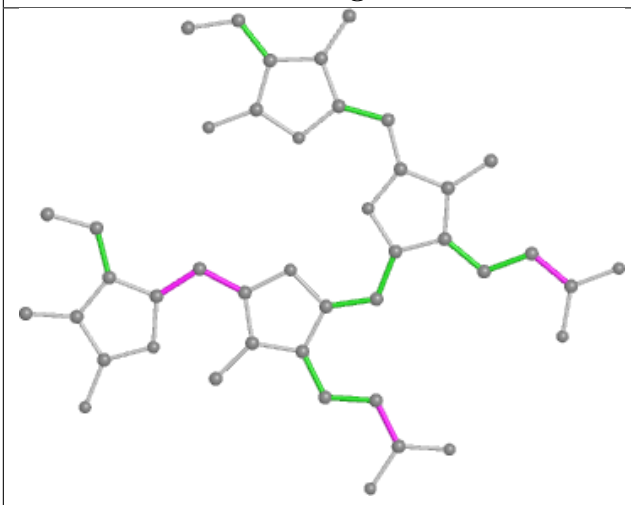

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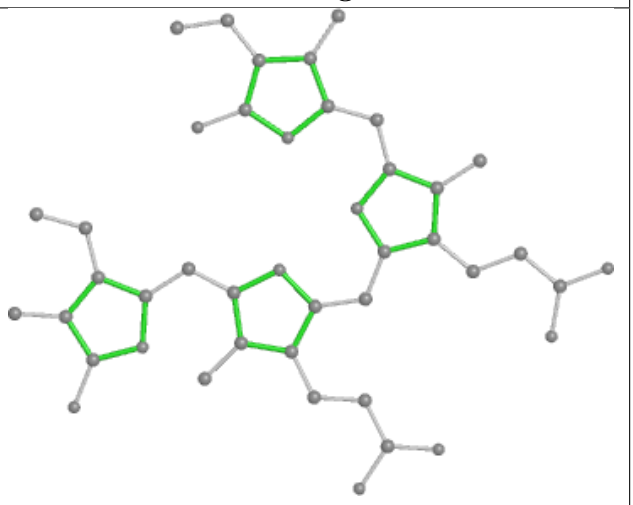
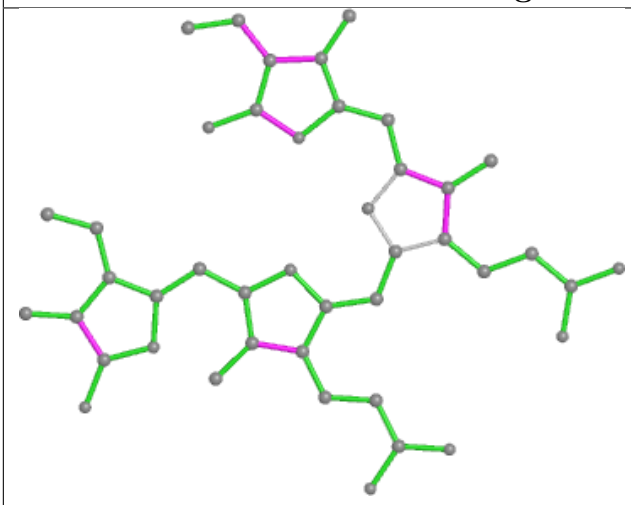


Rings

Ligand PEB H2 201



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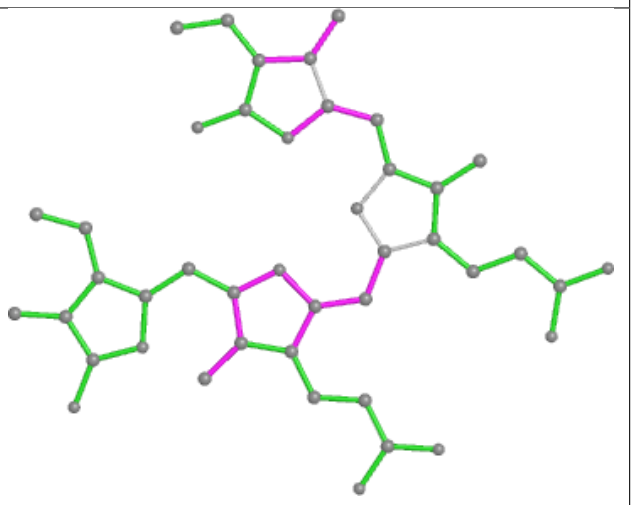
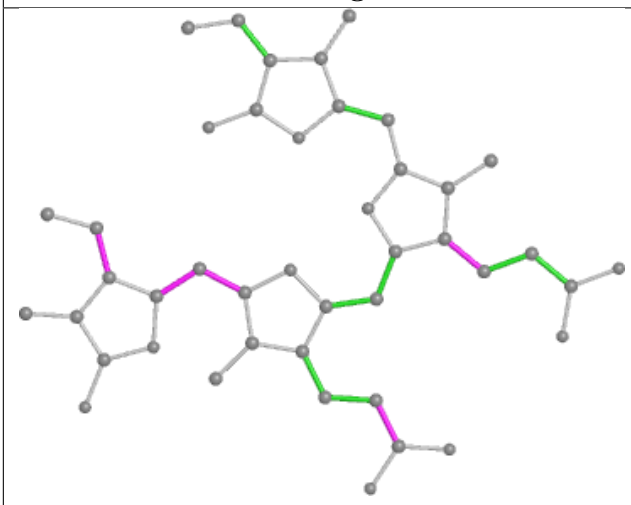


Bond angles



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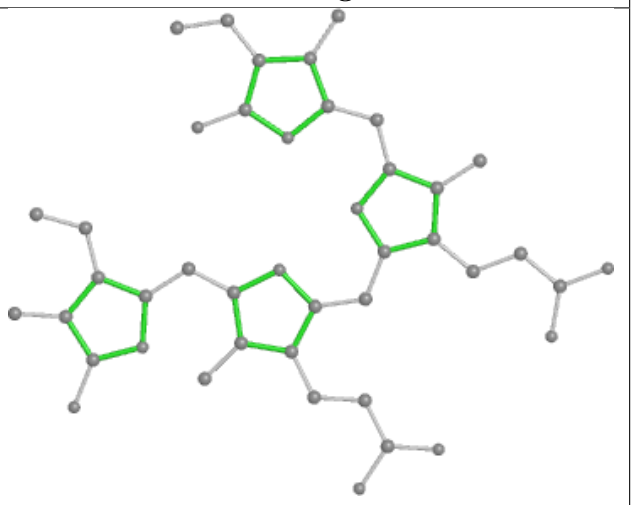
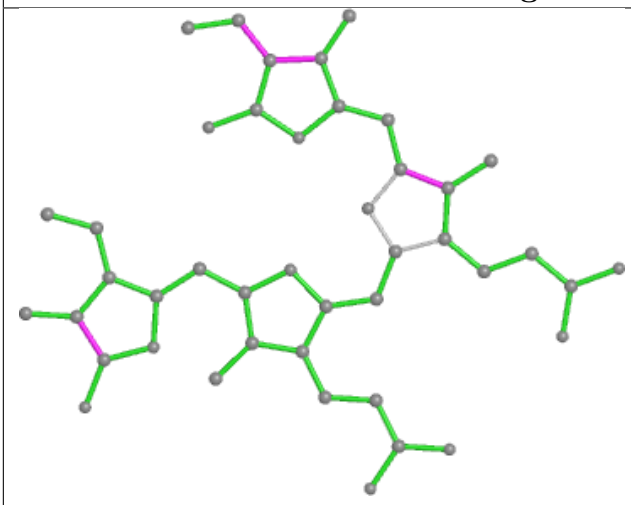


Rings

Ligand PEB cv 202



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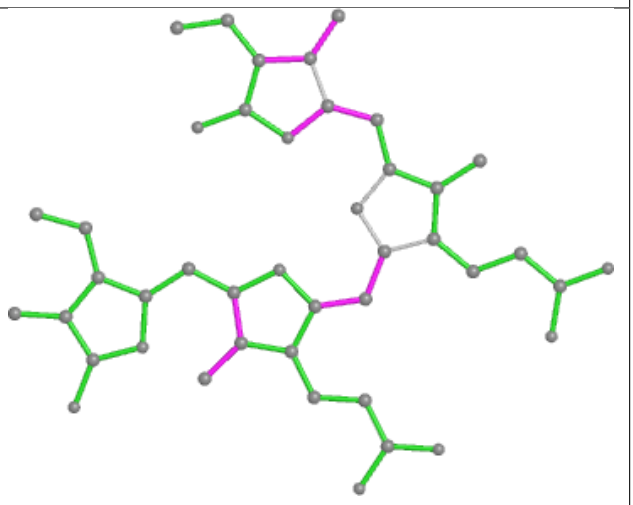

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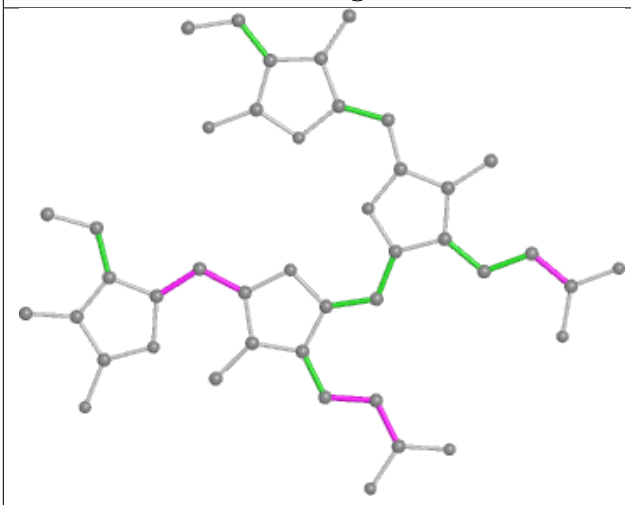

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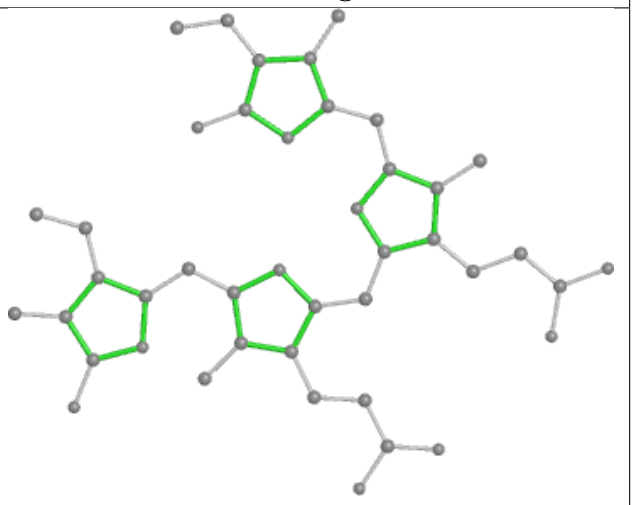
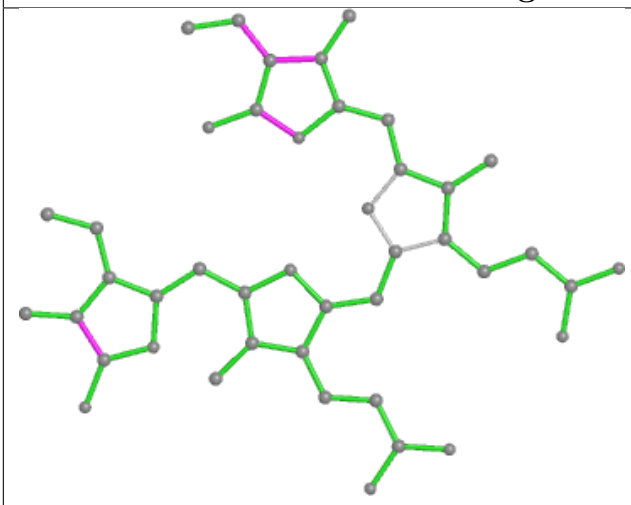


Rings

Ligand PEB L8 201



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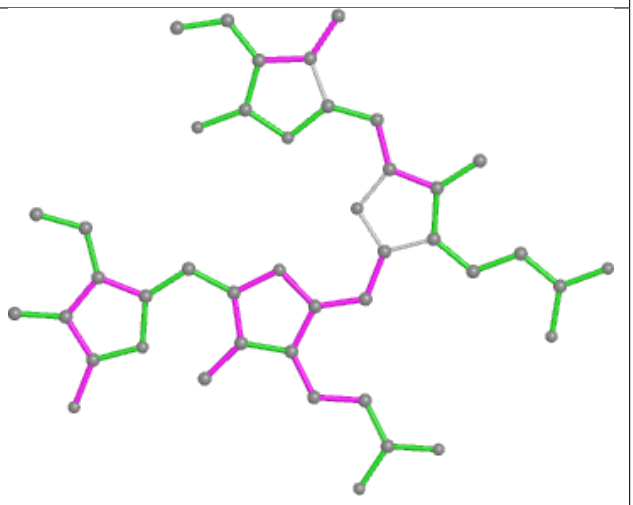

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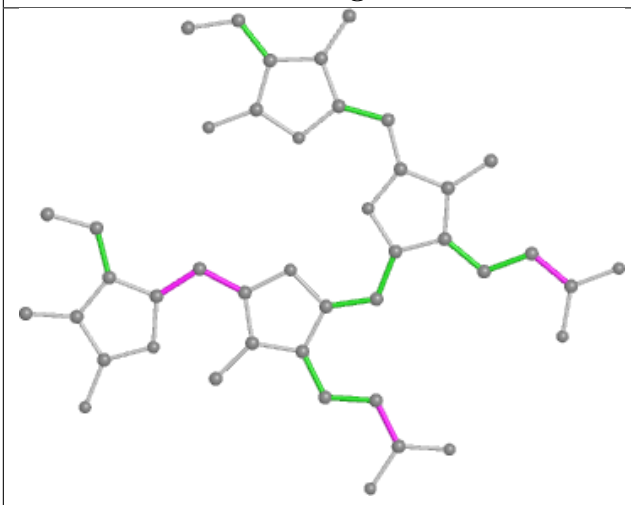

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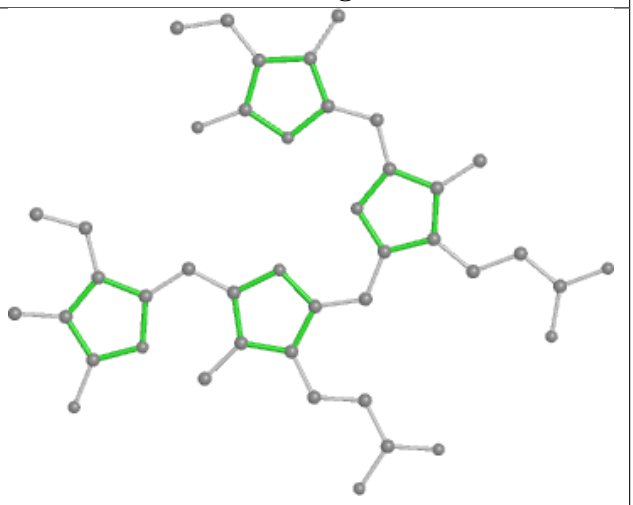
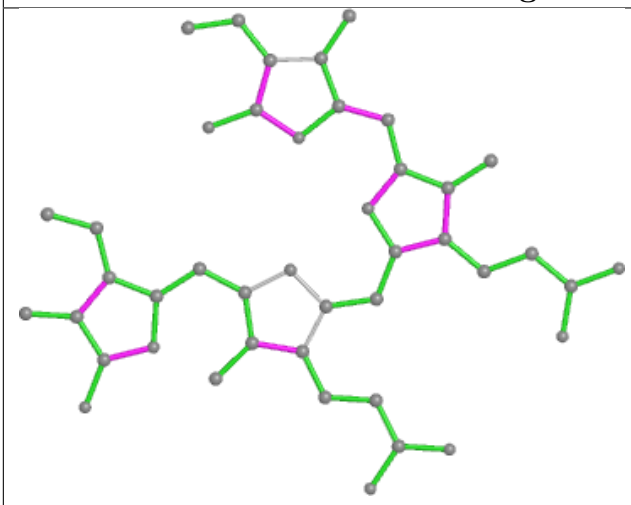


Rings

Ligand PUB r7 203



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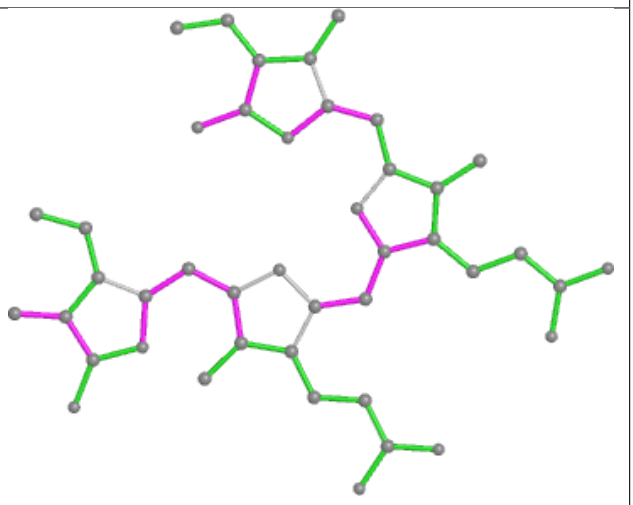

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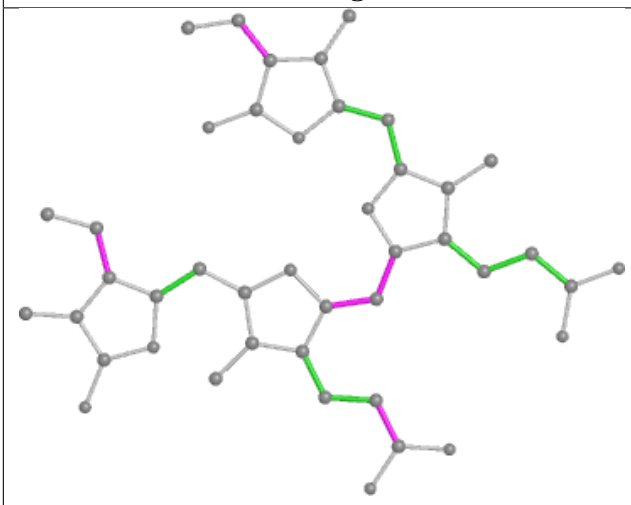

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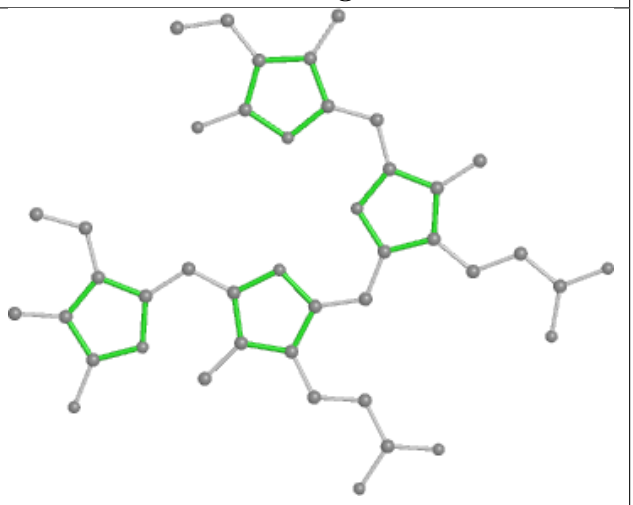
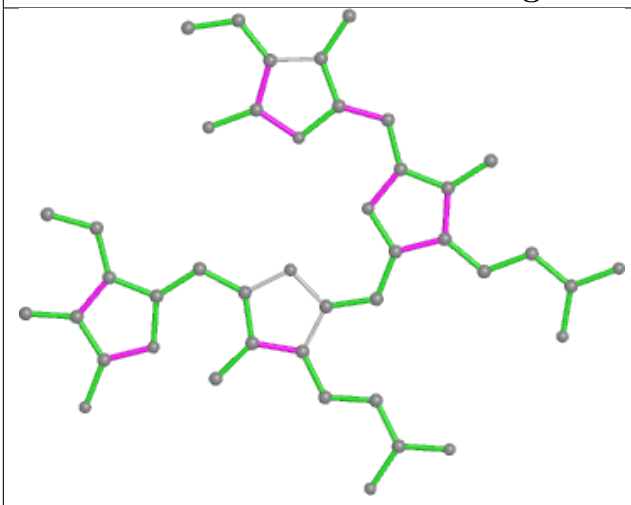


Rings

Ligand PUB lz 405



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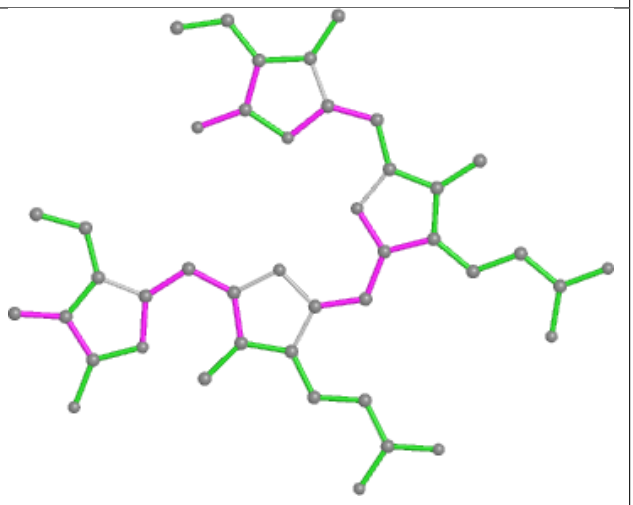

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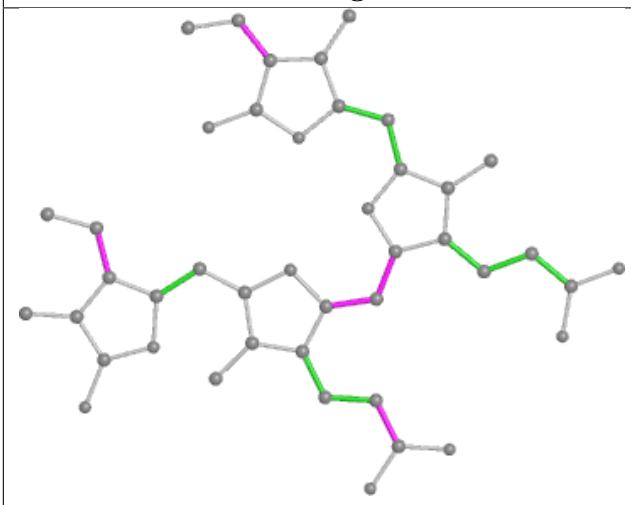

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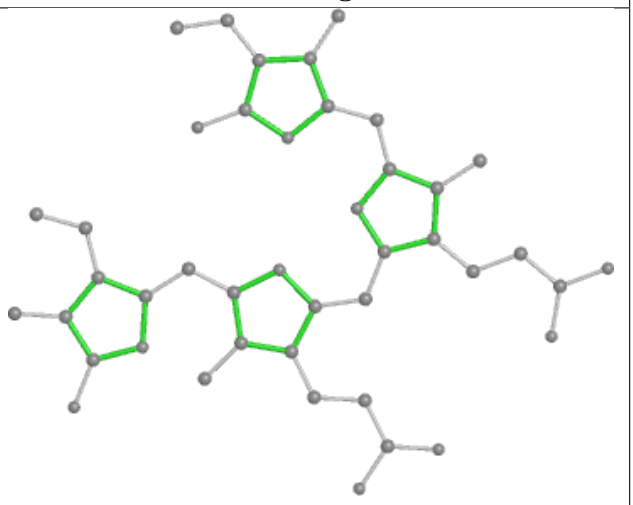
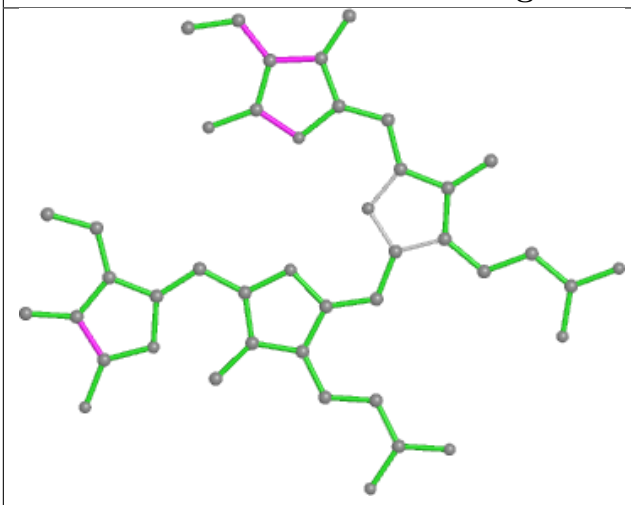


Rings

Ligand PEB T8 302



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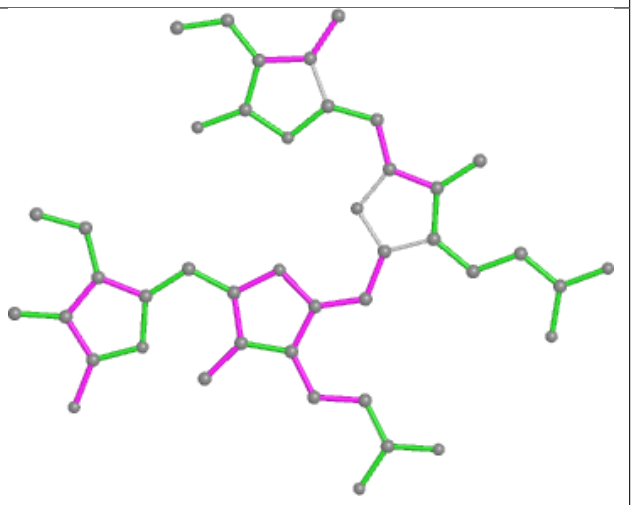
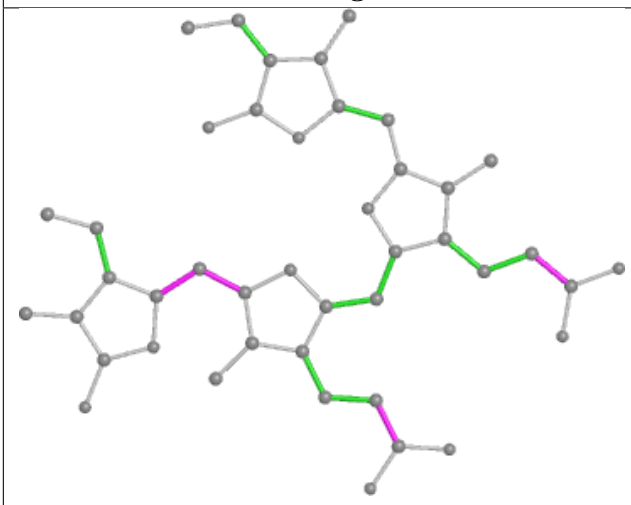


Bond angles



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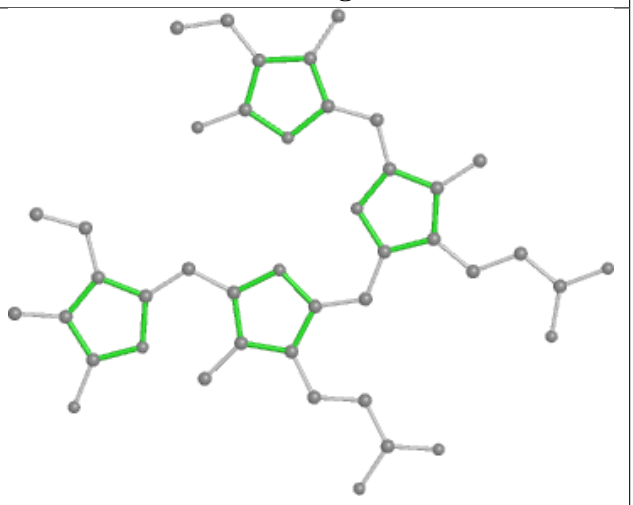
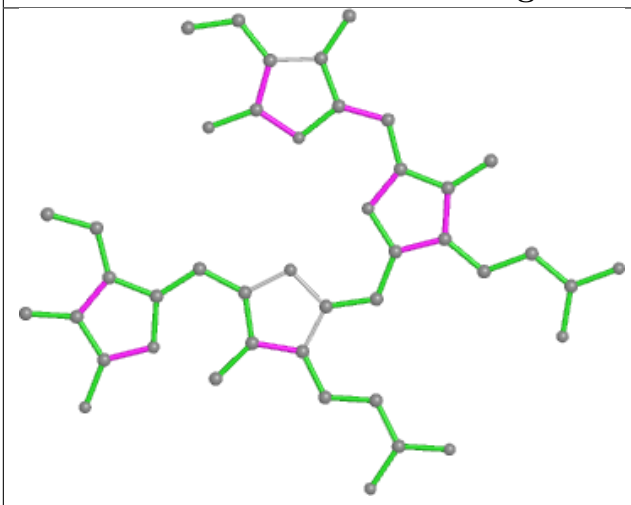


Rings

Ligand PUB v2 203



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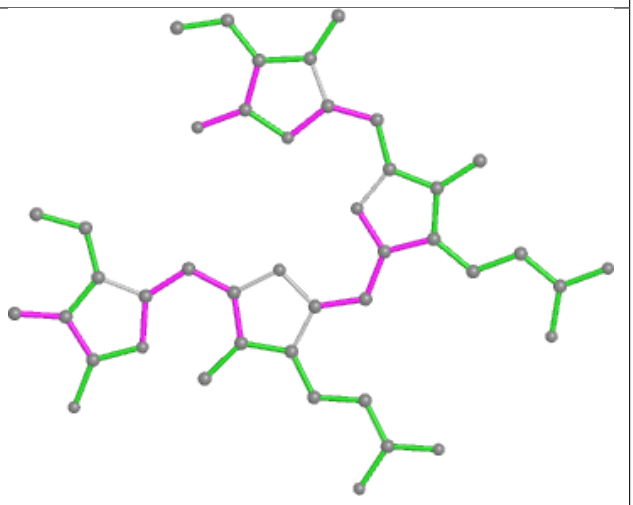

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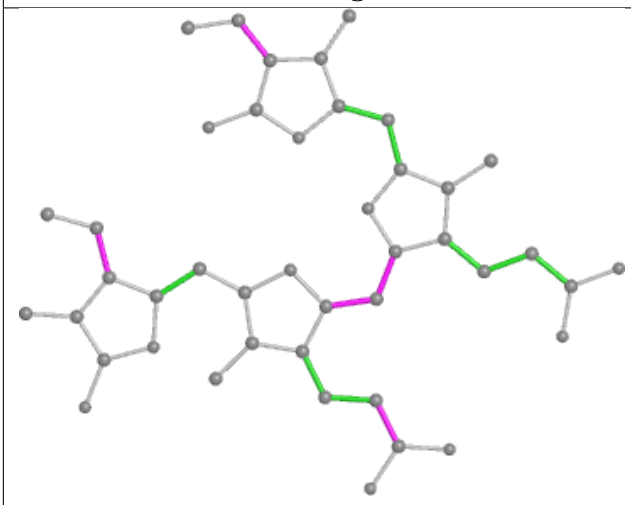

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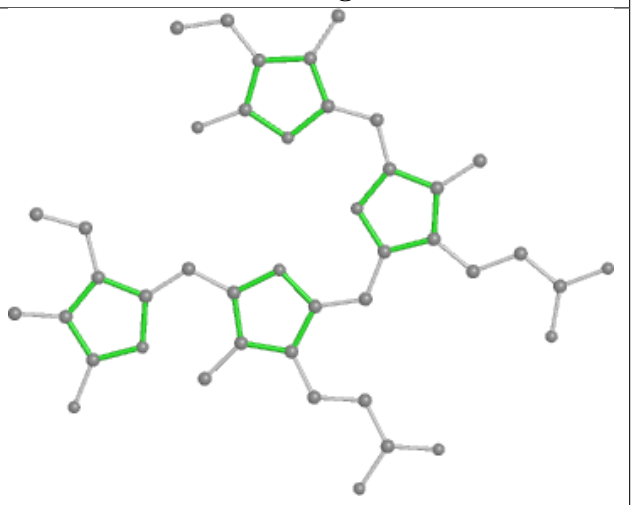
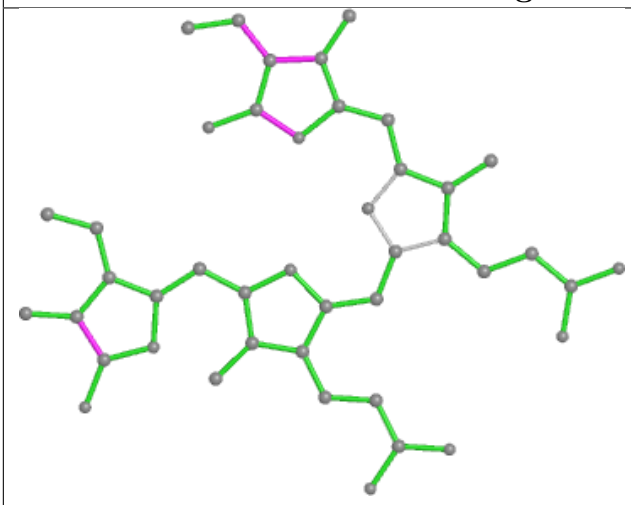


Rings

Ligand PEB X4 202



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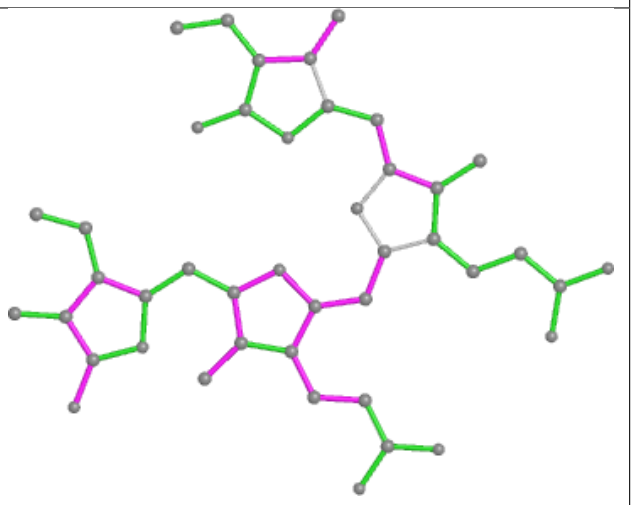

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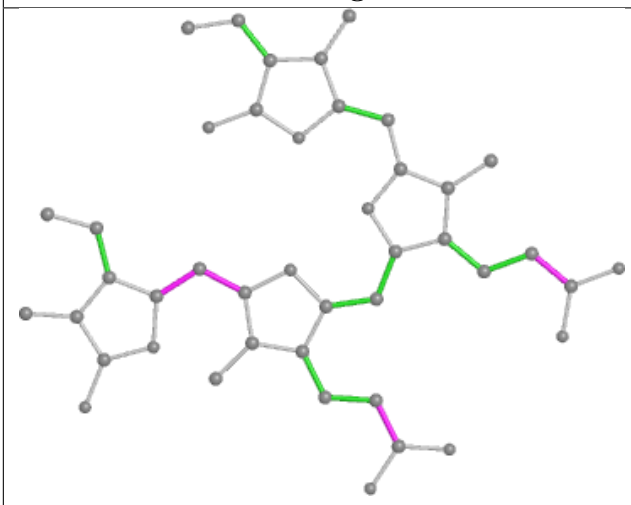

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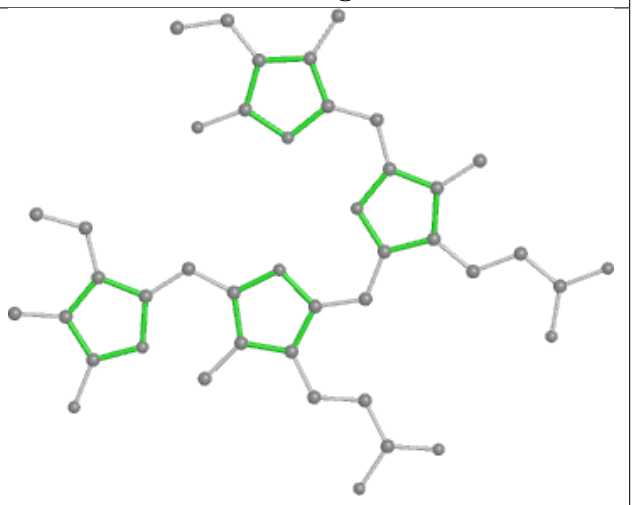
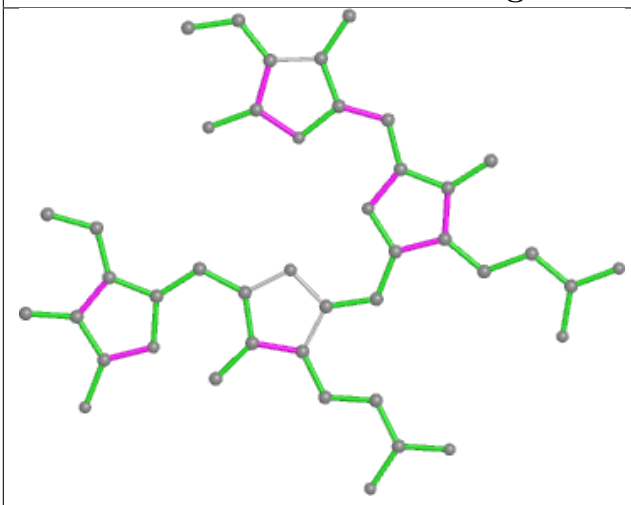


Rings

Ligand PUB Z9 1006



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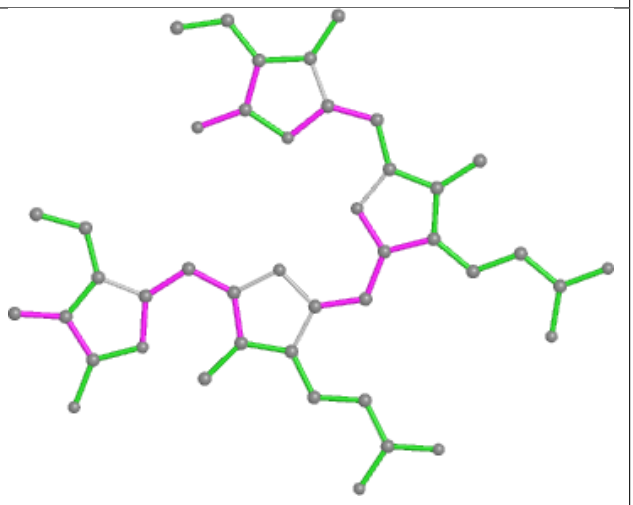
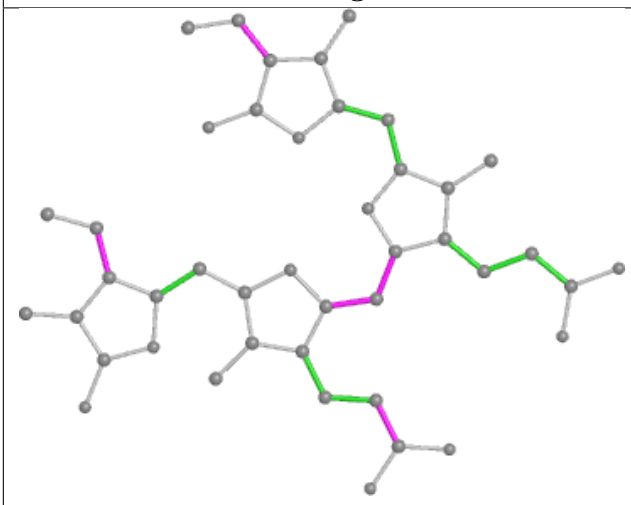


Bond angles



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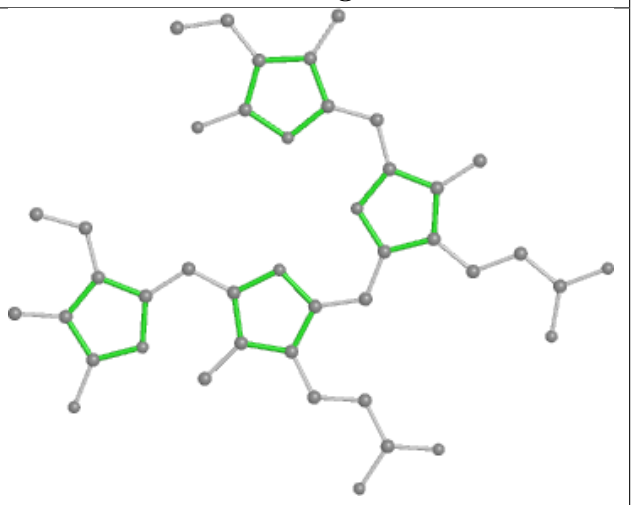
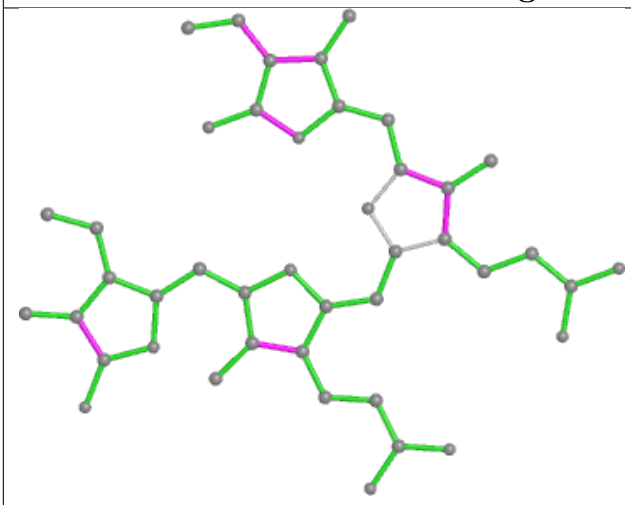


Rings

Ligand PEB cF 201



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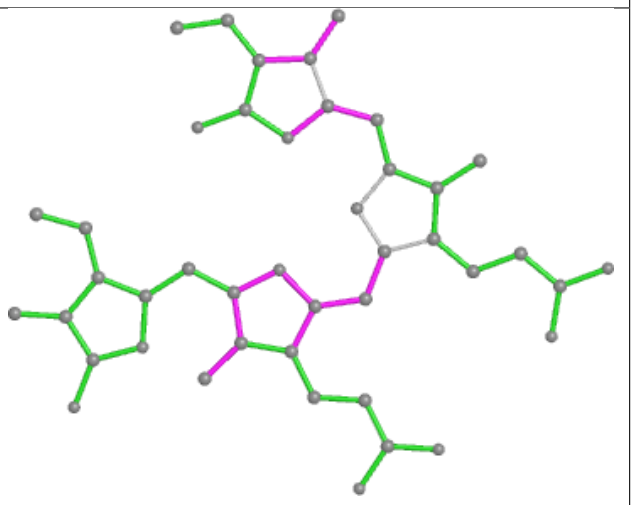
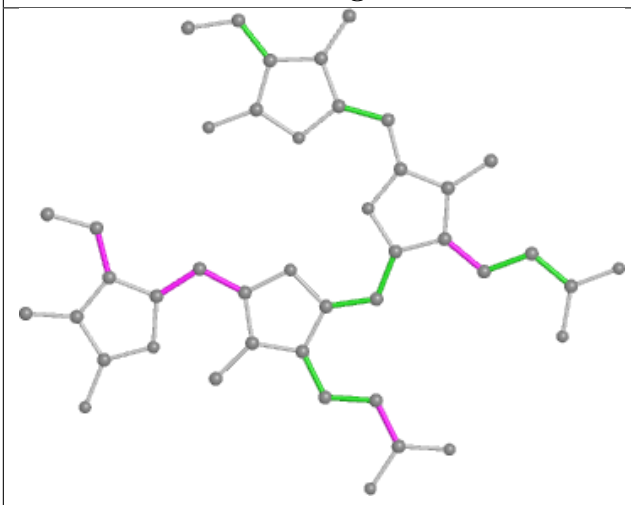


Bond angles



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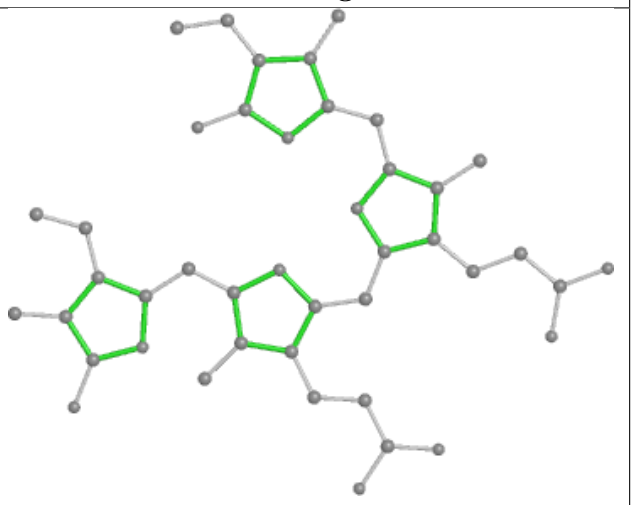
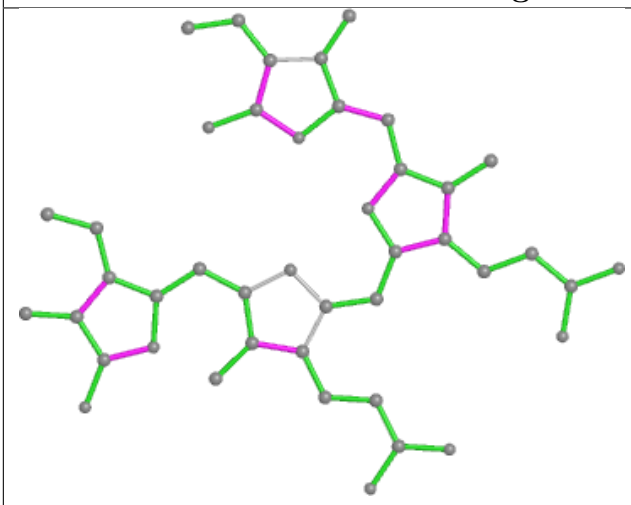


Rings

Ligand PUB jJ 1003



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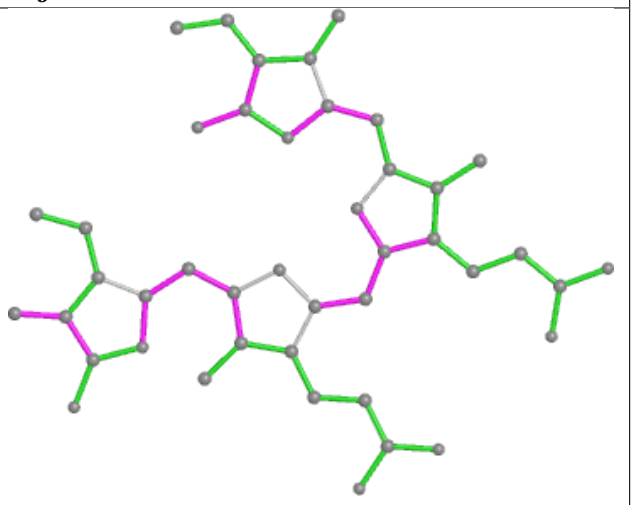
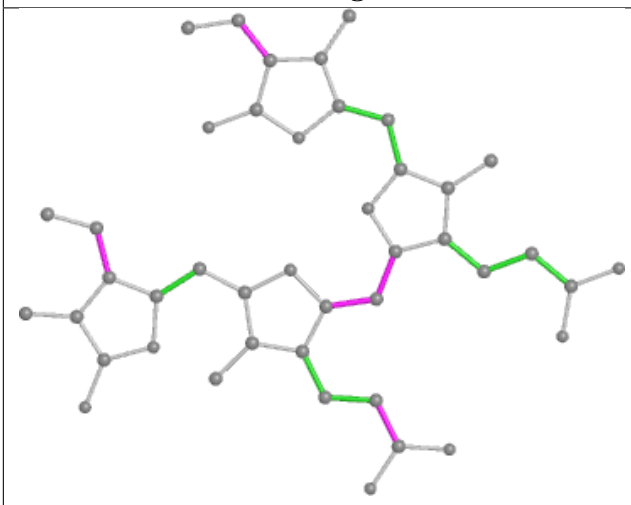
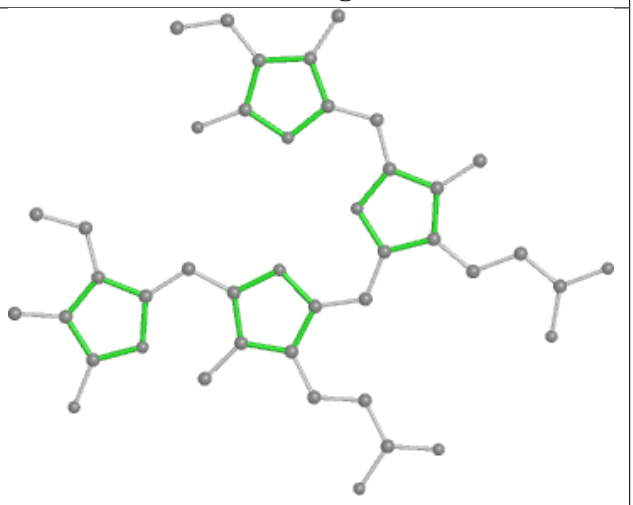


Bond angles

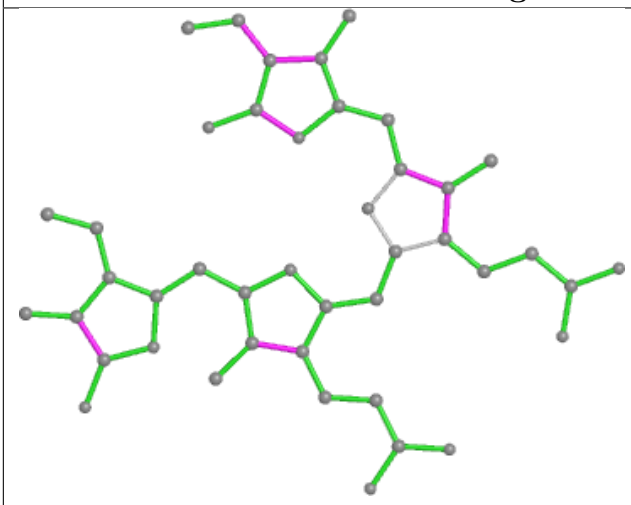


Torsions



Rings

Ligand PEB jN 1002



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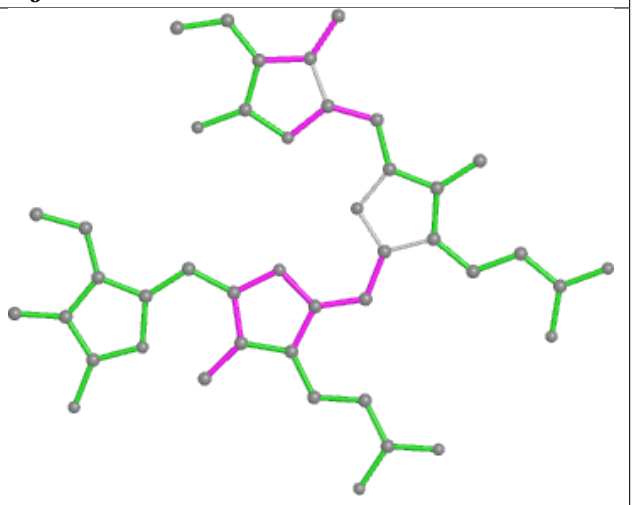

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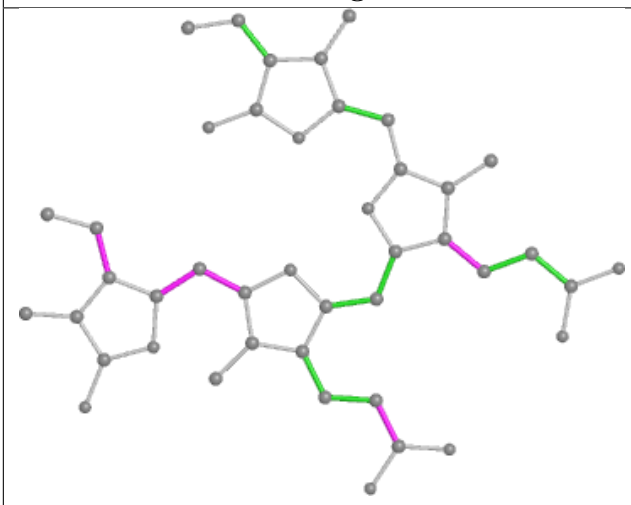

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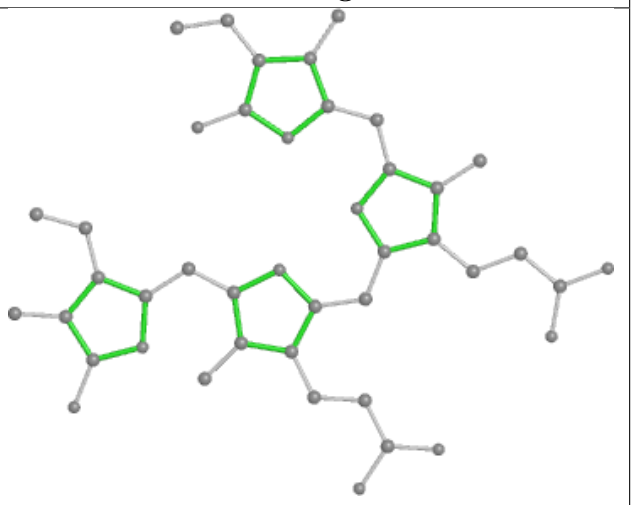
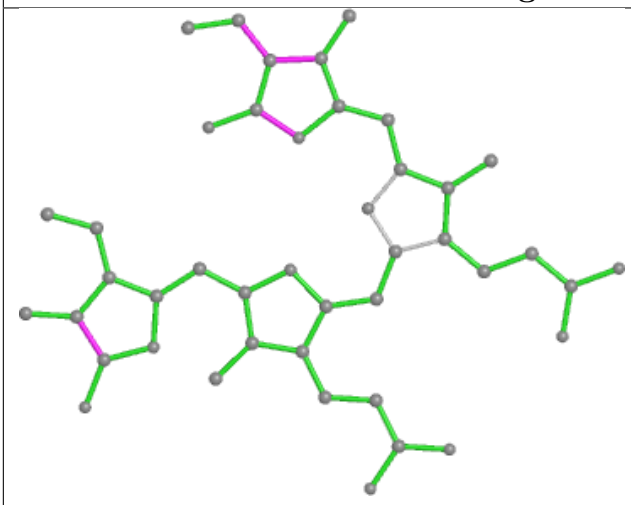


Rings

Ligand PEB aL 201



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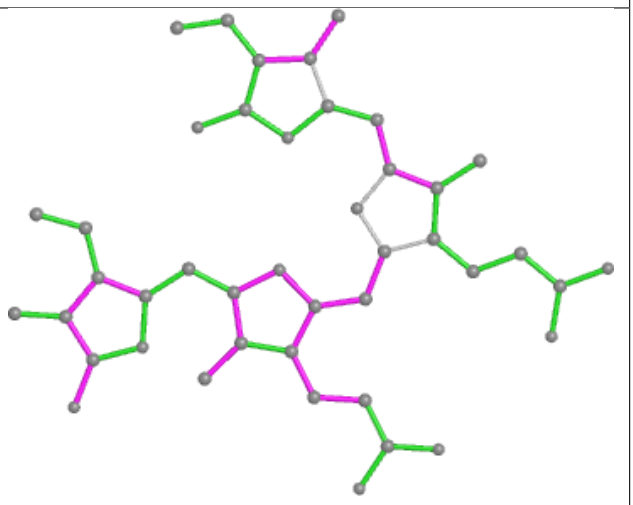

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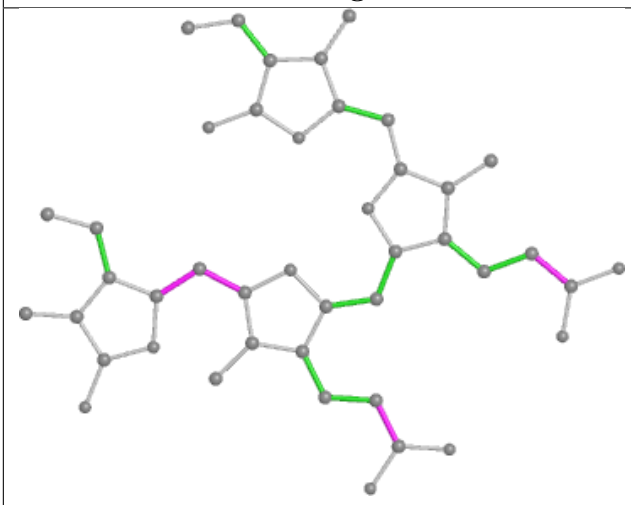

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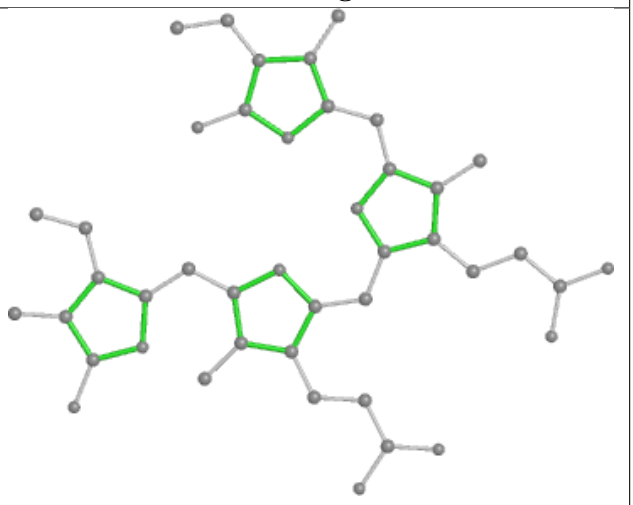
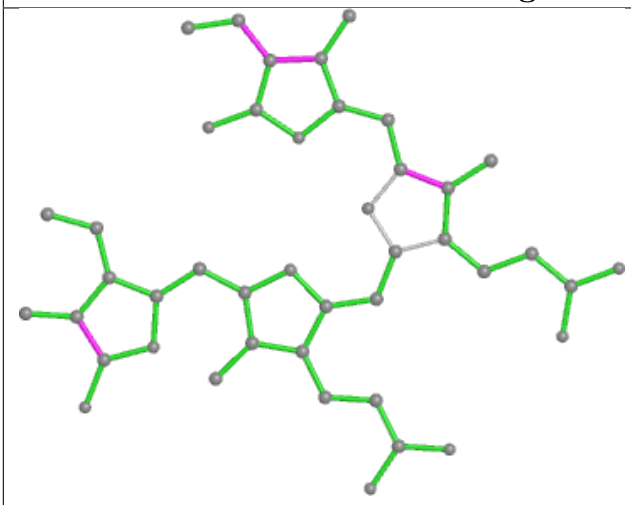


Rings

Ligand PEB S2 202



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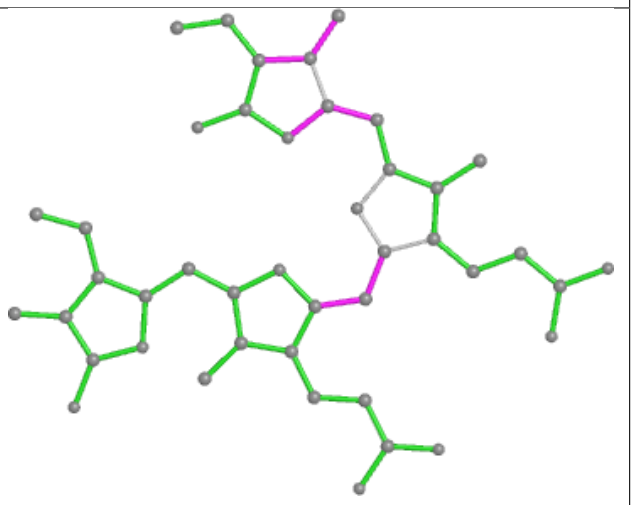

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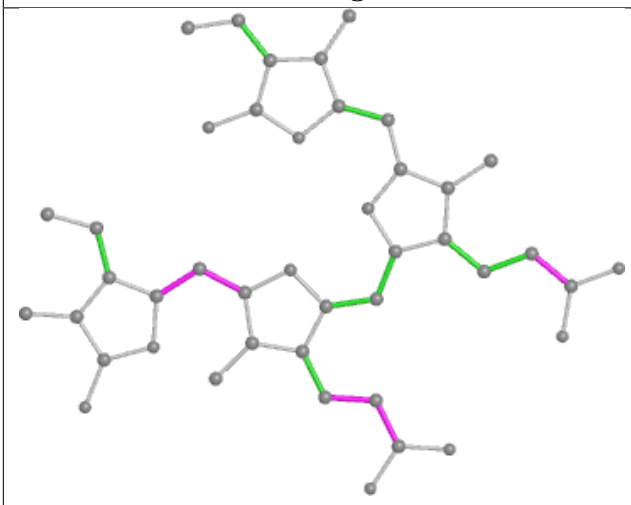

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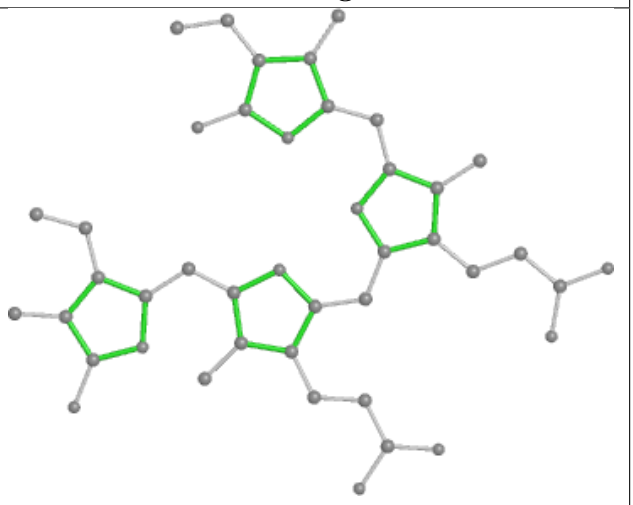
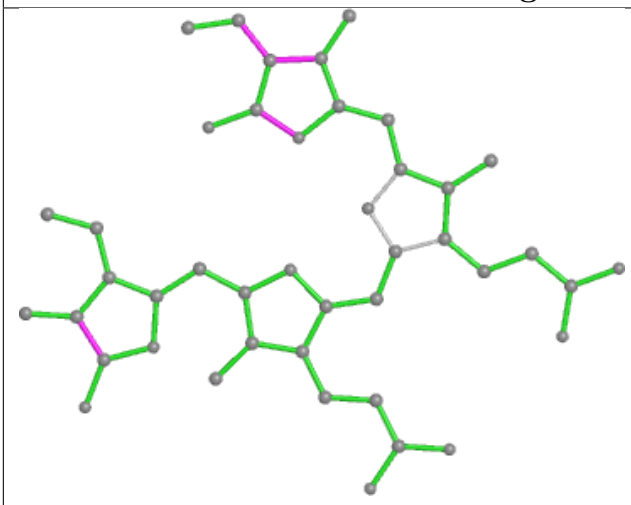


Rings

Ligand PEB g6 201



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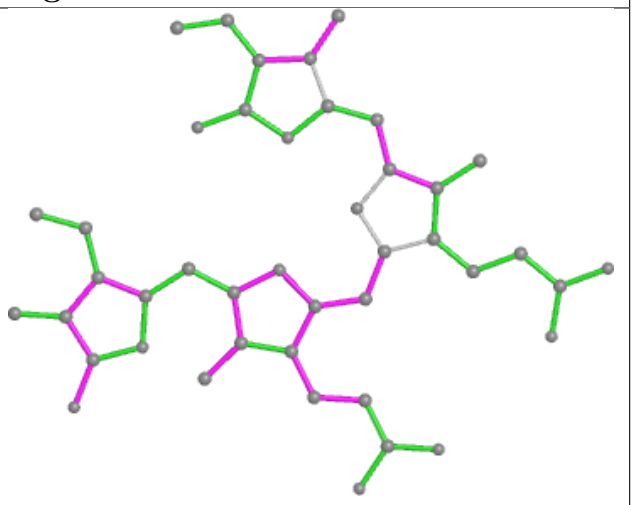

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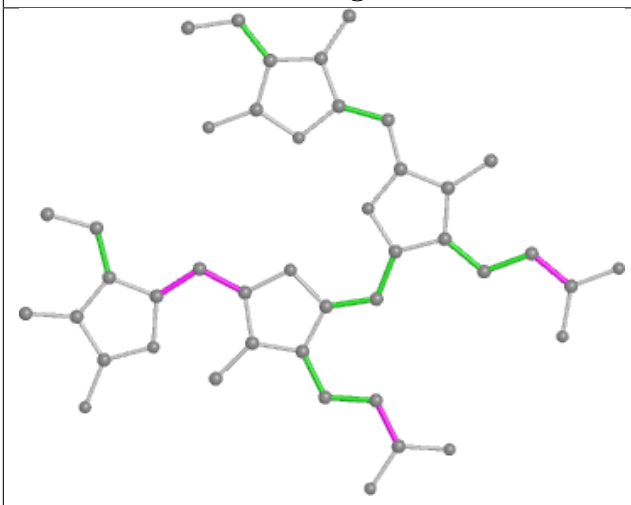

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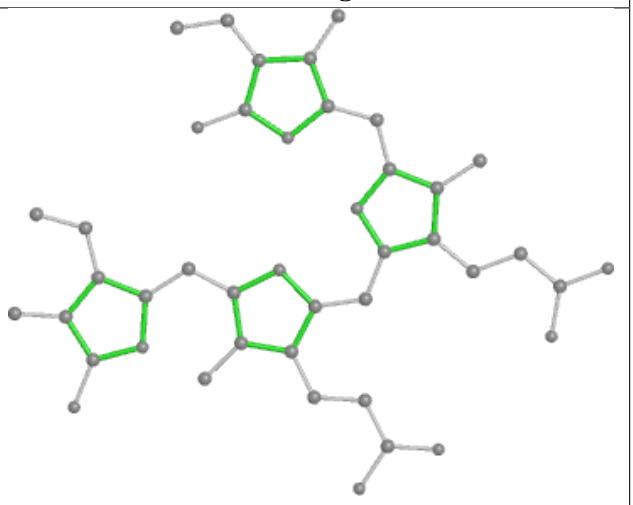
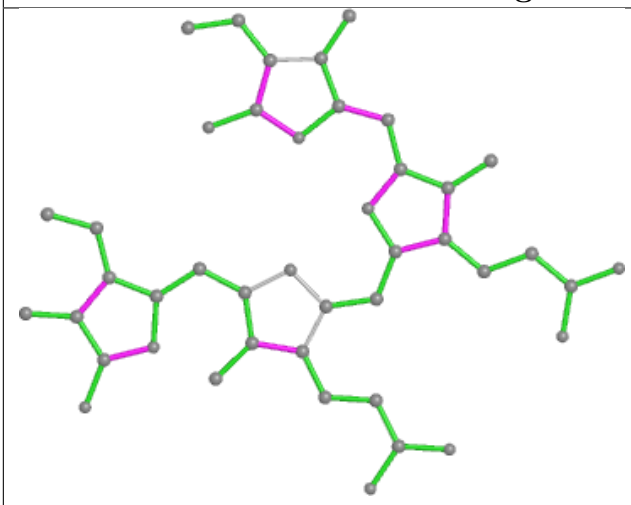


Rings

Ligand PUB hL 203



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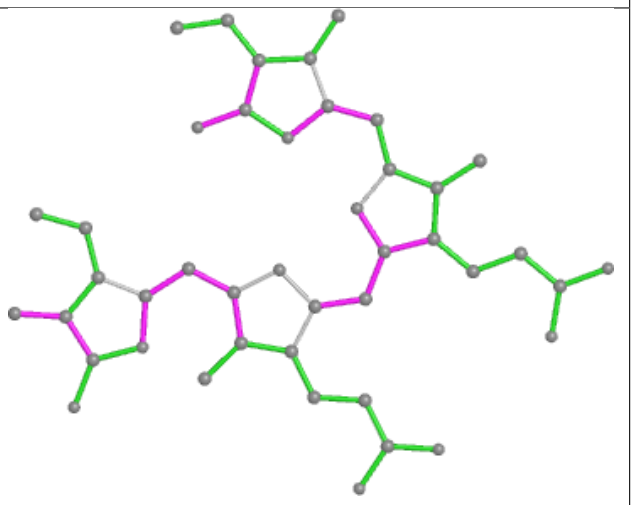

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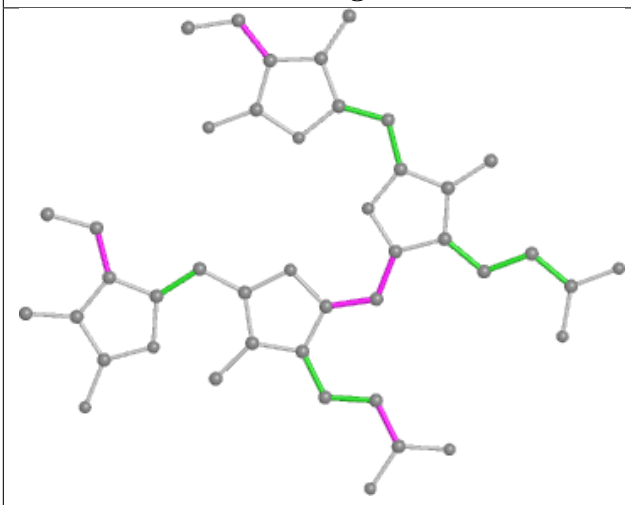

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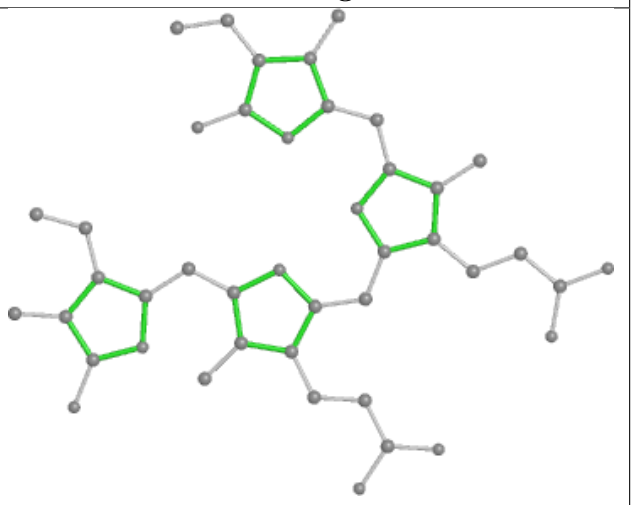
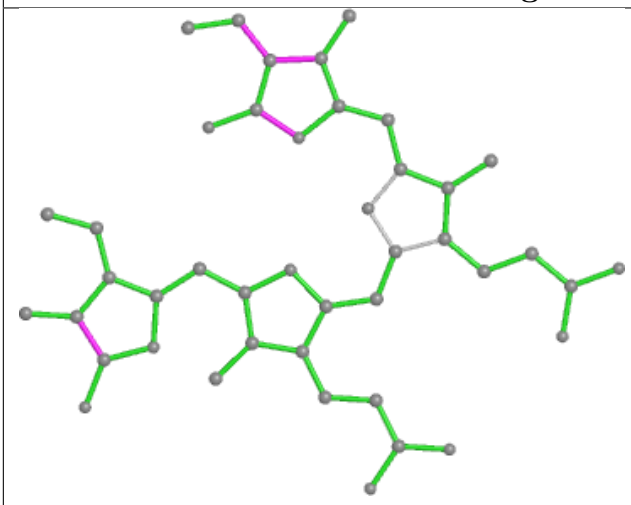


Rings

Ligand PEB ac 201



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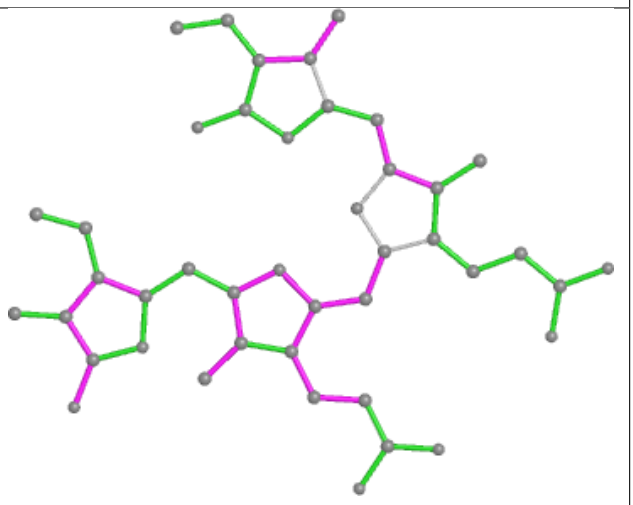

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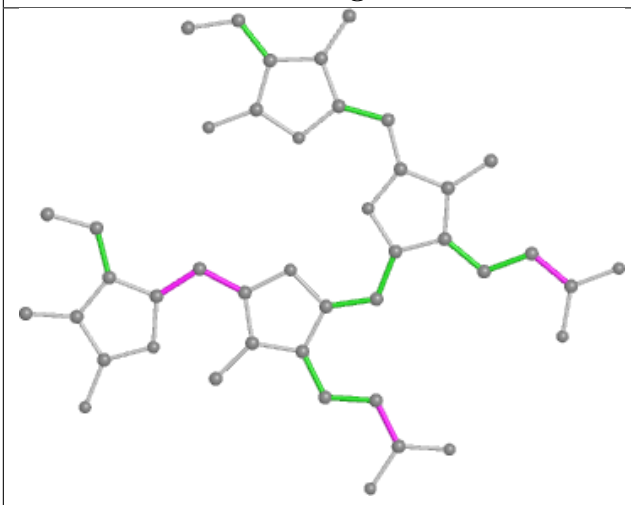

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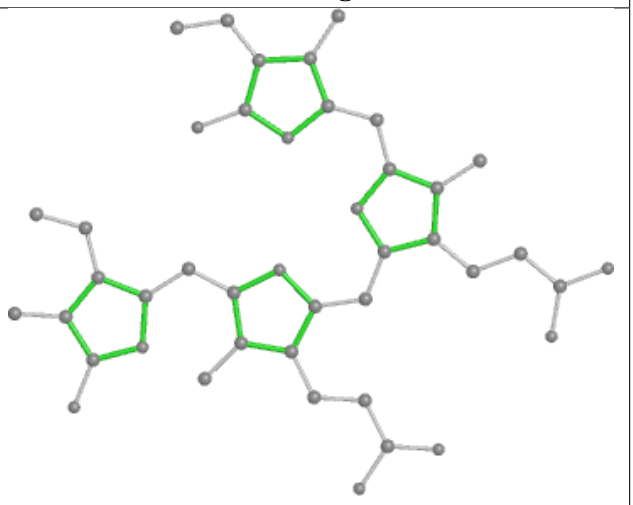

Rings

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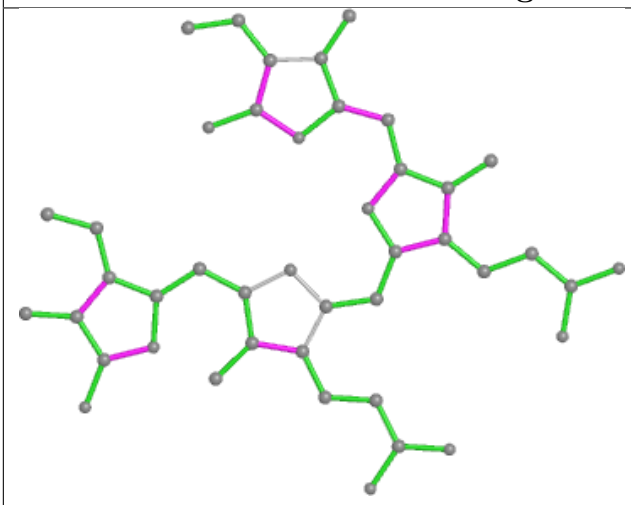

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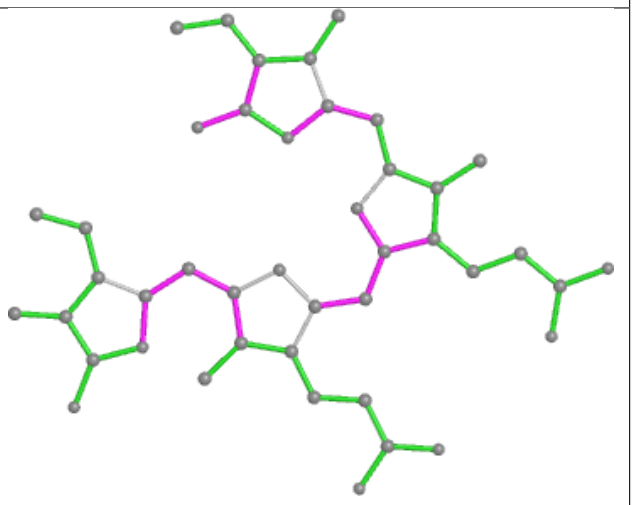

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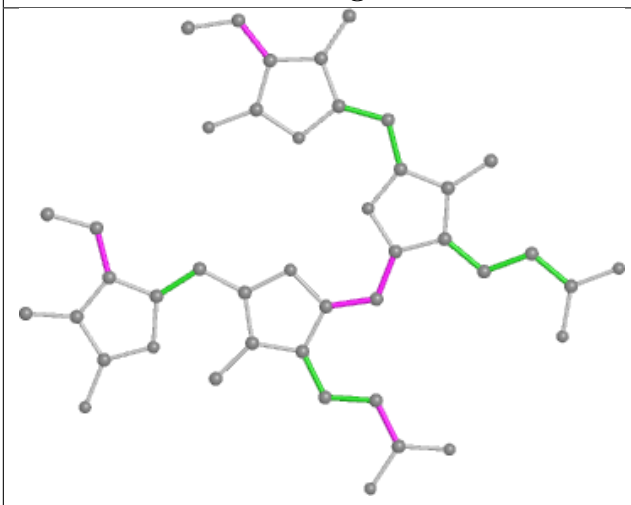

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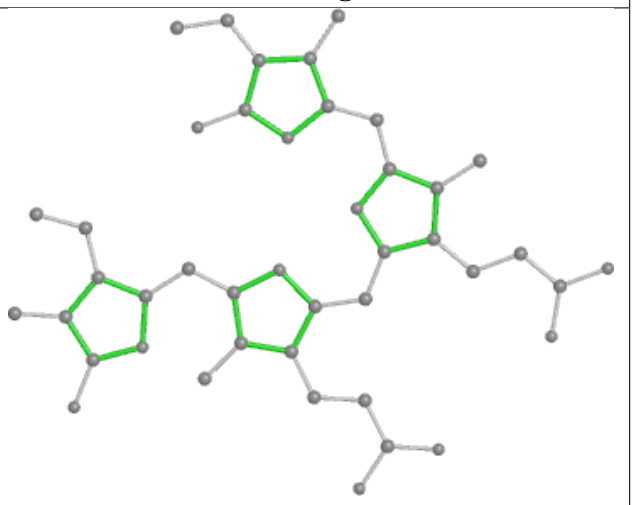
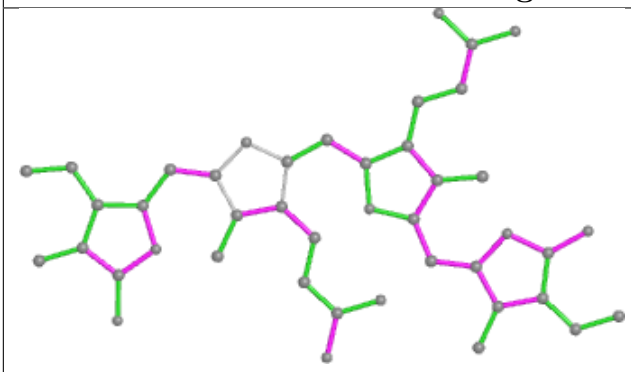


Rings

Ligand CYC S1 201



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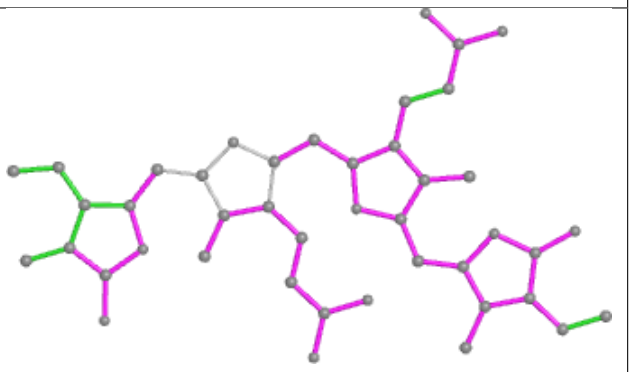

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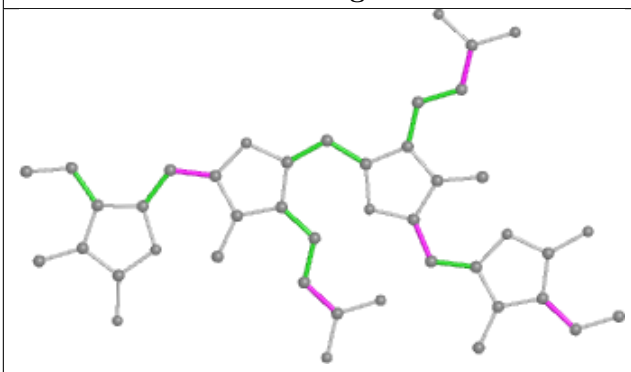

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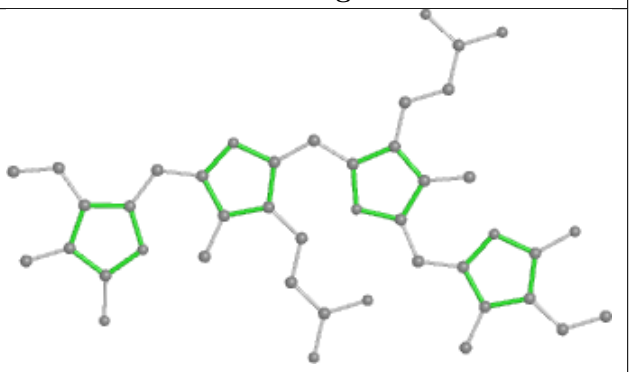
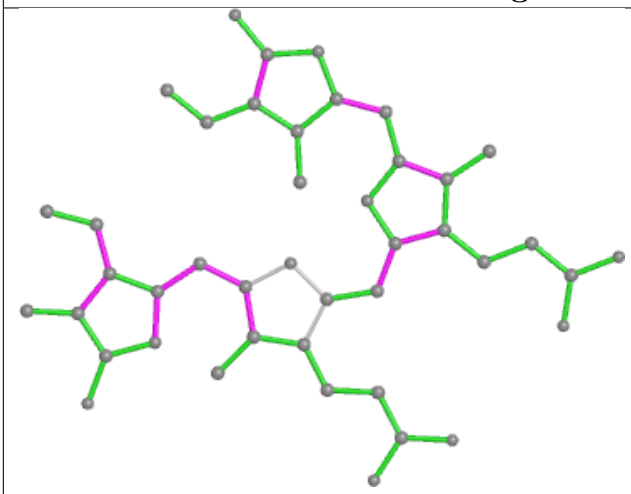


Rings

Ligand PVN hY 404



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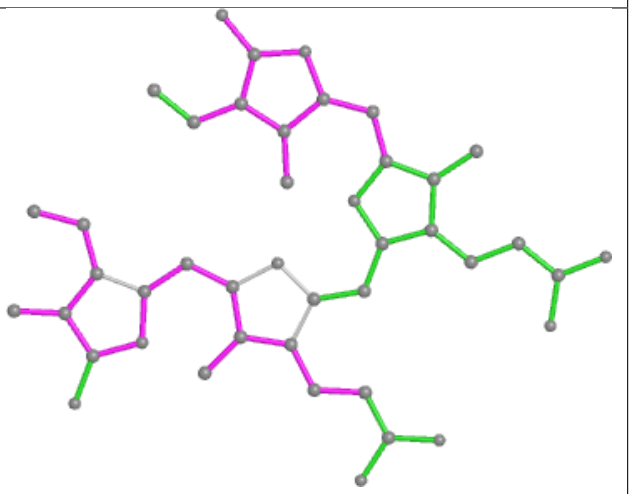

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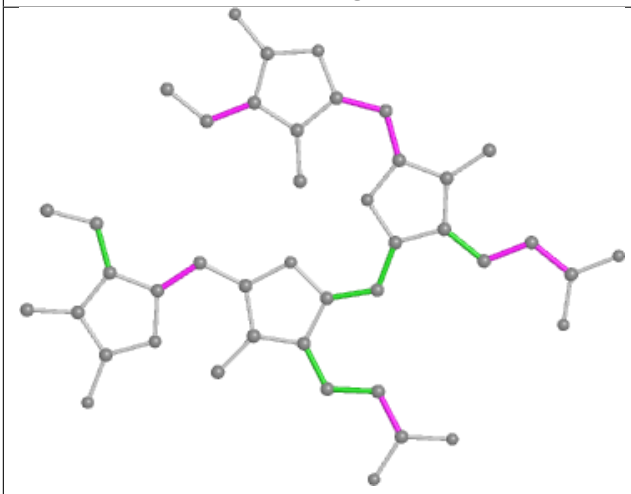

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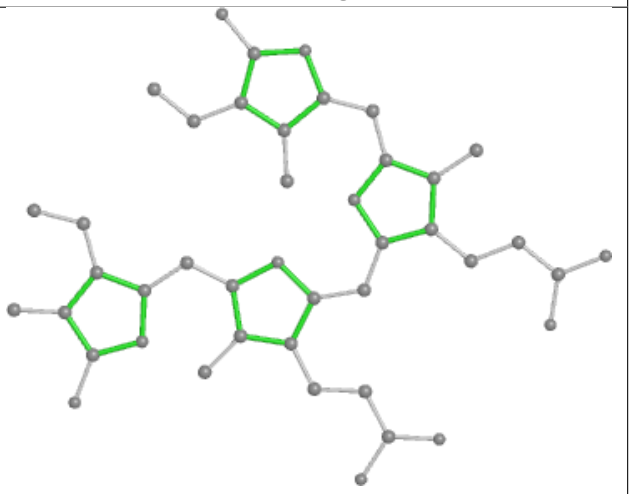

Rings

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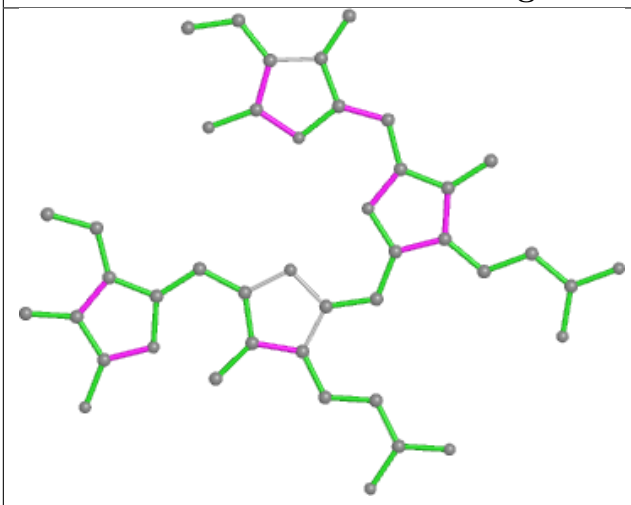

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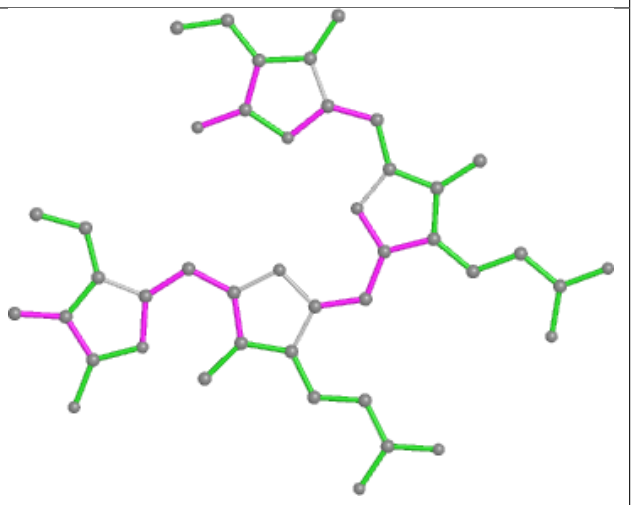

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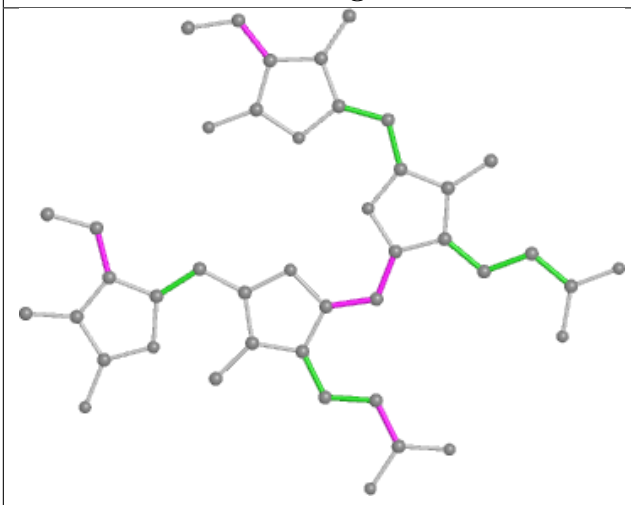

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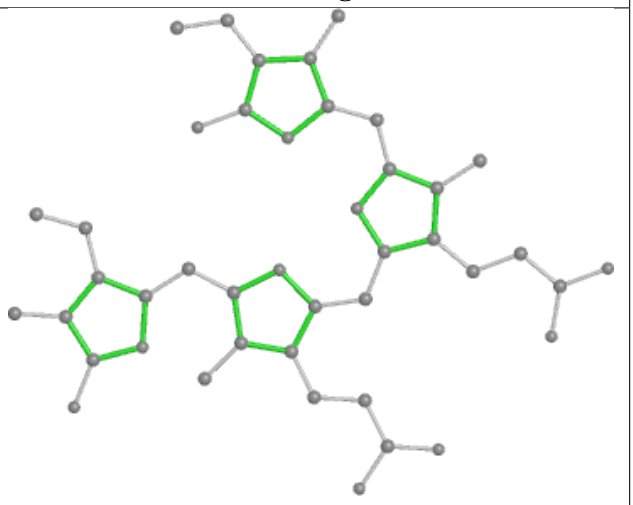
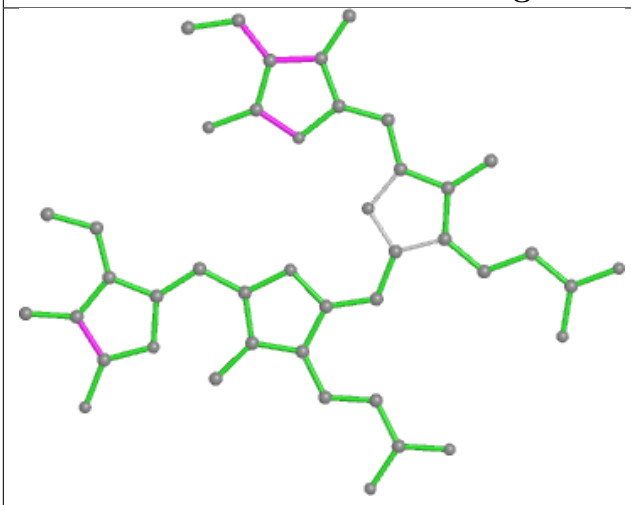


Rings

Ligand PEB fn 1001



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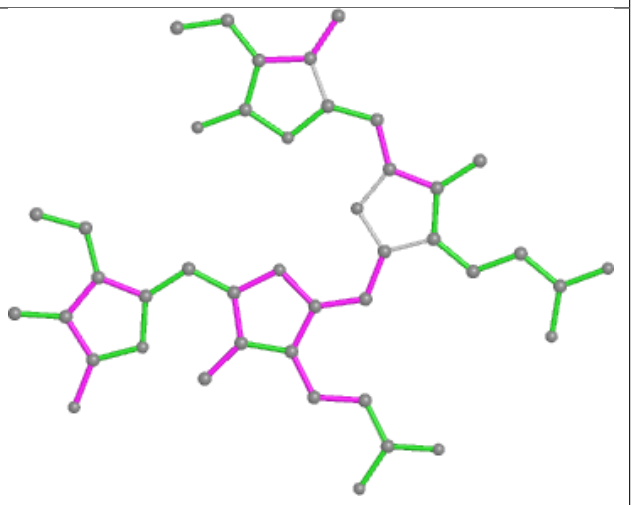

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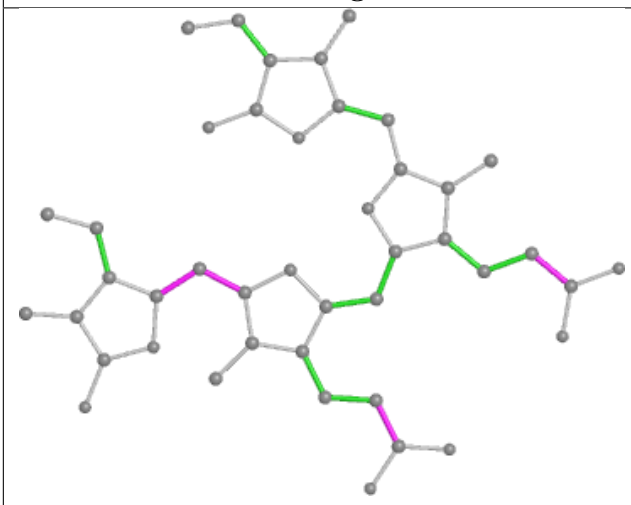

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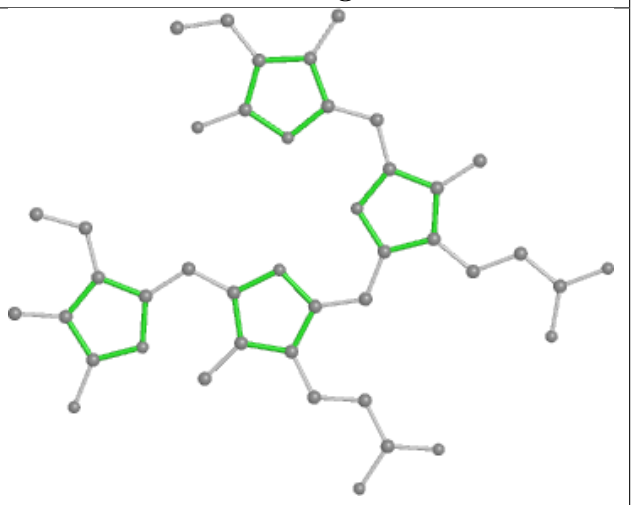
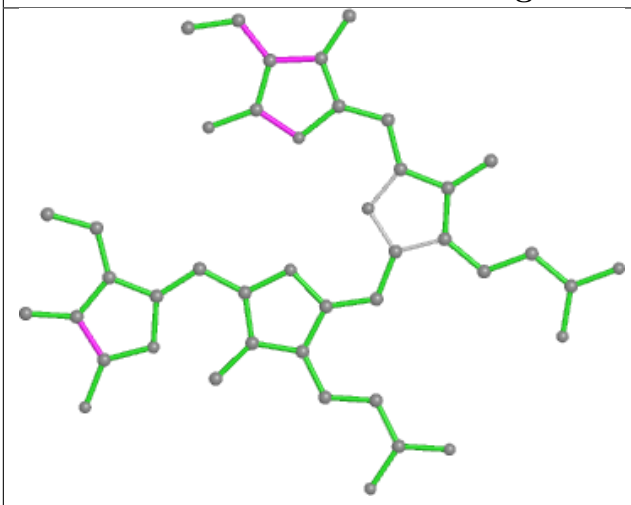


Rings

Ligand PEB X9 401



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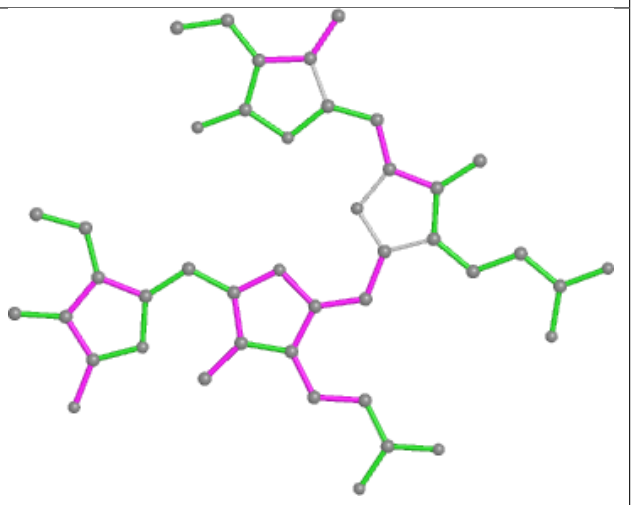

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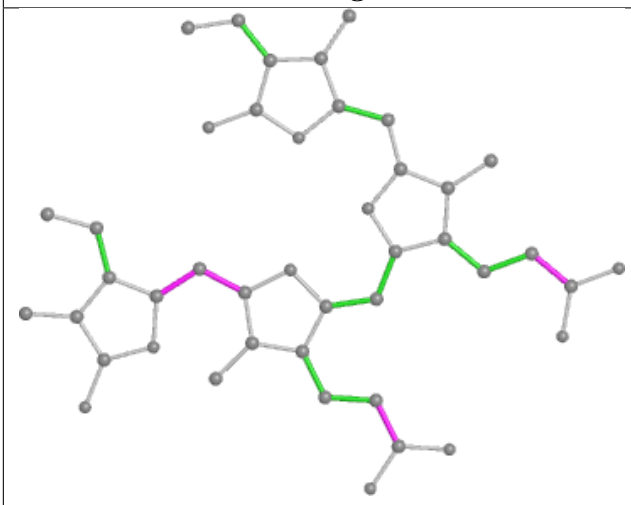

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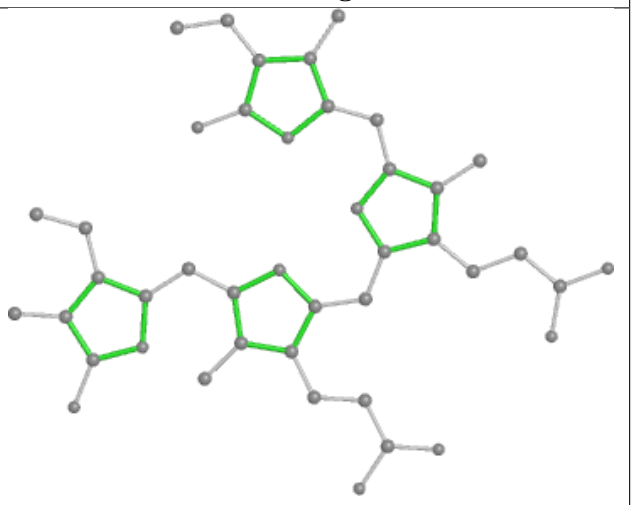

Rings

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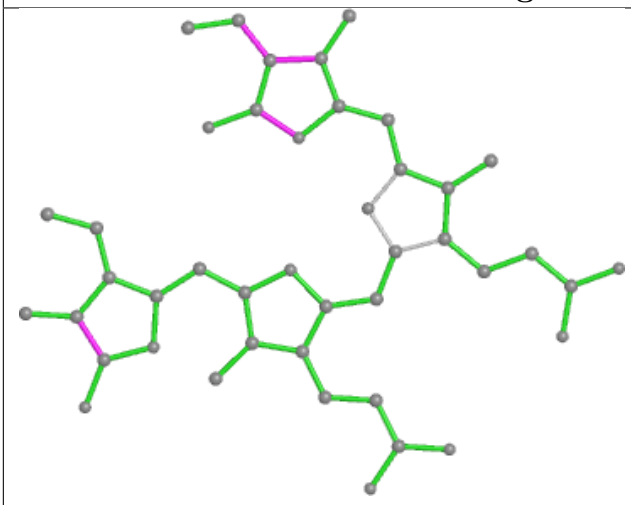

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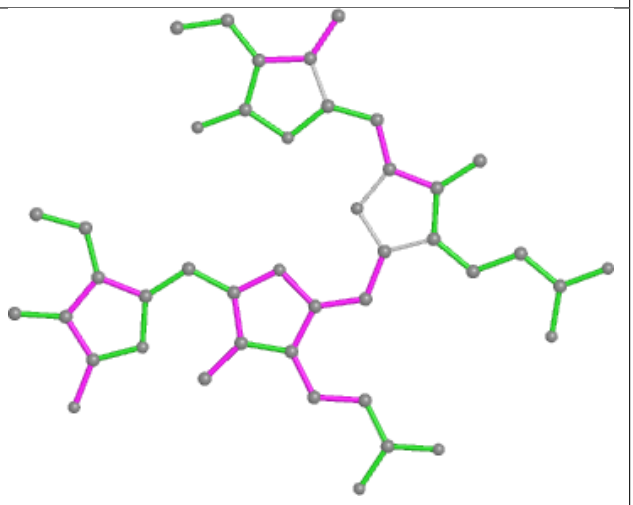
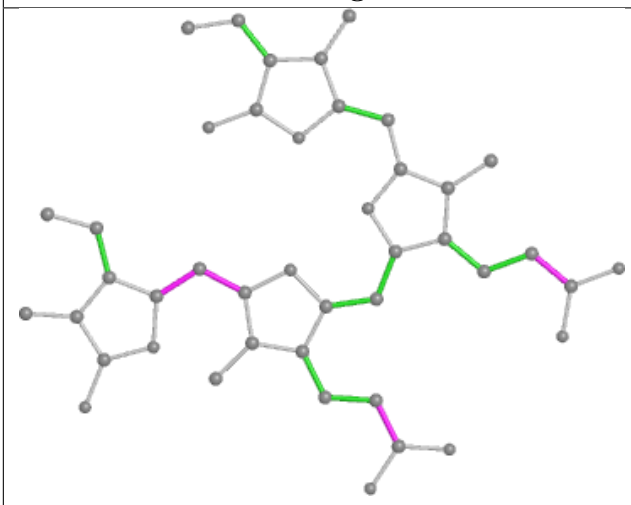


Bond angles



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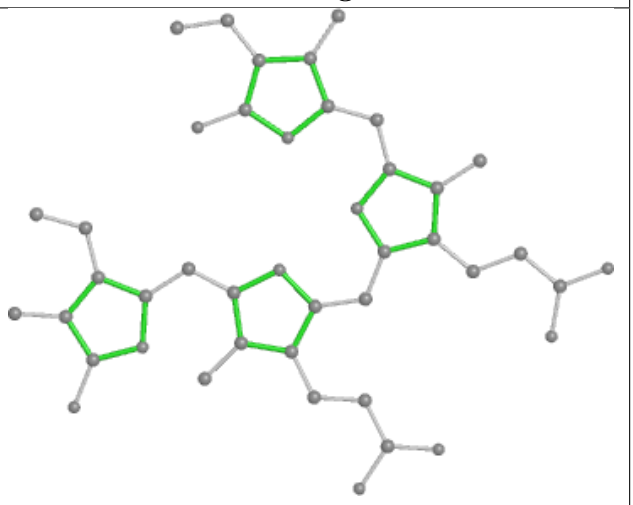
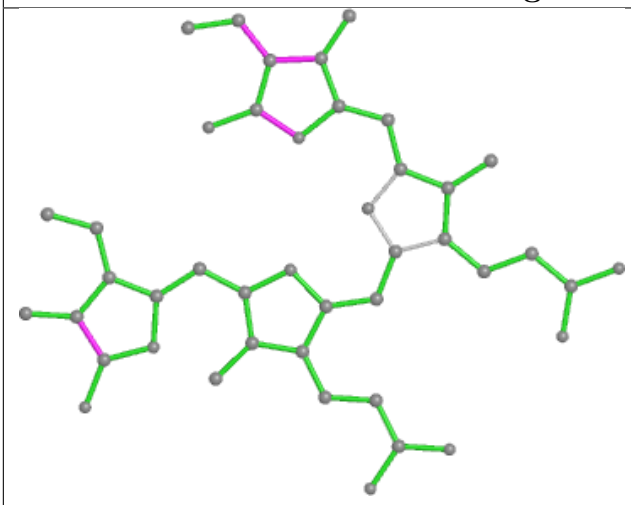
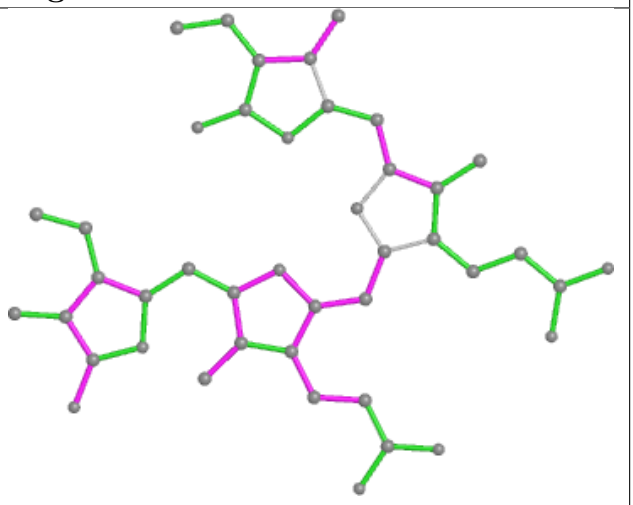


Rings

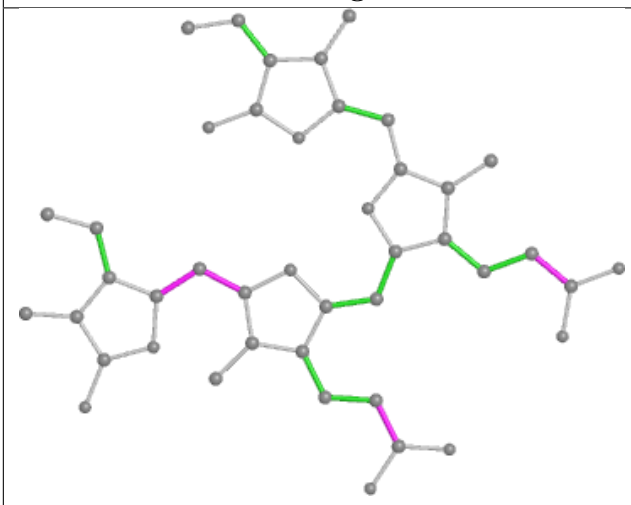
Ligand PEB gi 201



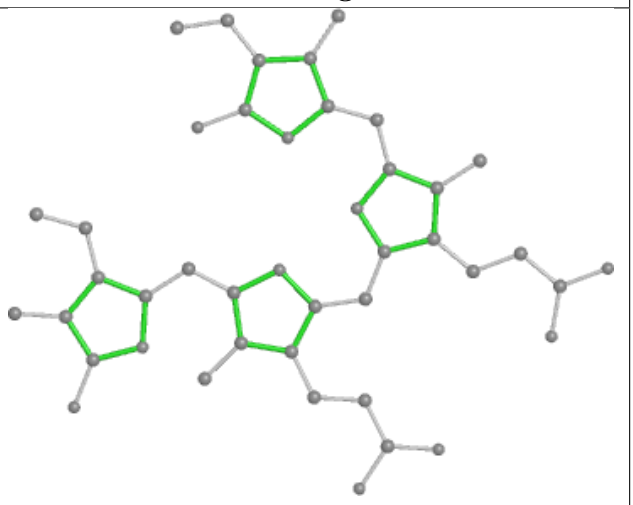
Bond lengths



Bond angles

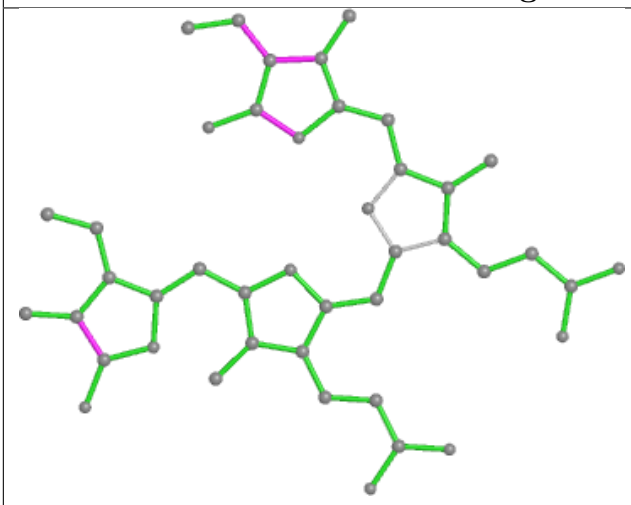


Torsions



Rings

Ligand PEB g2 201



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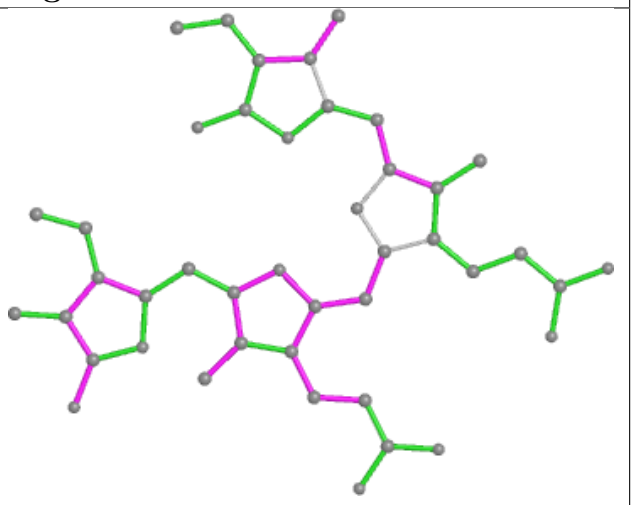

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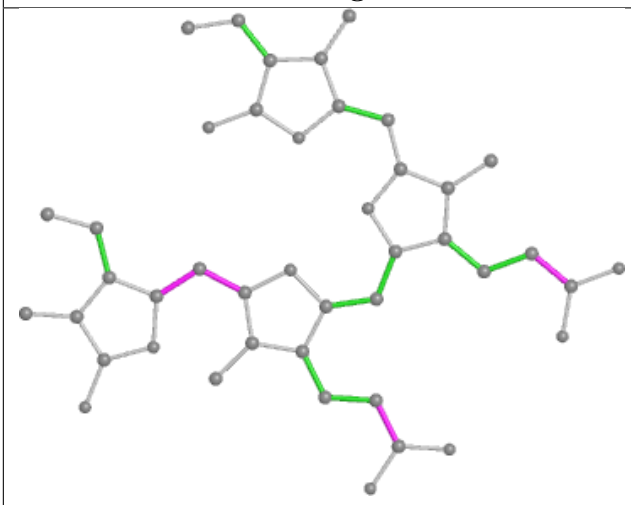

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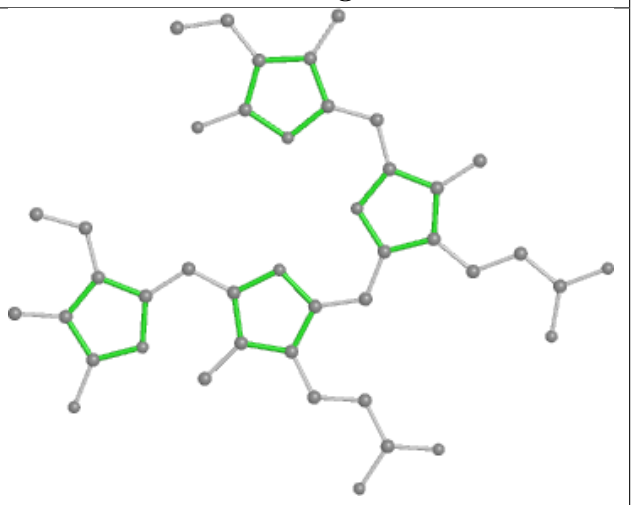
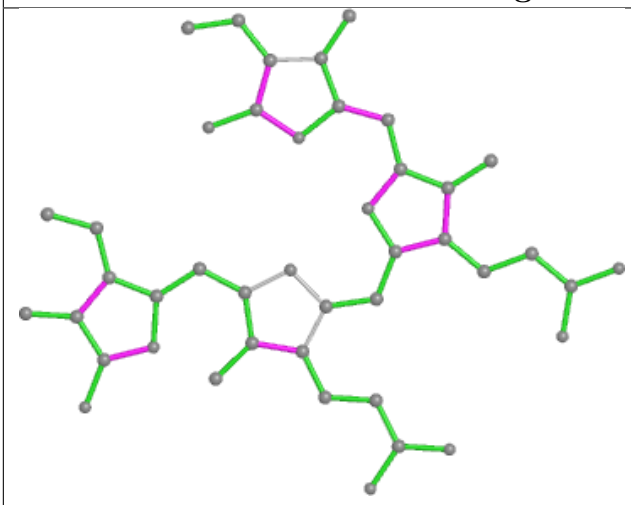


Rings

Ligand PUB T6 203



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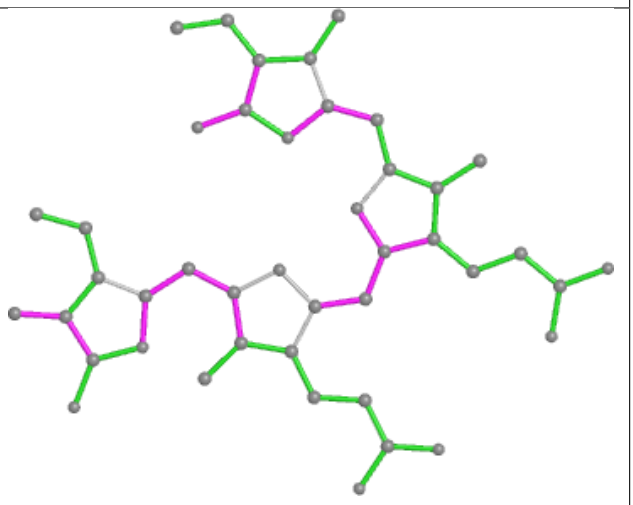

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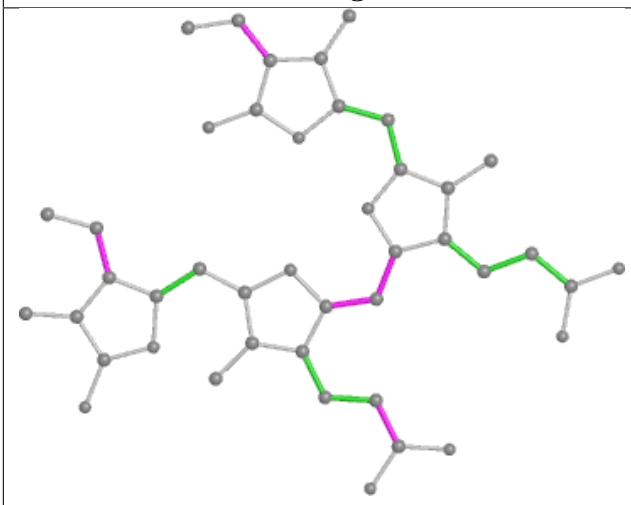

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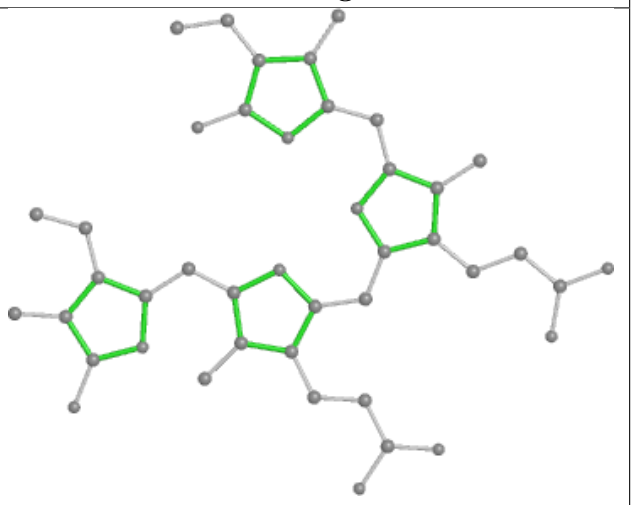
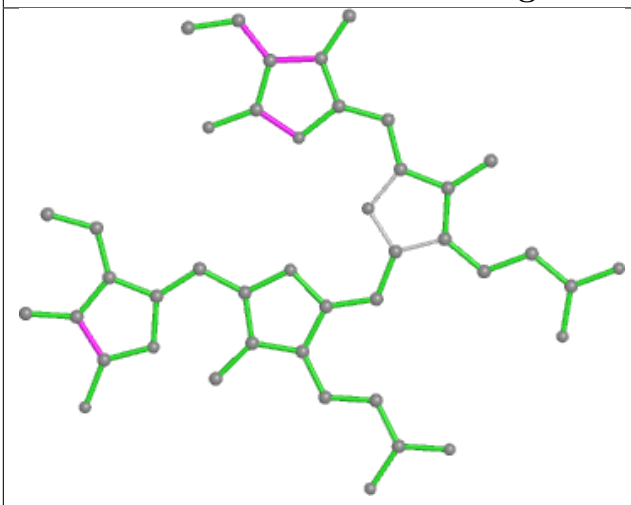


Rings

Ligand PEB hJ 201



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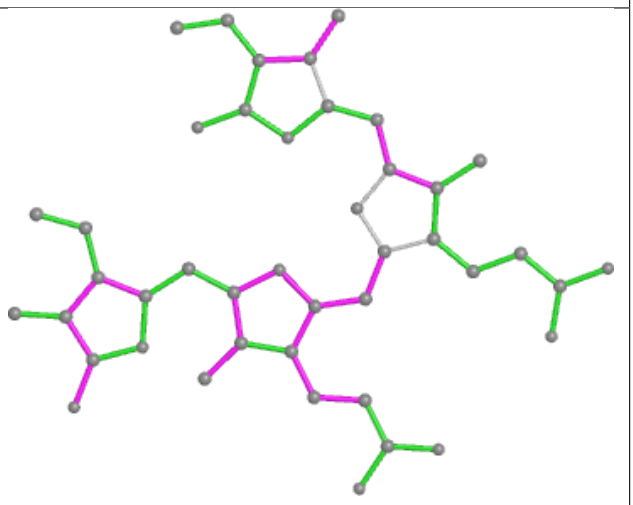

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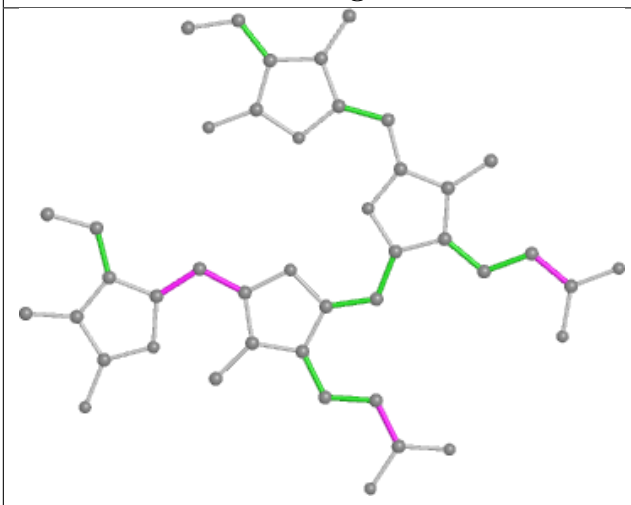

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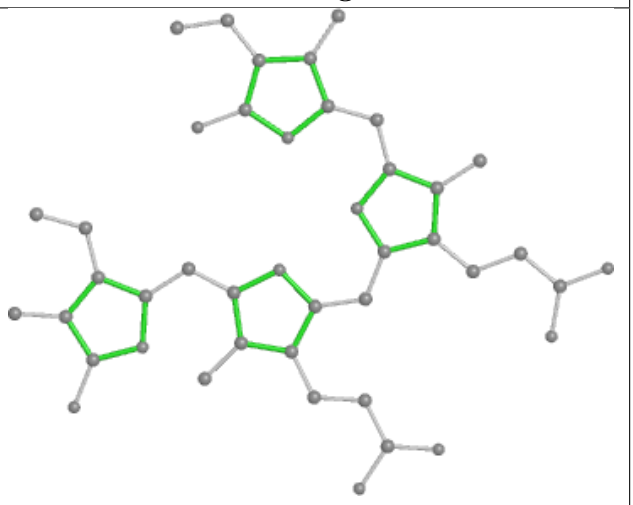

Rings

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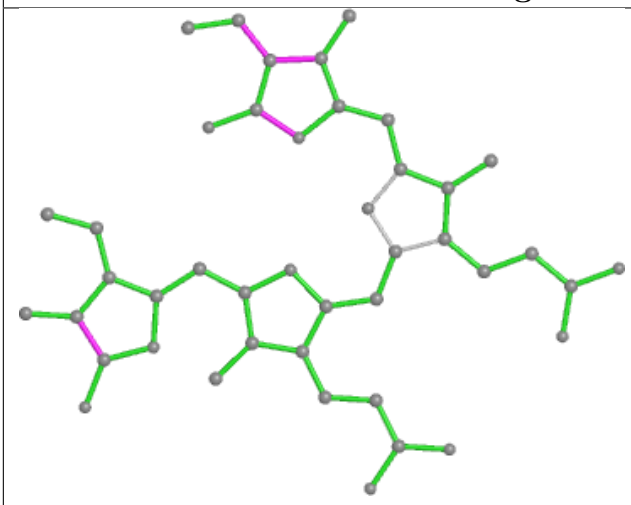

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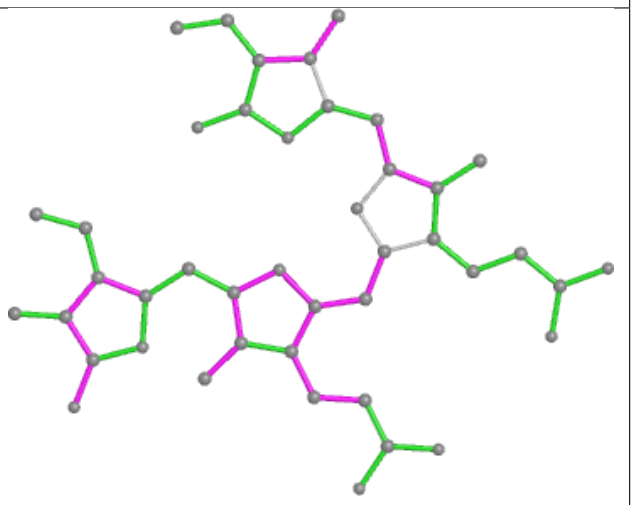

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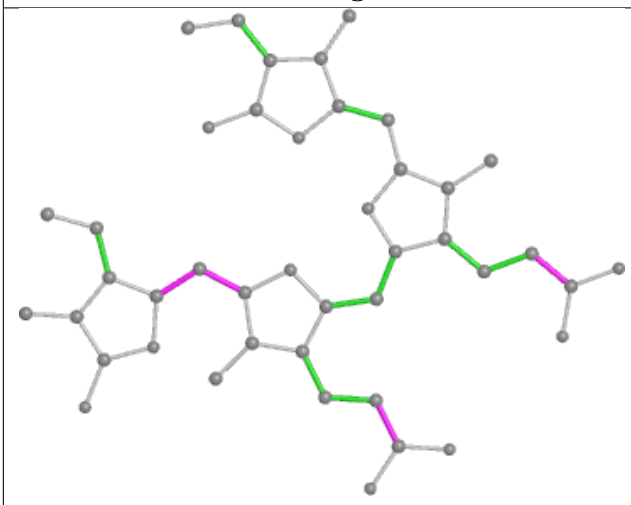

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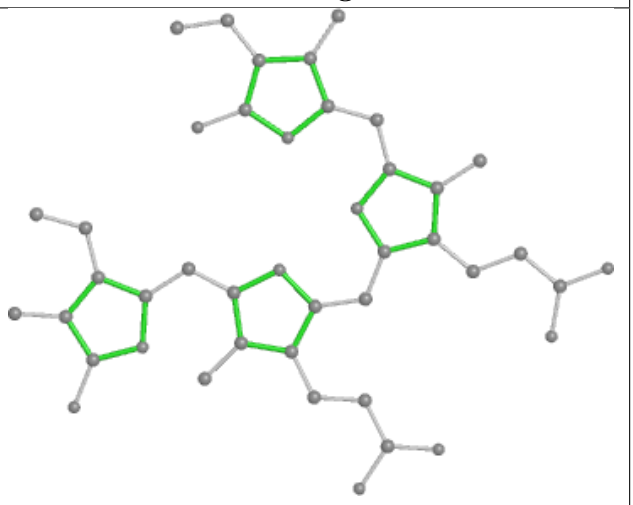

Rings

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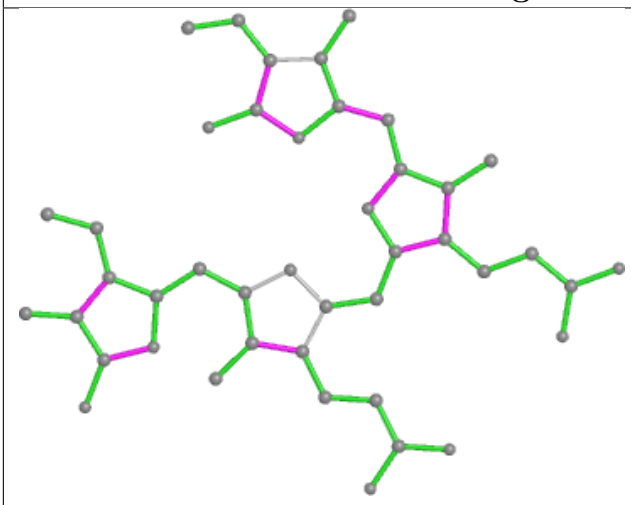

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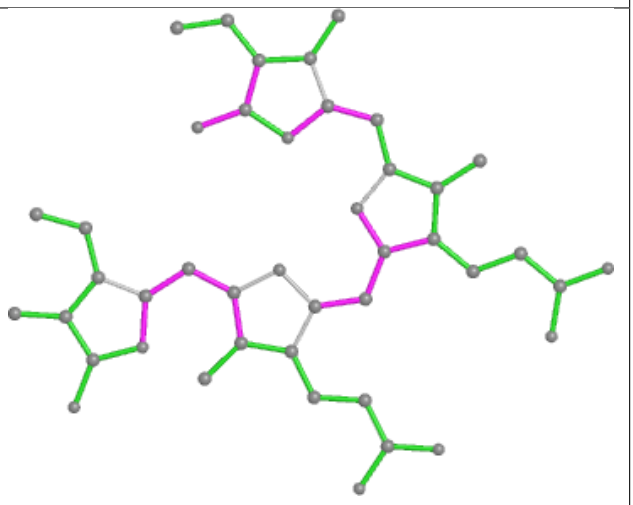

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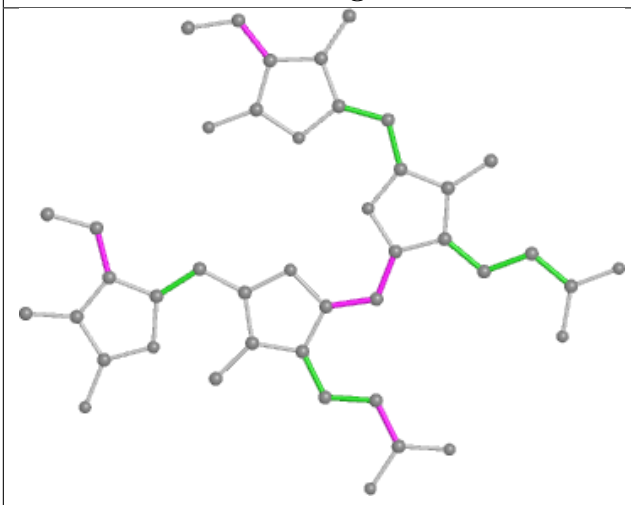

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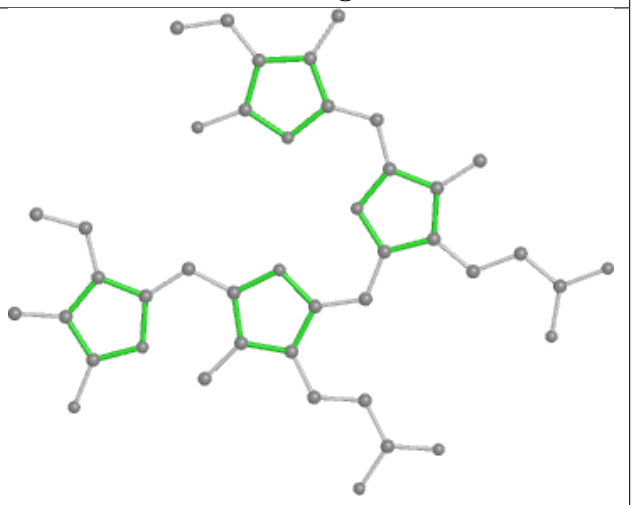

Rings

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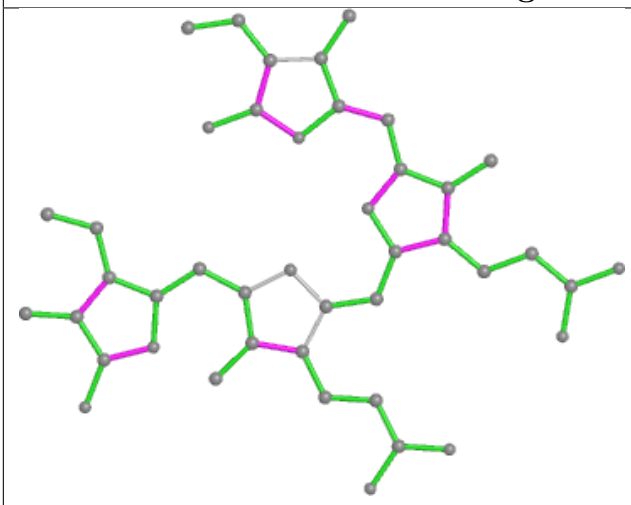

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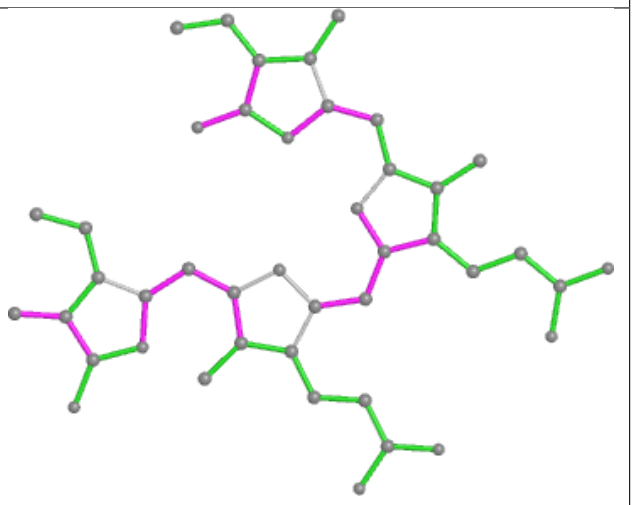

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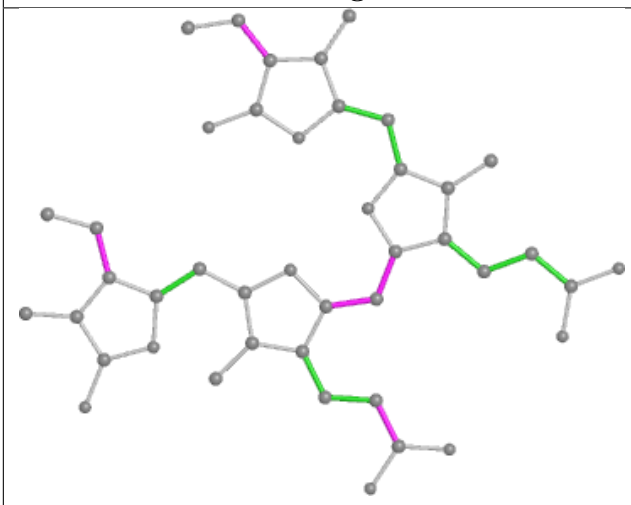

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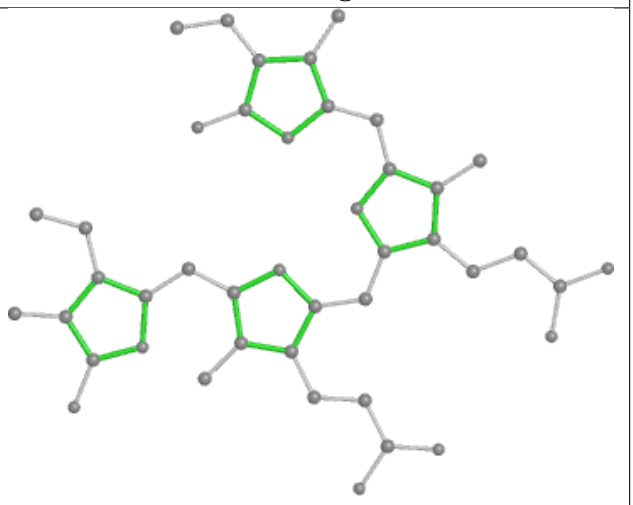

Rings

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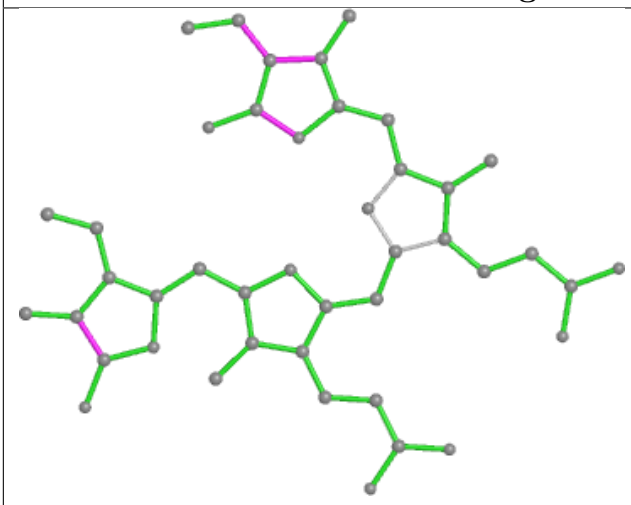

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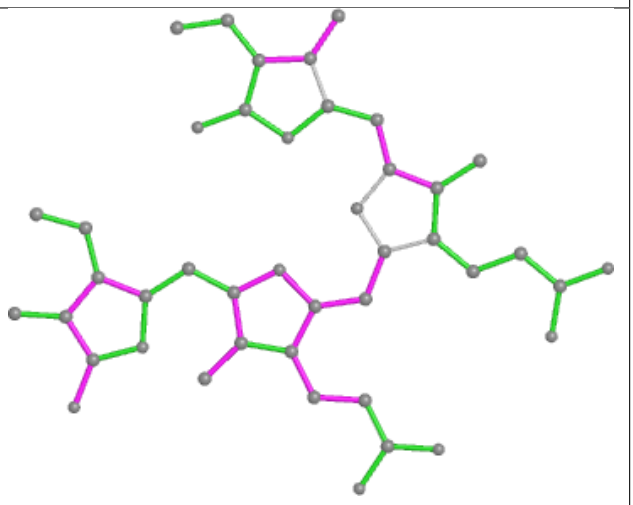

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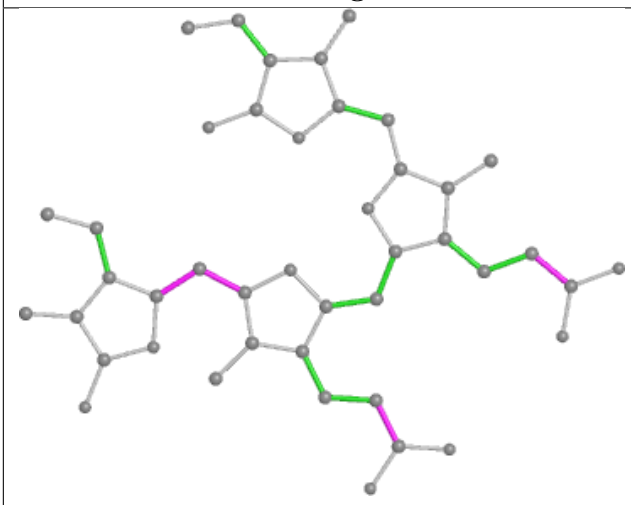

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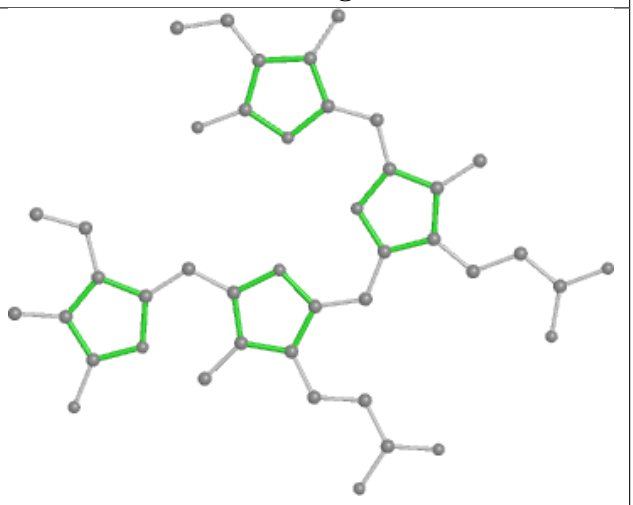

Rings

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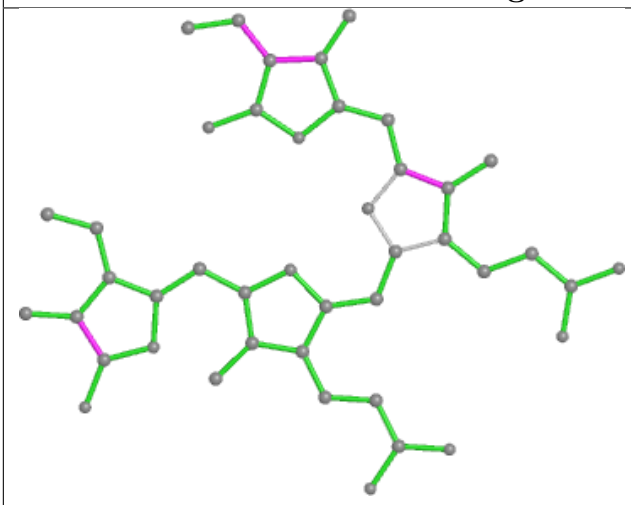

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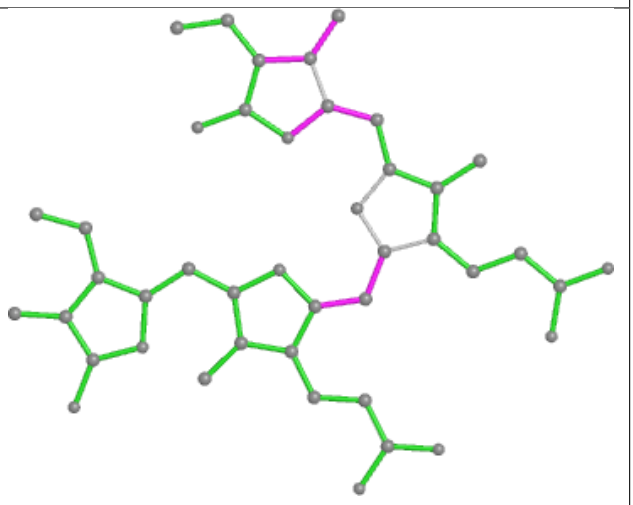

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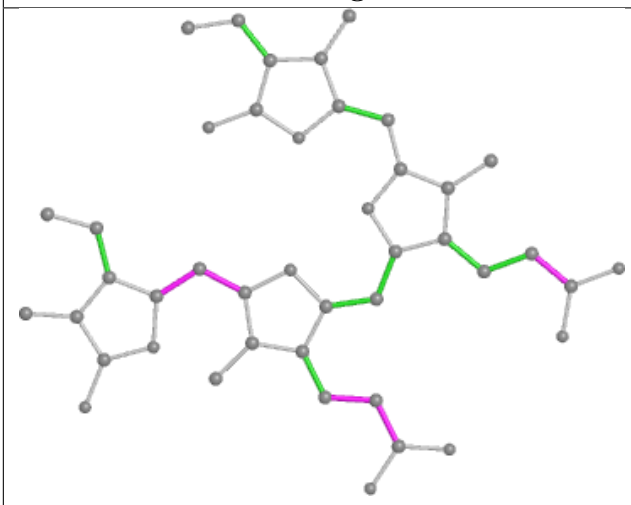

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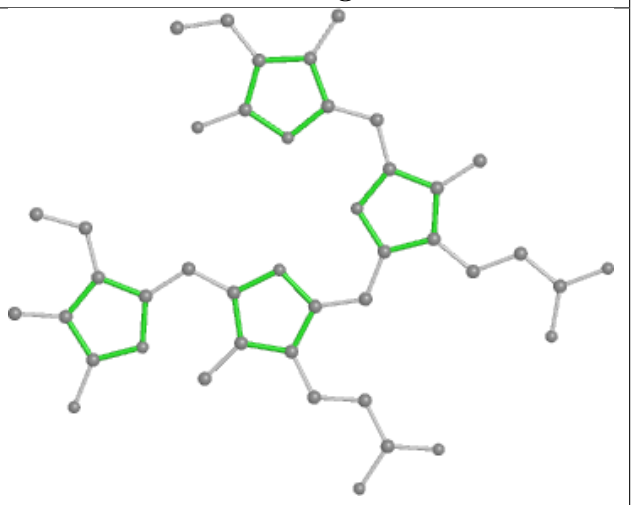

Rings

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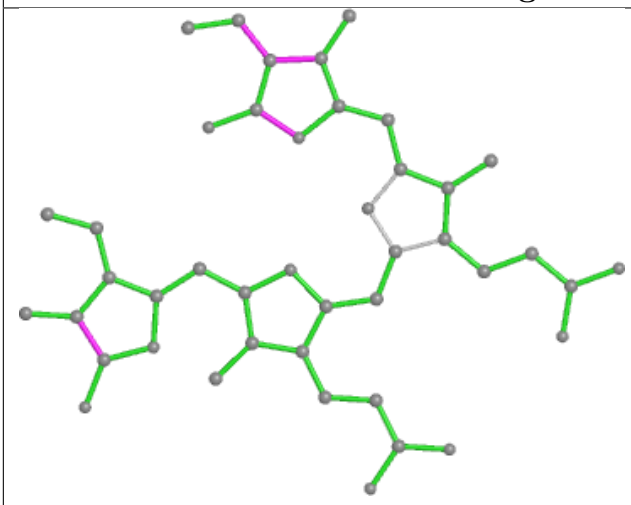

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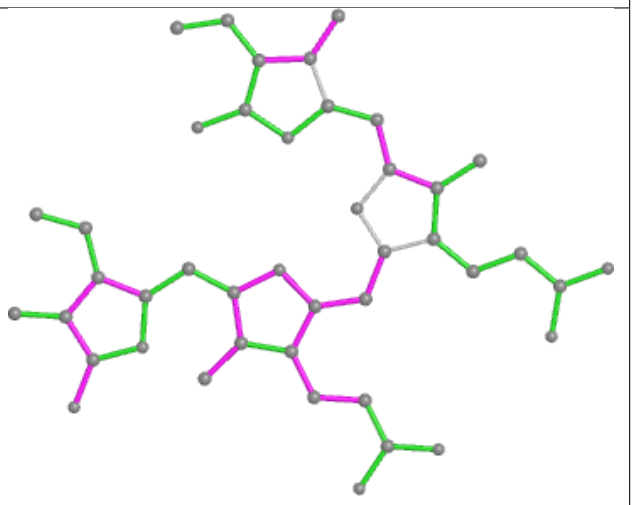

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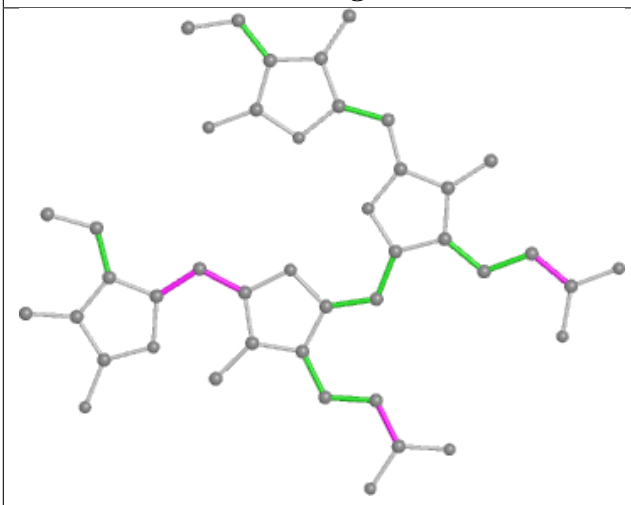

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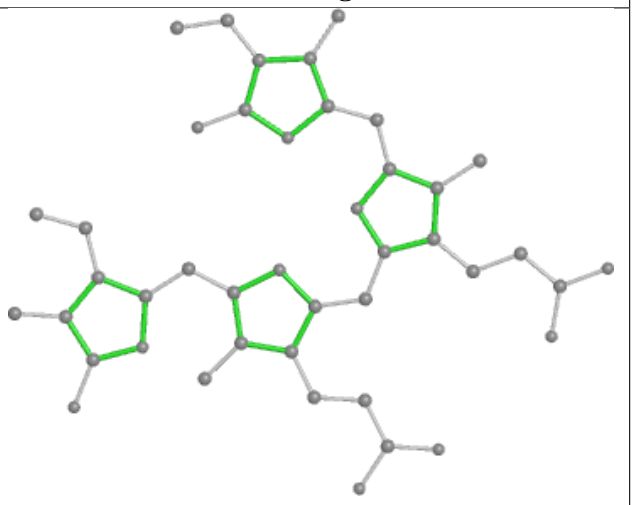

Rings

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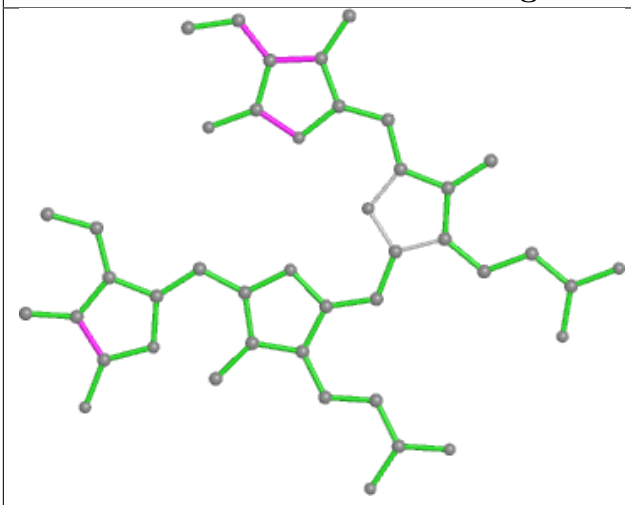

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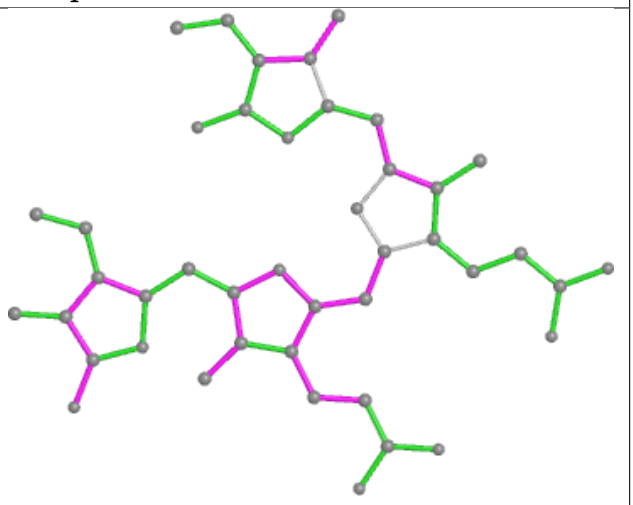

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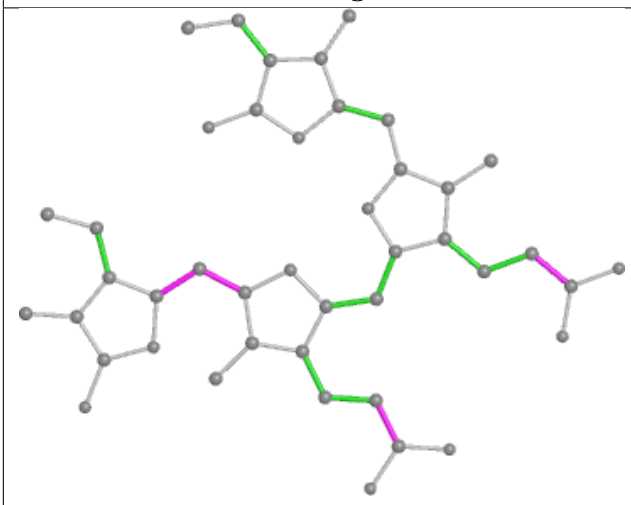

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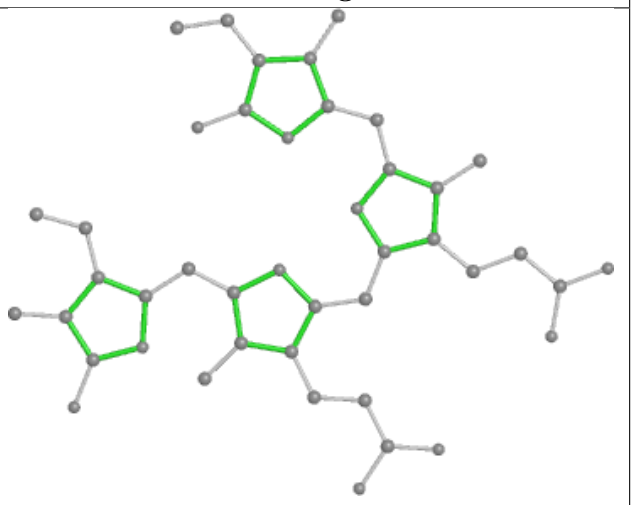

Rings

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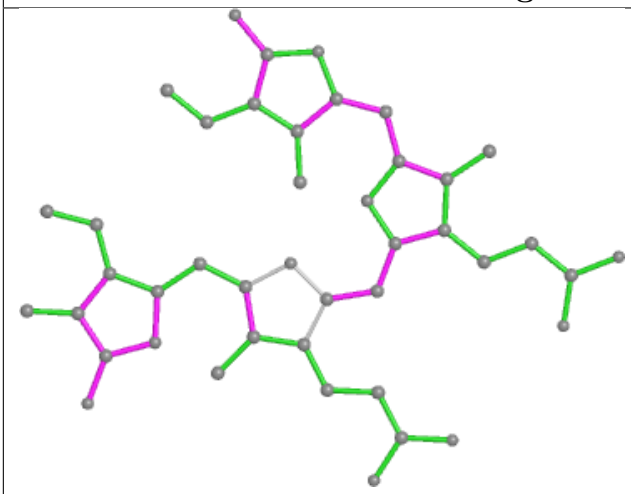

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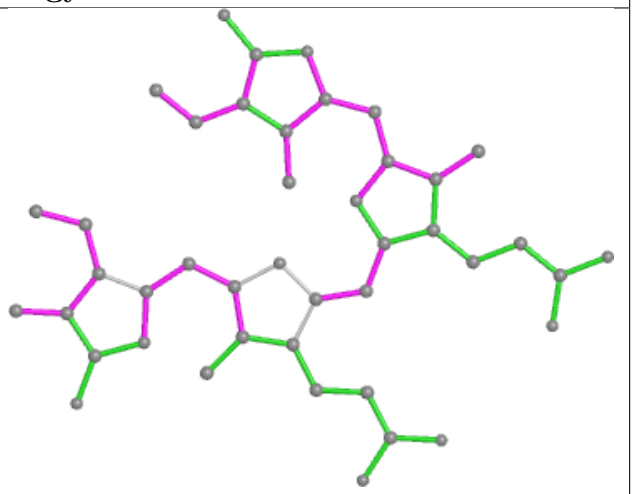

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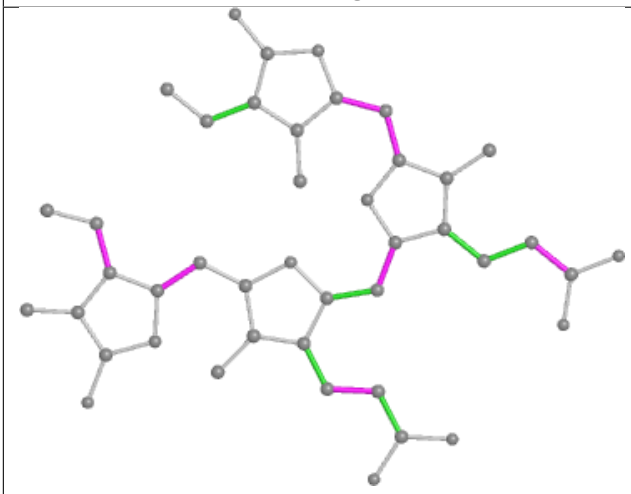

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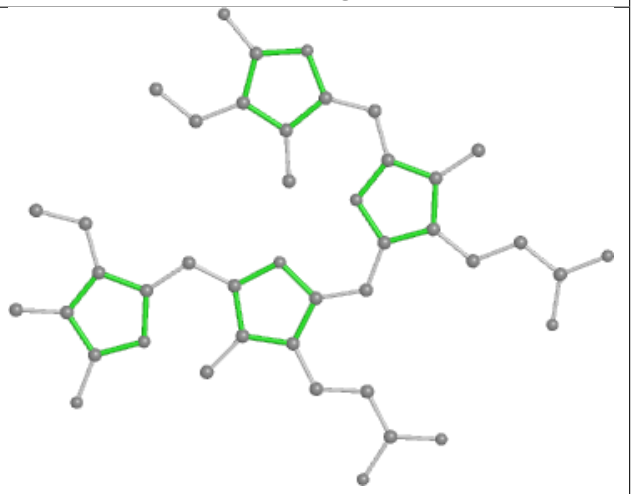
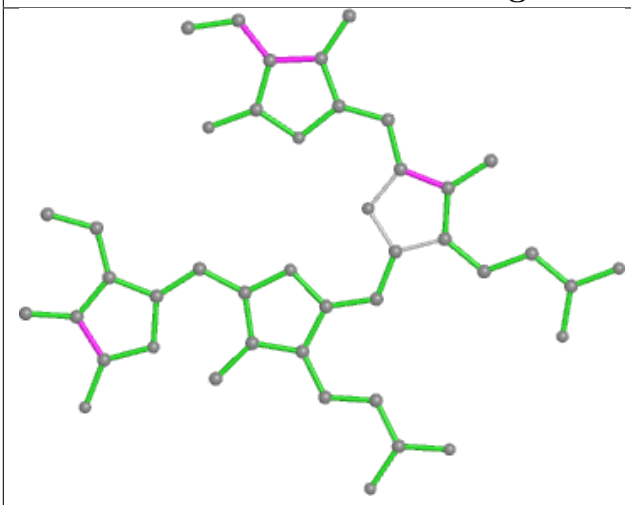


Rings

Ligand PEB lm 1002



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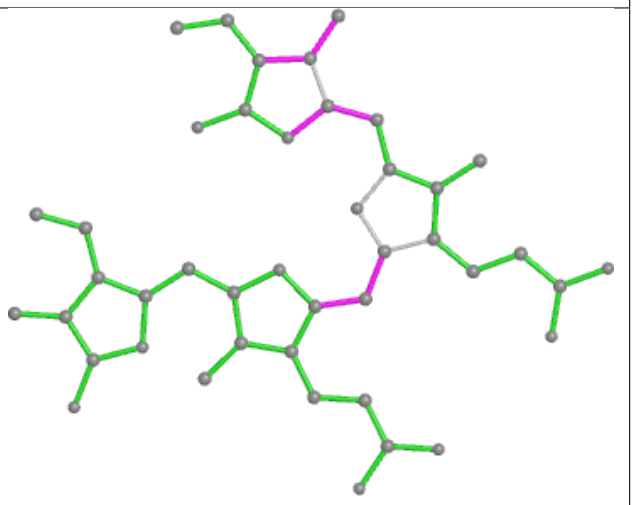

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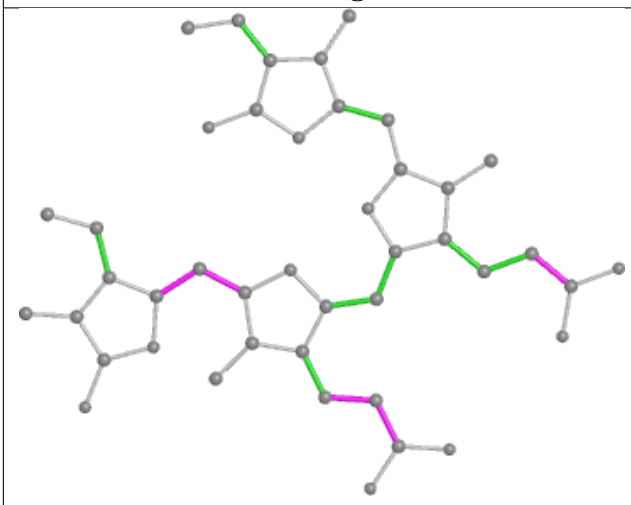

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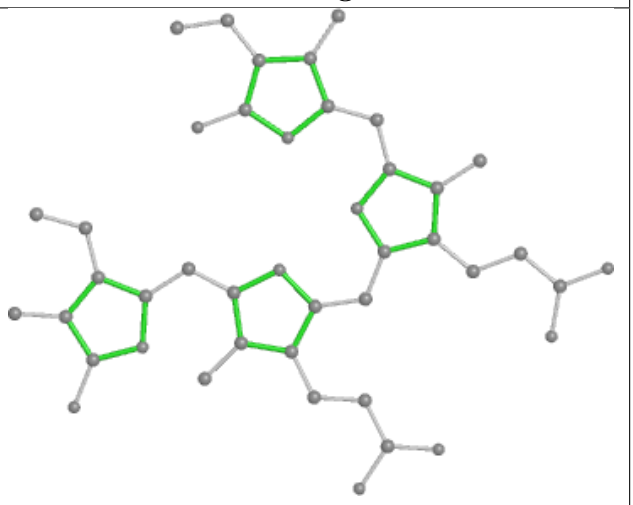

Rings

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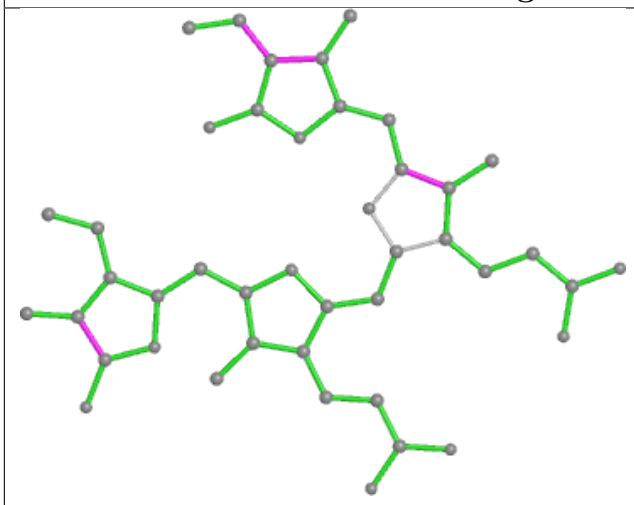

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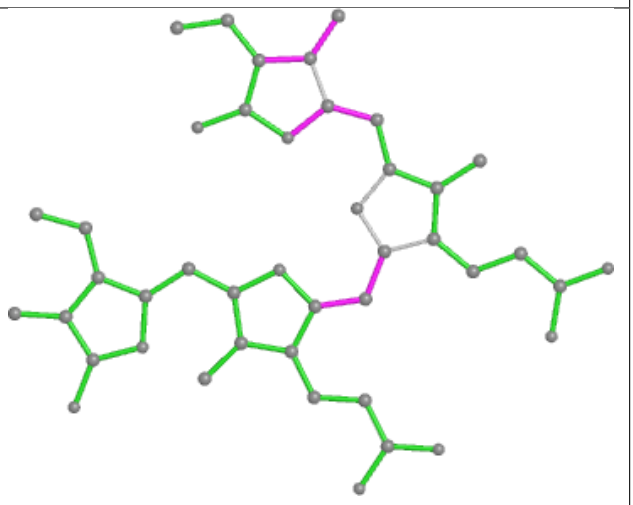
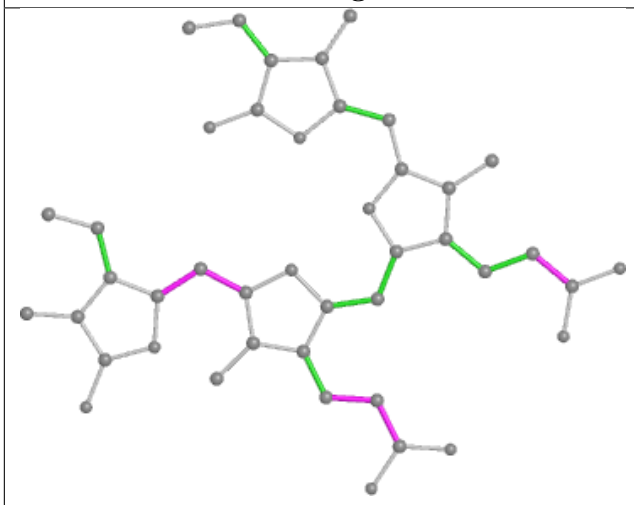
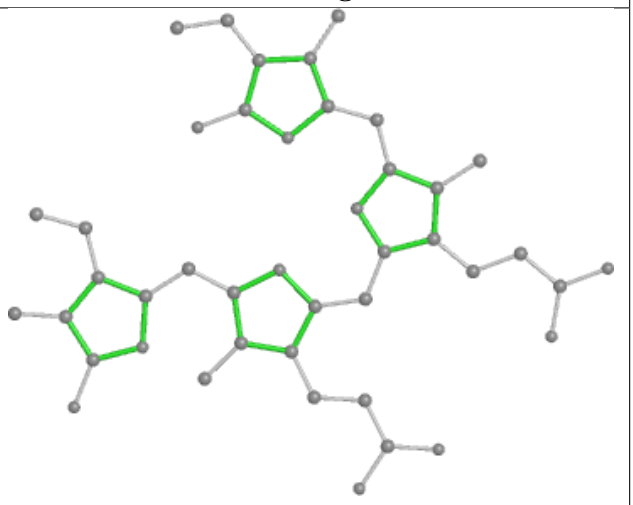


Bond angles

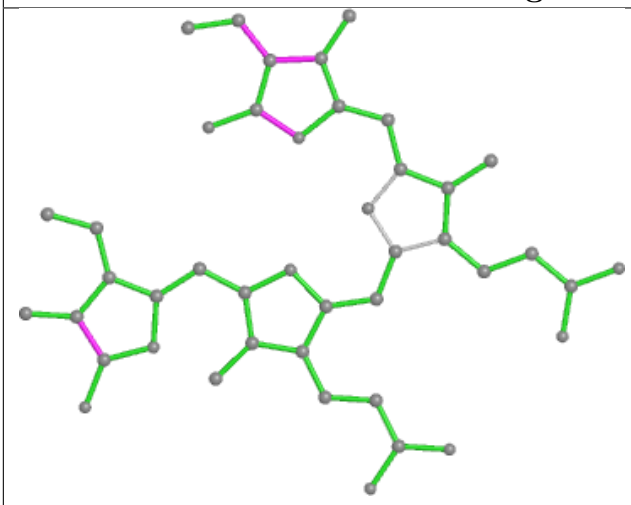


Torsions



Rings

Ligand PEB ls 201



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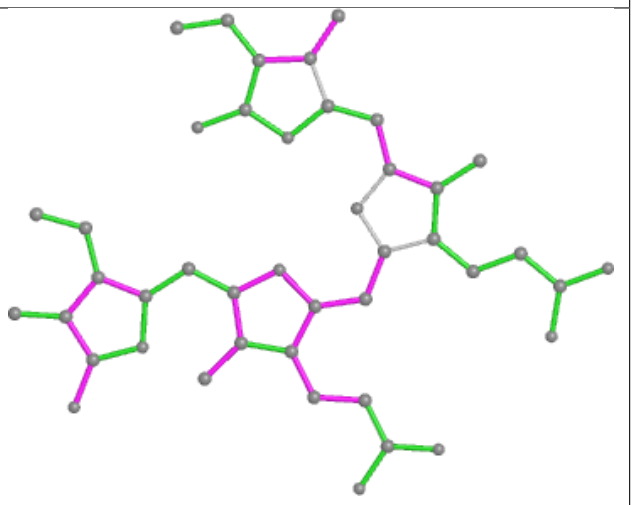

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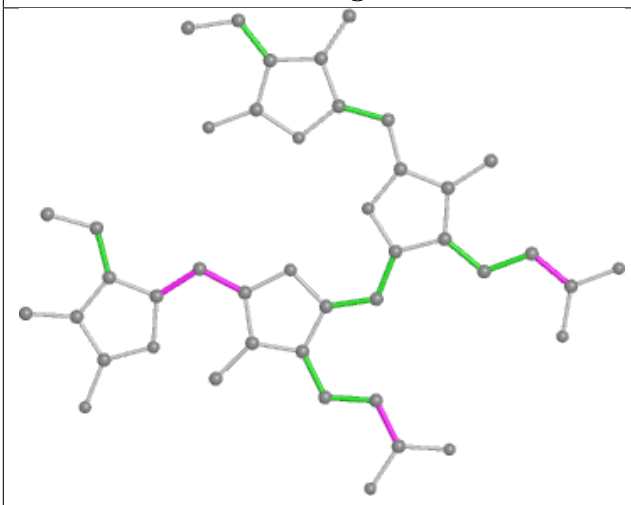

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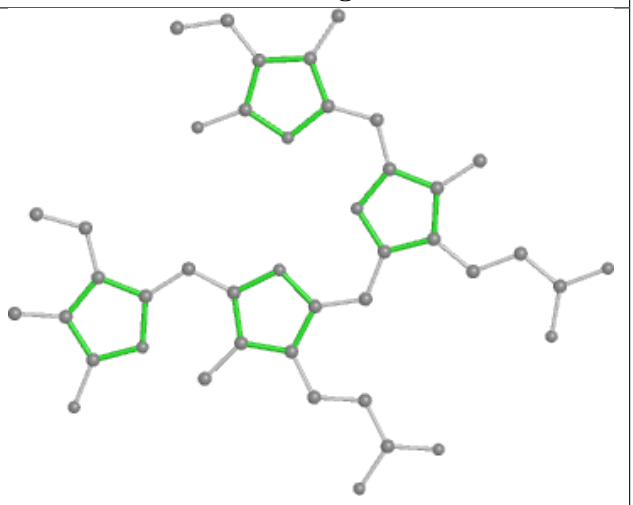
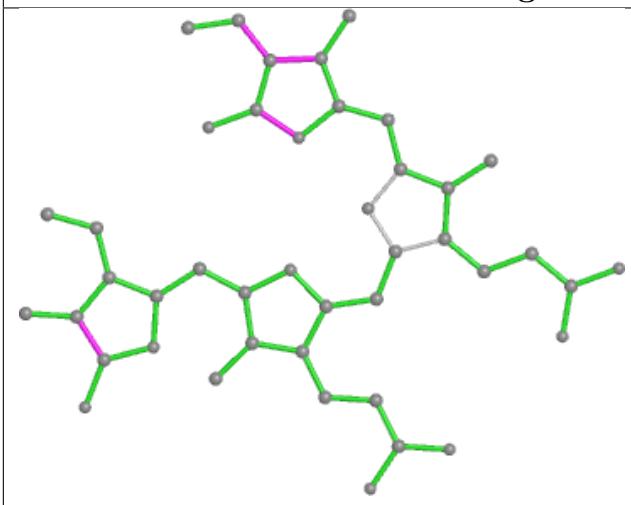


Rings

Ligand PEB aZ 301



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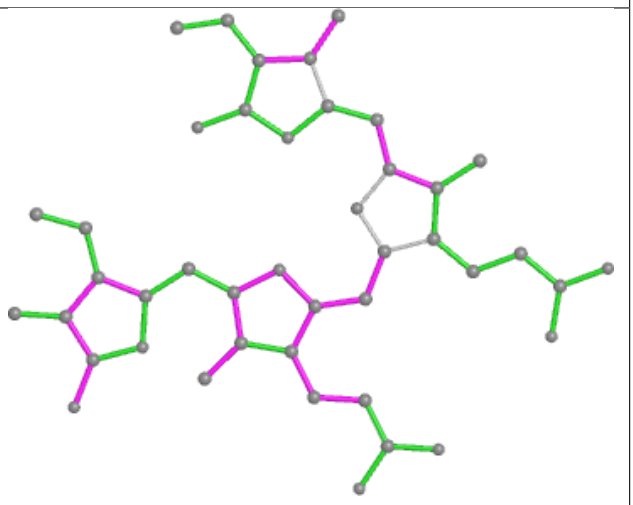

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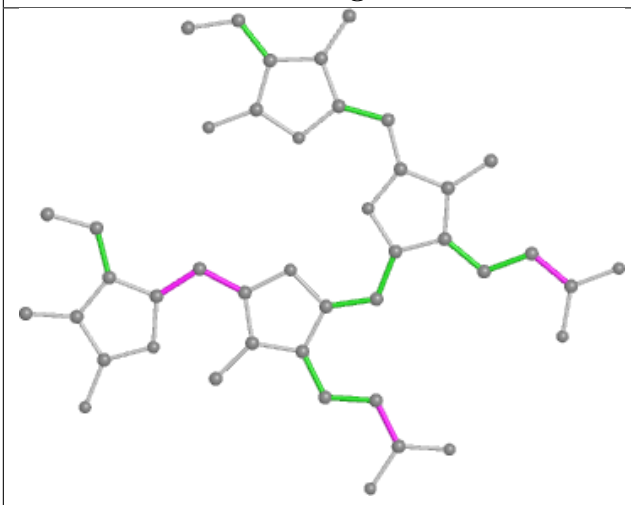

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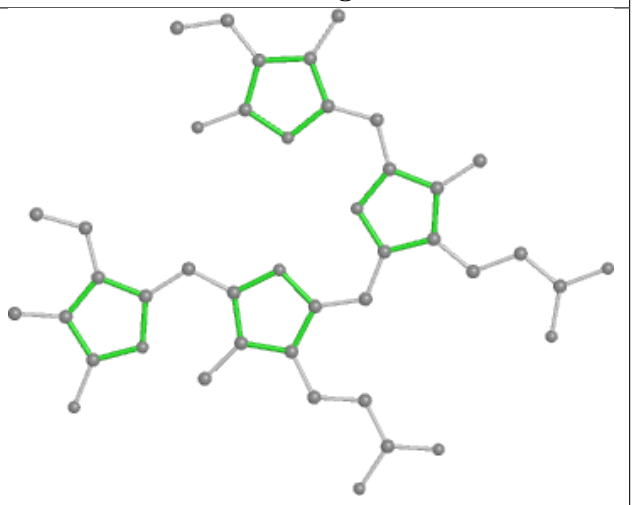

Rings

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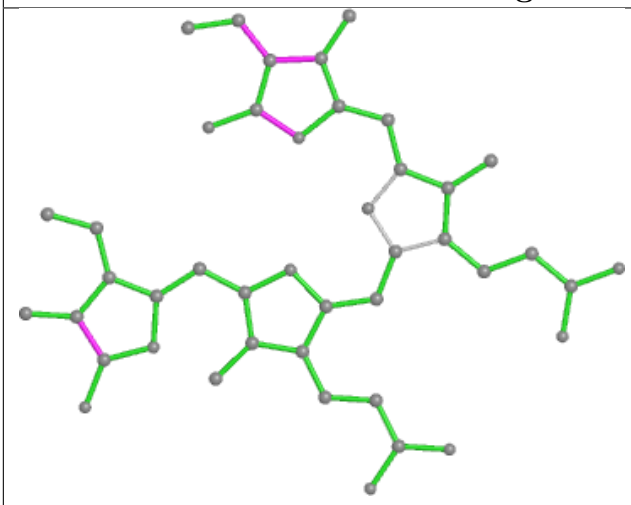

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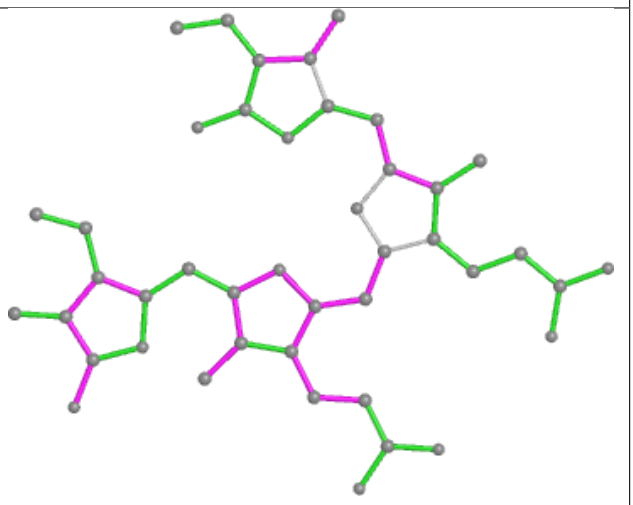

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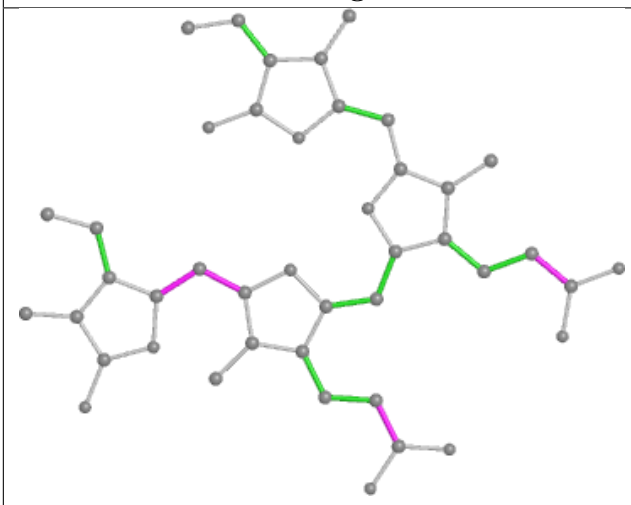

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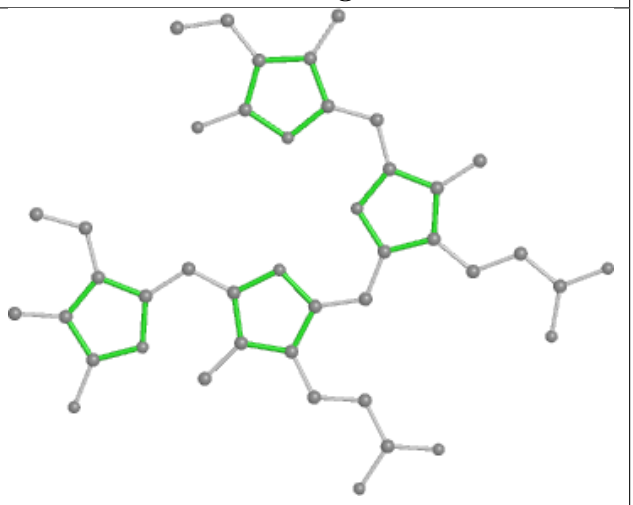
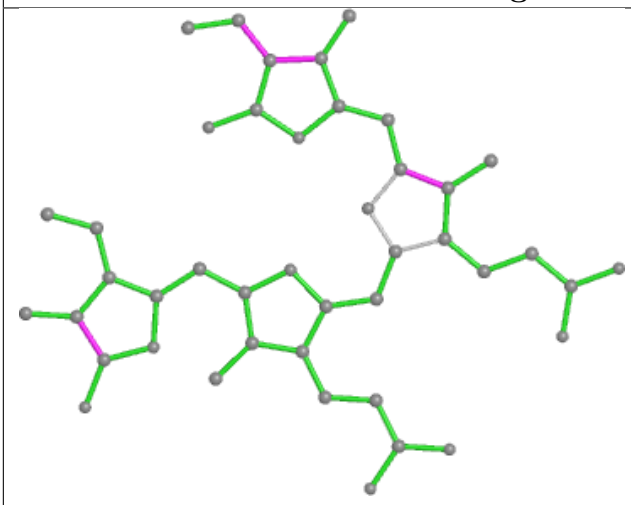


Rings

Ligand PEB da 1002



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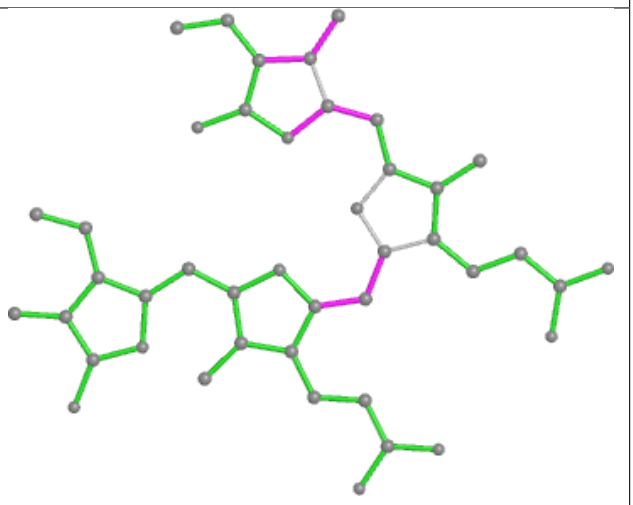

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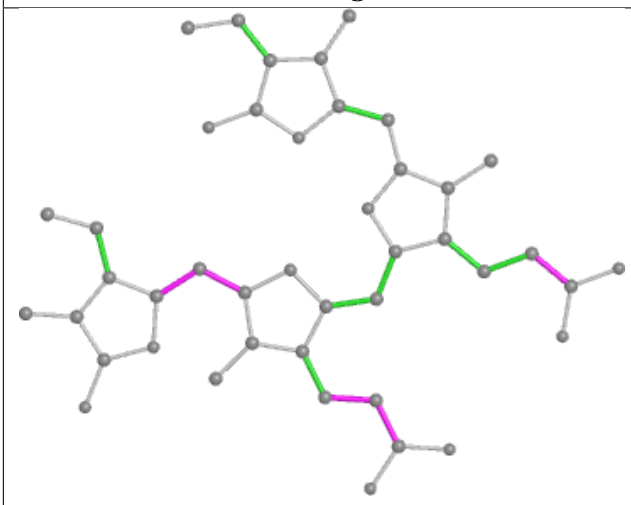

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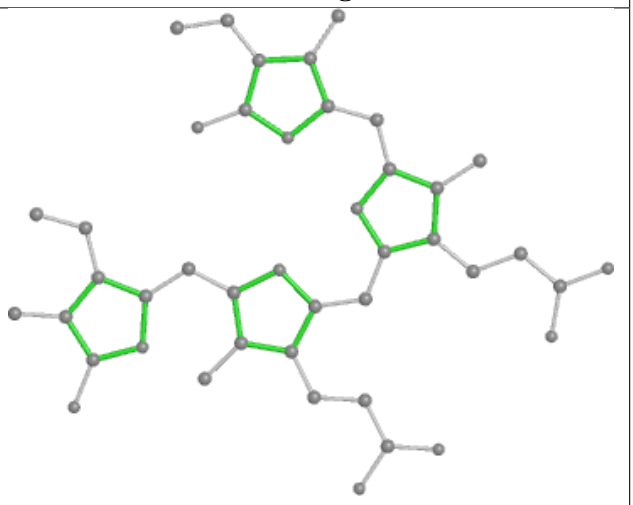

Rings

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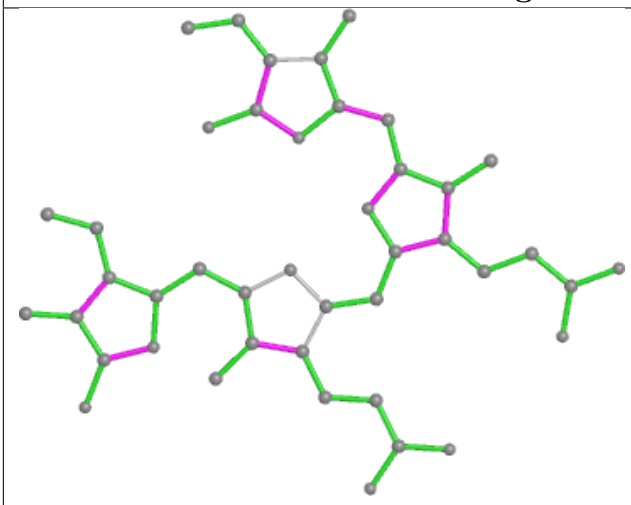

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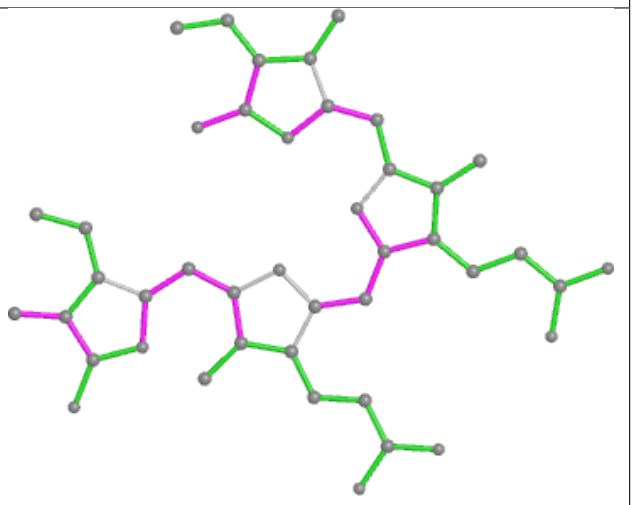

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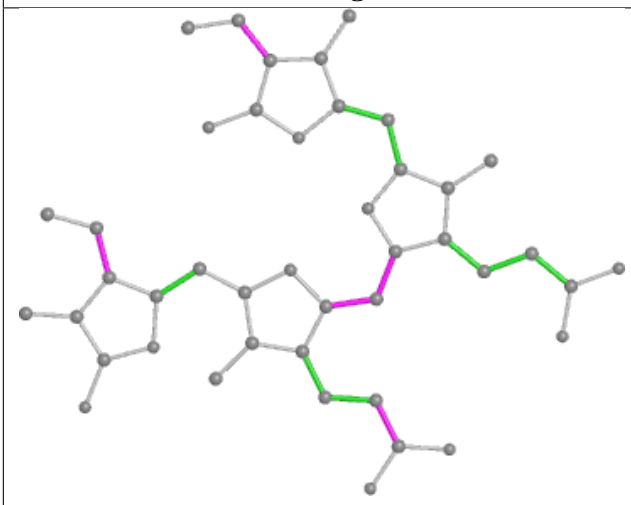

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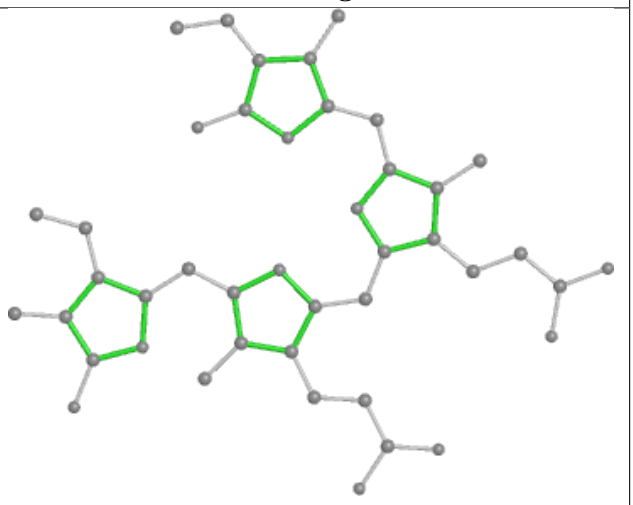

Rings

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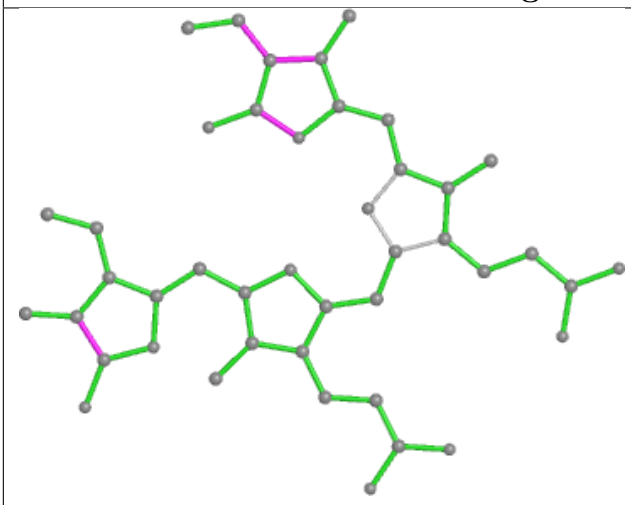

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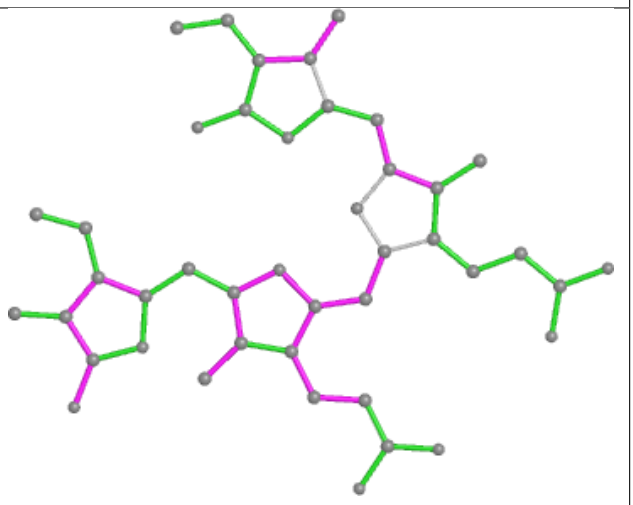

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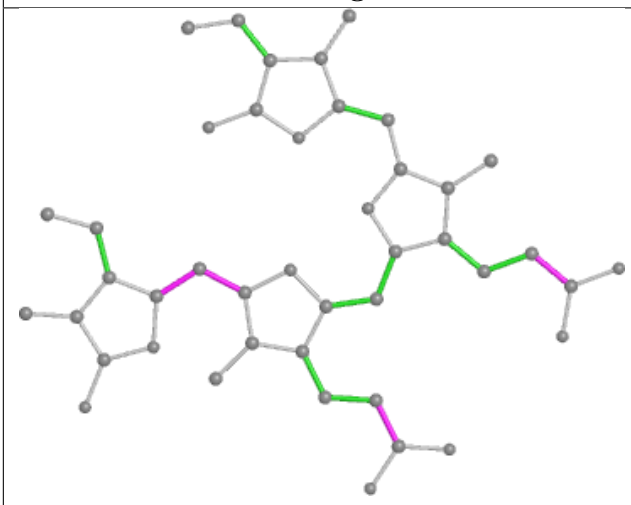

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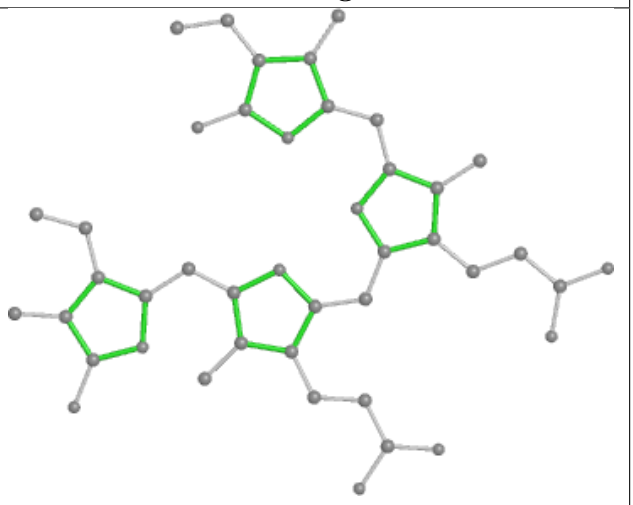

Rings

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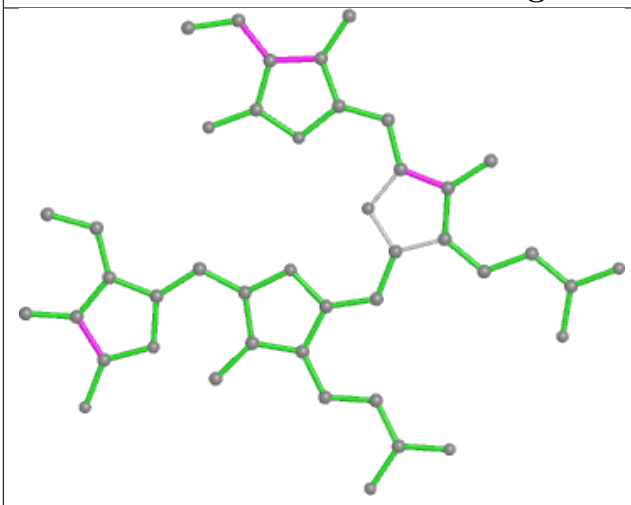

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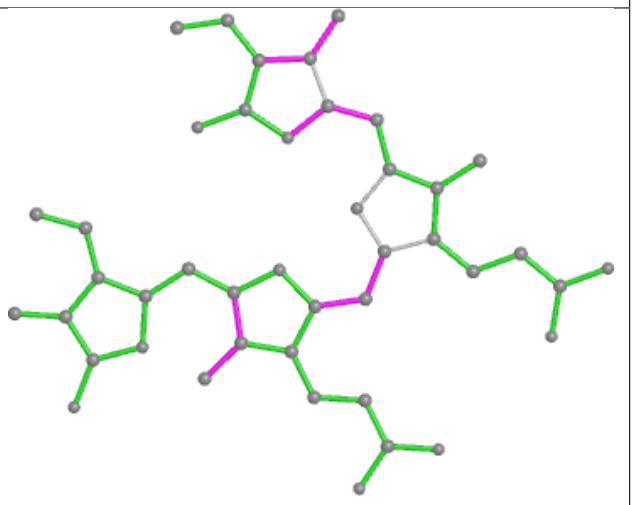

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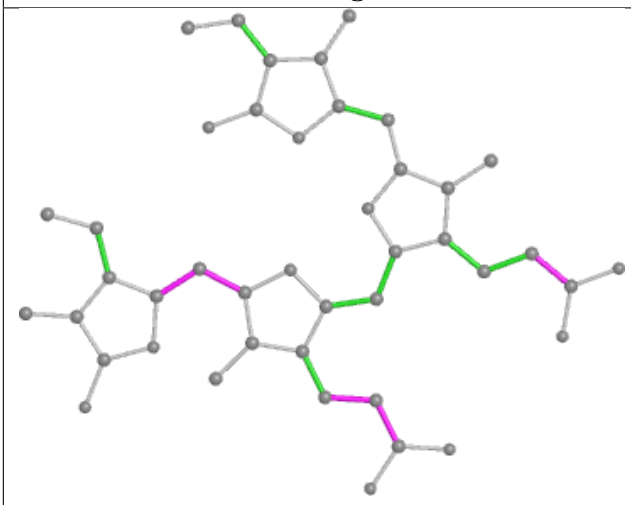

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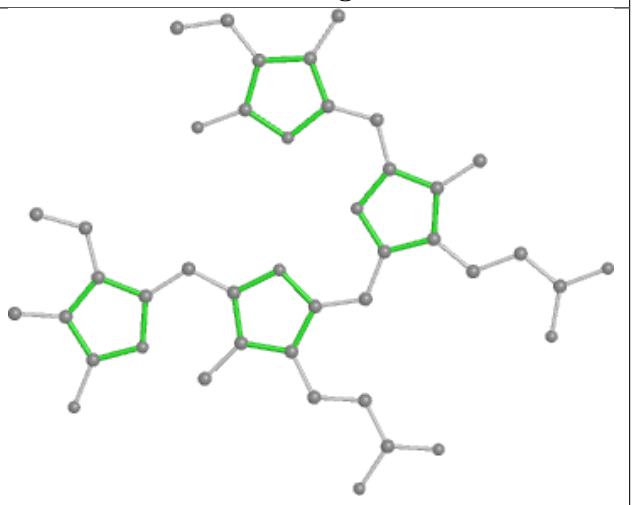

Rings

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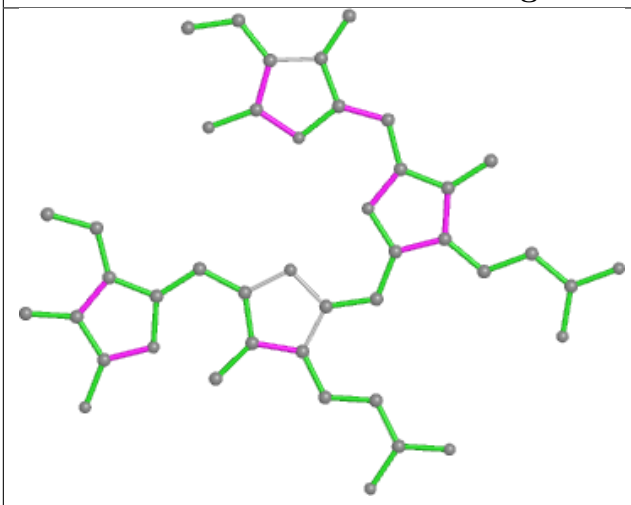

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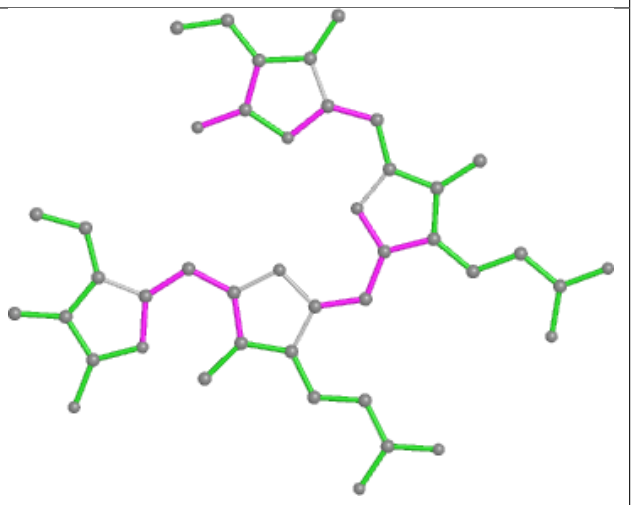

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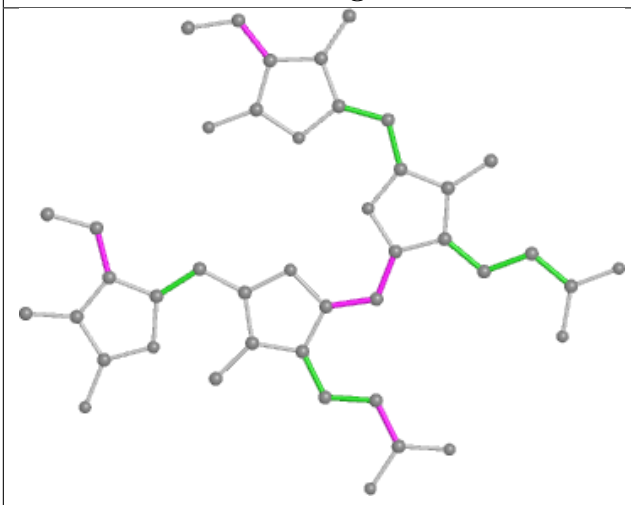

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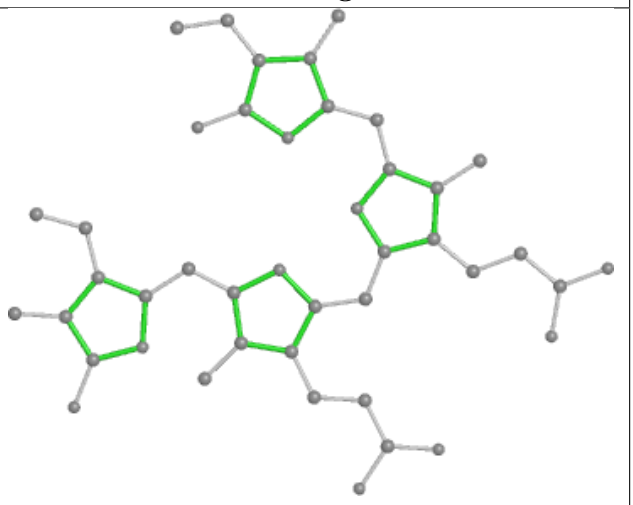
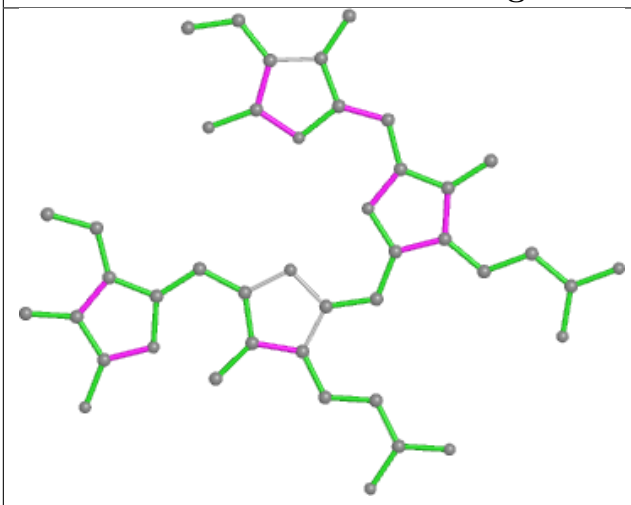


Rings

Ligand PUB iG 1002



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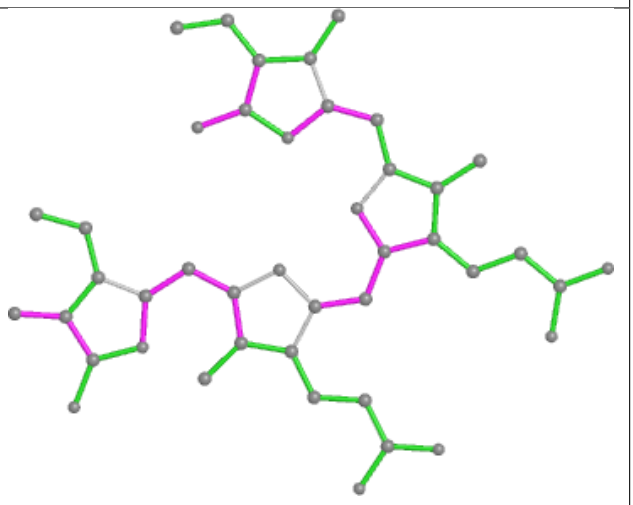

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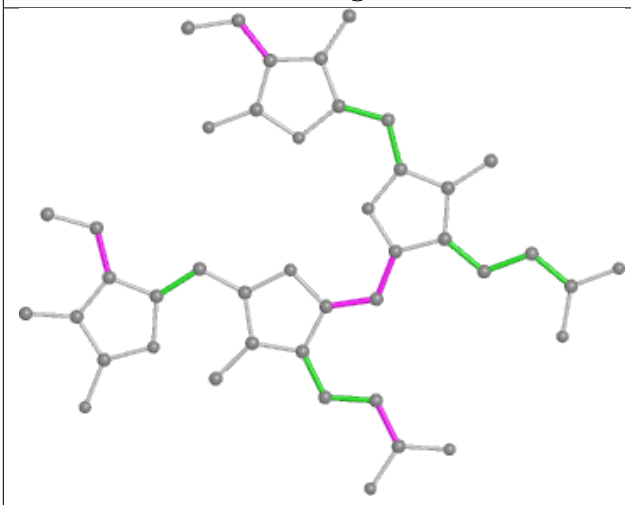

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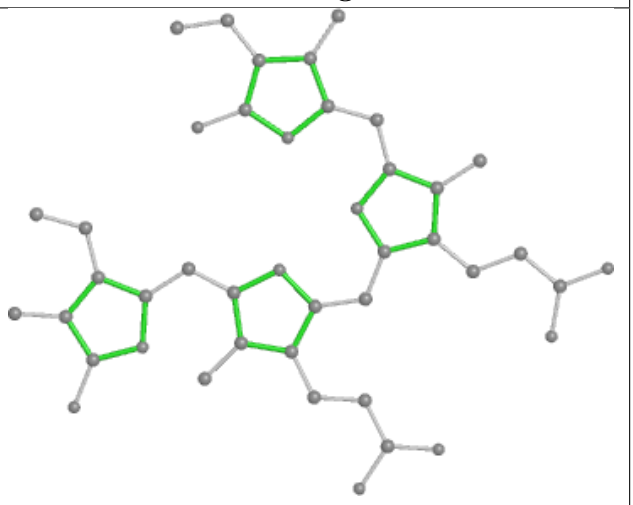
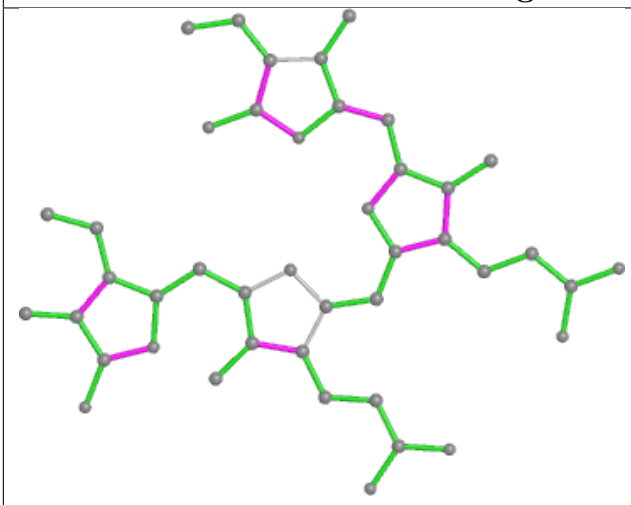


Rings

Ligand PUB n4 203



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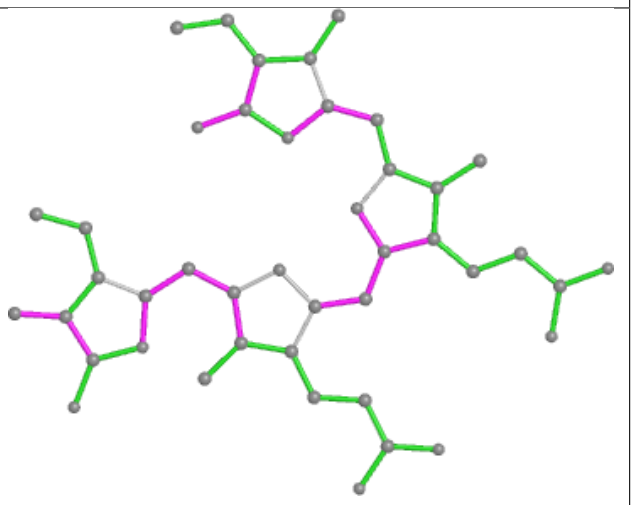

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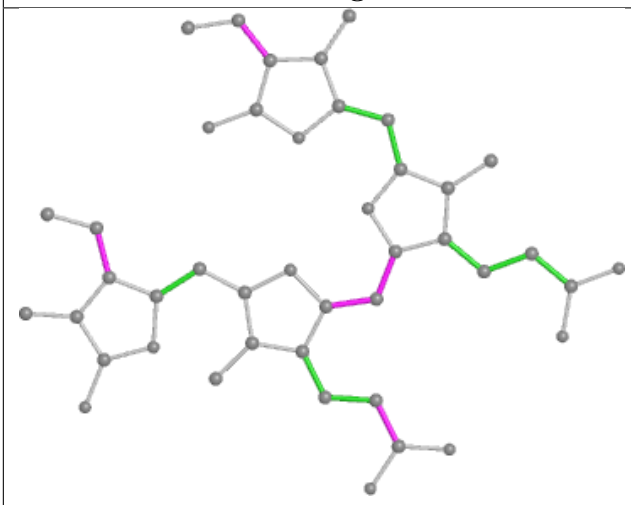

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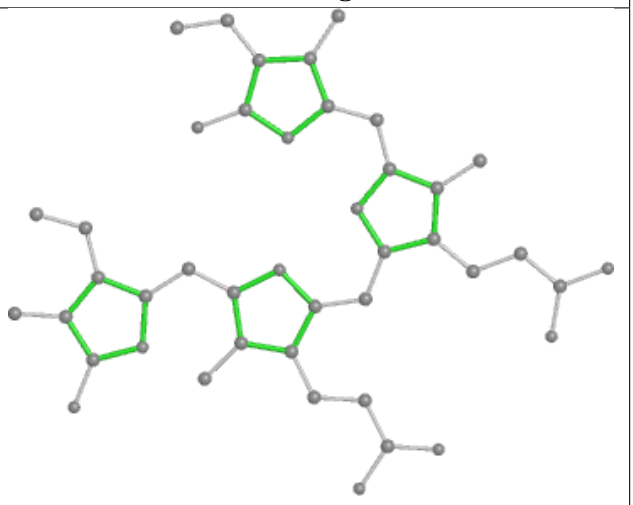

Rings

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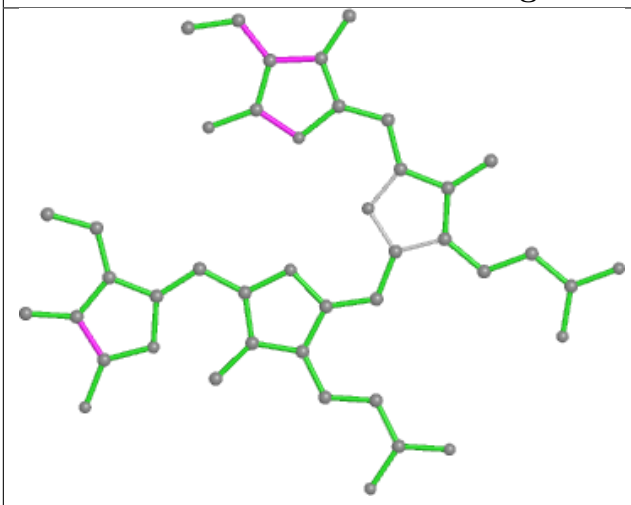

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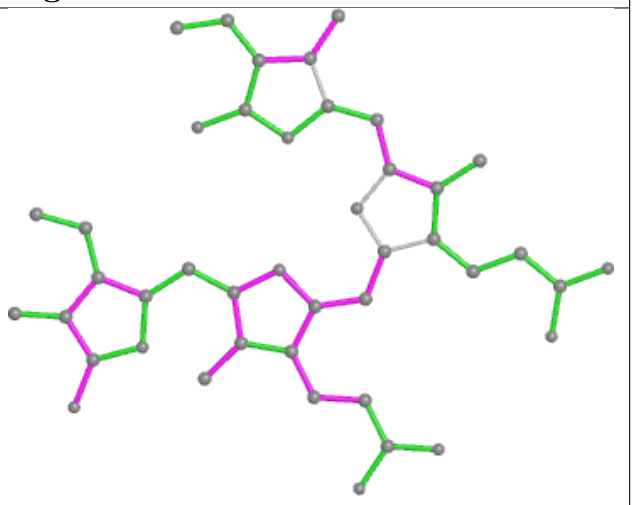

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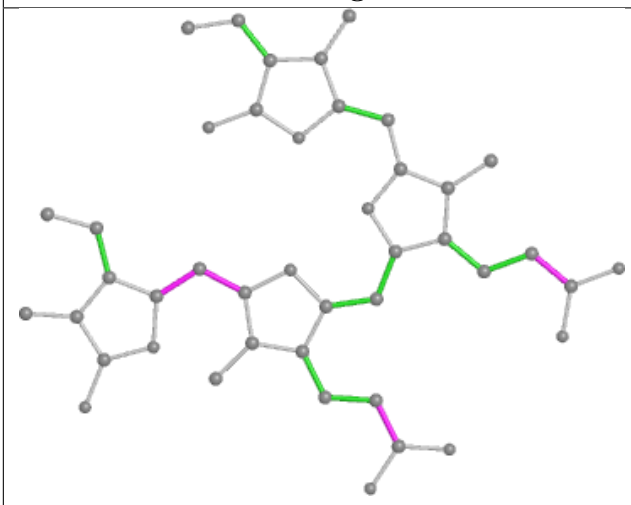

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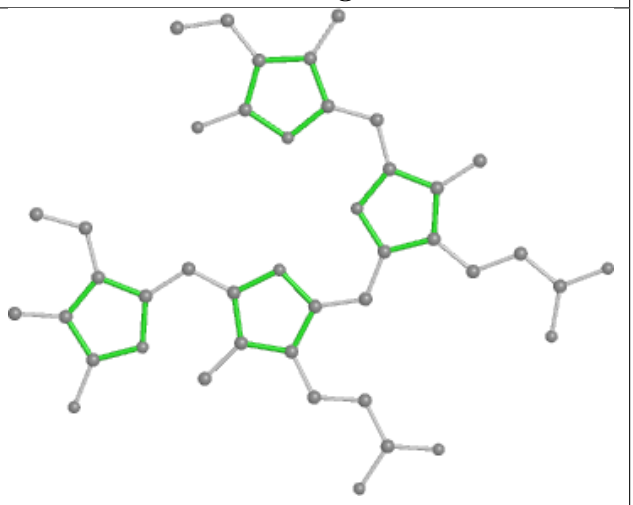

Rings

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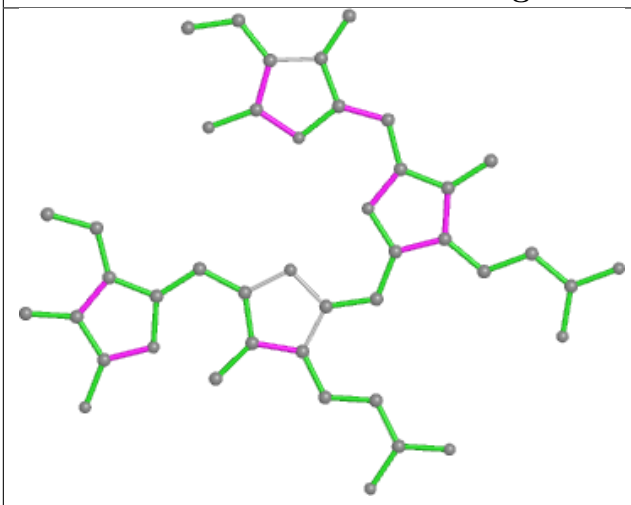

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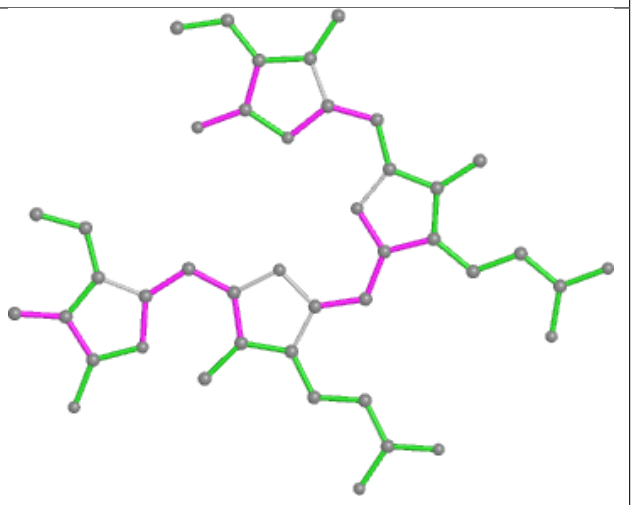

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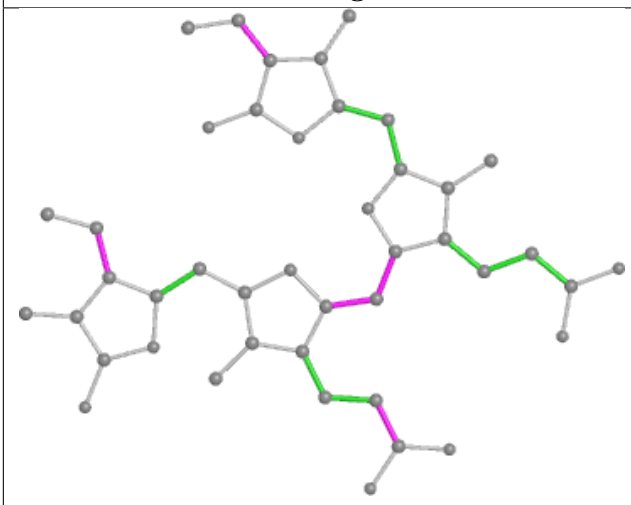

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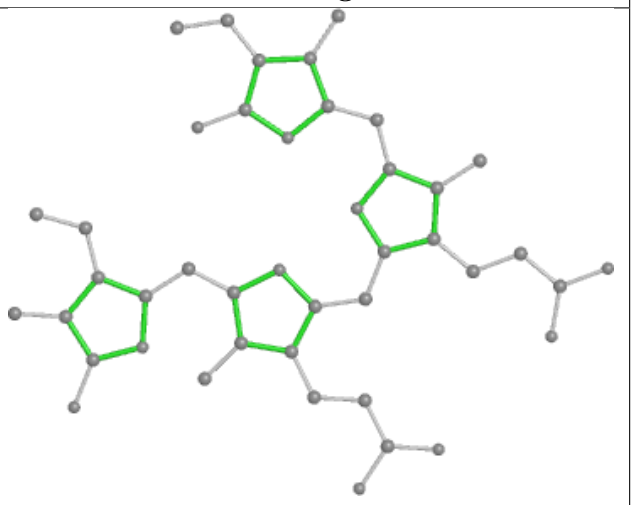
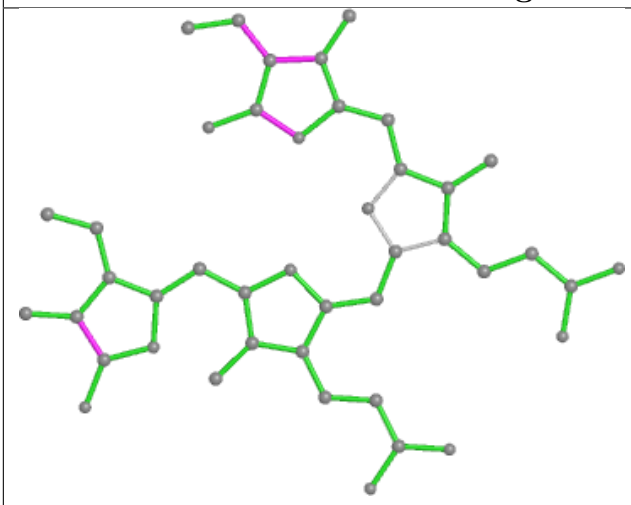


Rings

Ligand PEB aX 401



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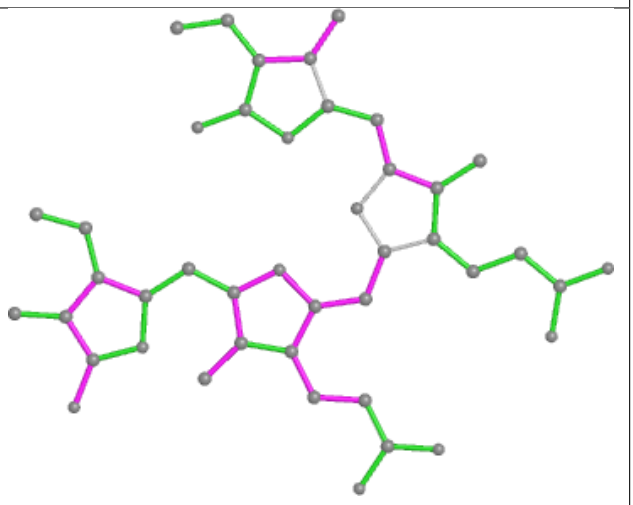

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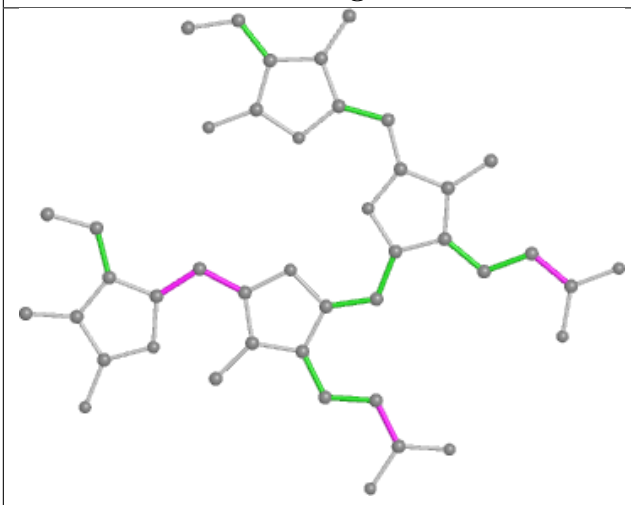
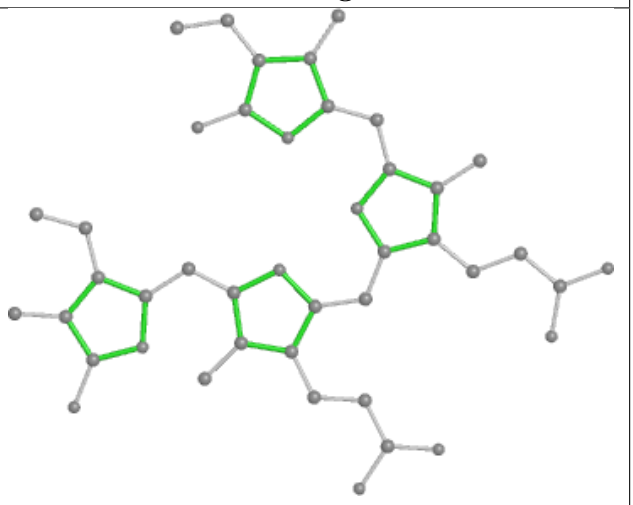
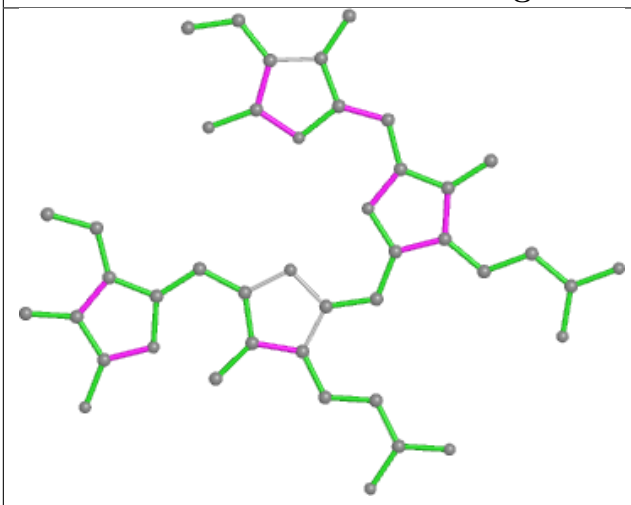


Torsions



Rings

Ligand PUB eD 203



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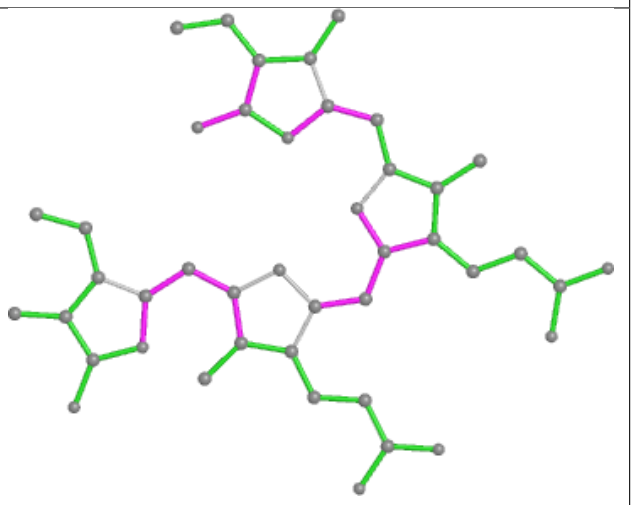

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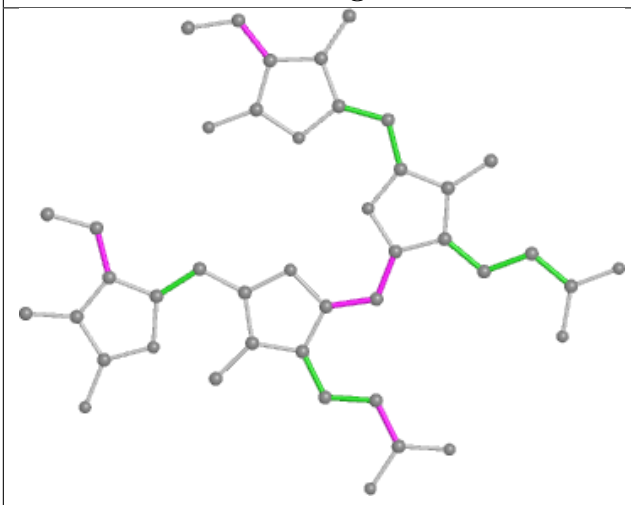

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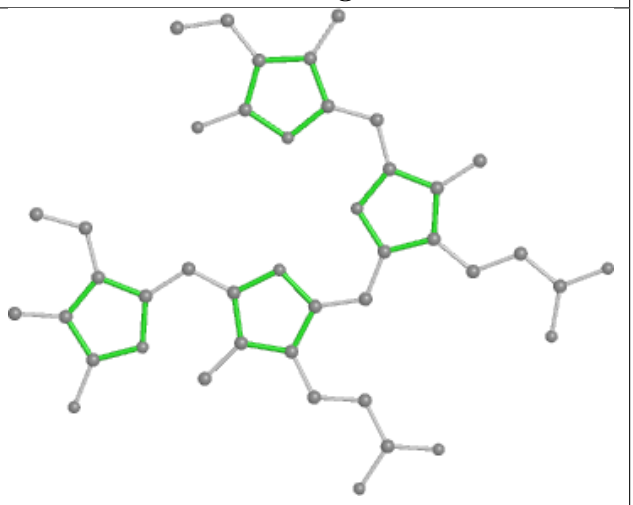
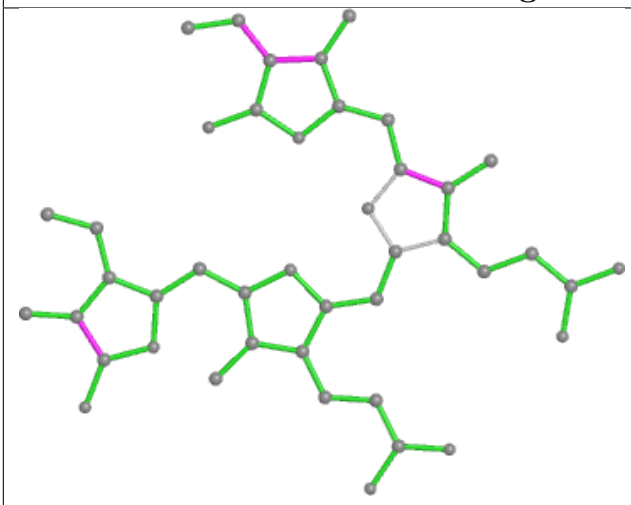


Rings

Ligand PEB q5 202



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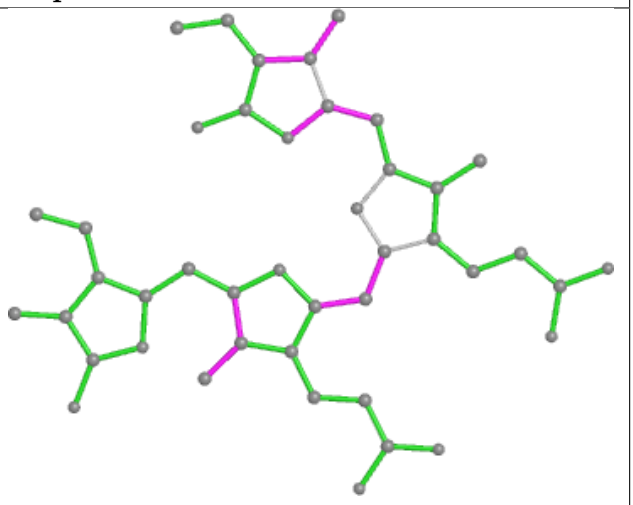

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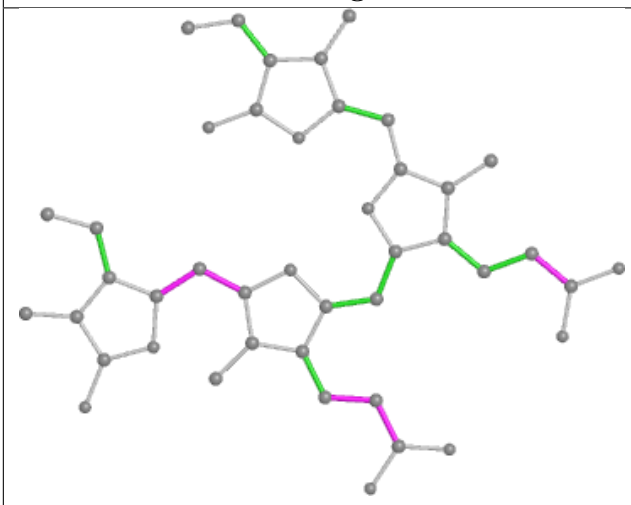

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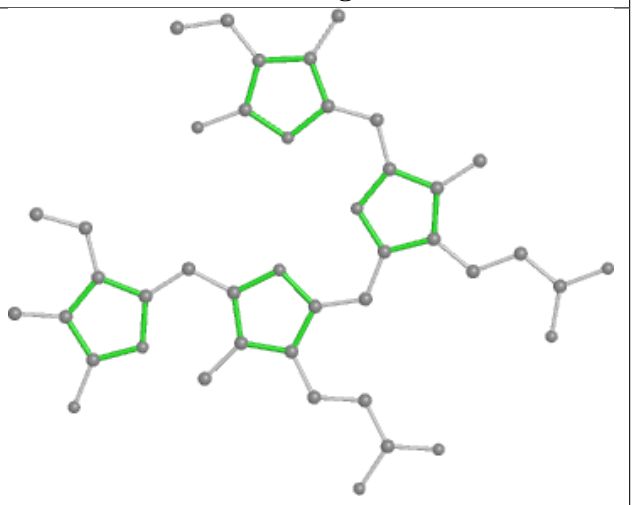
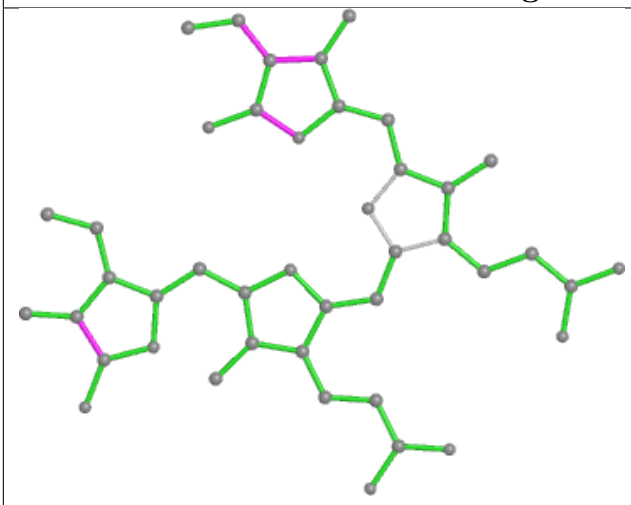


Rings

Ligand PEB s5 201



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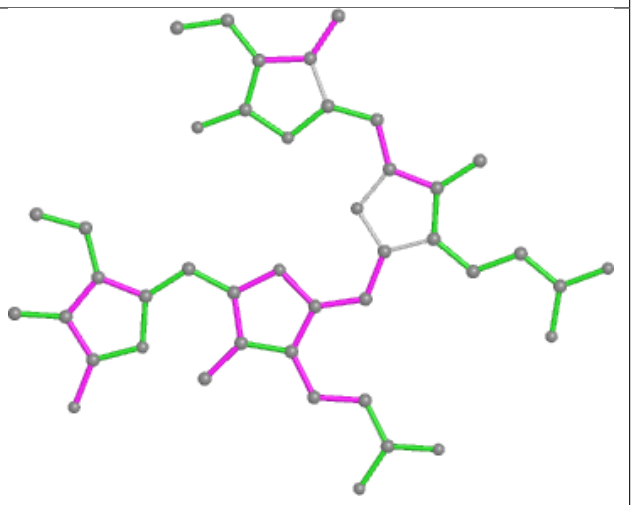

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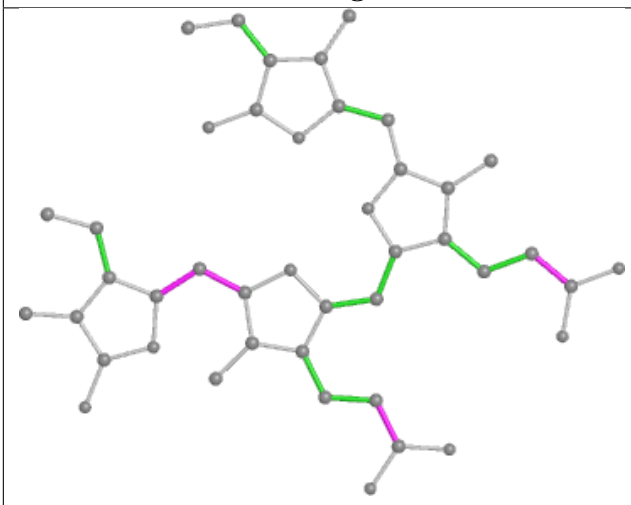

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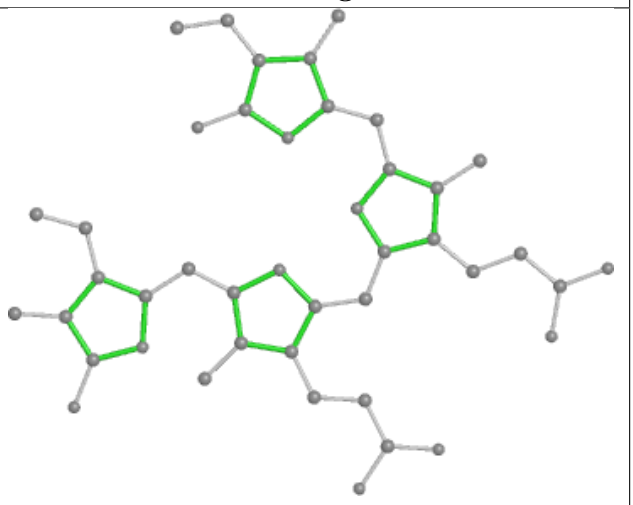
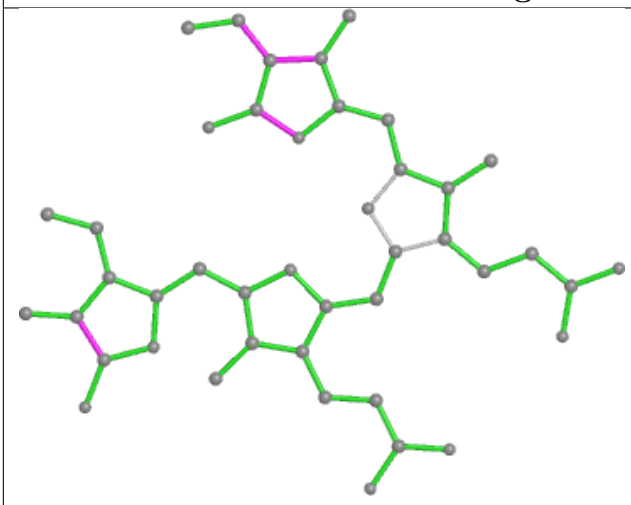


Rings

Ligand PEB dO 201



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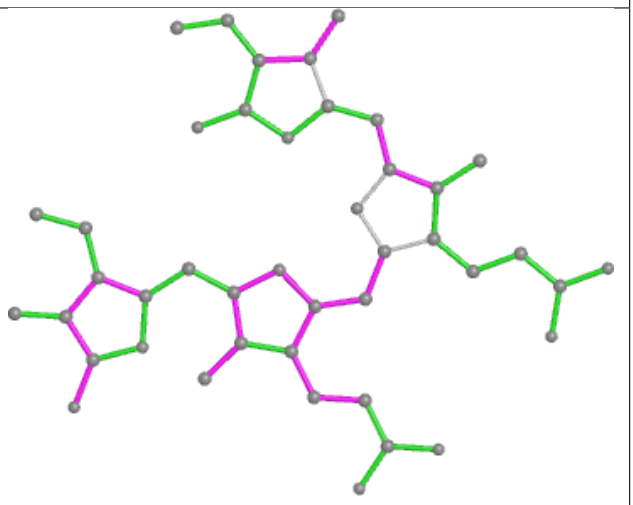

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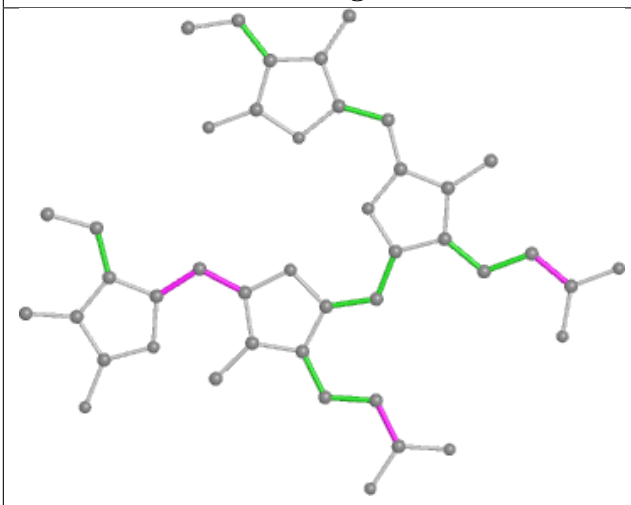

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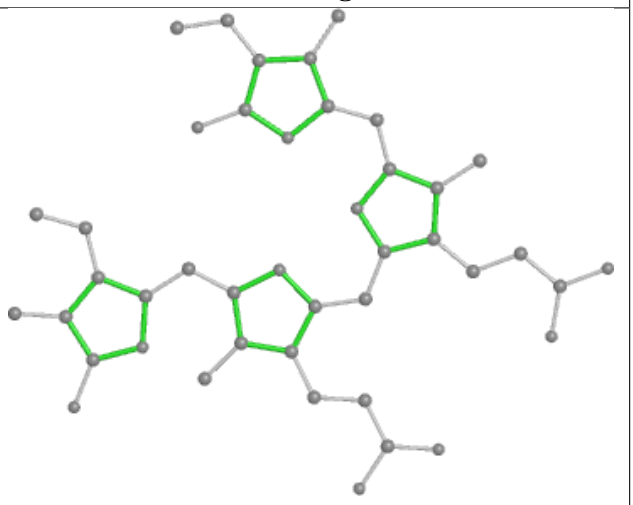
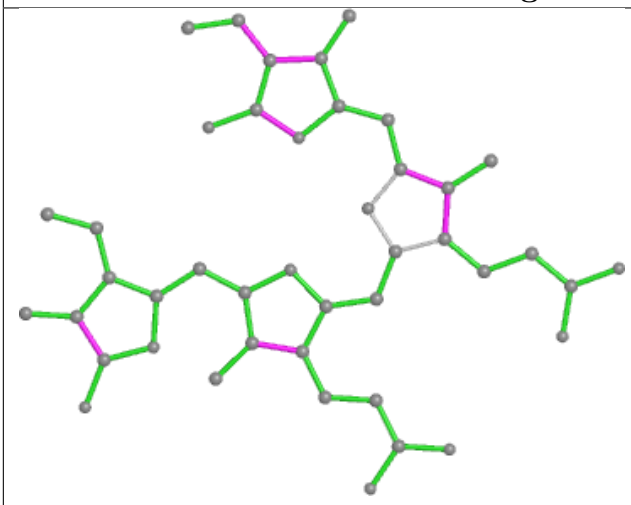


Rings

Ligand PEB z5 202



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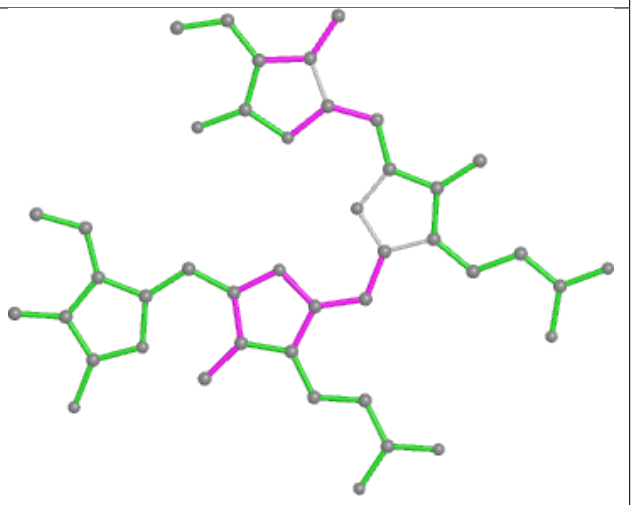

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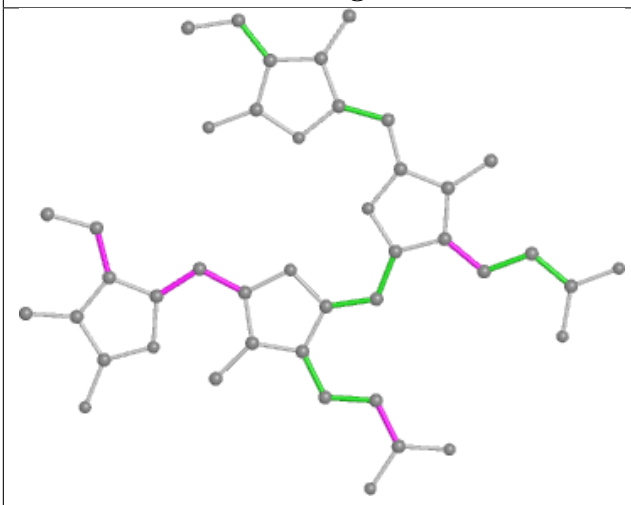

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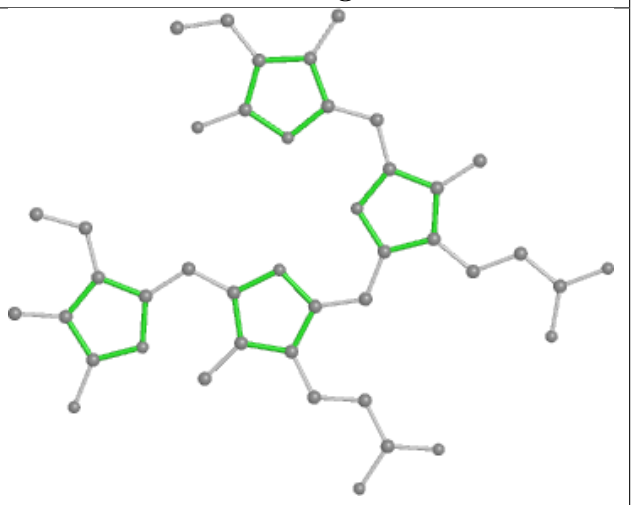

Rings

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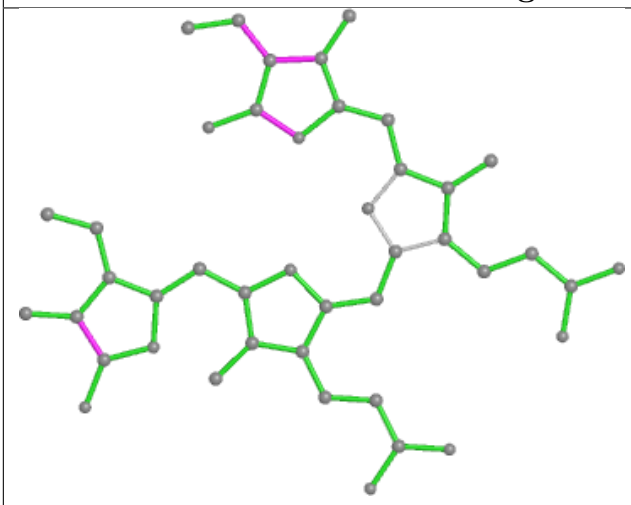

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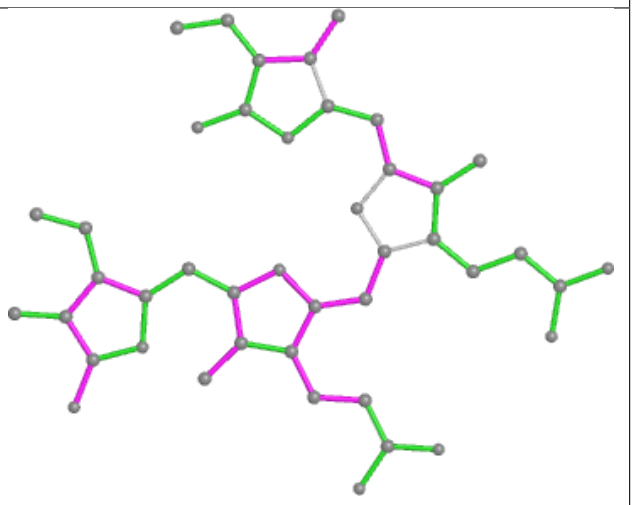

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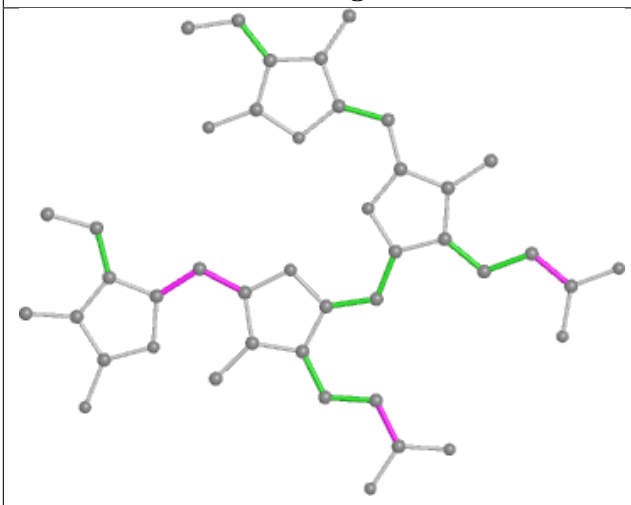

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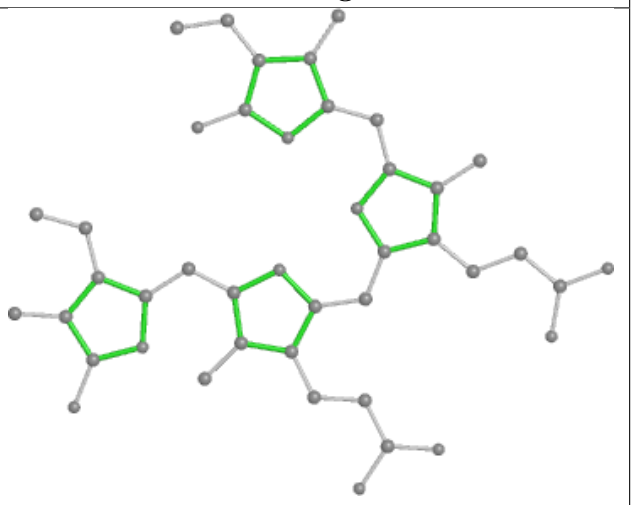
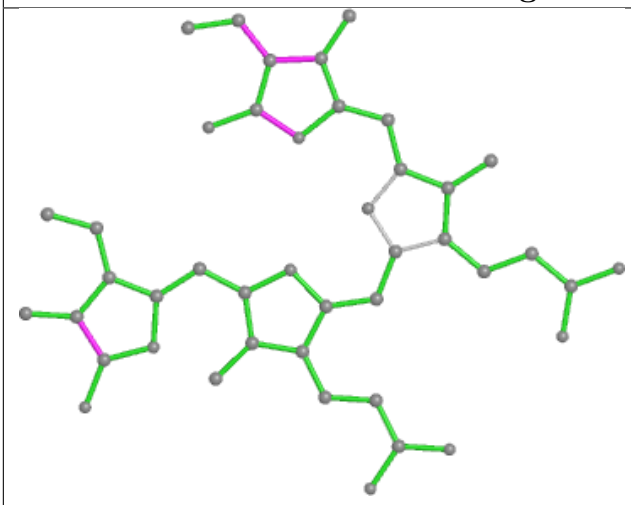


Rings

Ligand PEB k2 202



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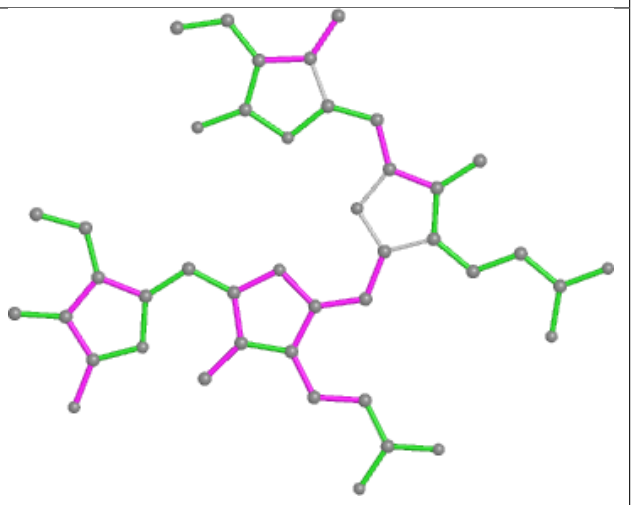

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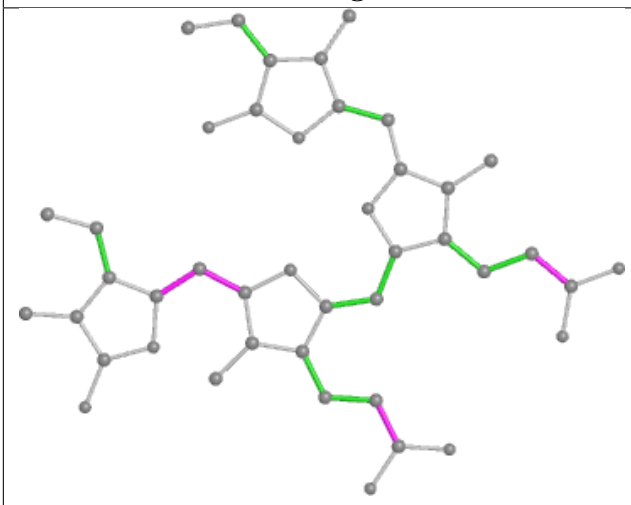

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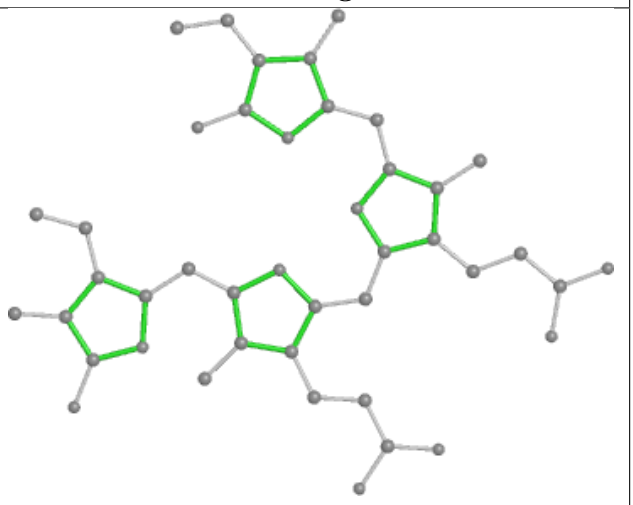
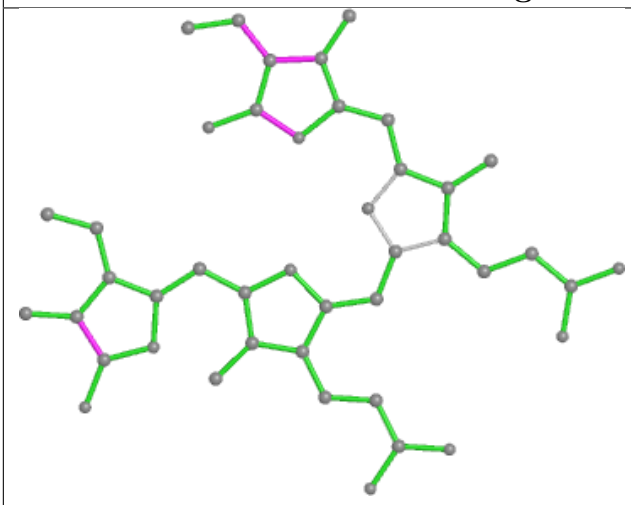


Rings

Ligand PEB dw 402



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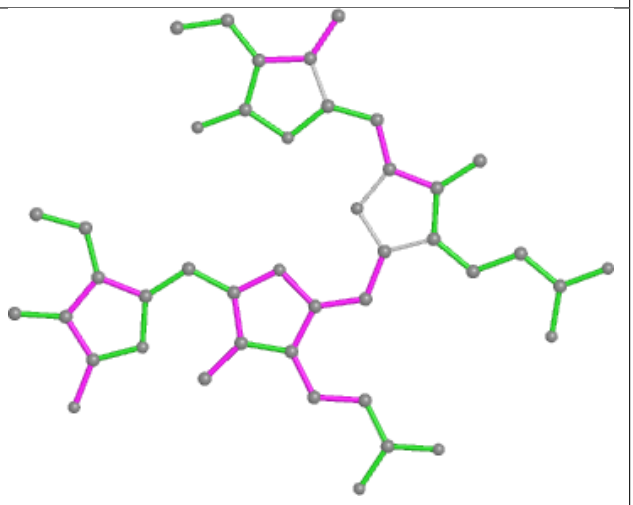

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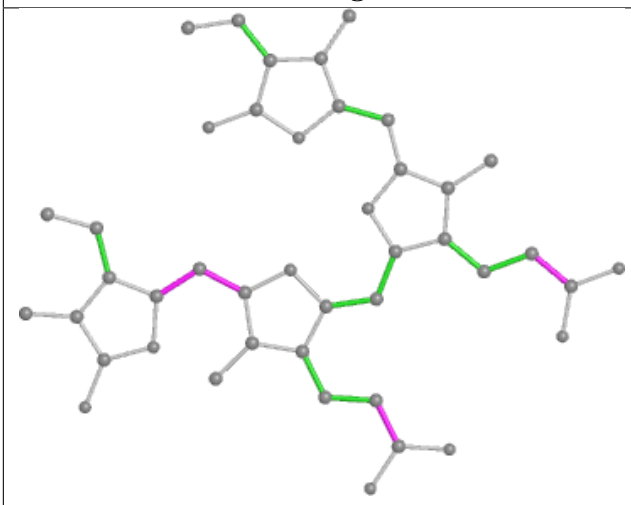

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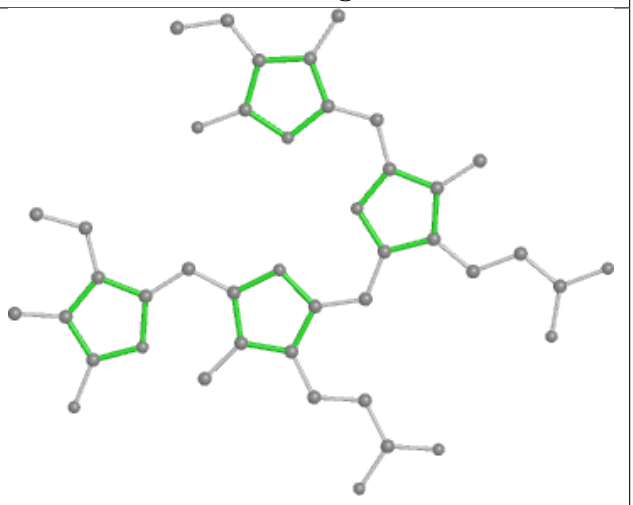
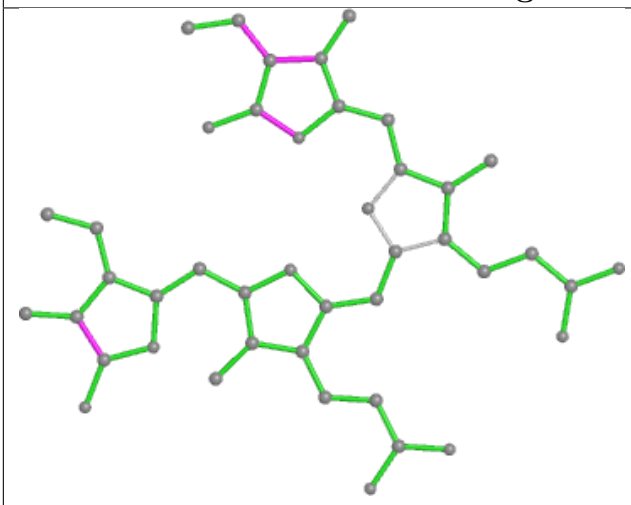


Rings

Ligand PEB cO 201



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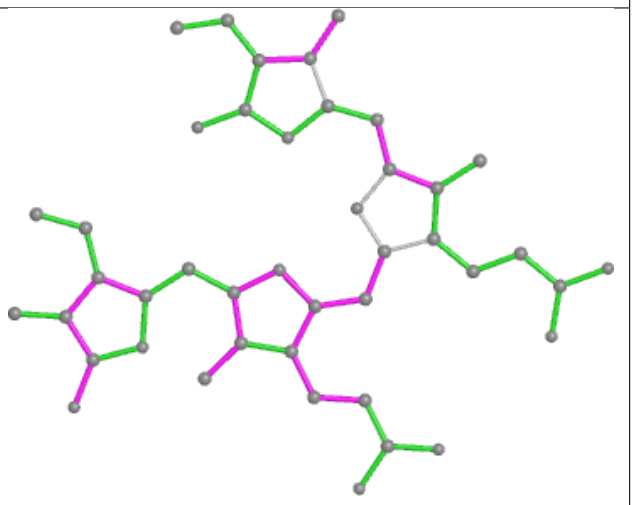

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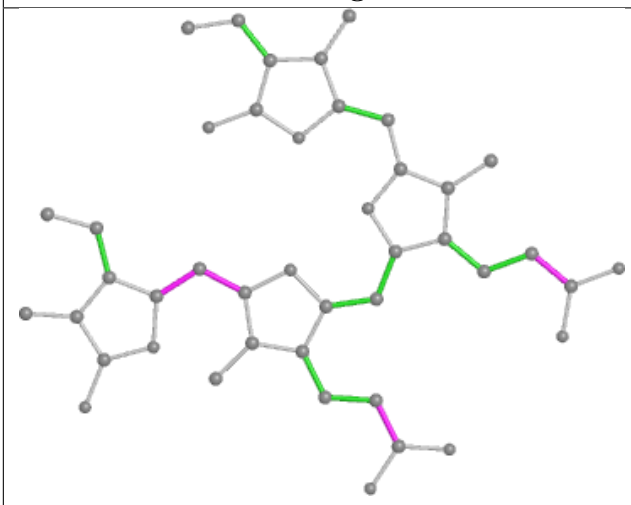

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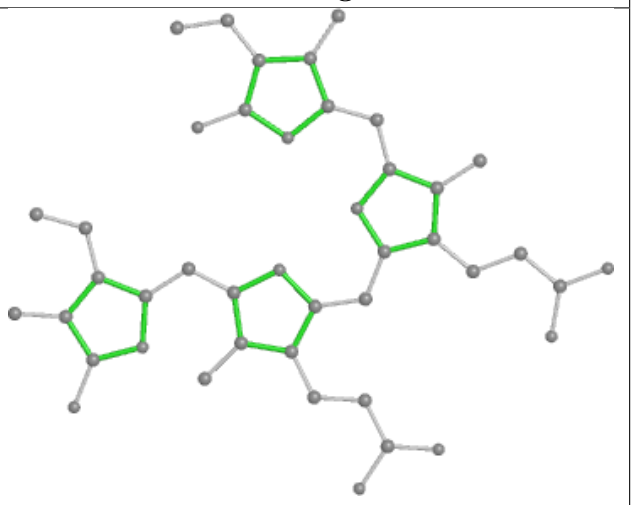
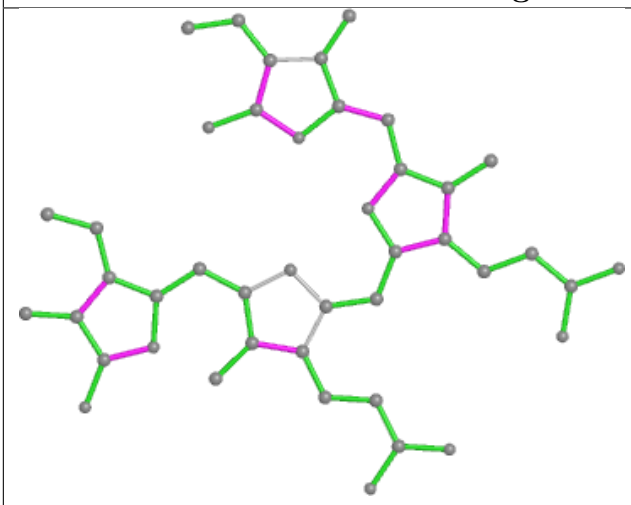


Rings

Ligand PUB hY 405



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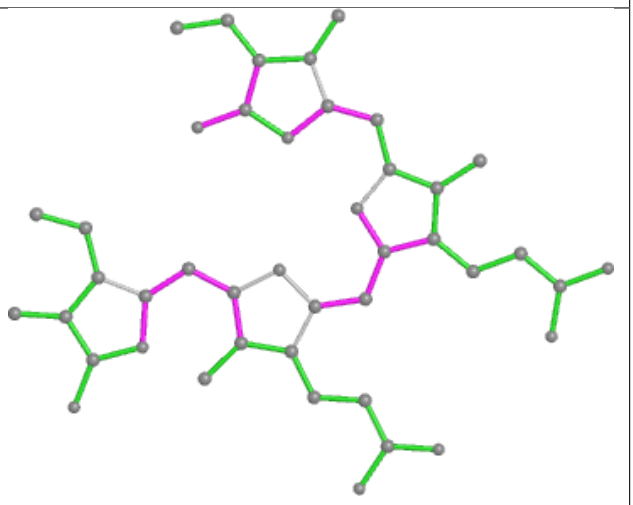

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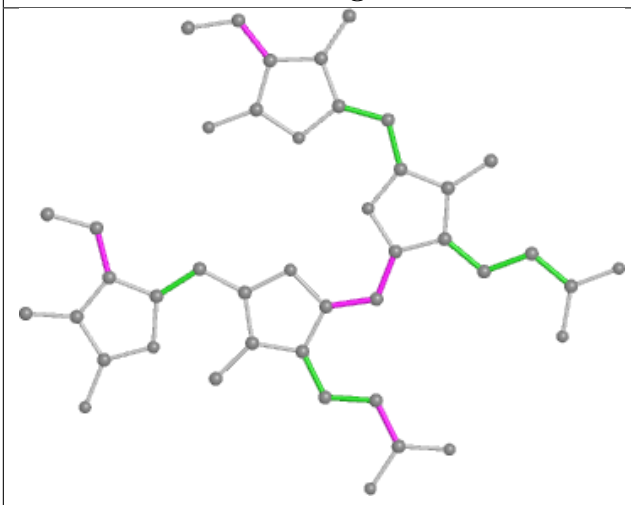

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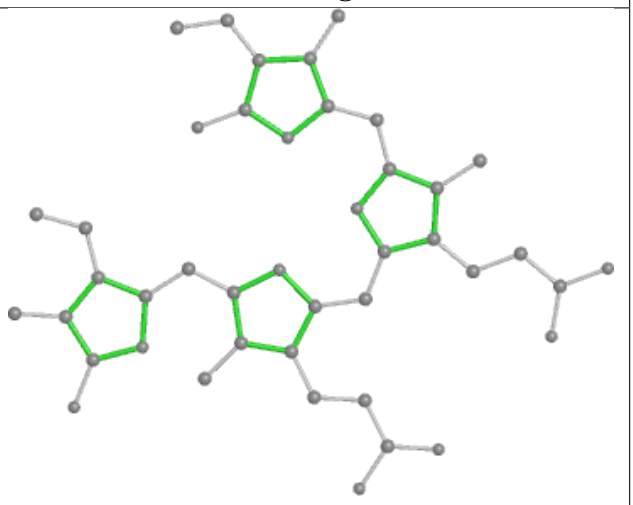
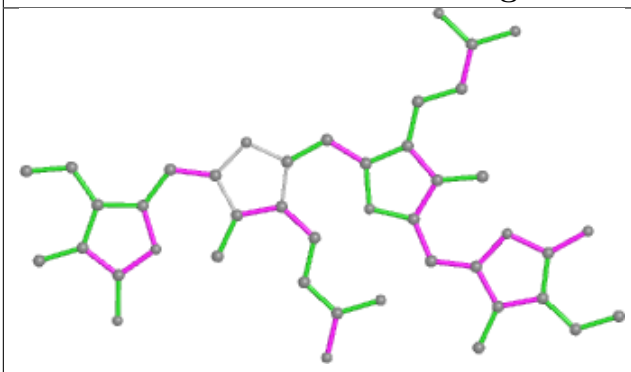


Rings

Ligand CYC M1 1001



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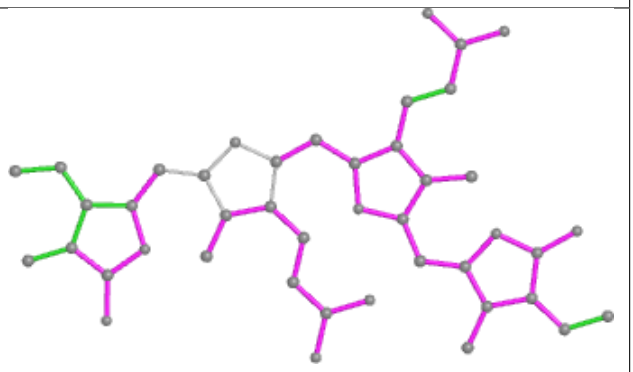

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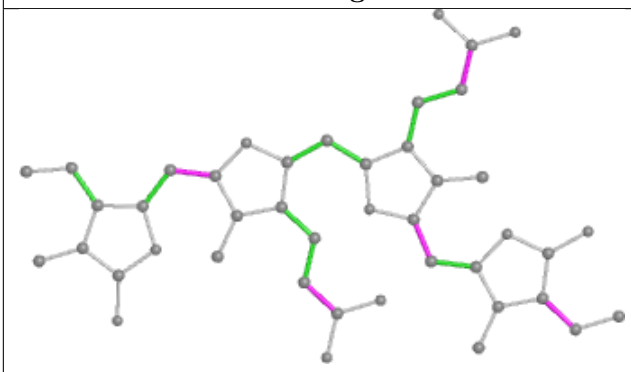

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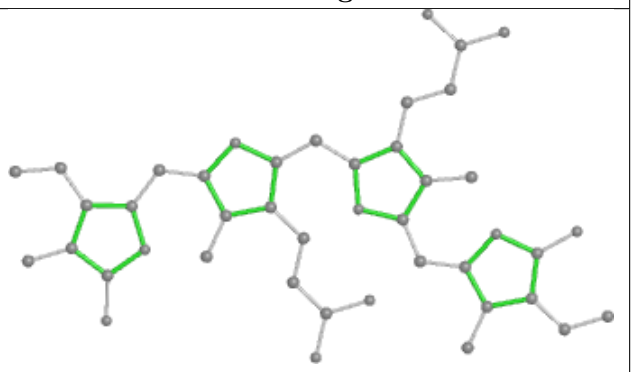
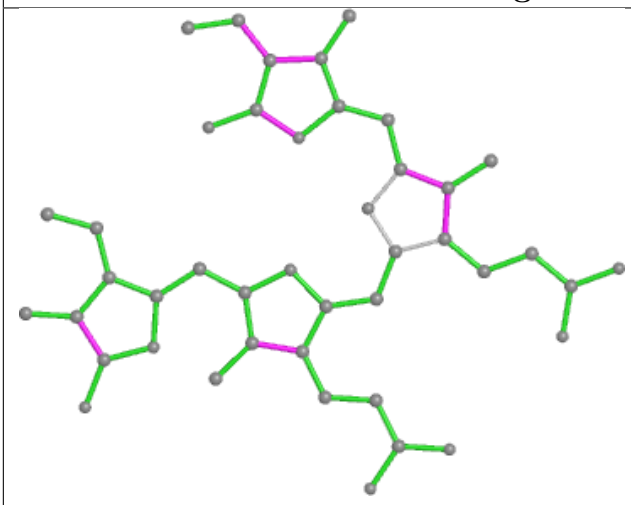


Rings

Ligand PEB hN 202



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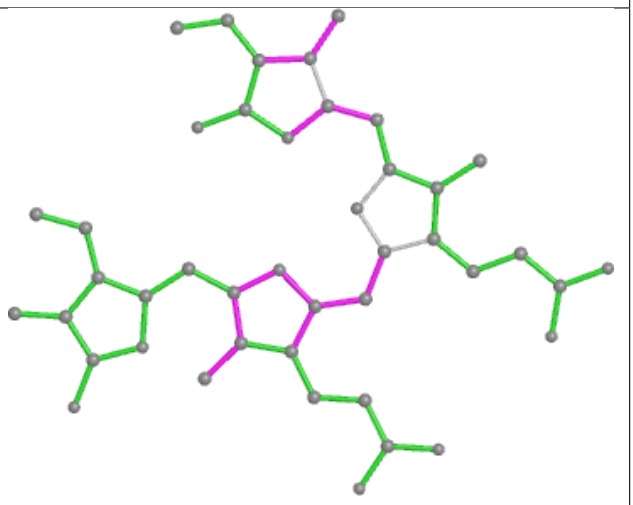
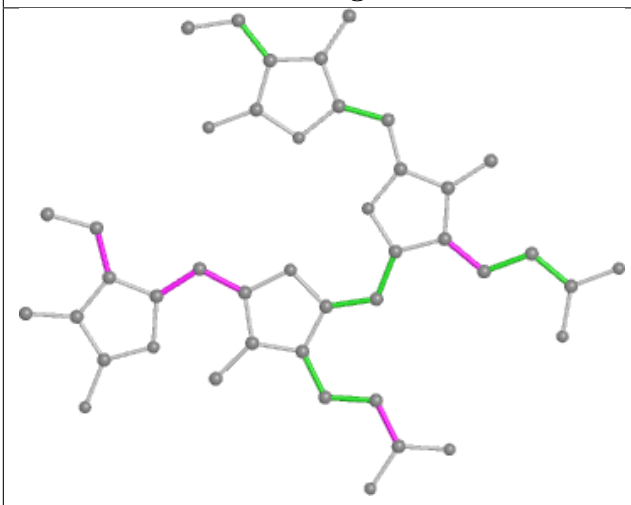


Bond angles



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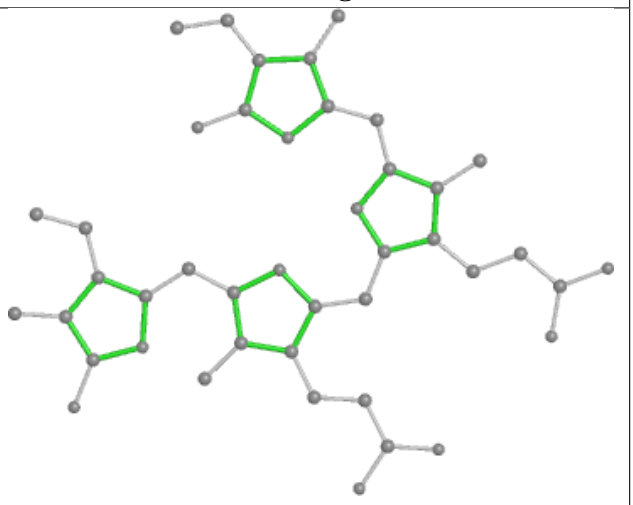
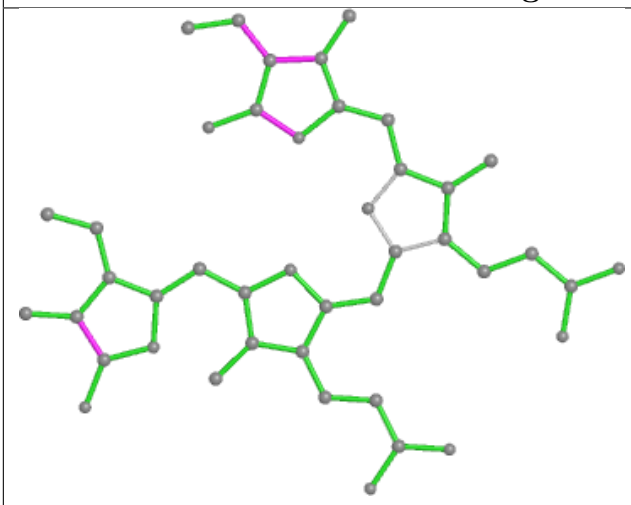


Rings

Ligand PEB I4 202



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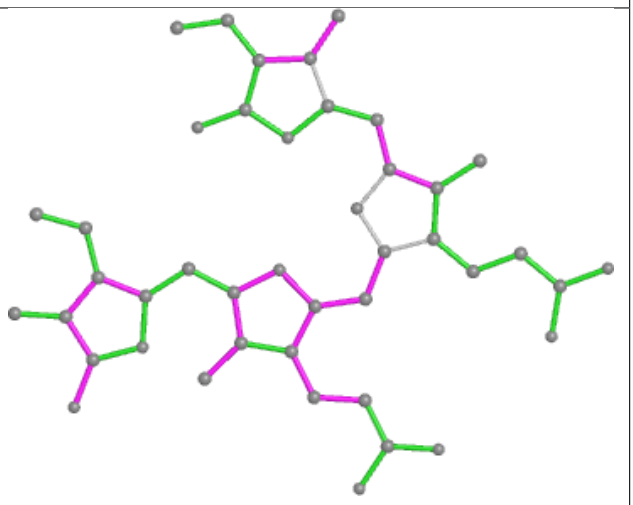
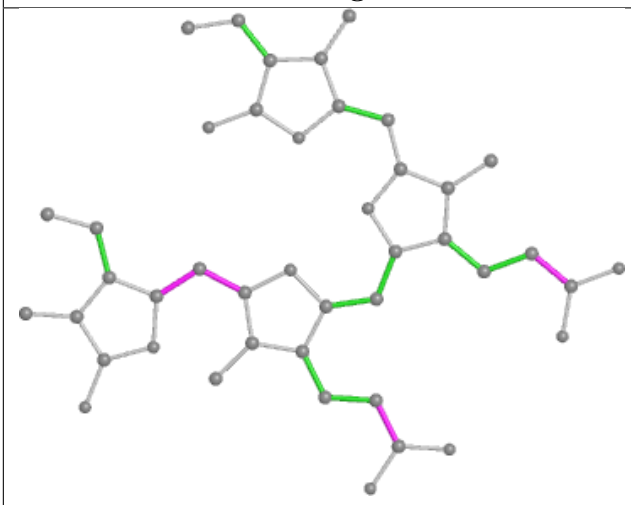


Bond angles



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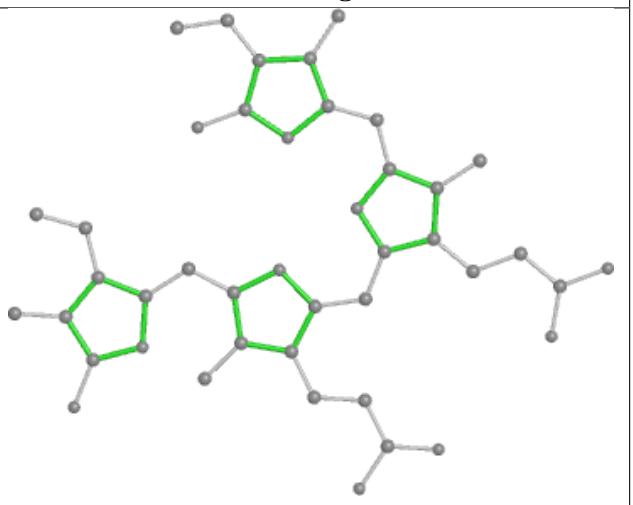
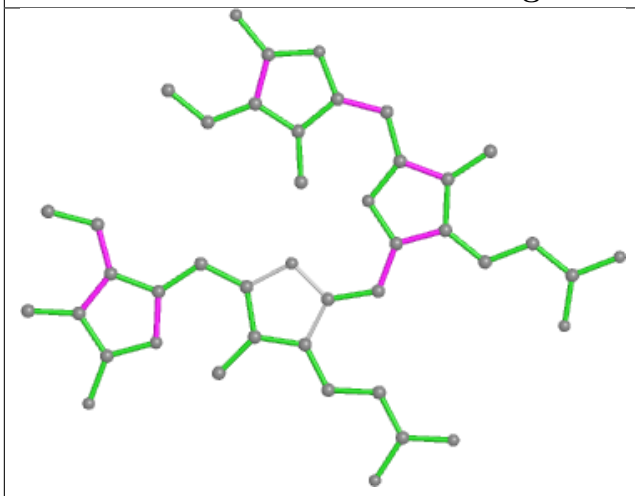


Rings

Ligand PVN lz 403



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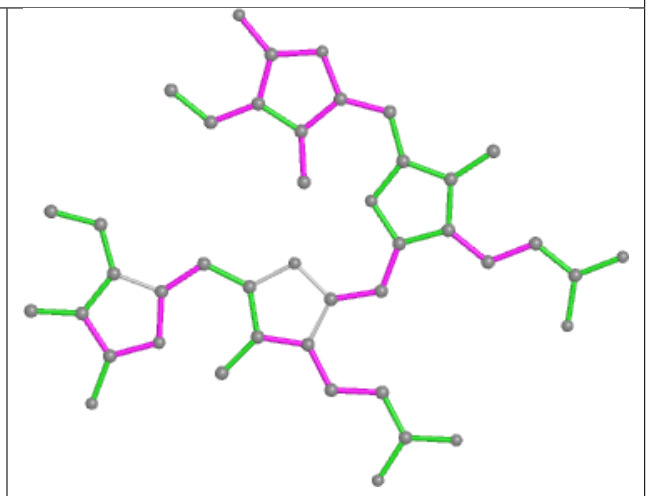

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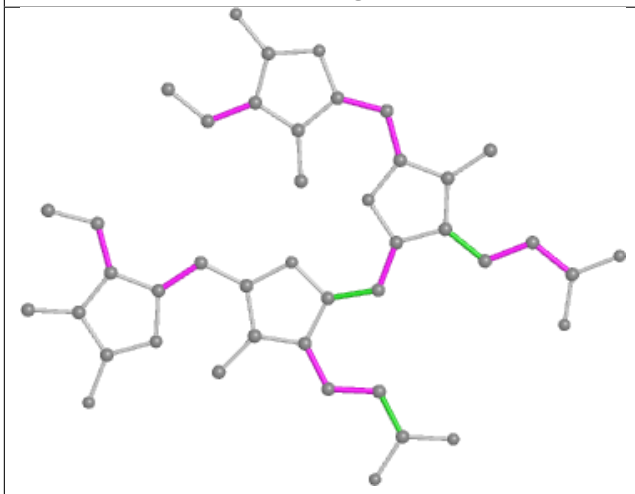
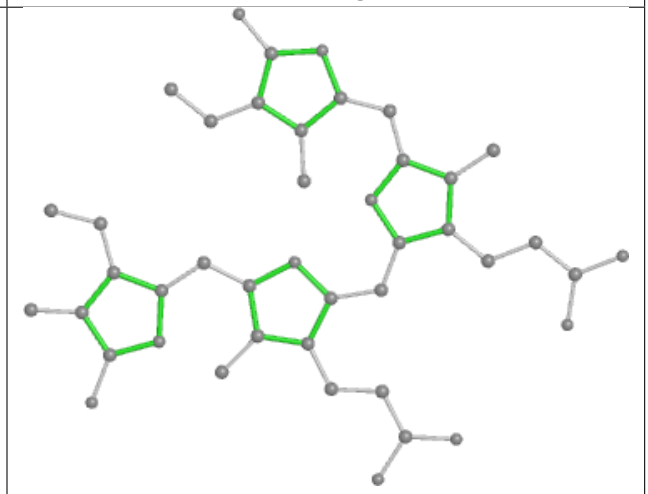


Torsions



Rings

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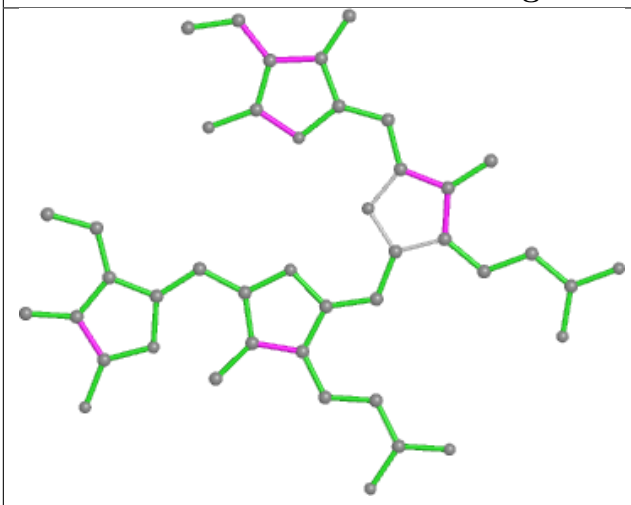

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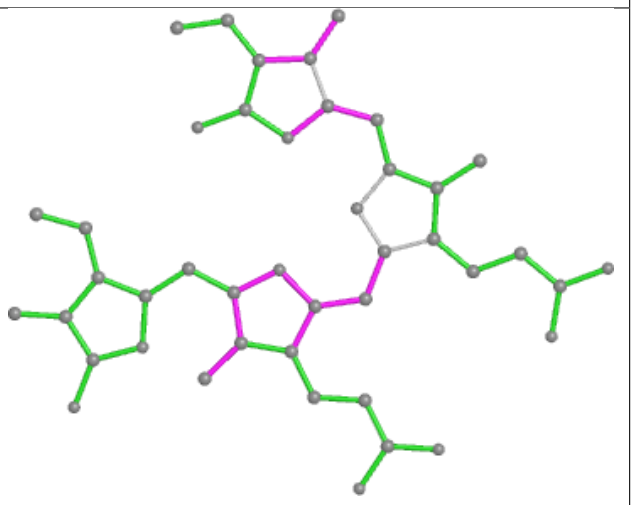

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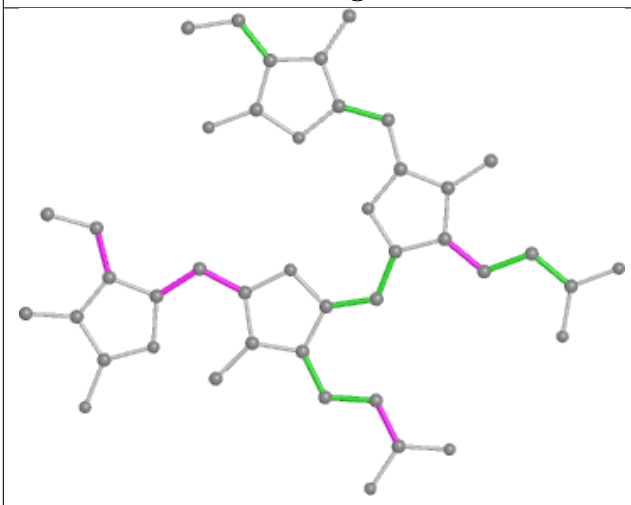

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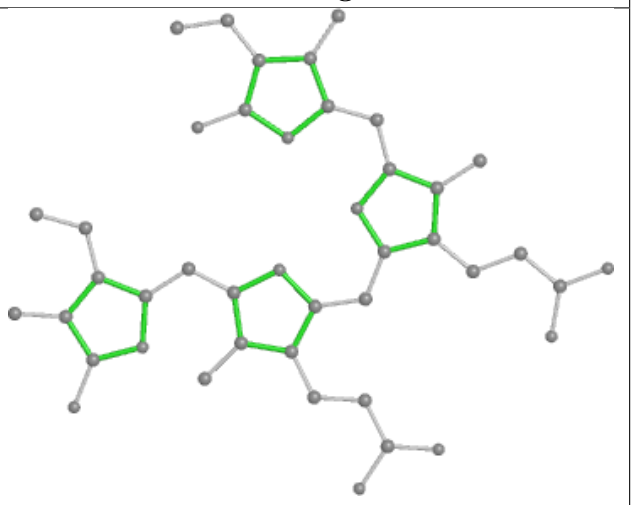

Rings

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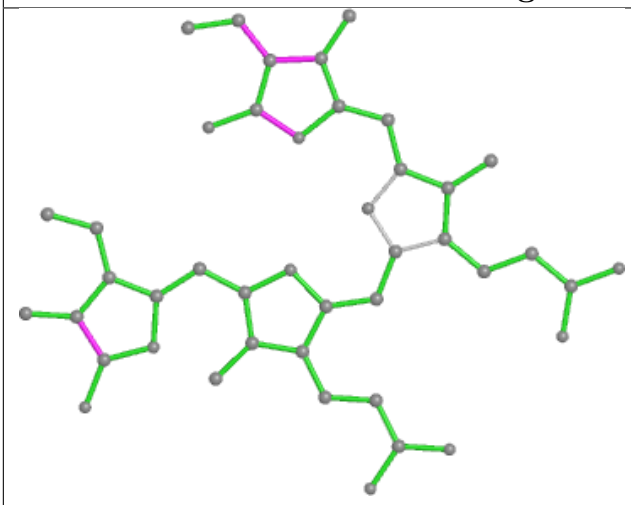

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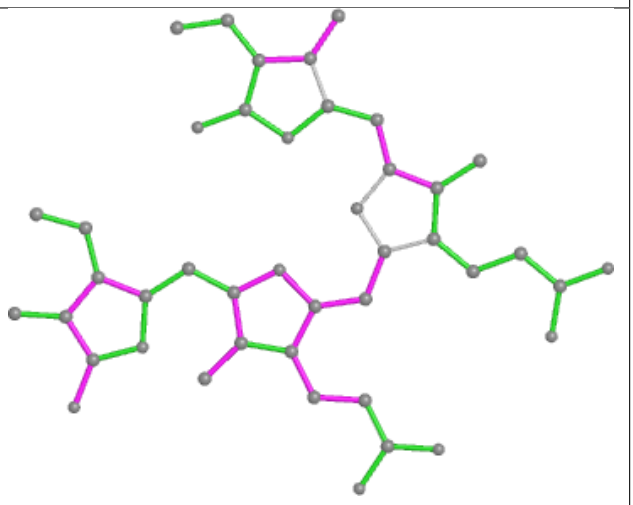

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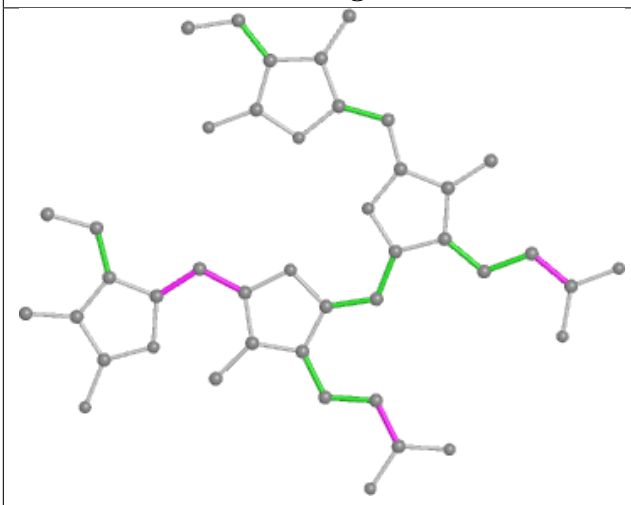

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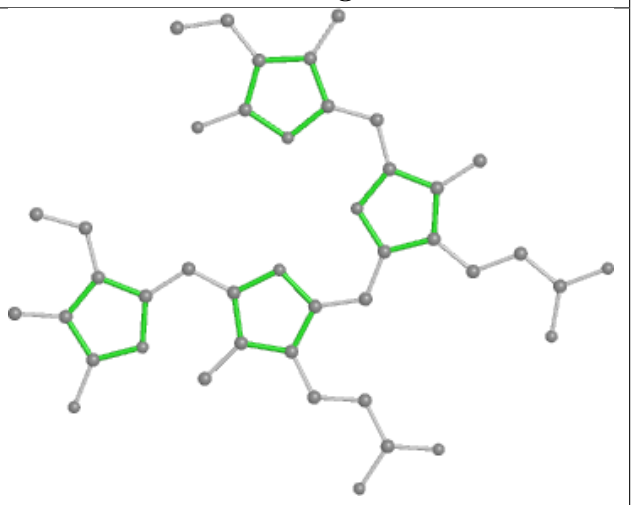

Rings

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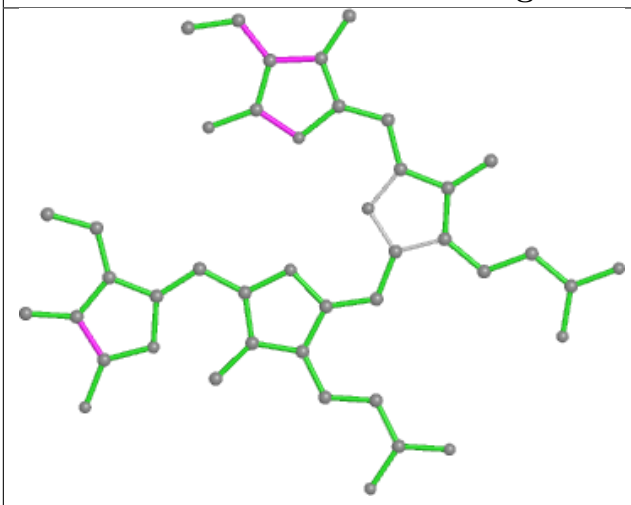

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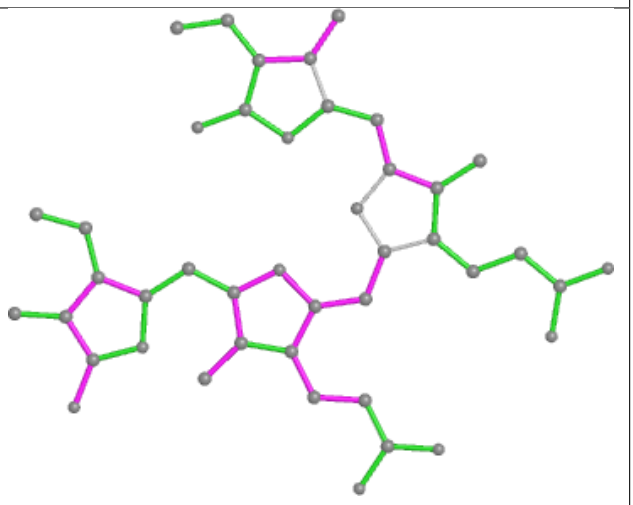

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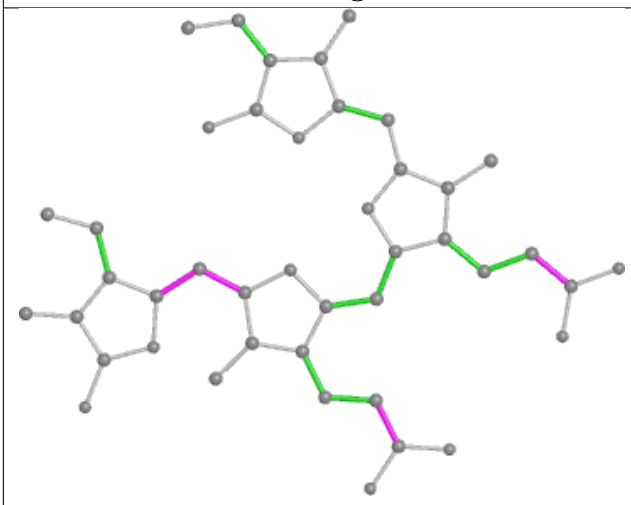

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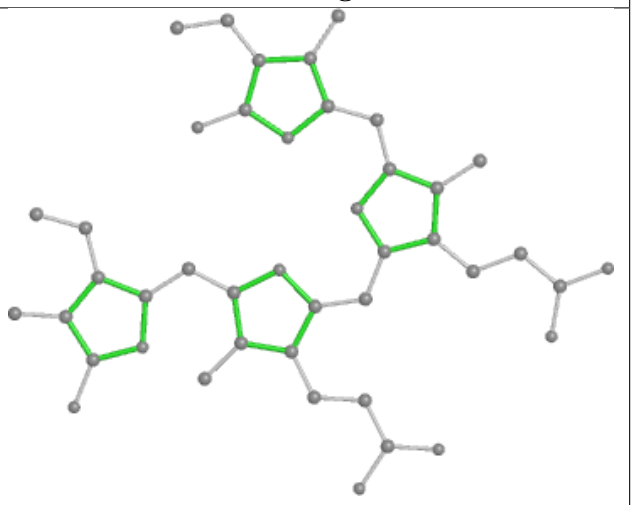

Rings

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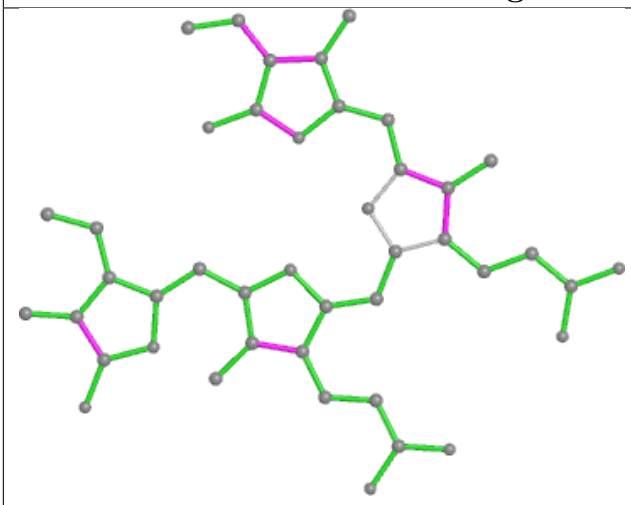

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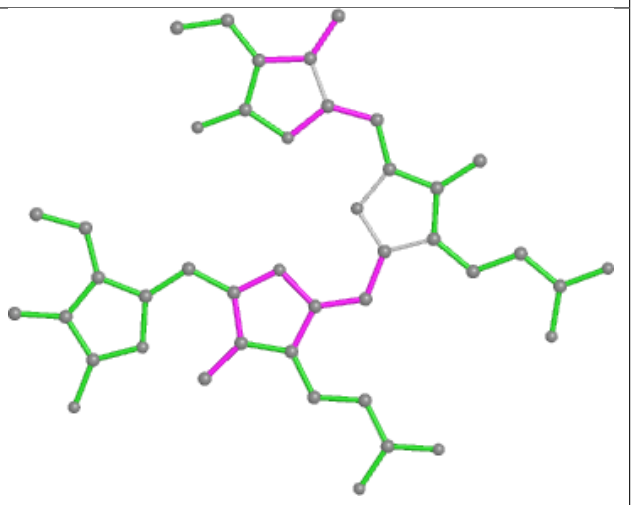

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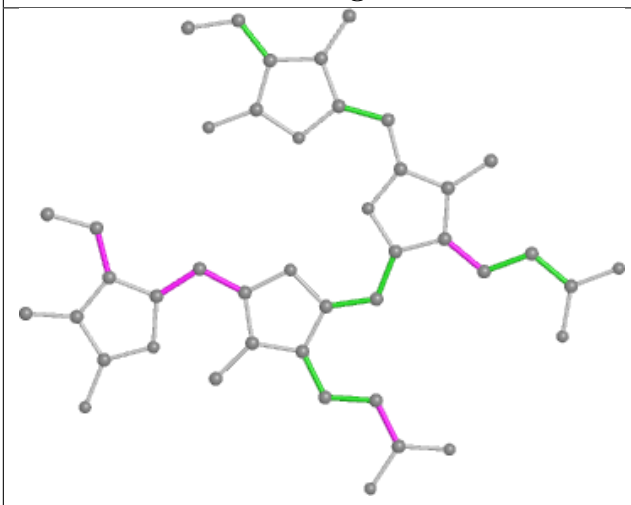

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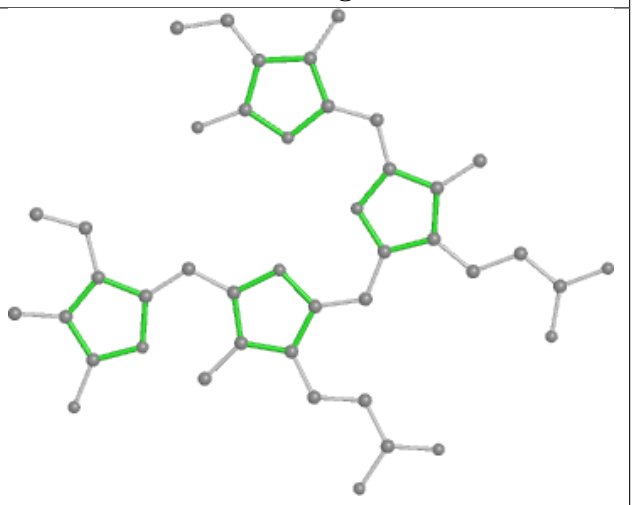

Rings

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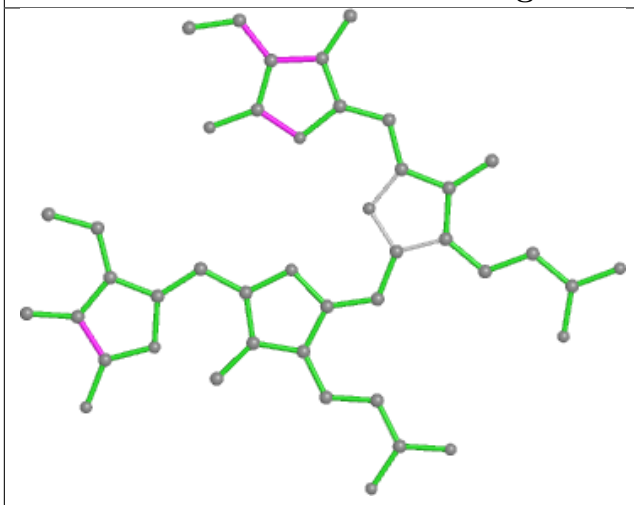

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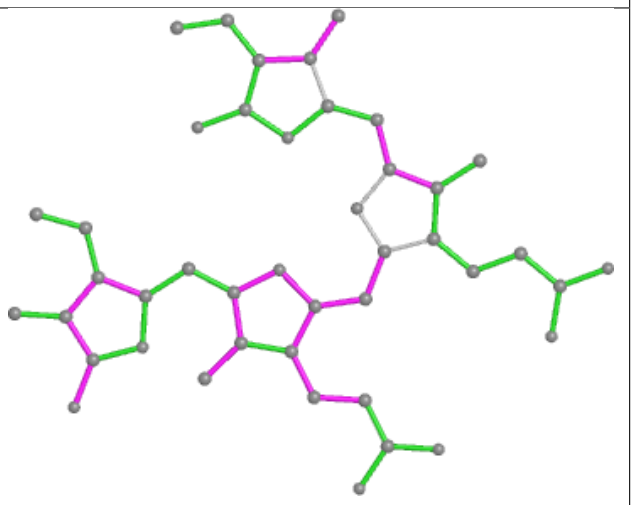

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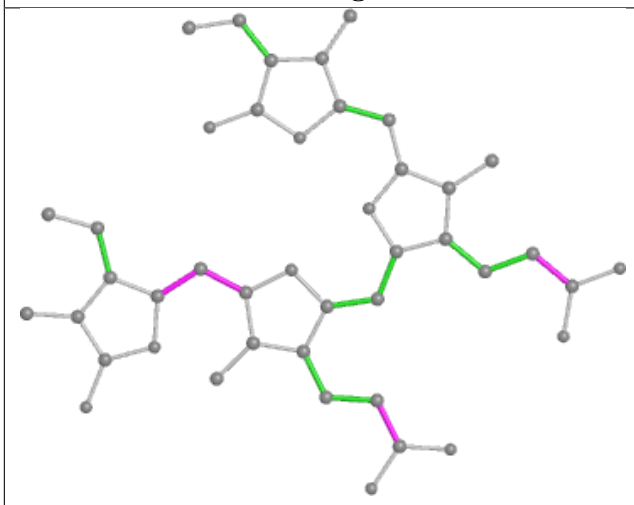

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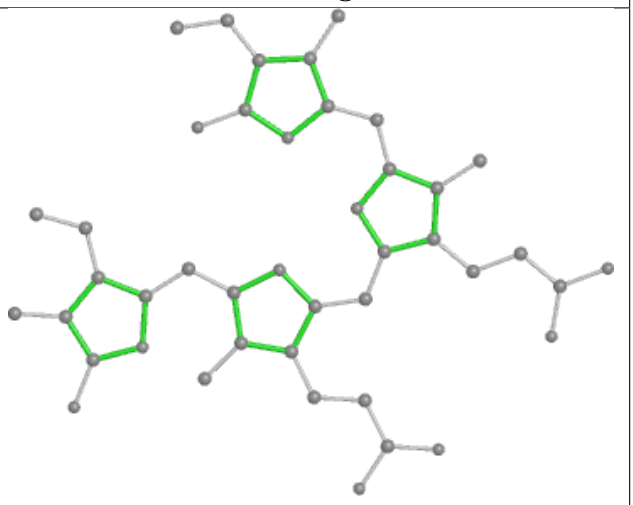

Rings

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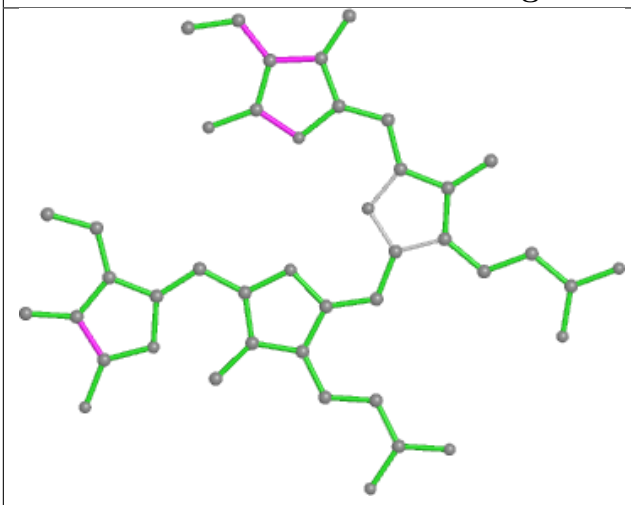

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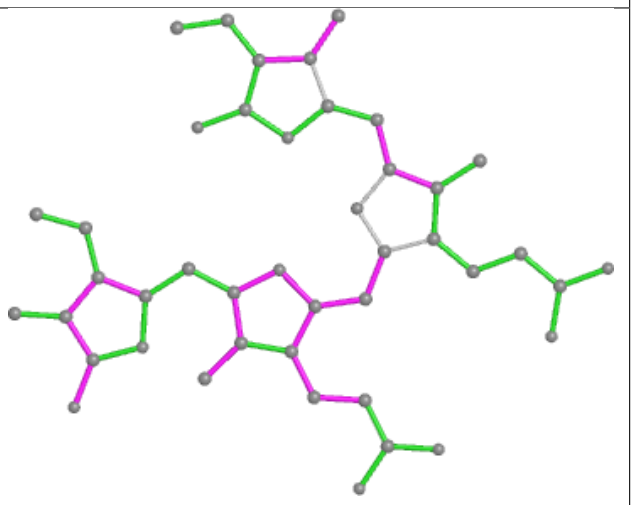

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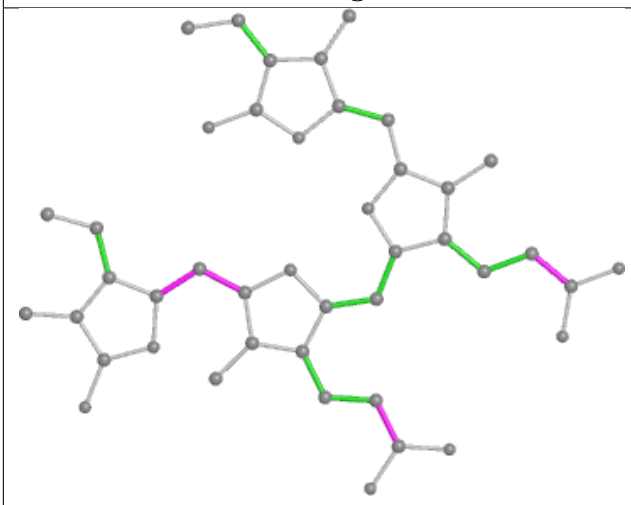

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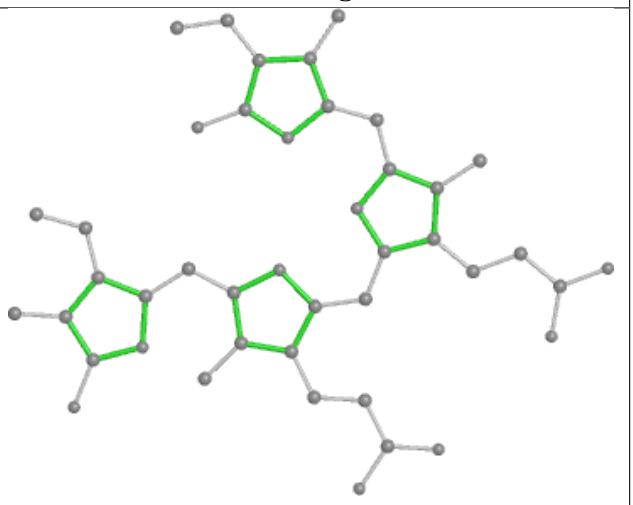

Rings

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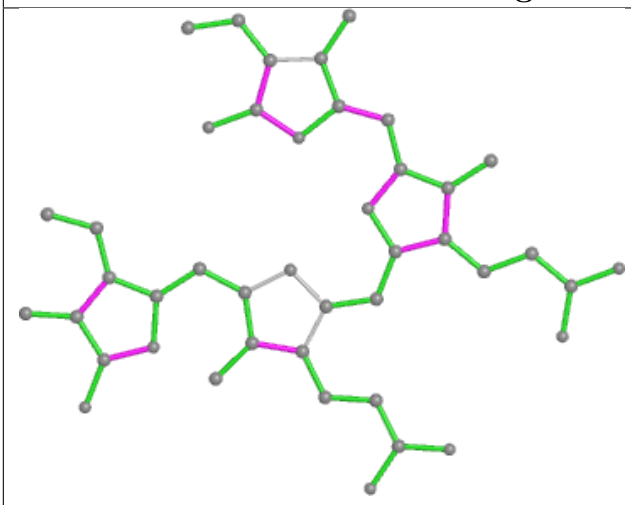

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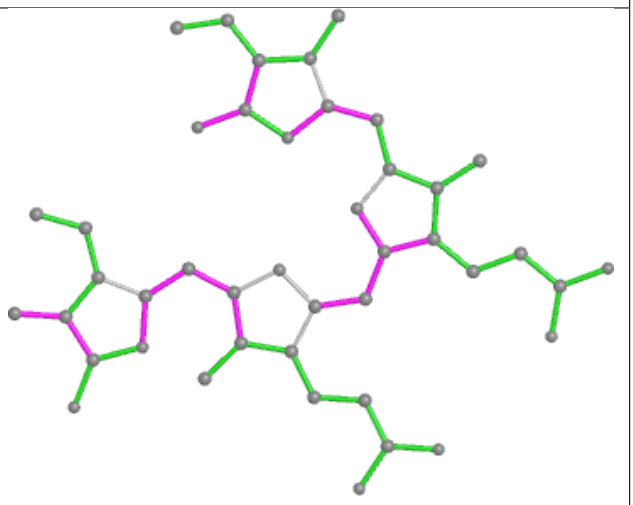

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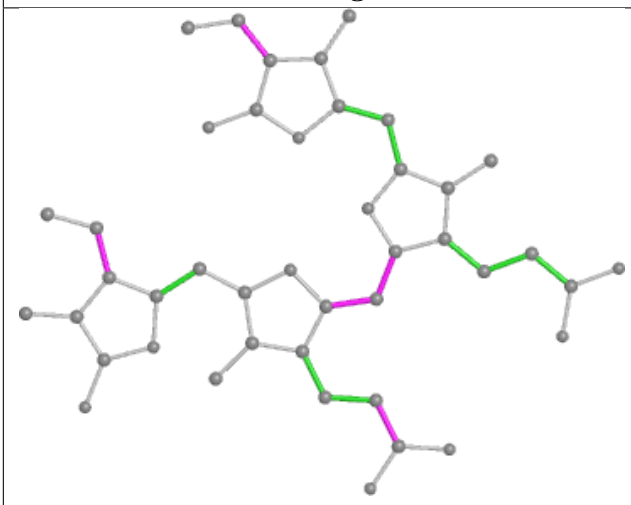

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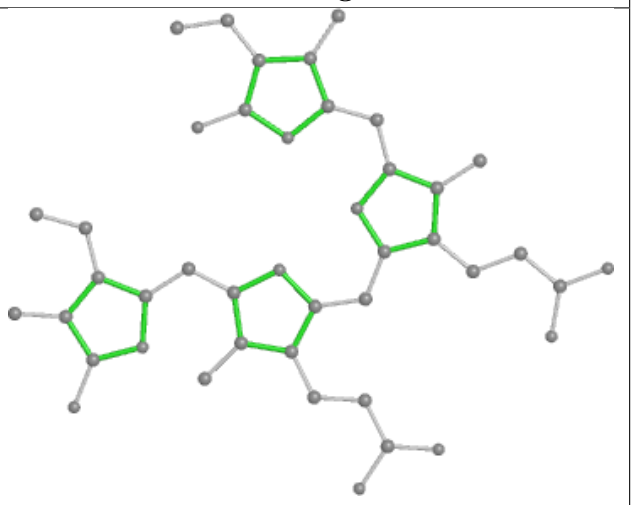

Rings

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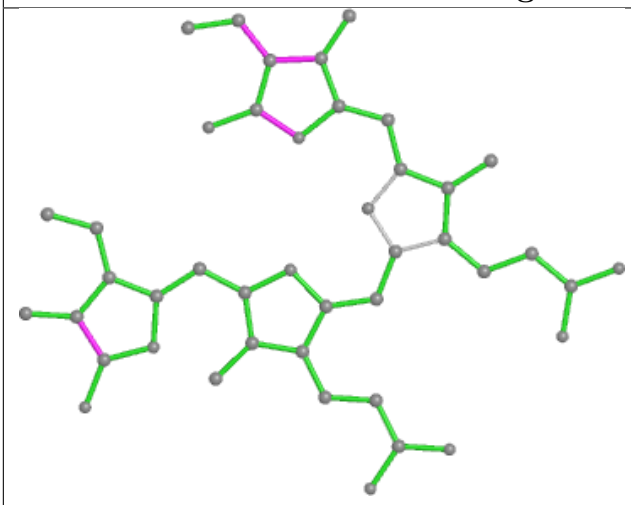

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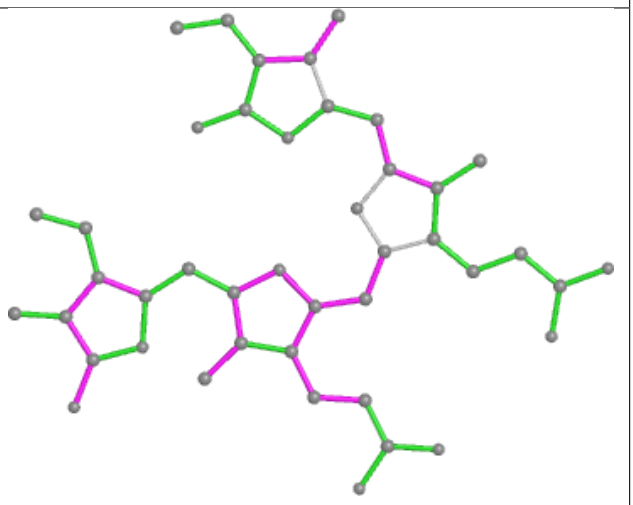

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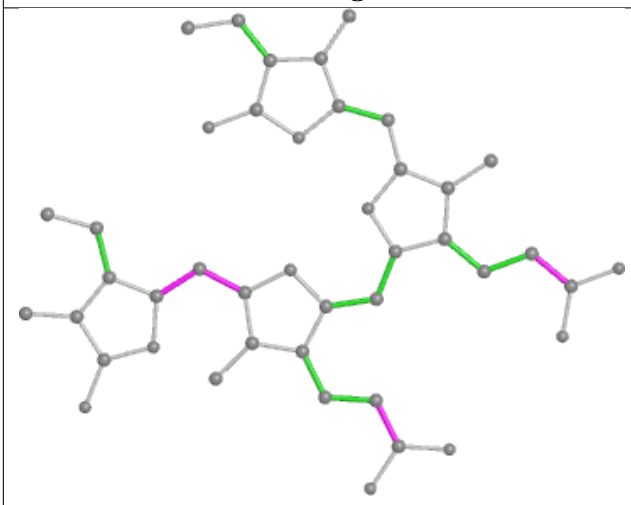

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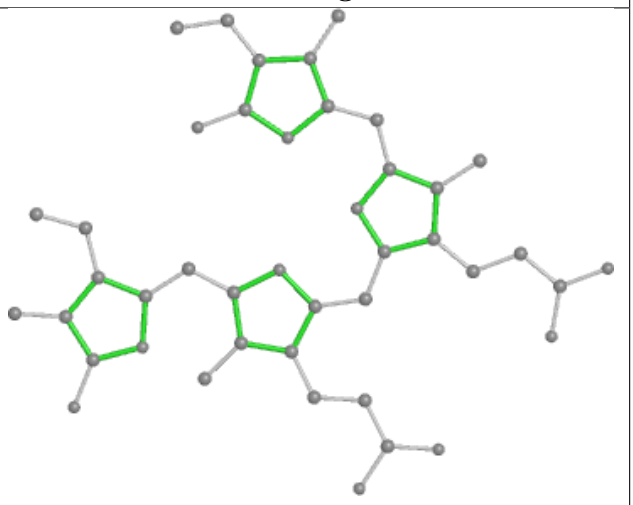

Rings

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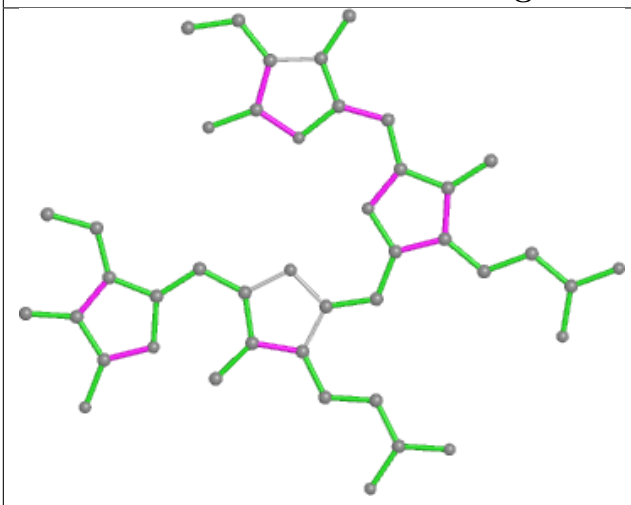

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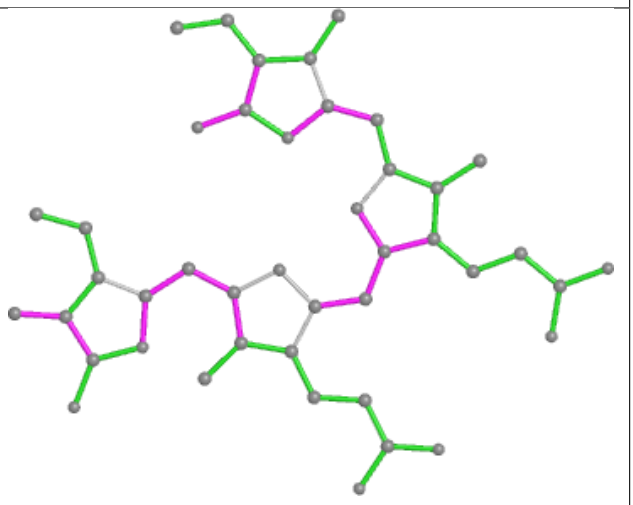

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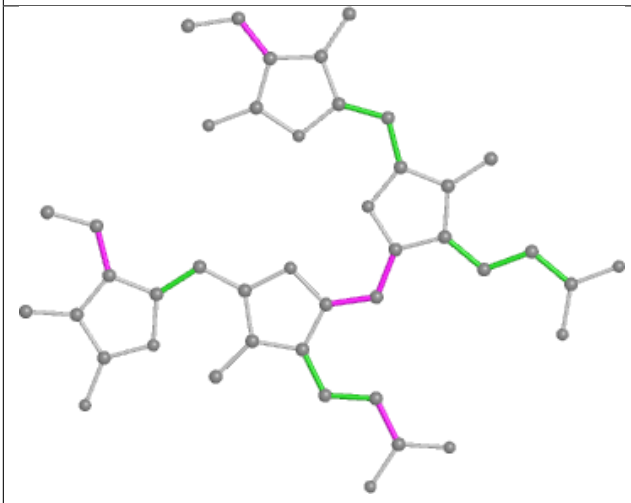

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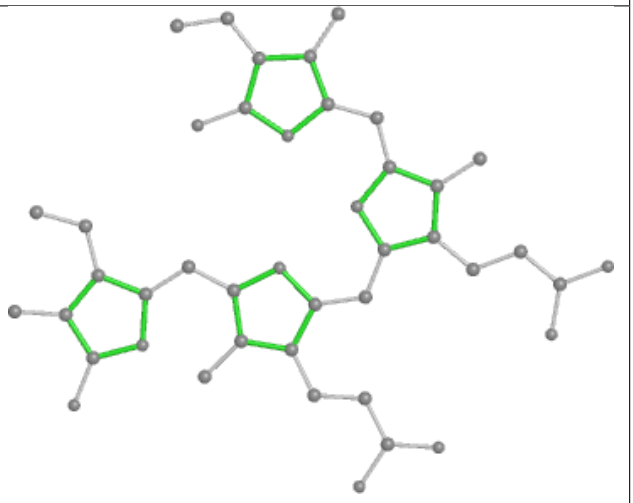

Rings

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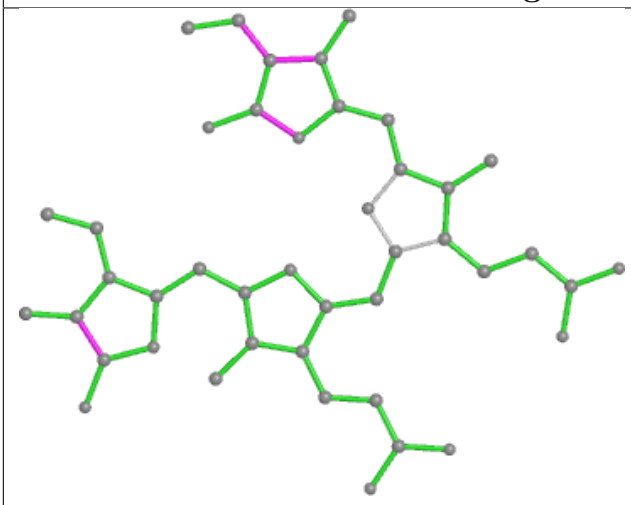

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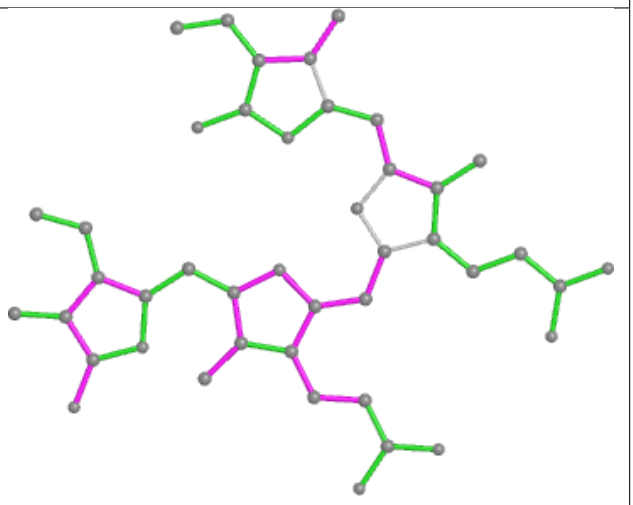

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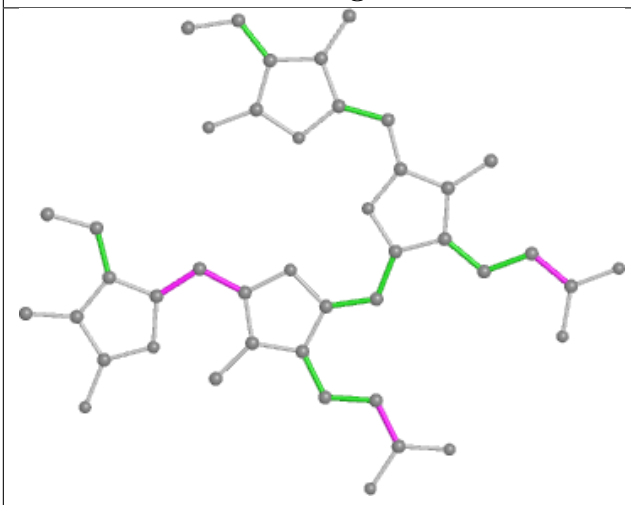

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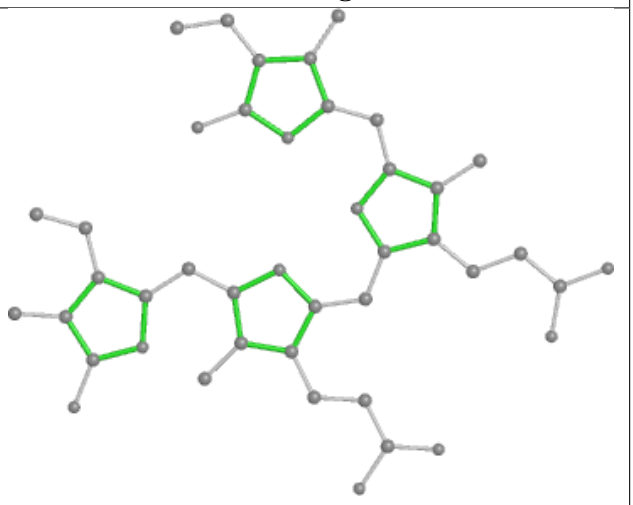
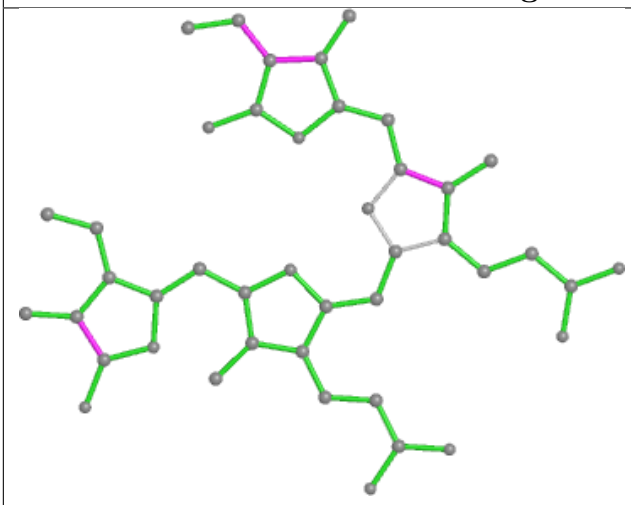


Rings

Ligand PEB c8 301



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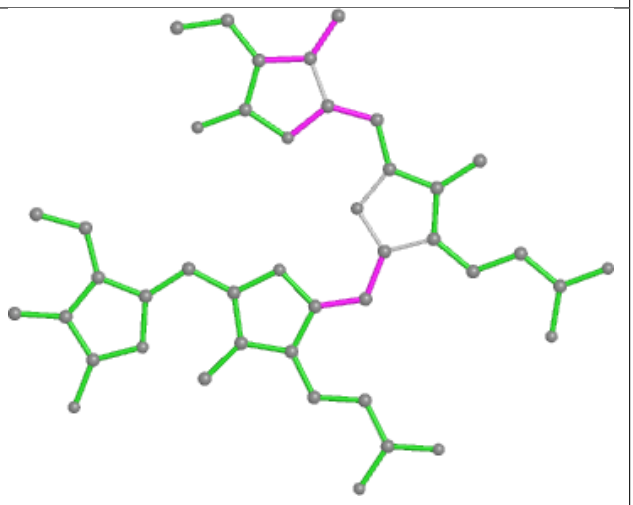

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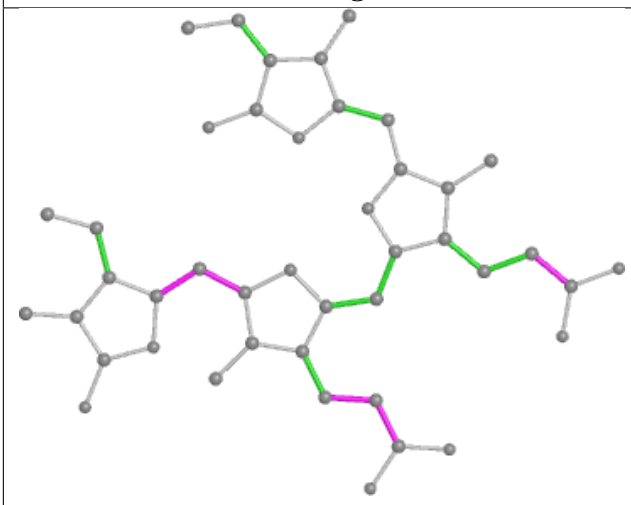

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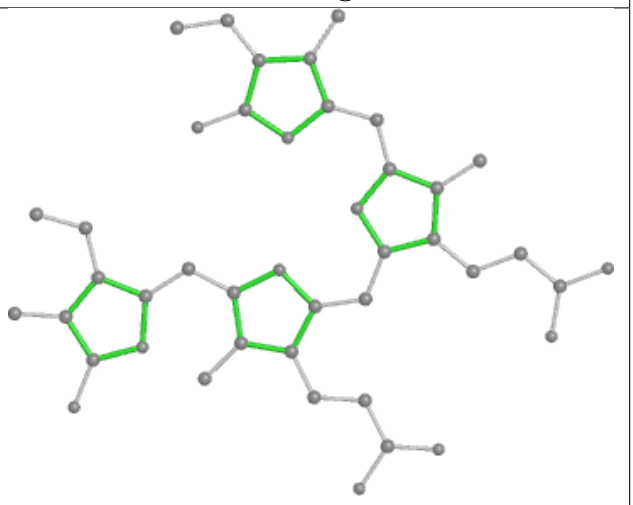
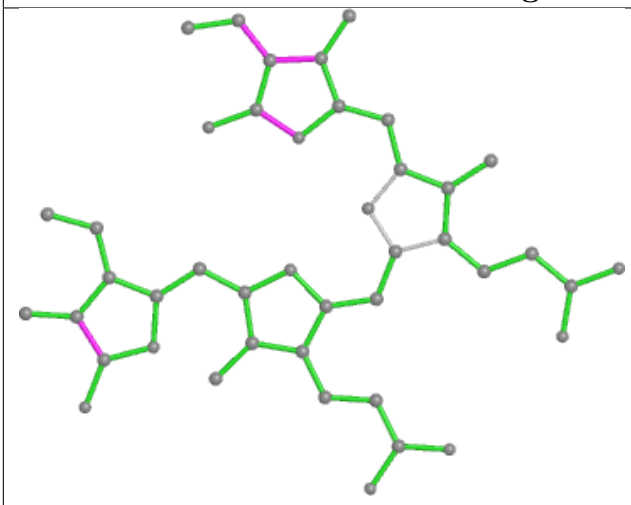


Rings

Ligand PEB ar 201



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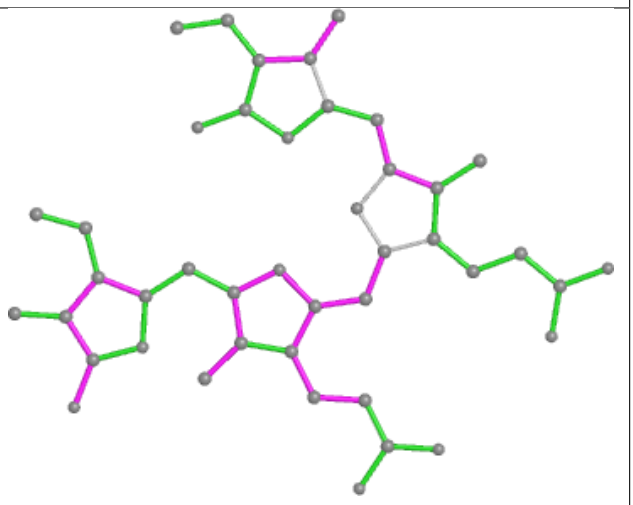

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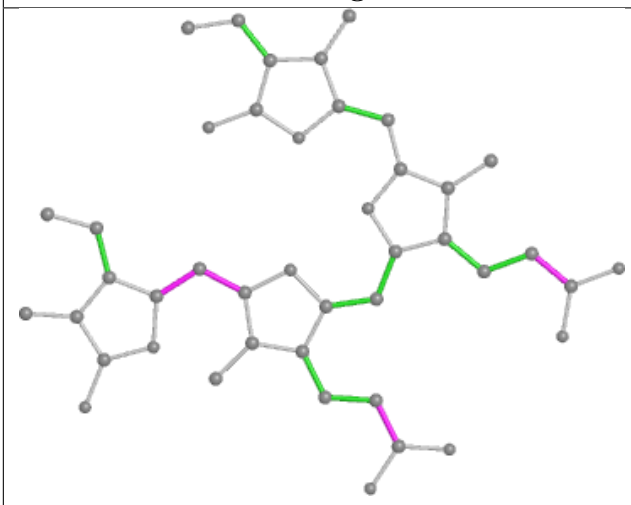

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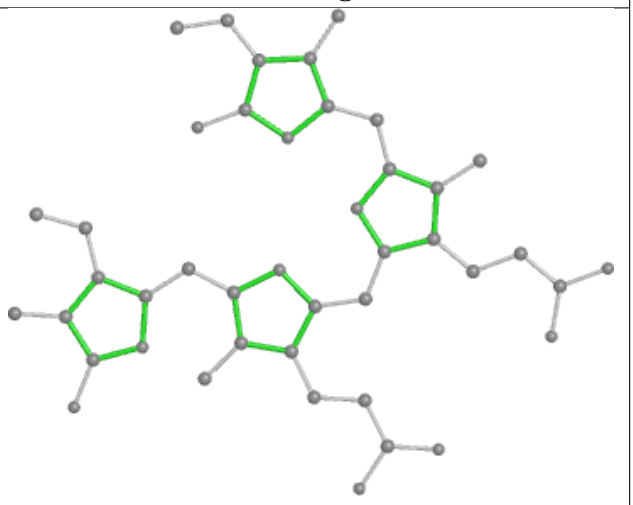
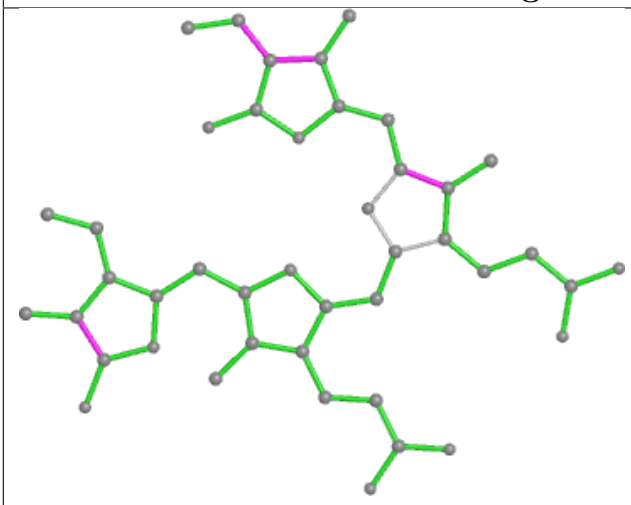
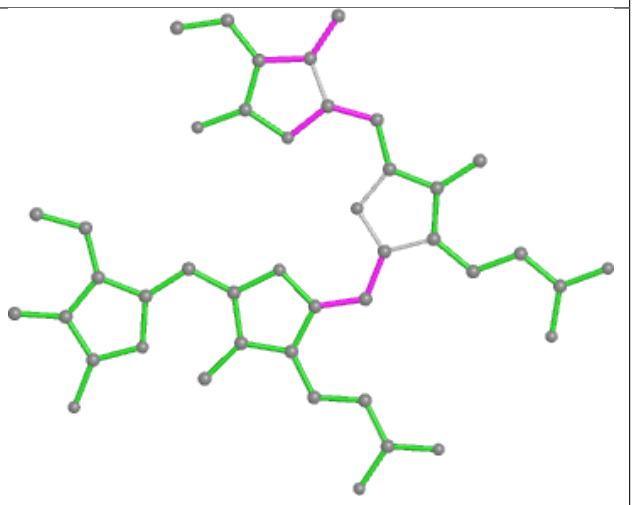


Rings

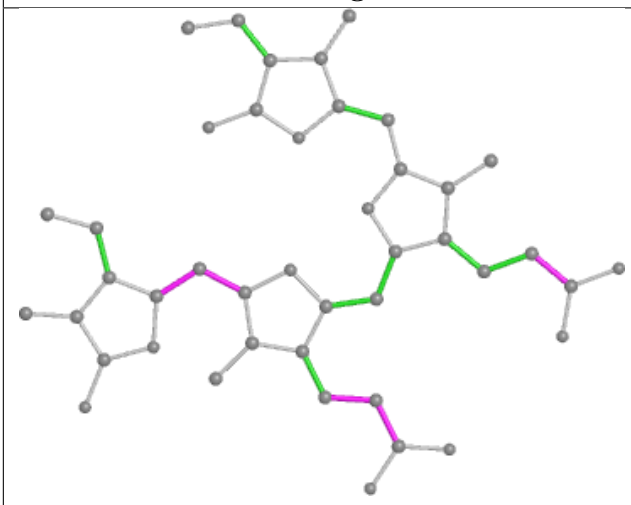
Ligand PEB I3 202



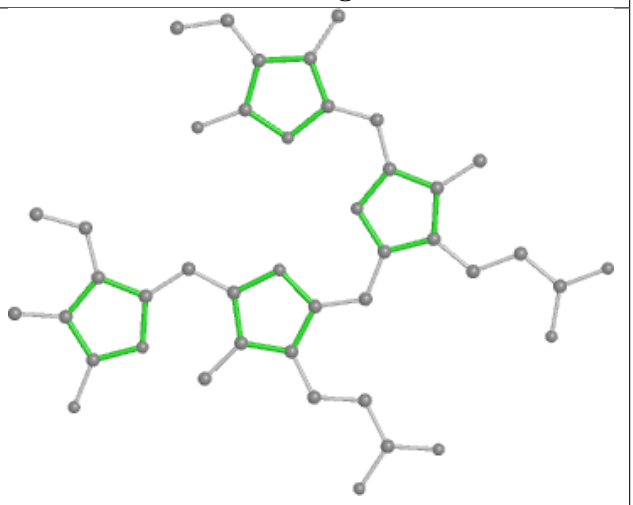
Bond lengths



Bond angles

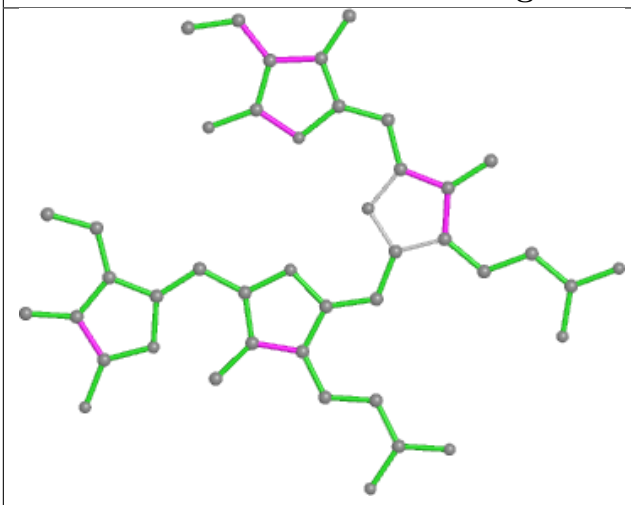


Torsions



Rings

Ligand PEB bF 202



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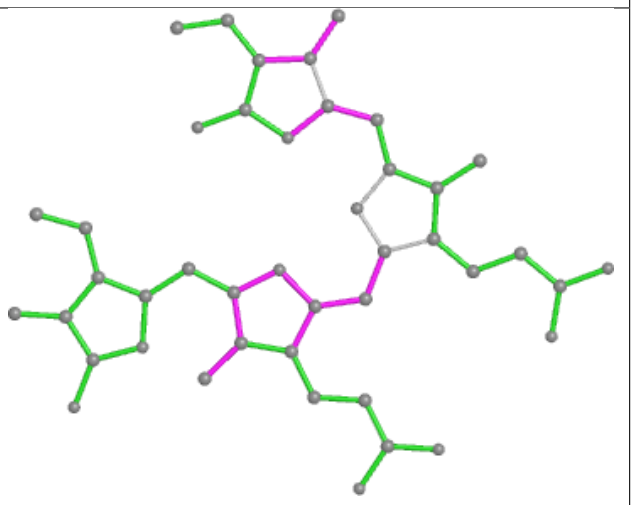

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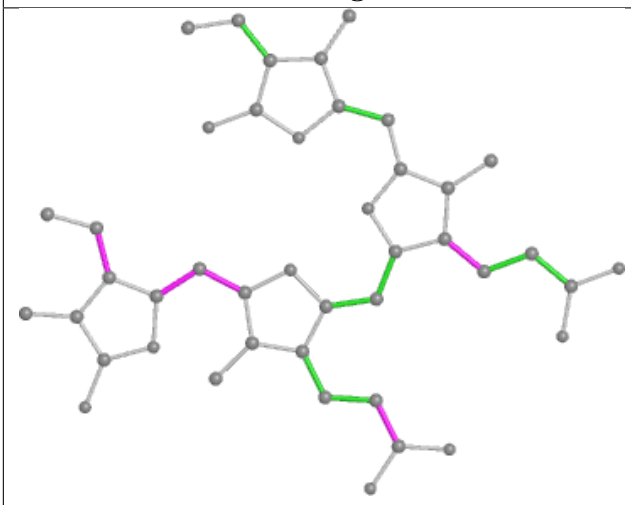

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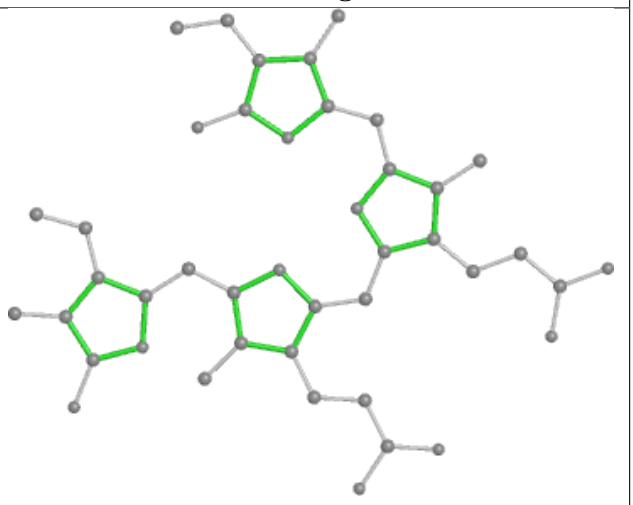
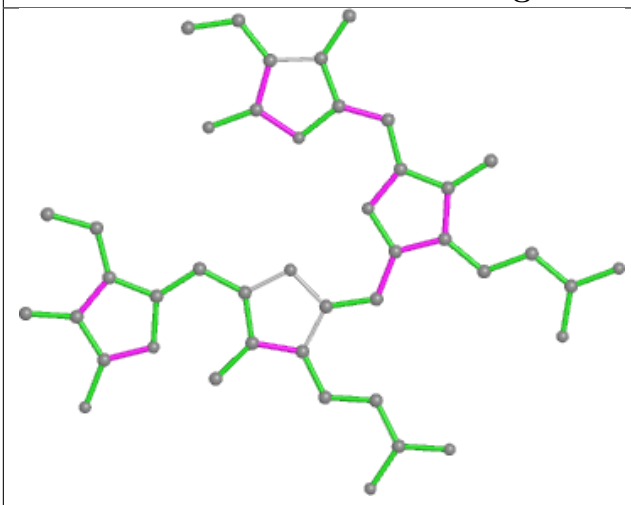


Rings

Ligand PUB X2 203



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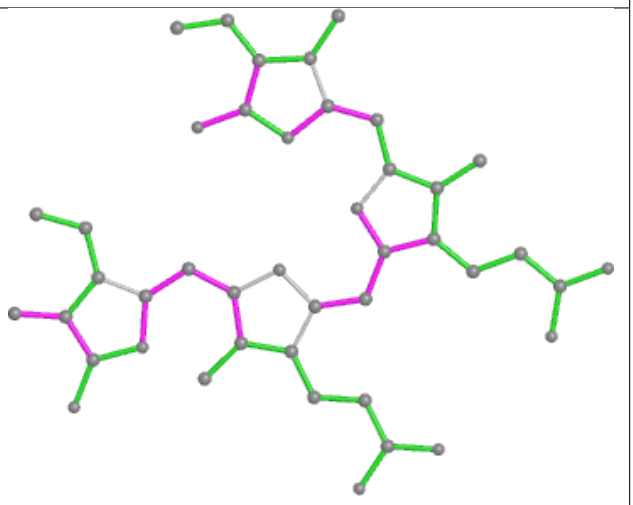

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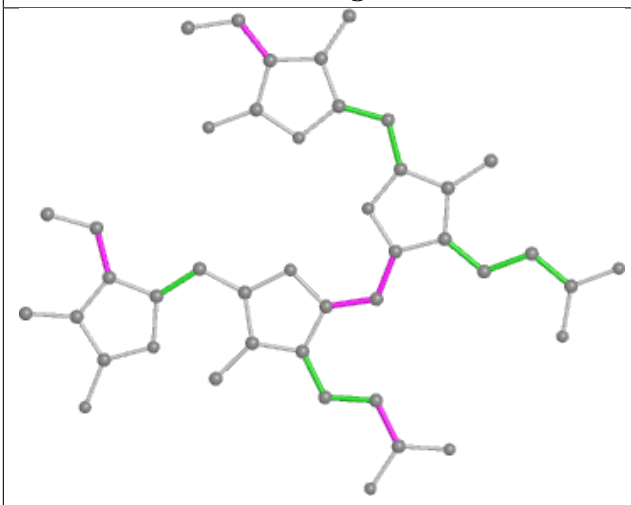

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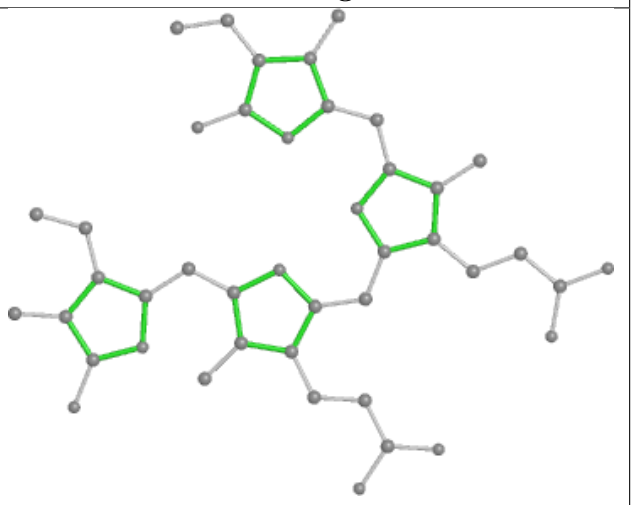
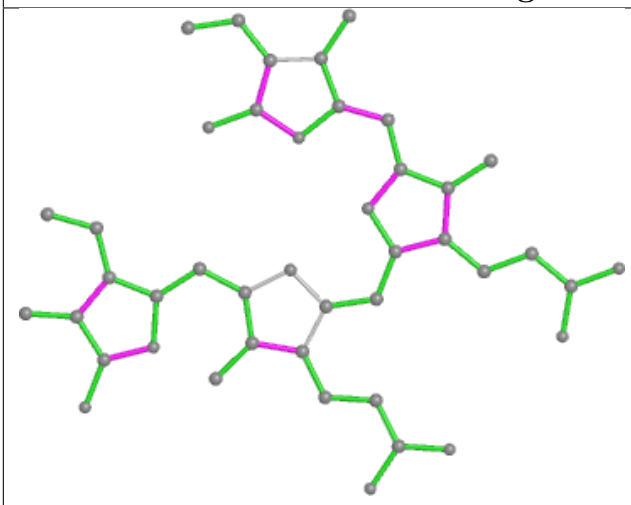


Rings

Ligand PUB v6 203



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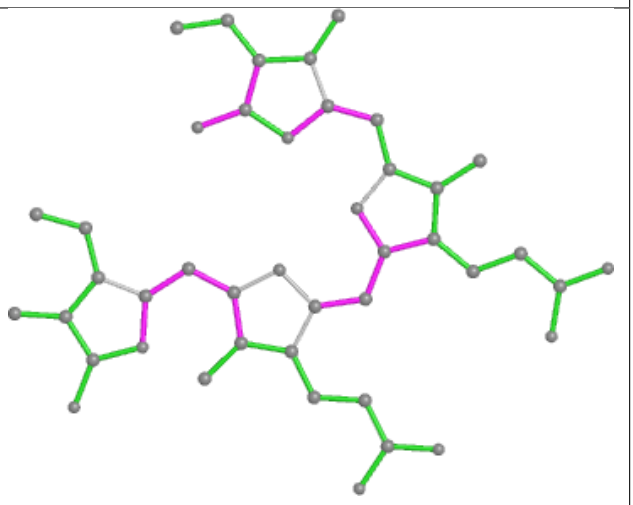

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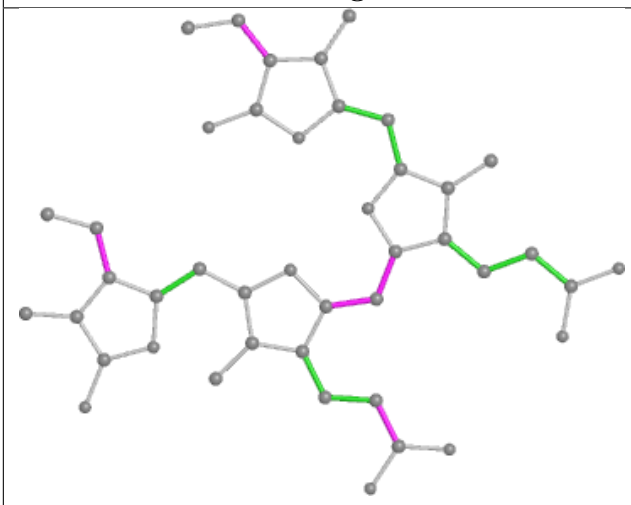

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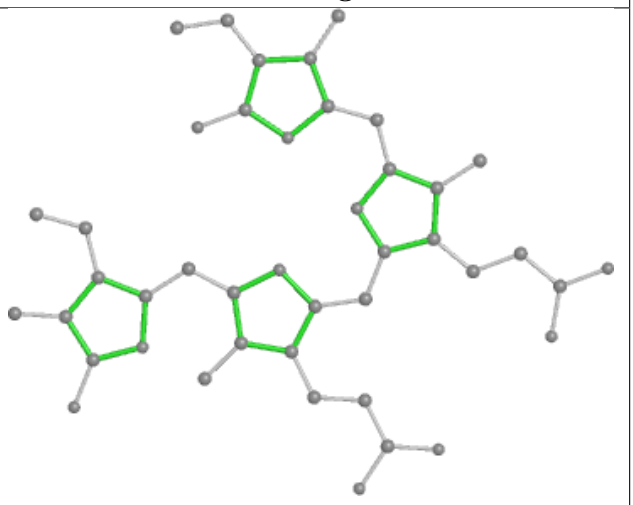
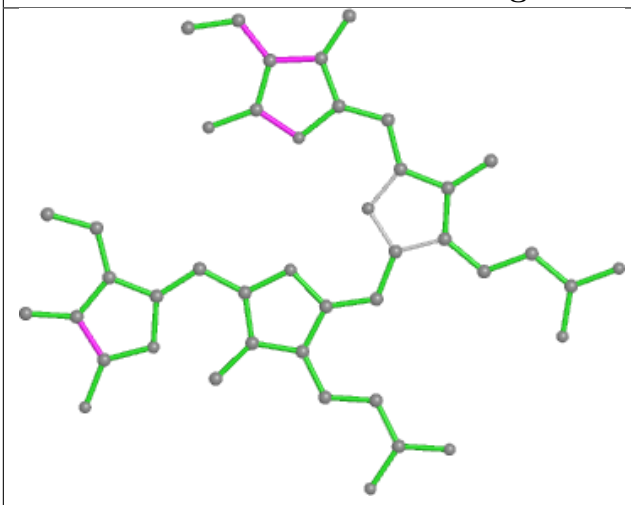


Rings

Ligand PEB iG 1001



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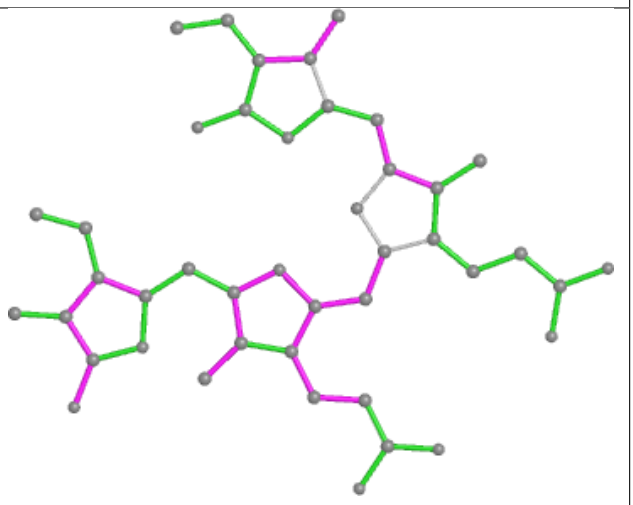

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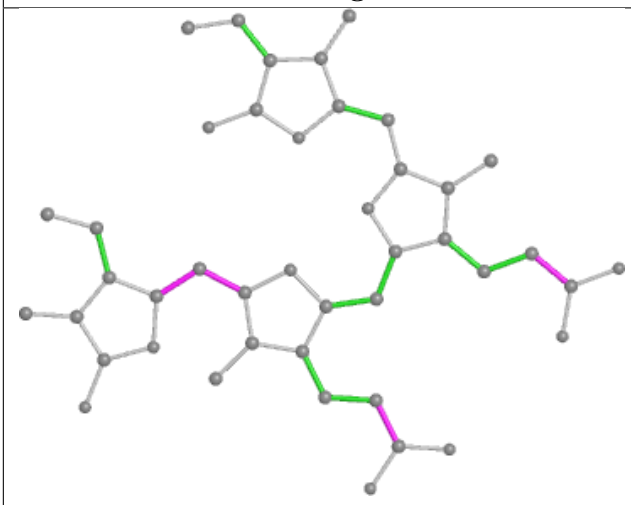

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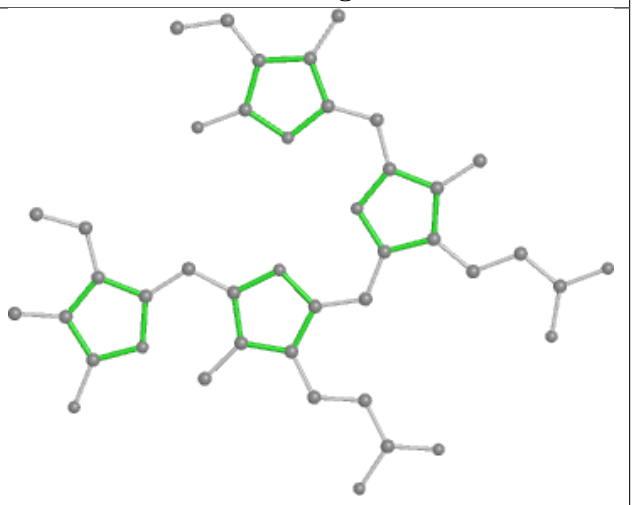
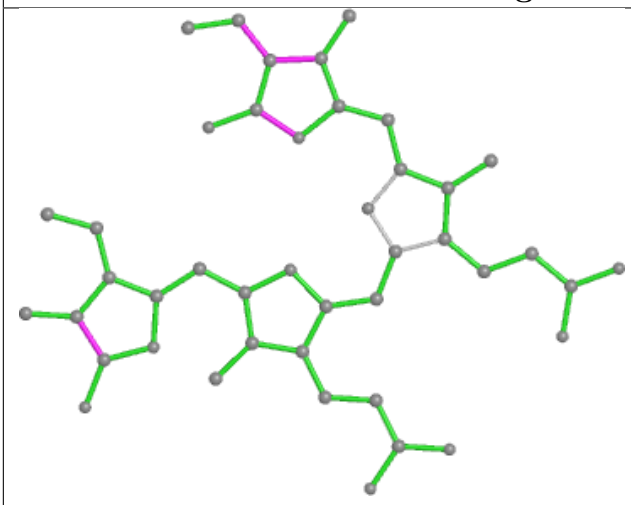


Rings

Ligand PEB Q4 202



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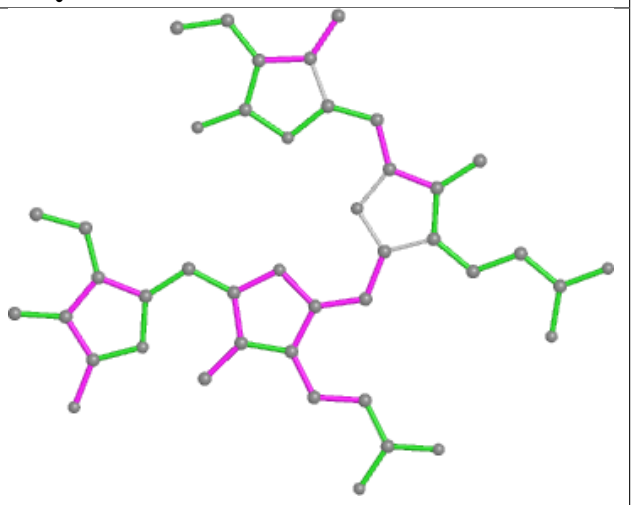

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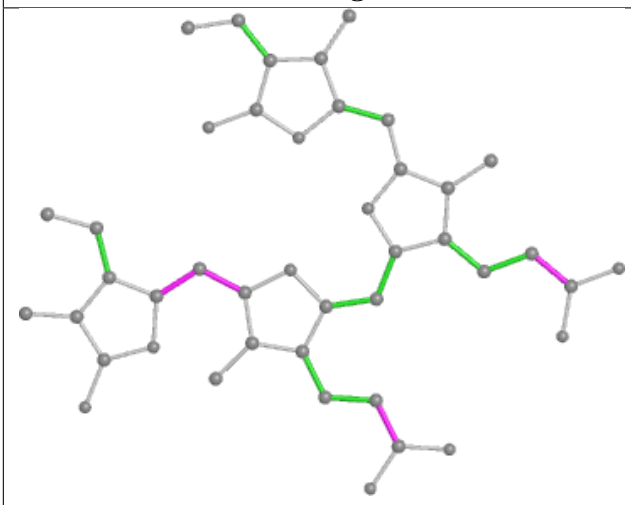

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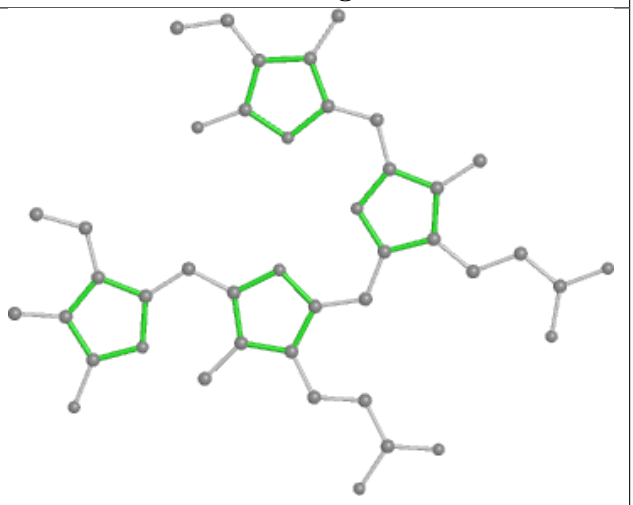
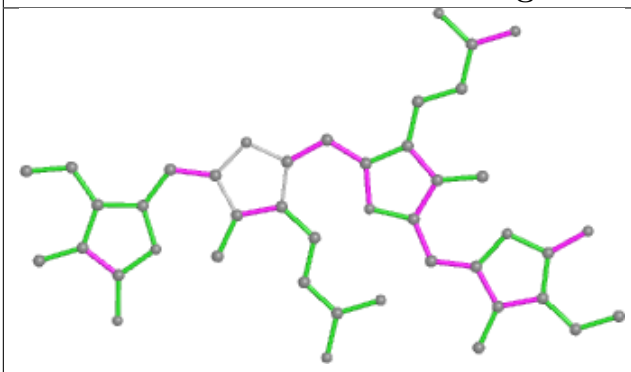


Rings

Ligand CYC q1 201



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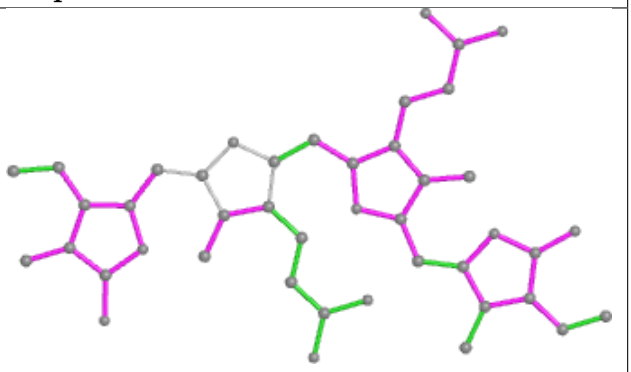

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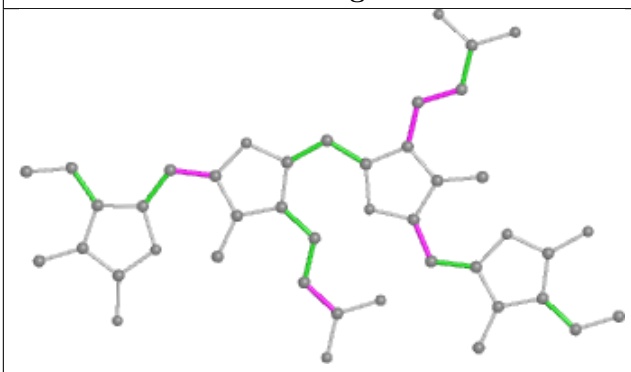

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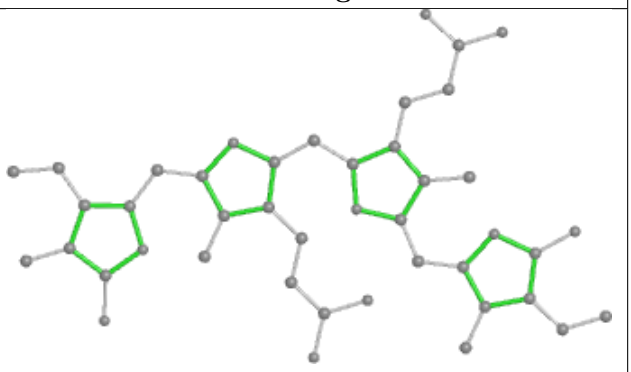
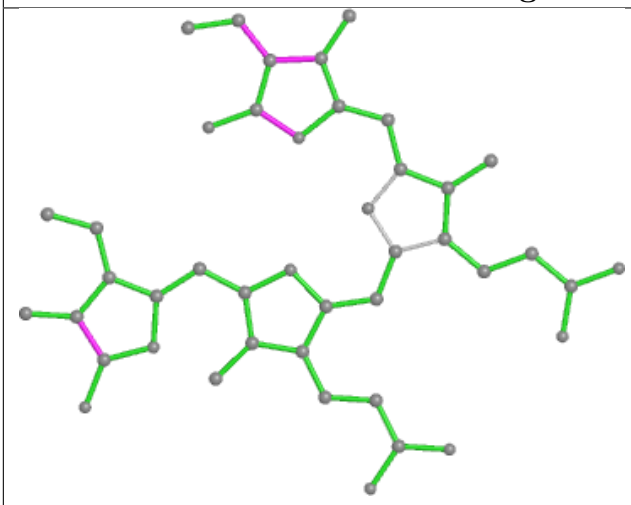


Rings

Ligand PEB gq 201



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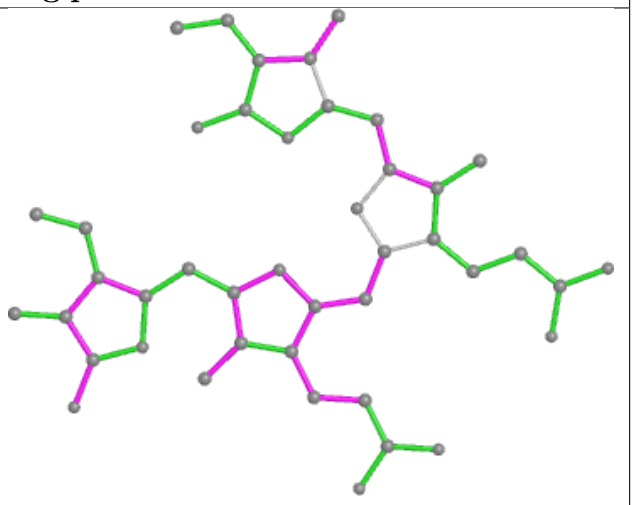

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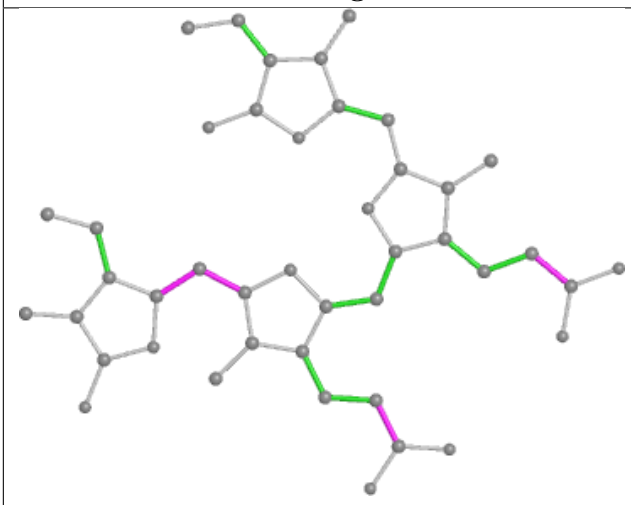

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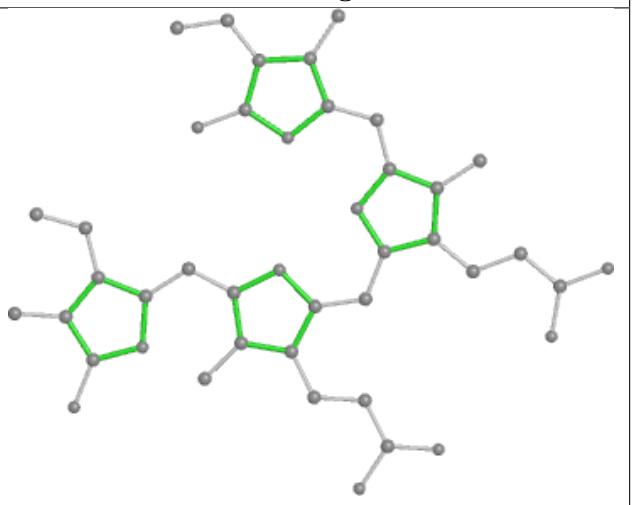
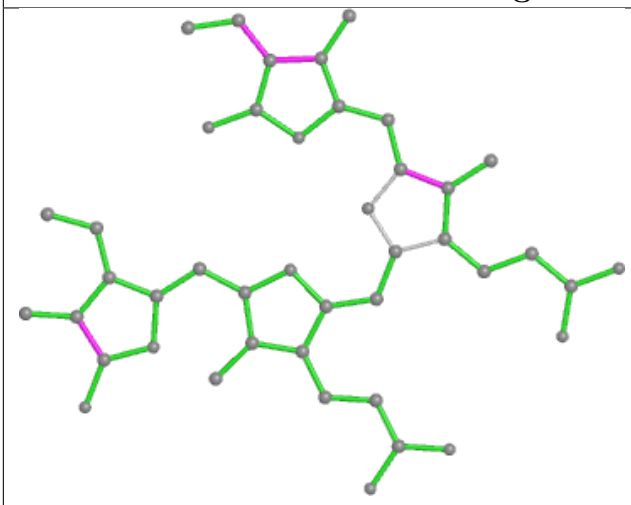


Rings

Ligand PEB fh 1002



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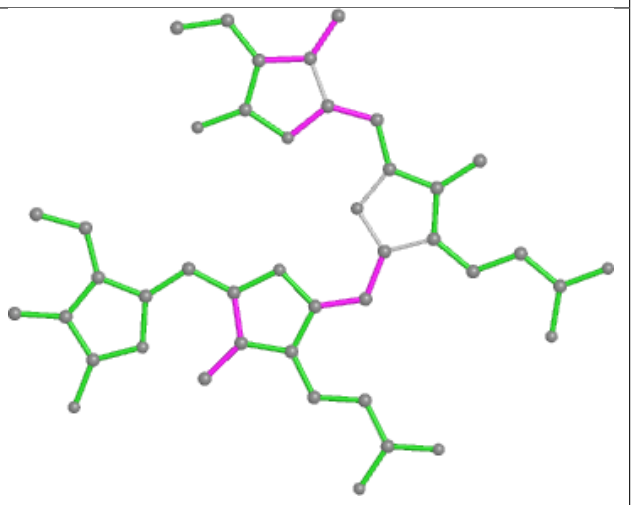

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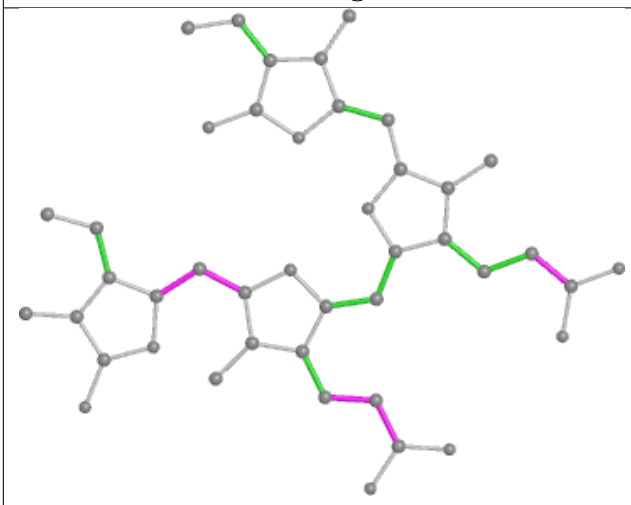

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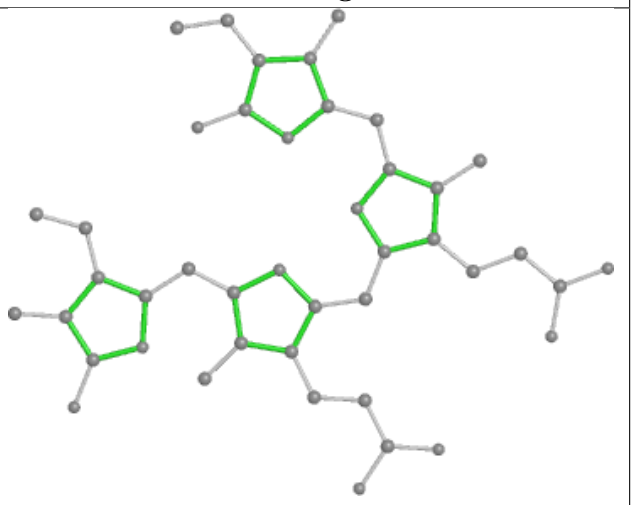
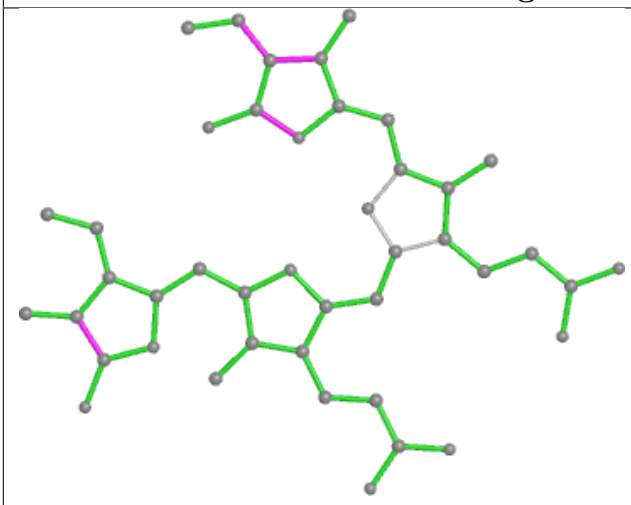


Rings

Ligand PEB Z4 202



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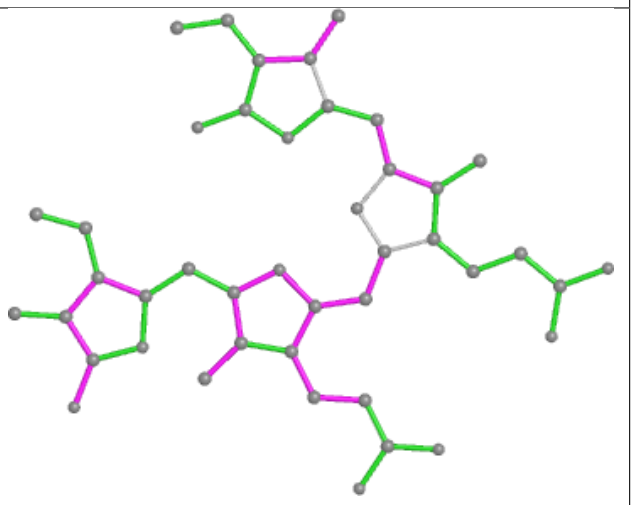
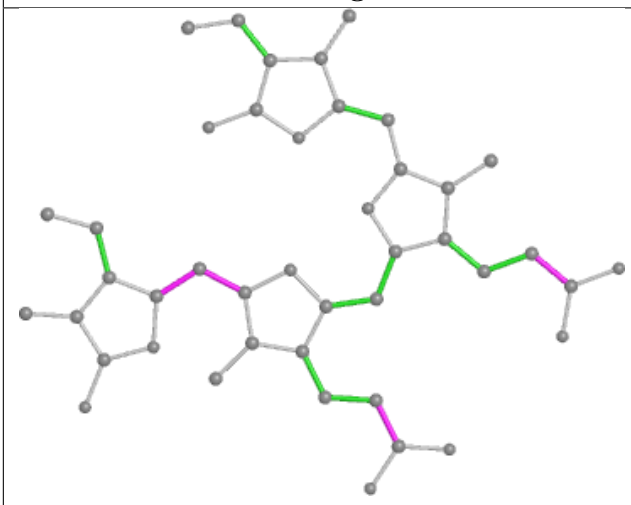


Bond angles



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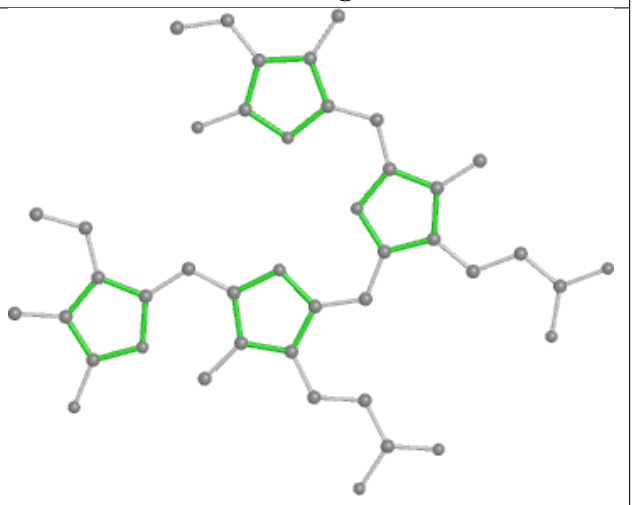
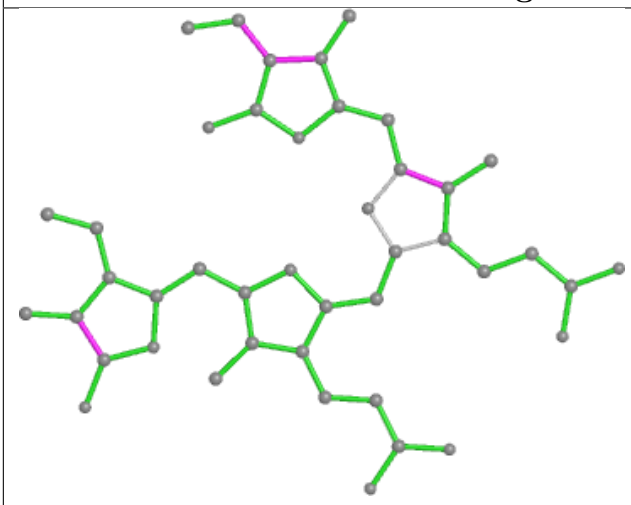


Rings

Ligand PEB C7 202



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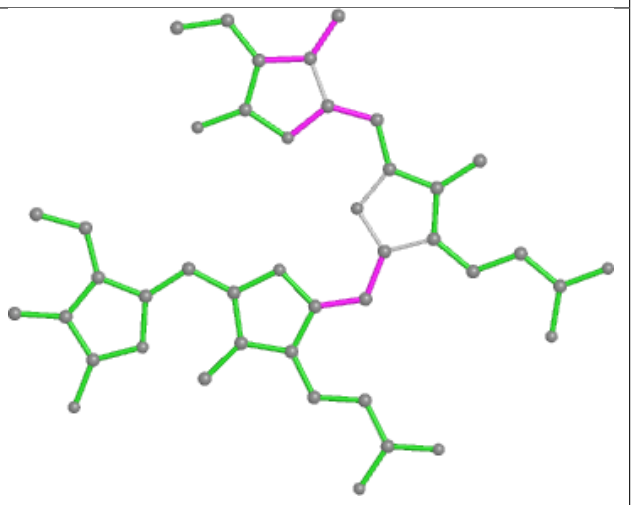

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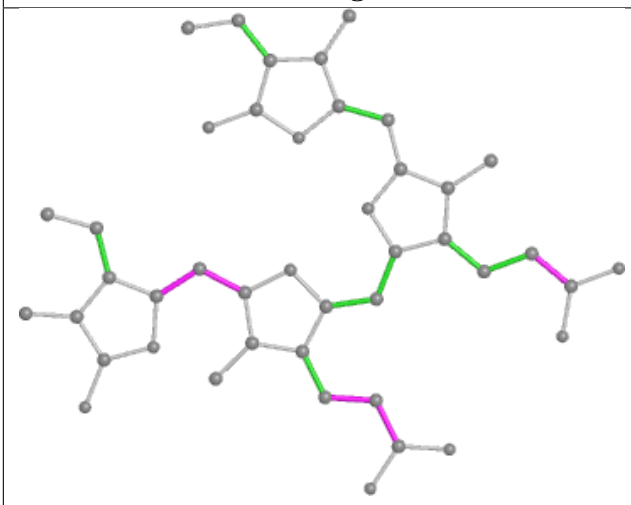

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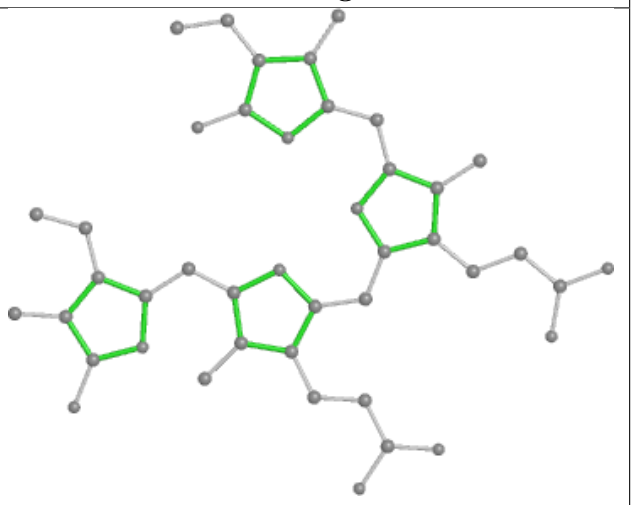
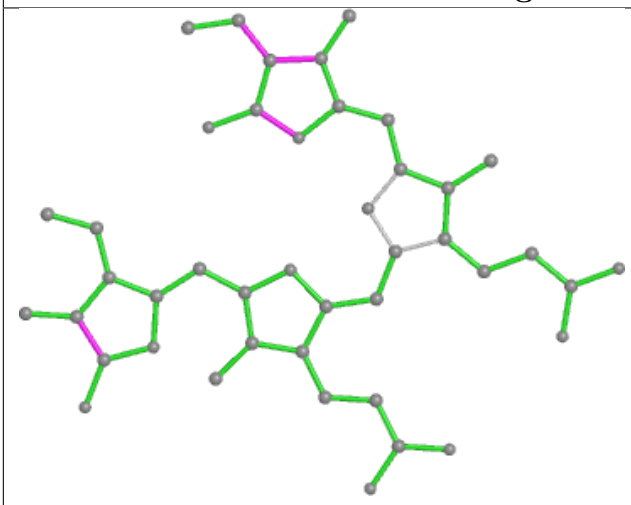


Rings

Ligand PEB R7 201



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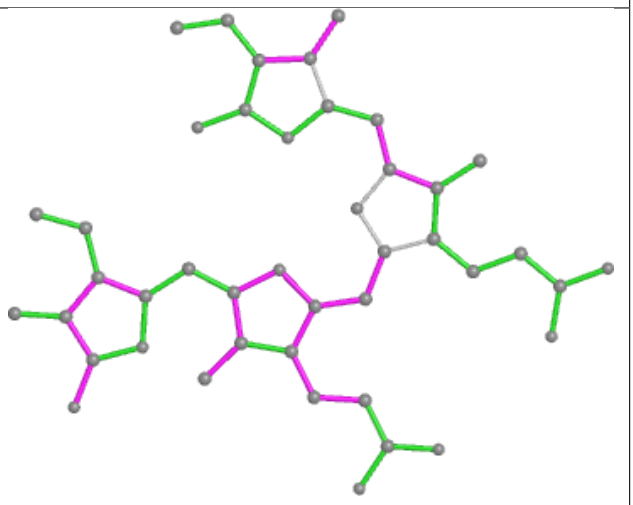

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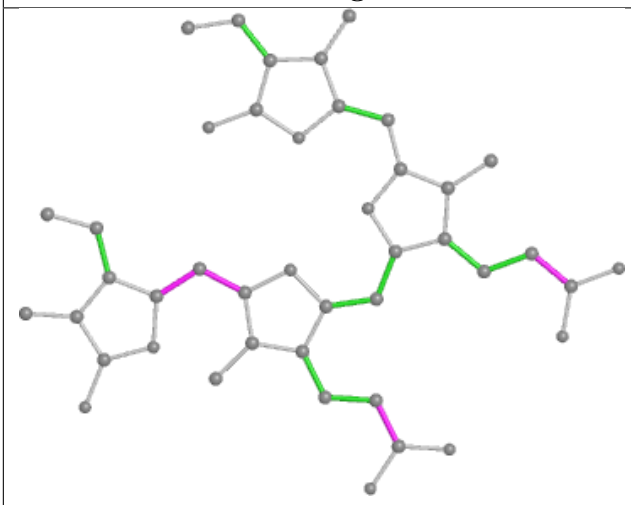

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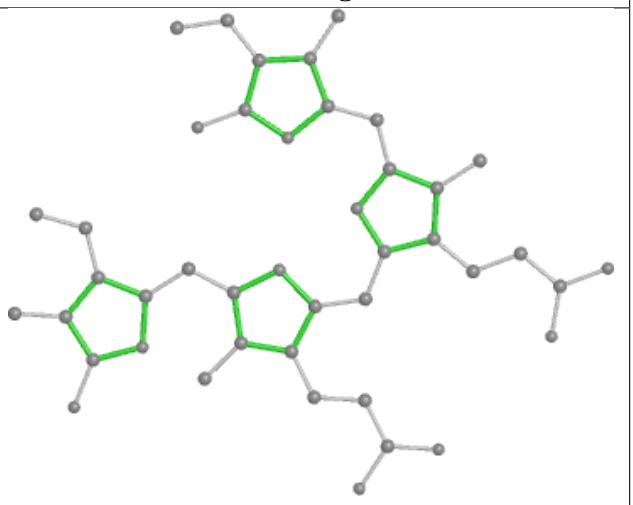
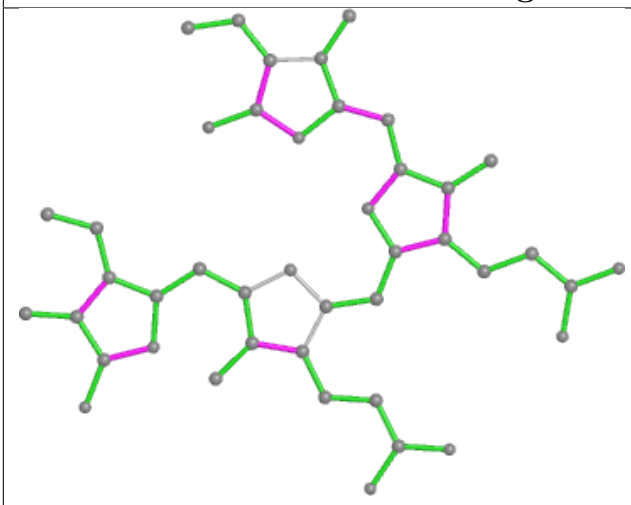


Rings

Ligand PUB b9 407



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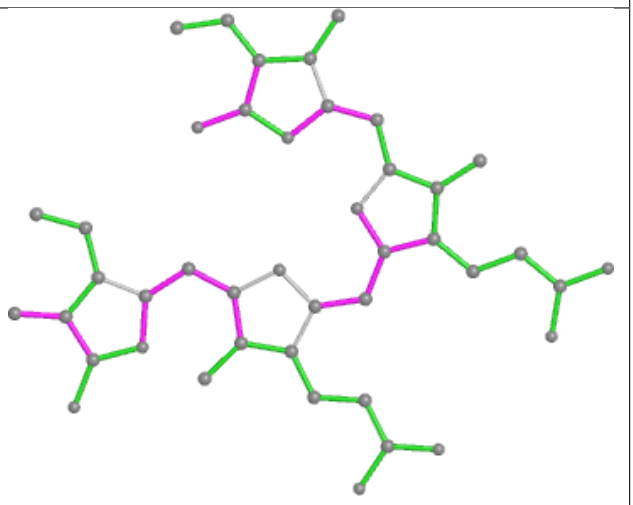
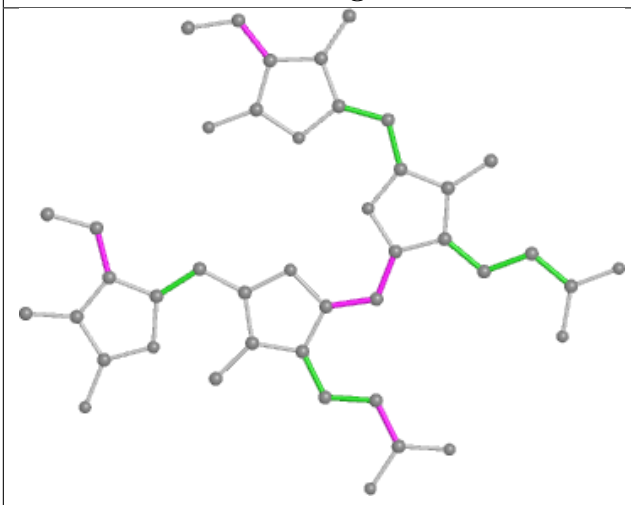


Bond angles



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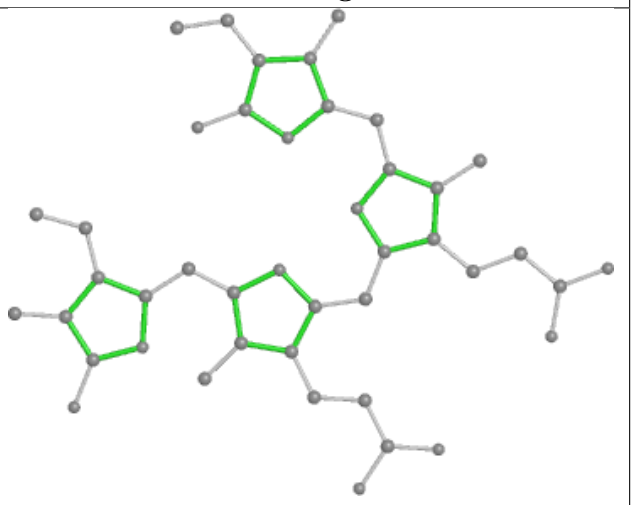
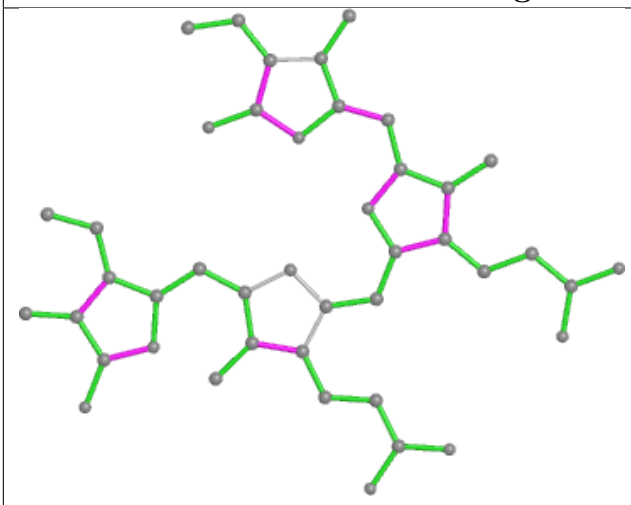


Rings

Ligand PUB cH 202



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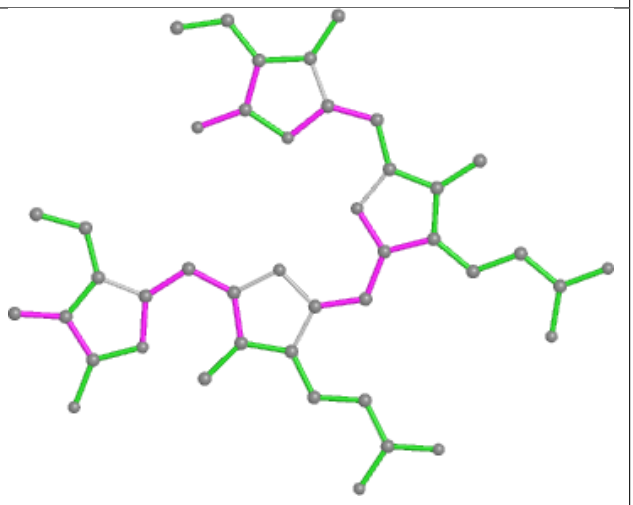
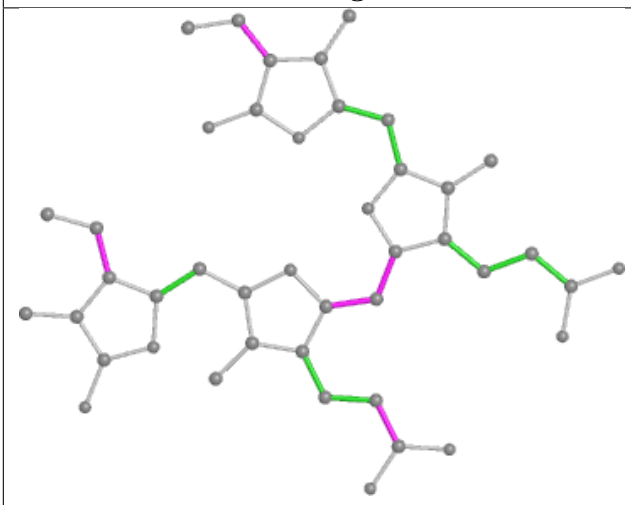
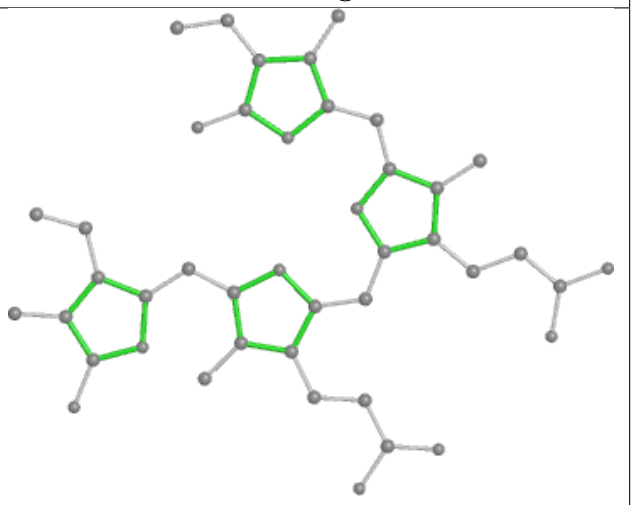


Bond angles

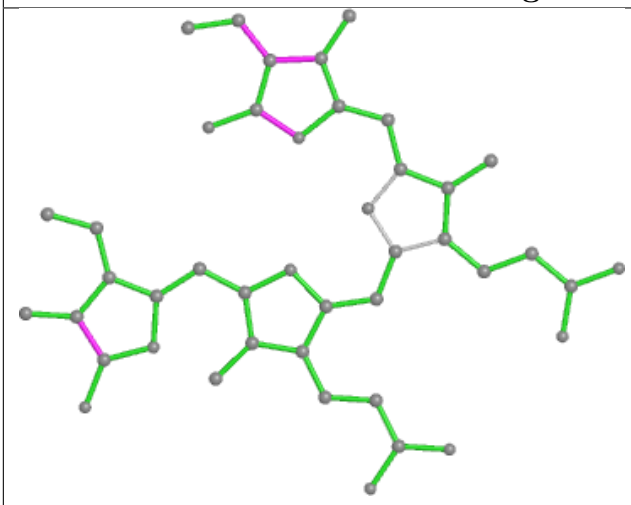


Torsions



Rings

Ligand PEB fb 201



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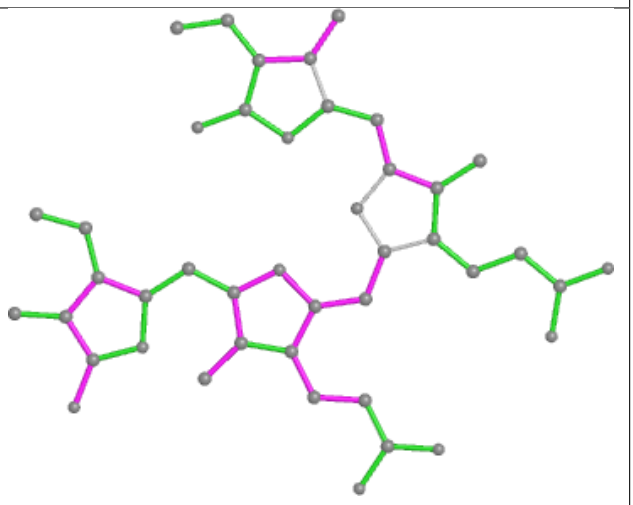

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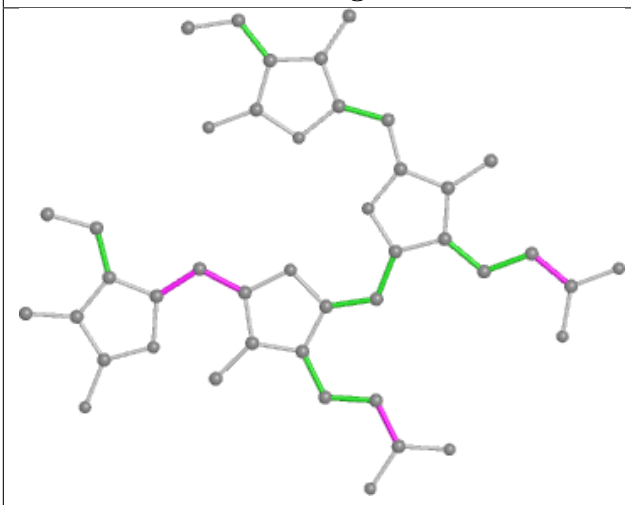

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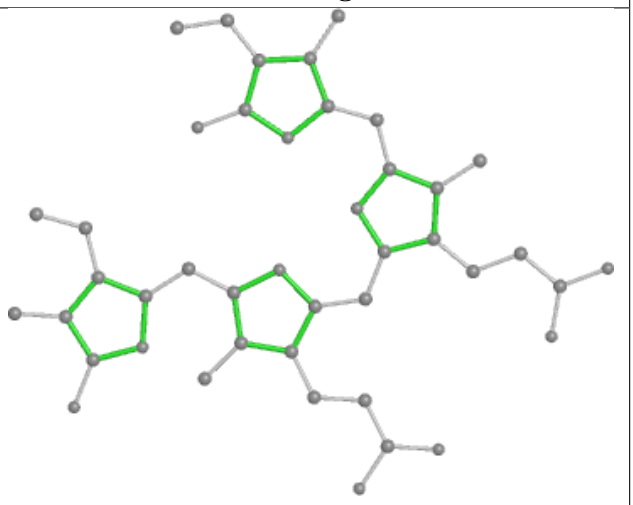

Rings

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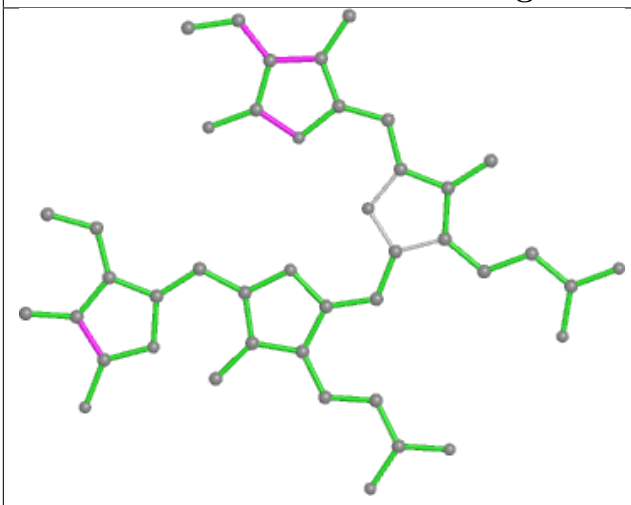

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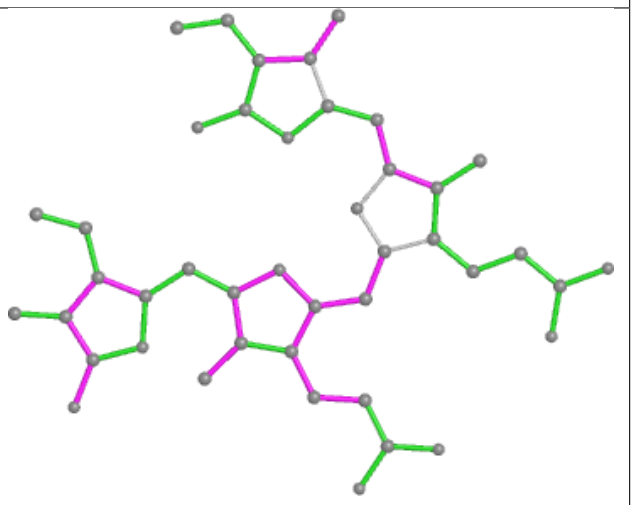

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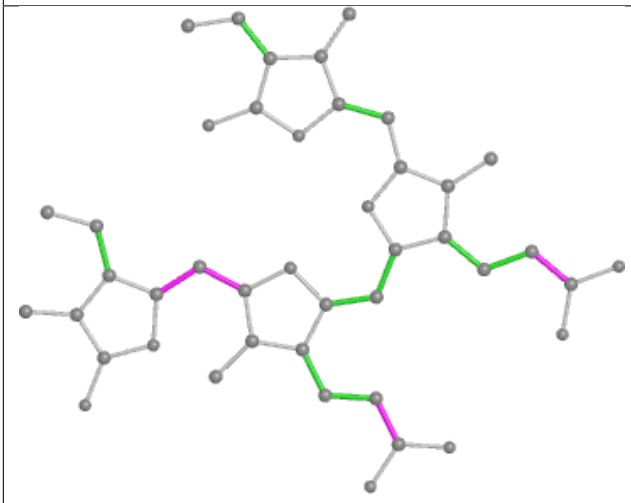

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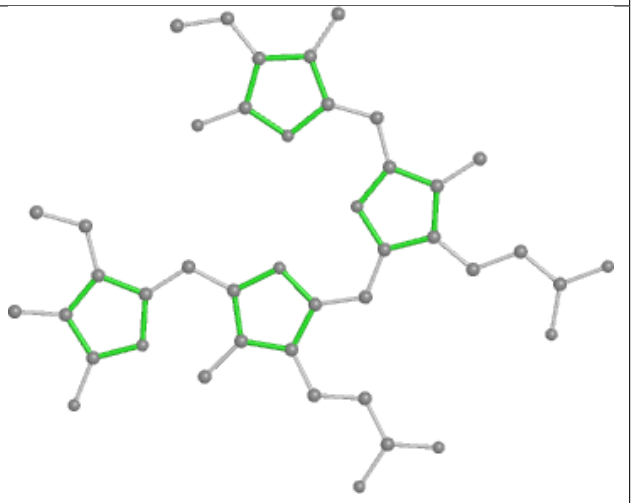

Rings

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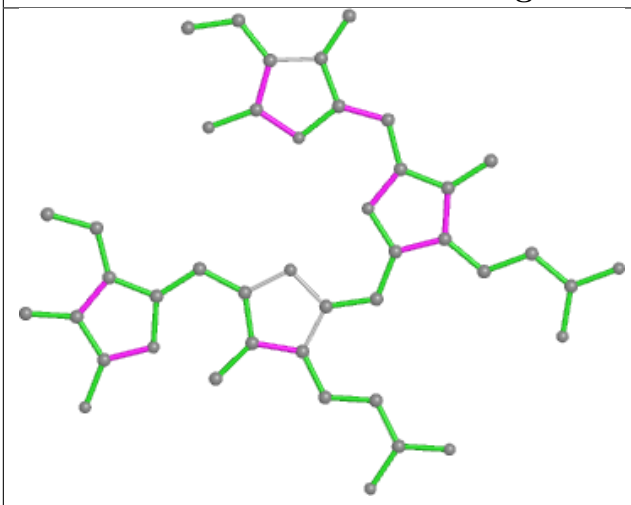

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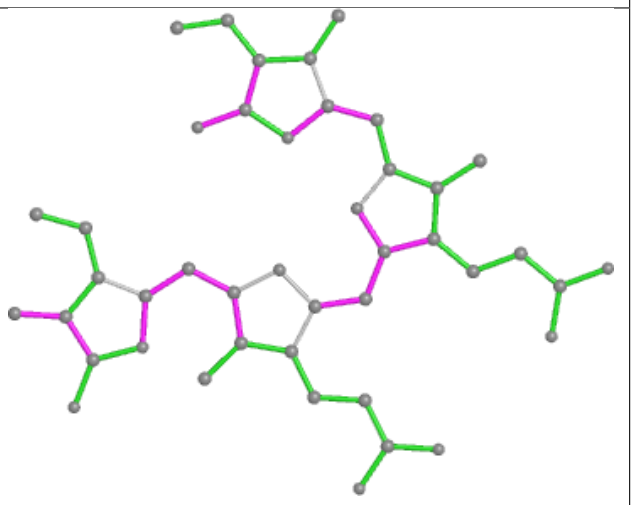

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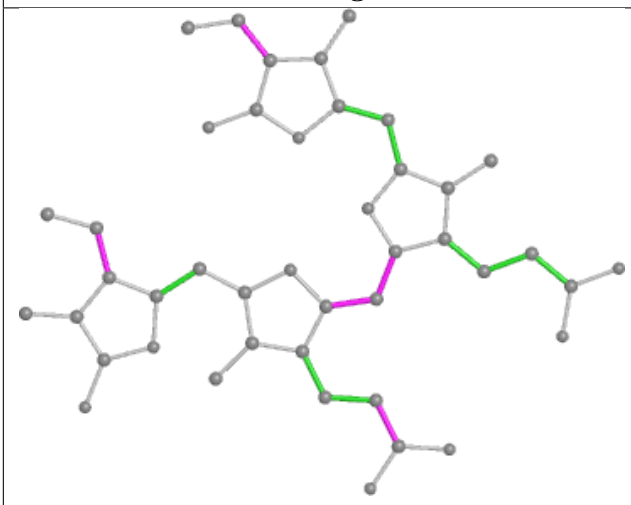

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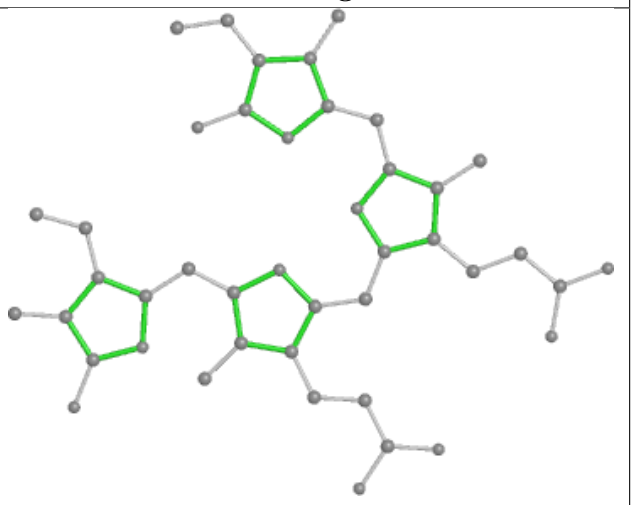
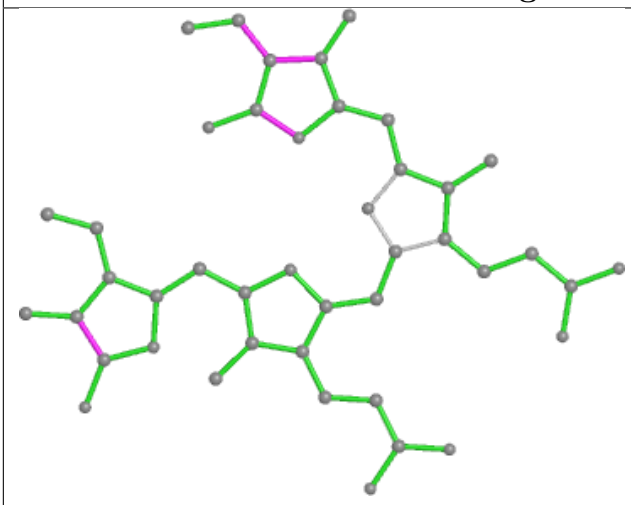


Rings

Ligand PEB x8 201



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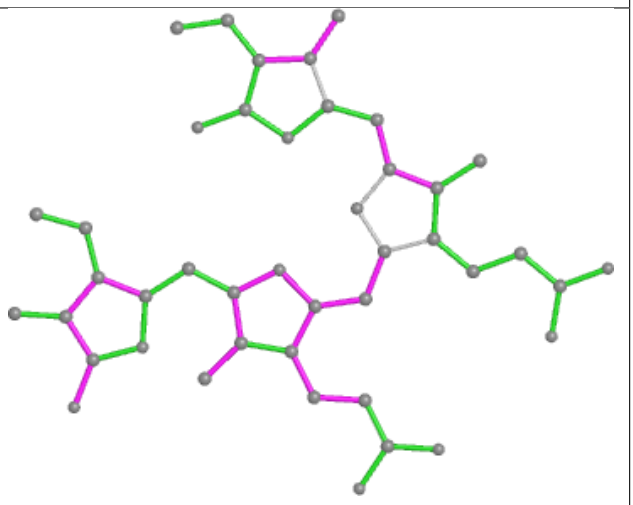

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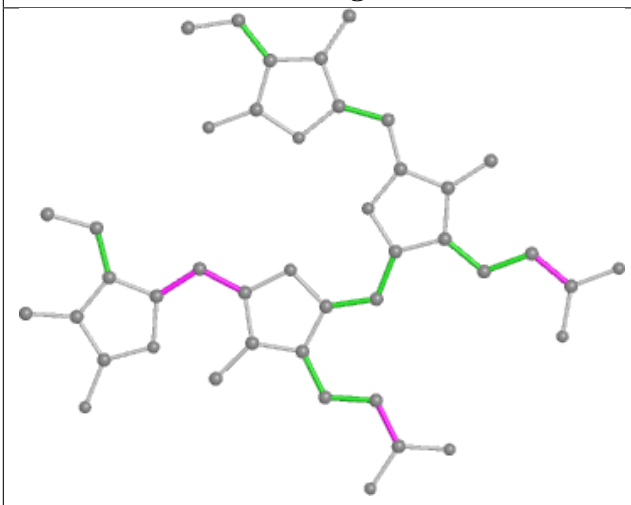

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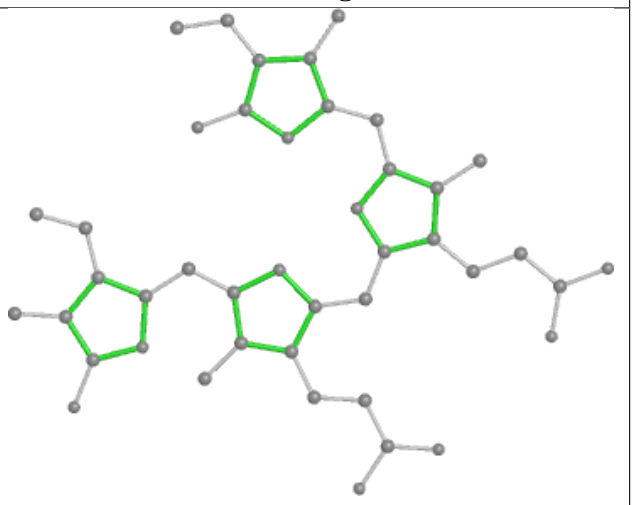

Rings

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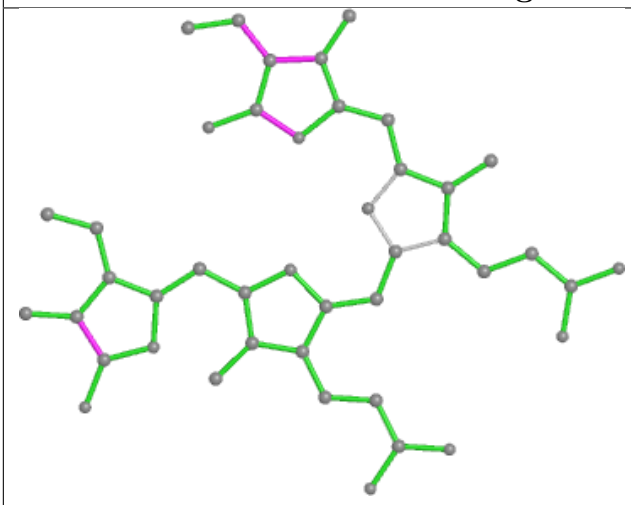

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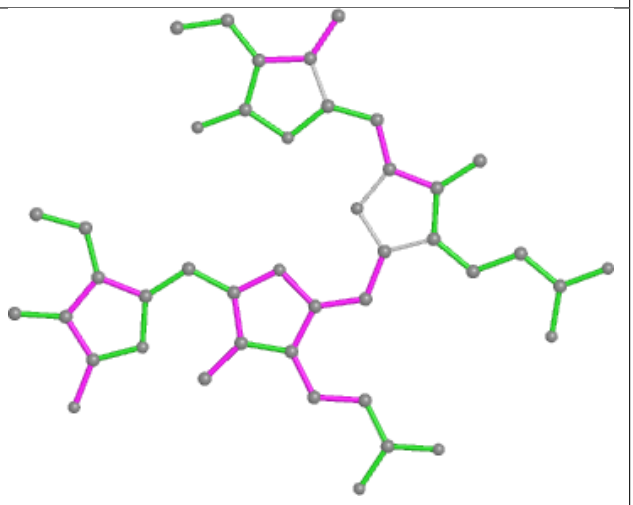

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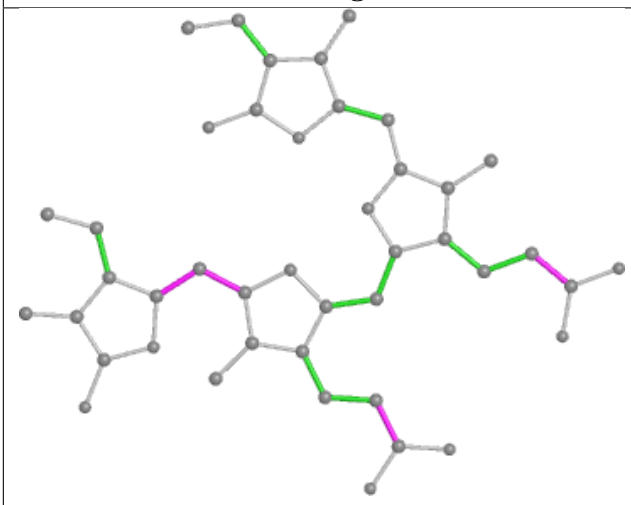

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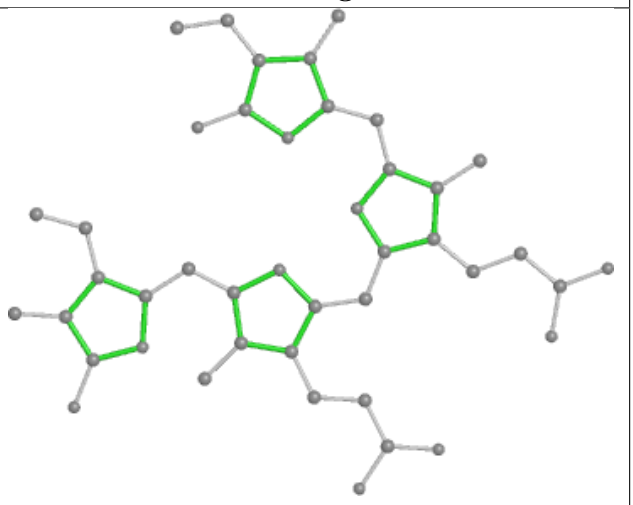

Rings

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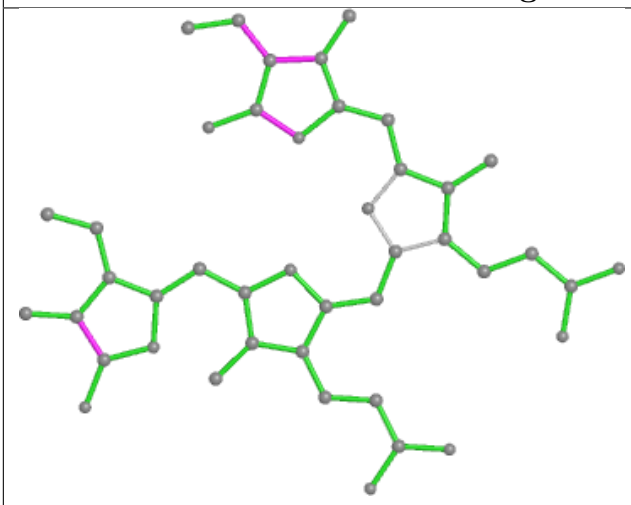

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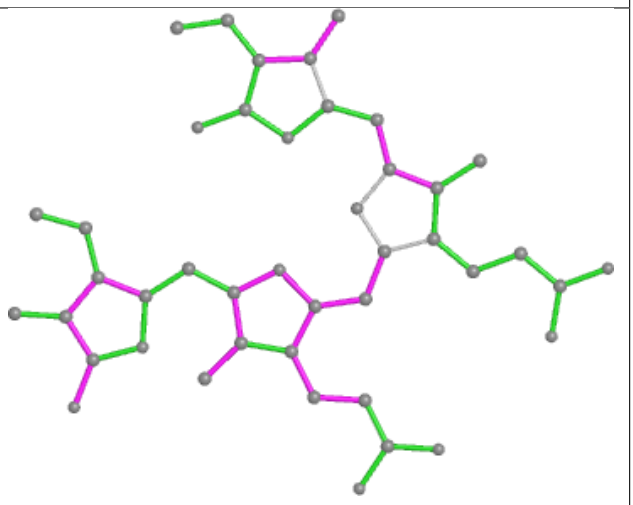

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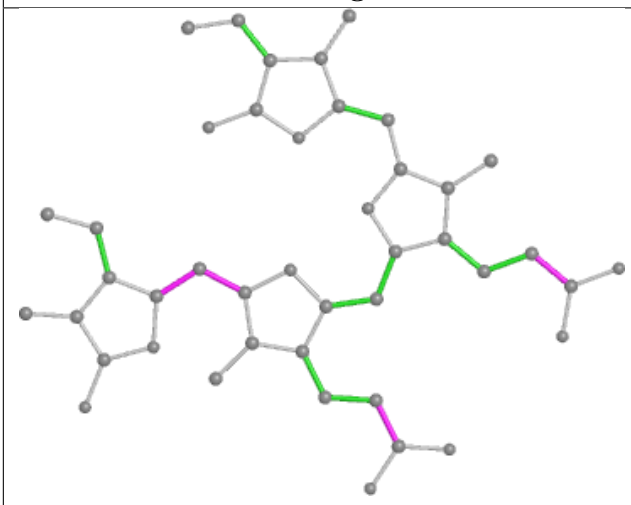

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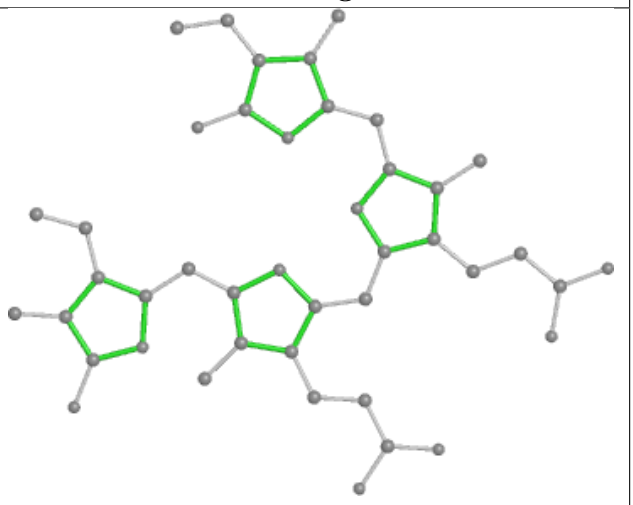

Rings

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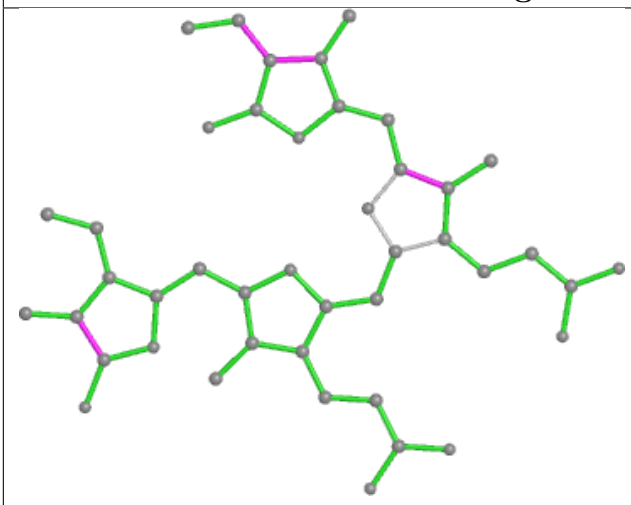

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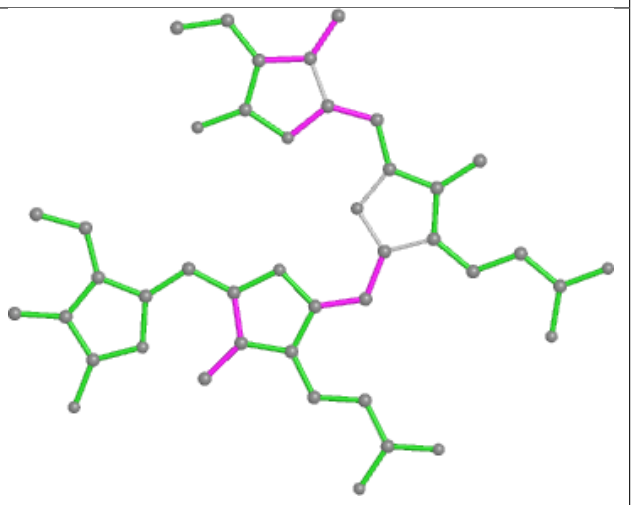

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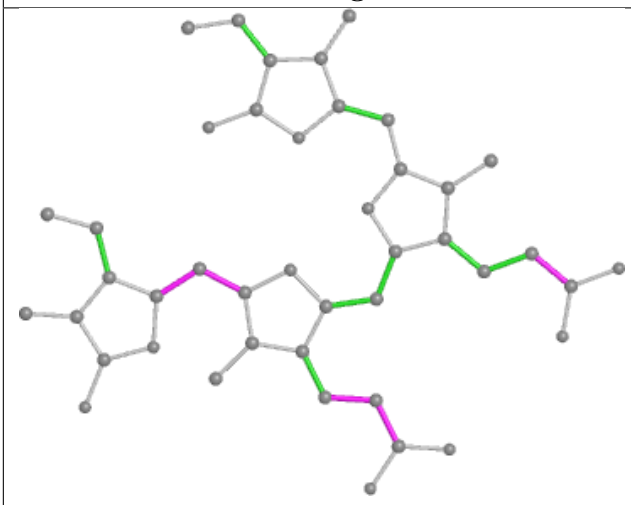

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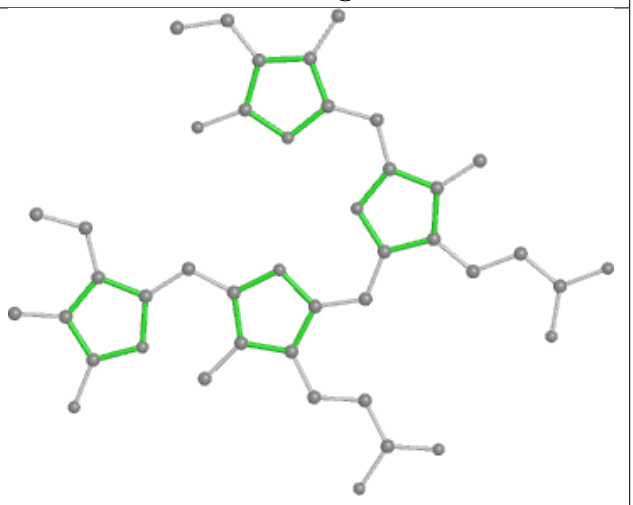
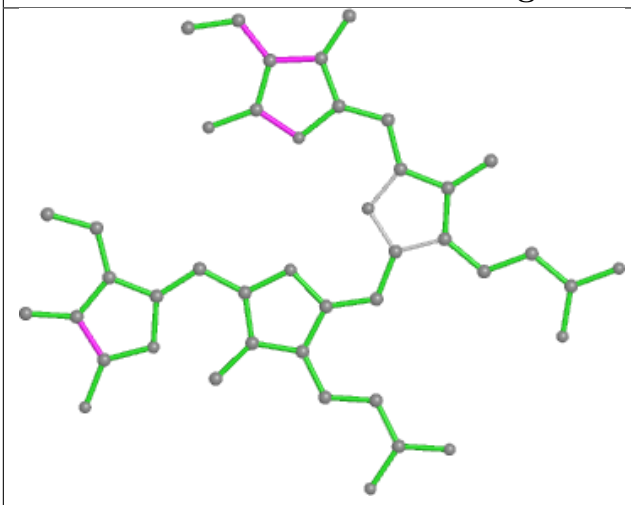


Rings

Ligand PEB bq 201



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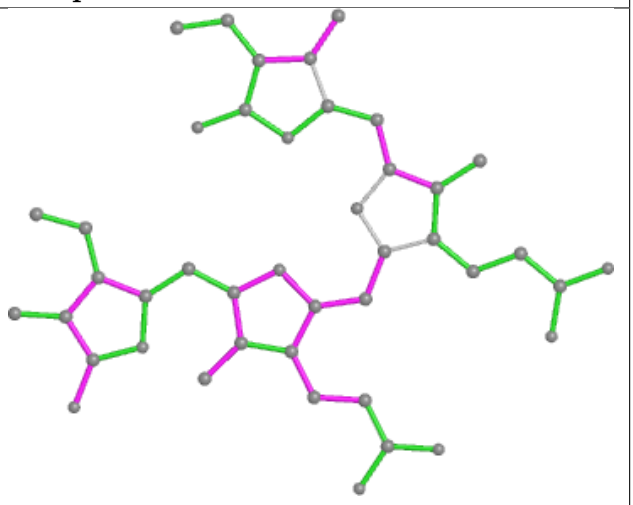
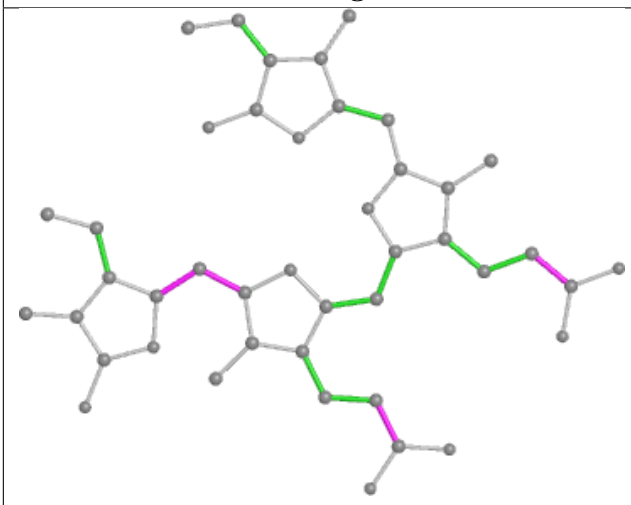


Bond angles



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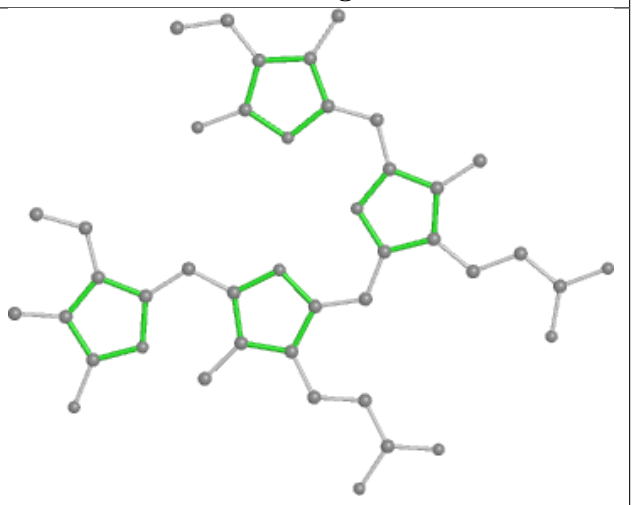

Rings

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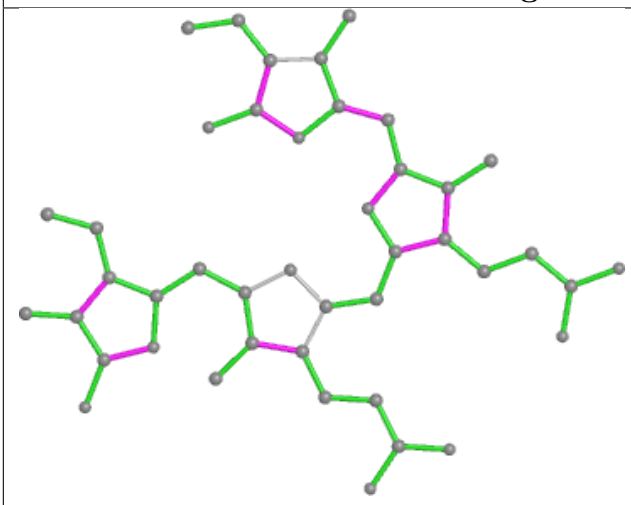

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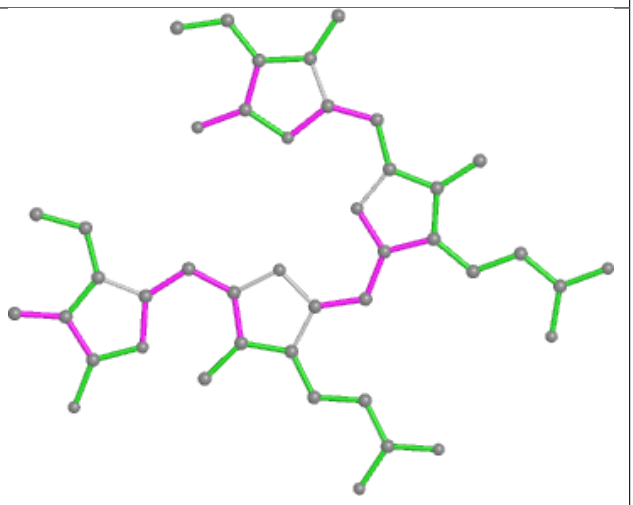

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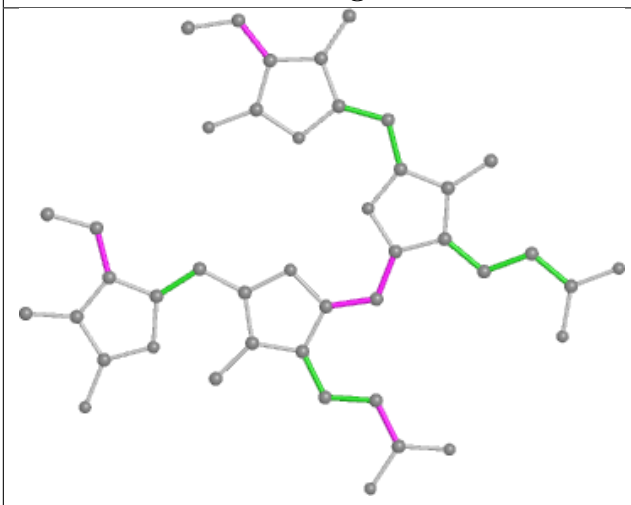

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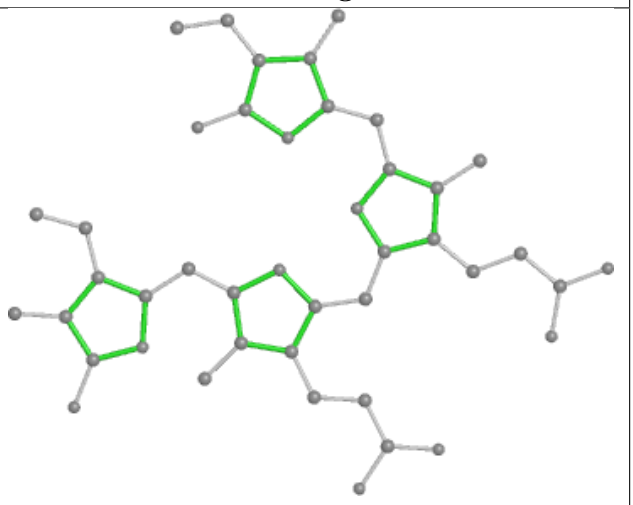
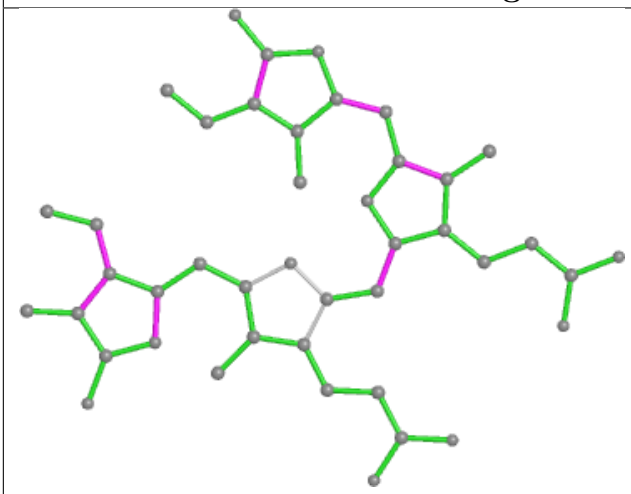


Rings

Ligand PVN U8 1004



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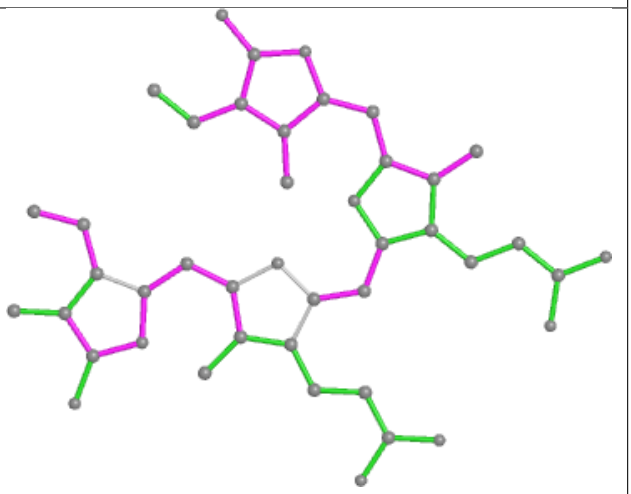

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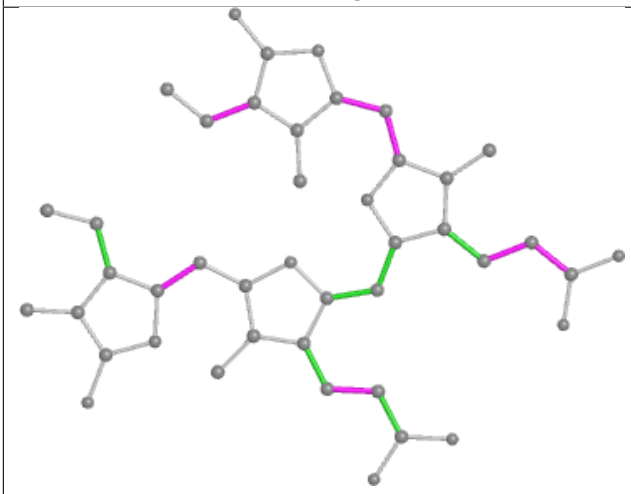

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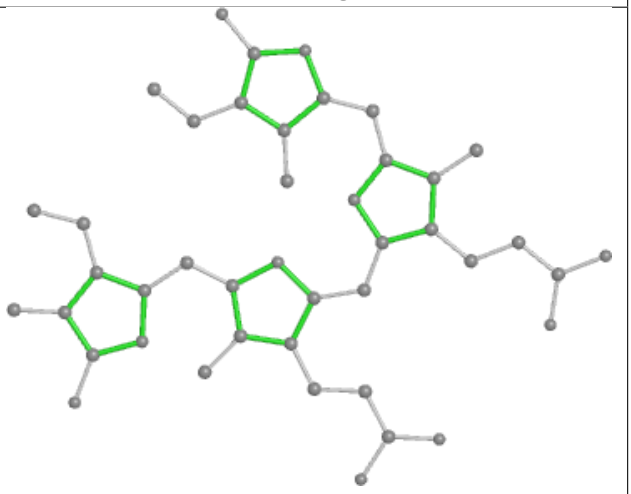

Rings

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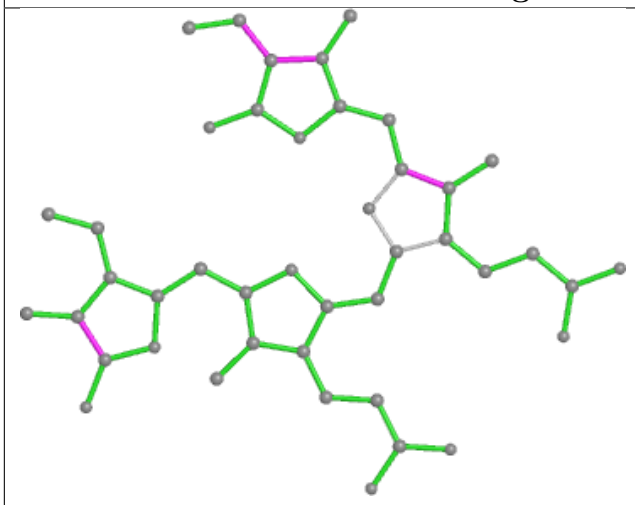

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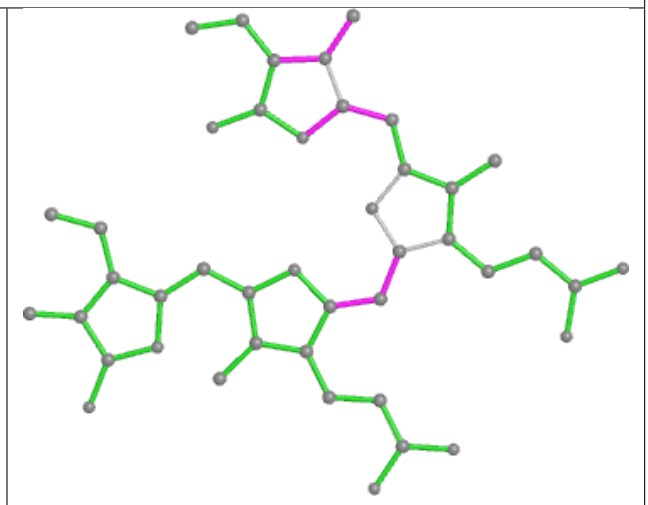

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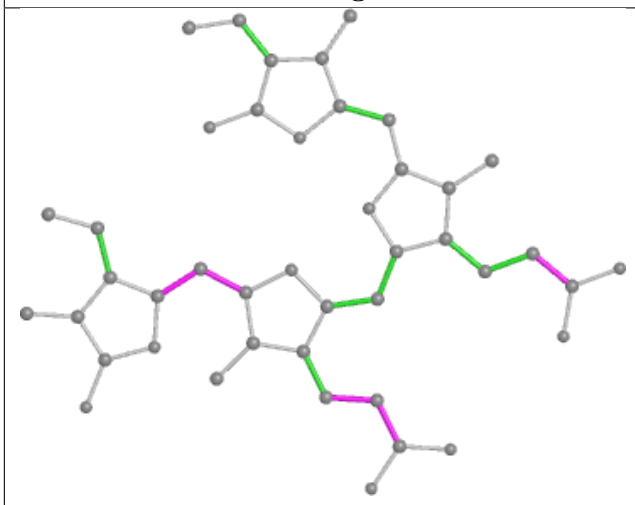

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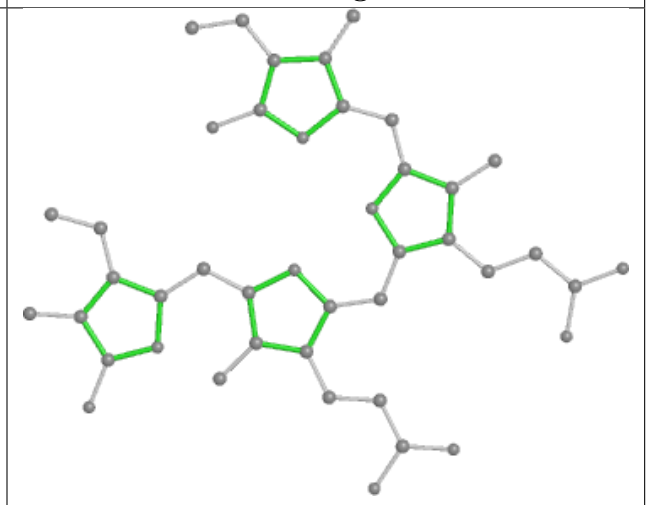
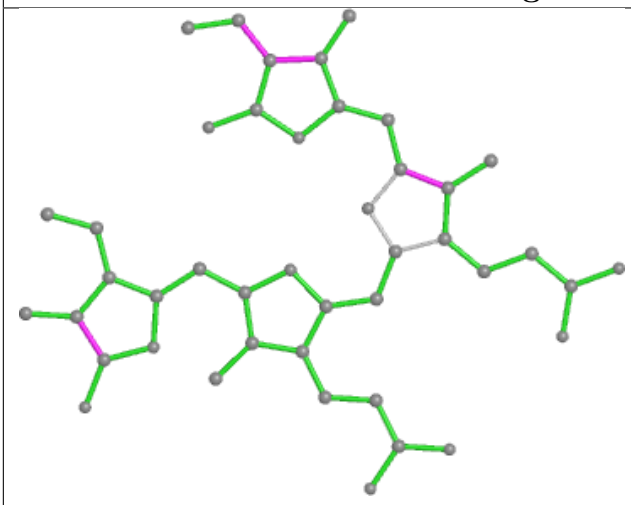


Rings

Ligand PEB fv 202



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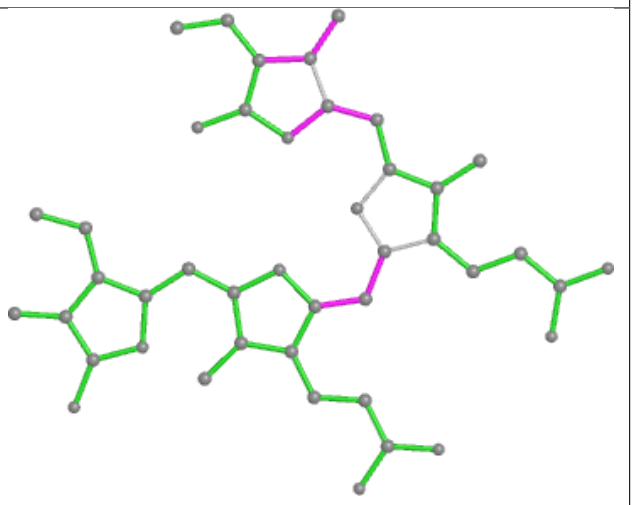

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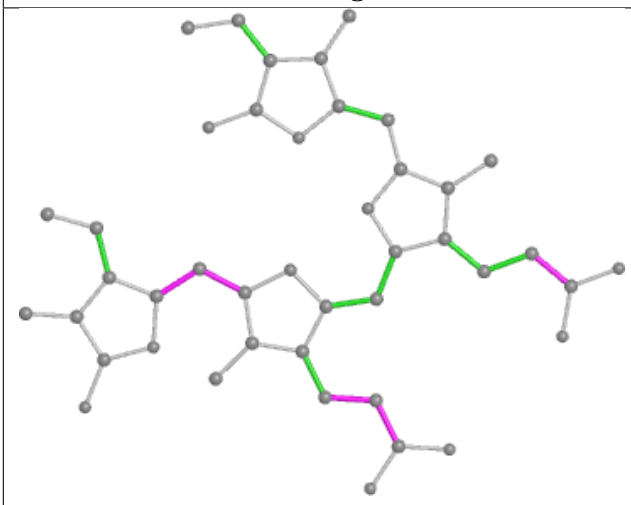

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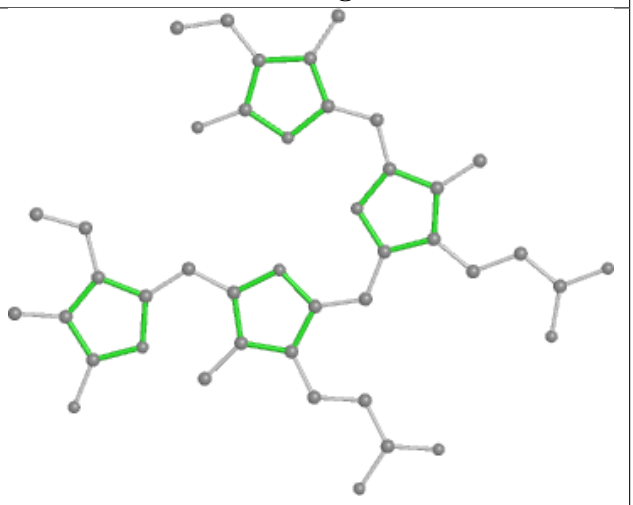
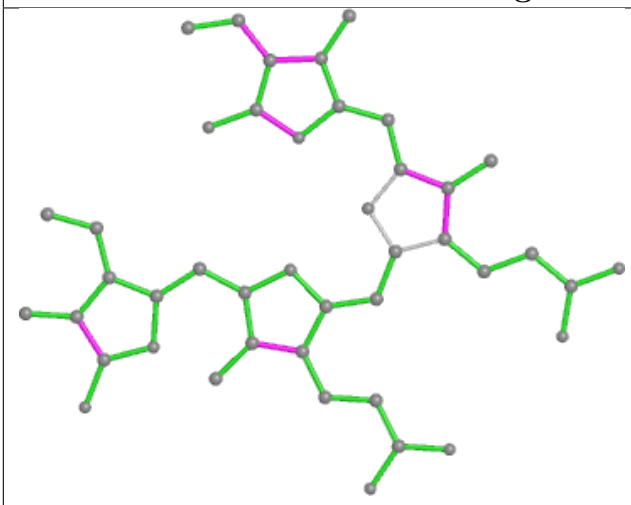


Rings

Ligand PEB bV 202



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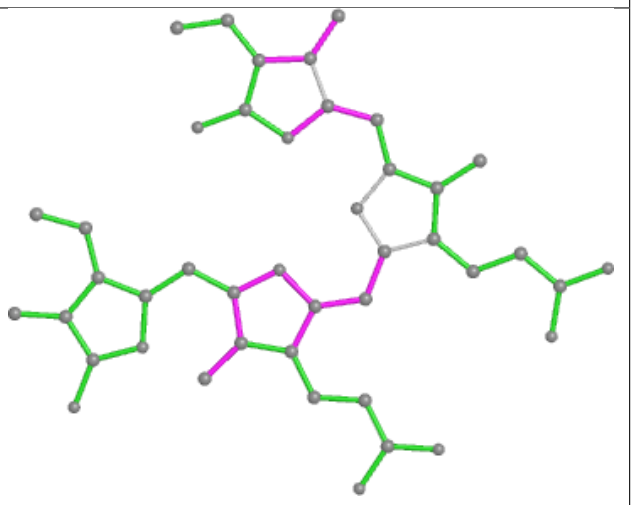

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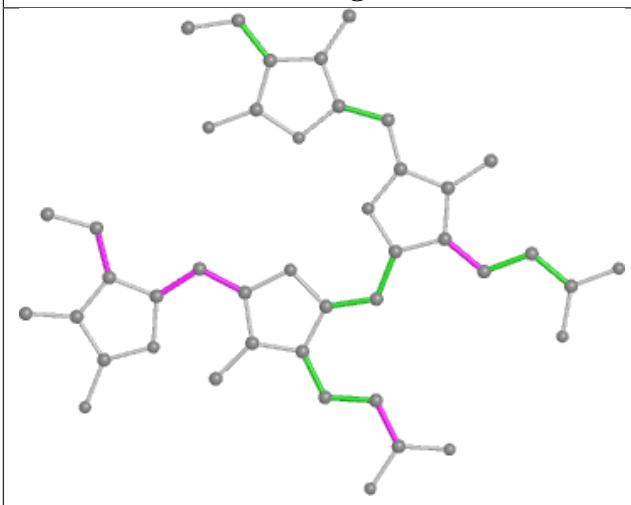
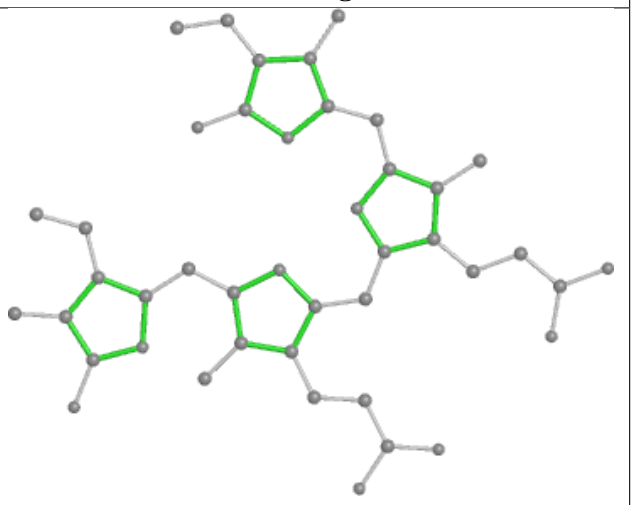
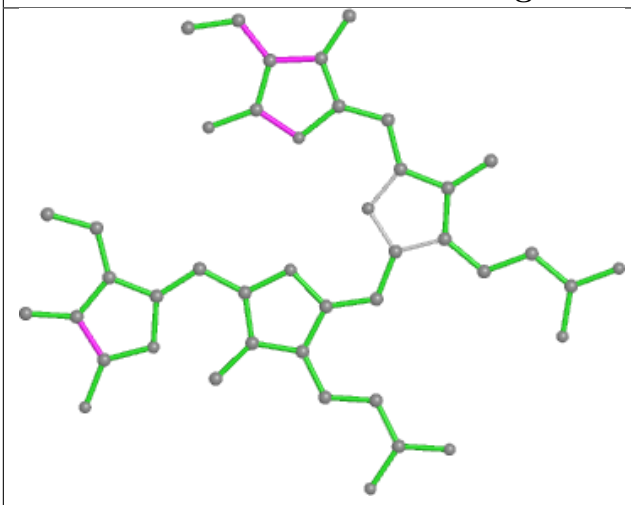


Torsions



Rings

Ligand PEB D4 201



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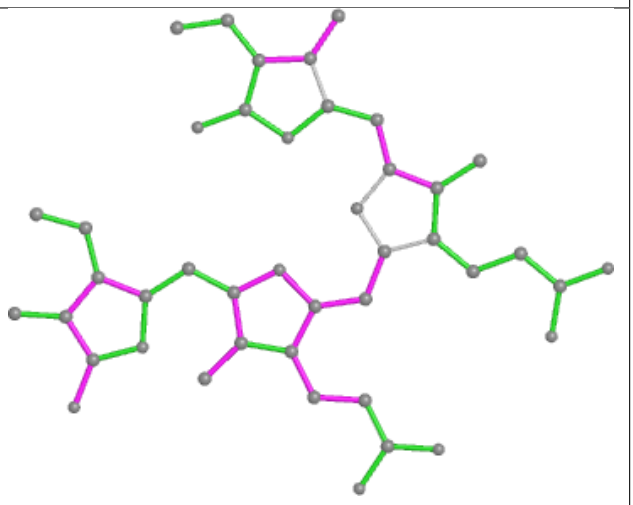

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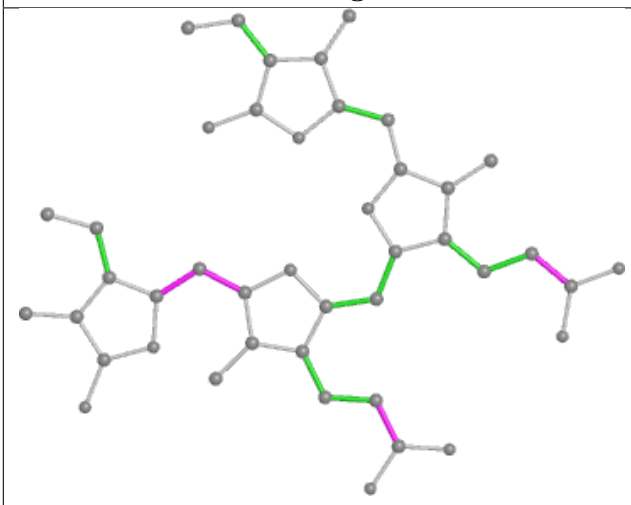

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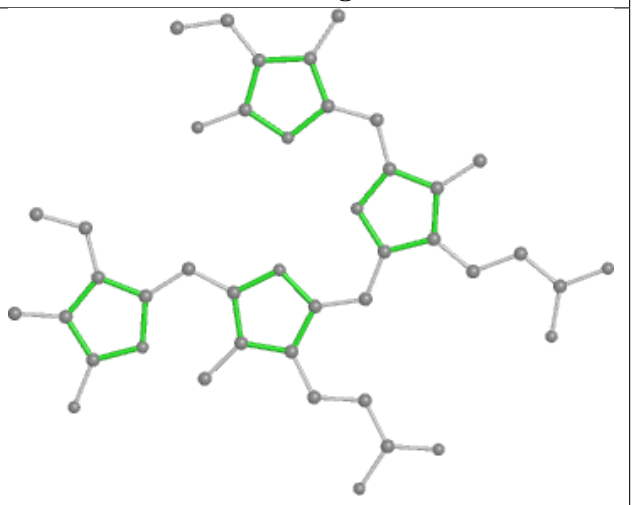
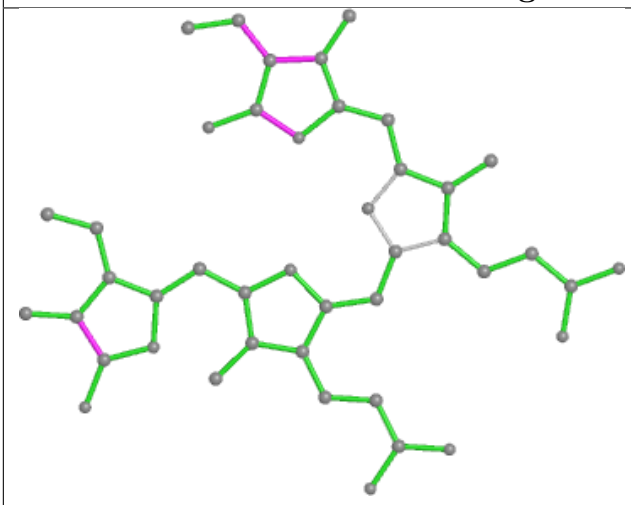


Rings

Ligand PEB dv 201



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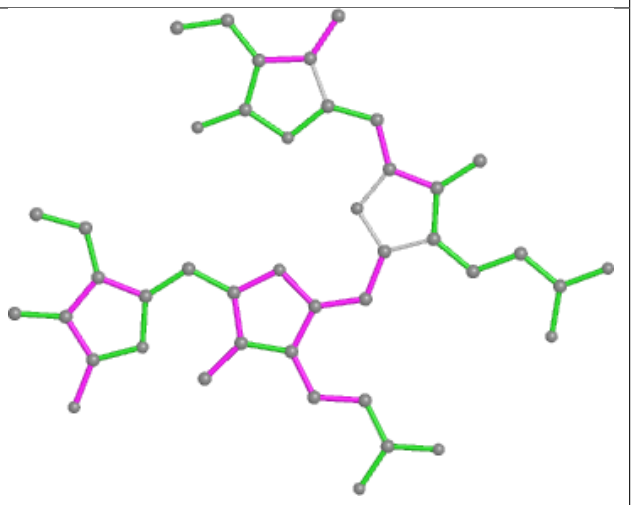

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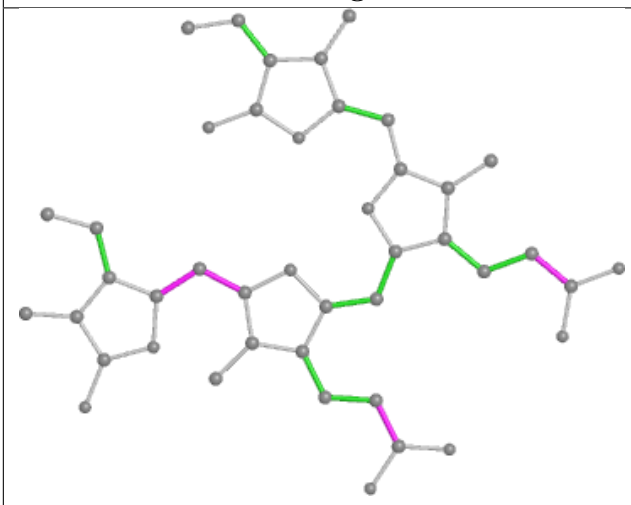

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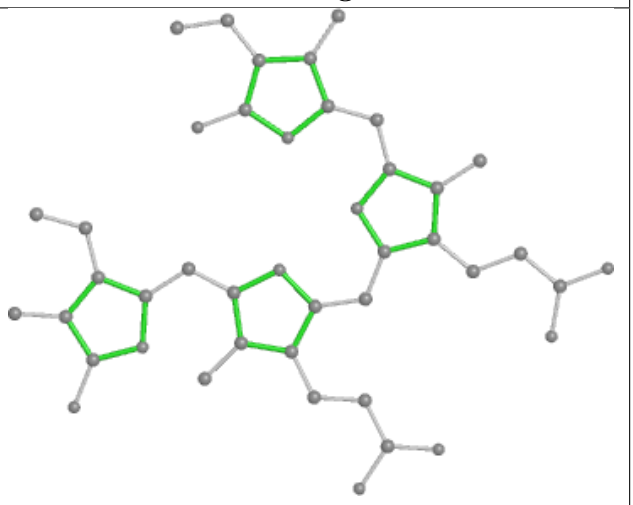
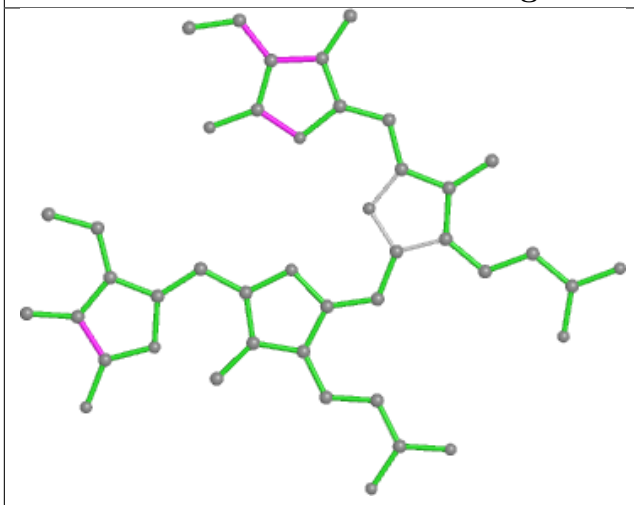


Rings

Ligand PEB J3 201



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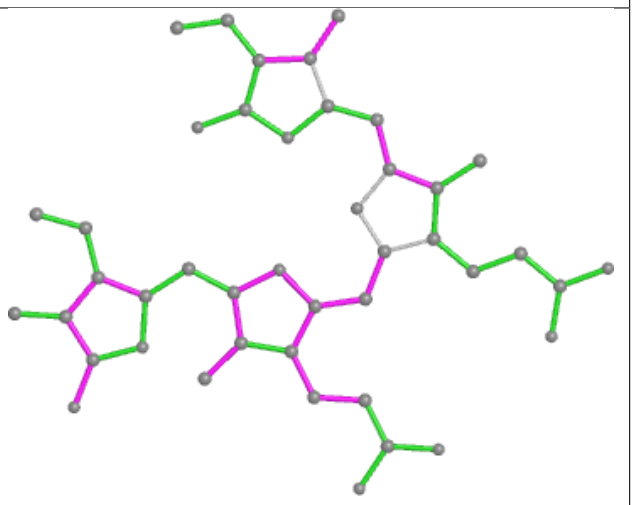

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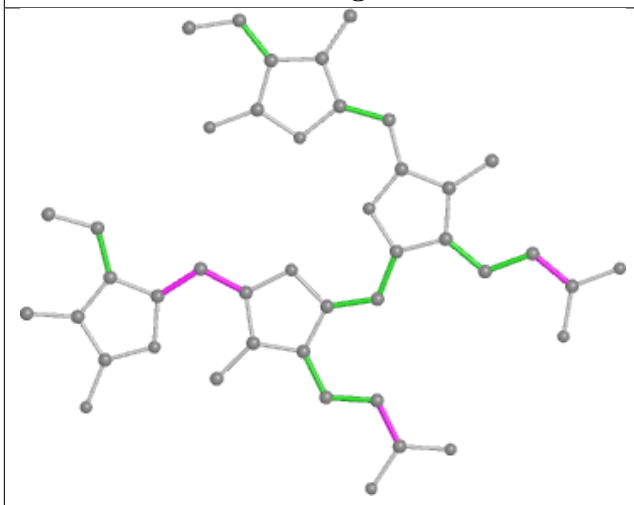

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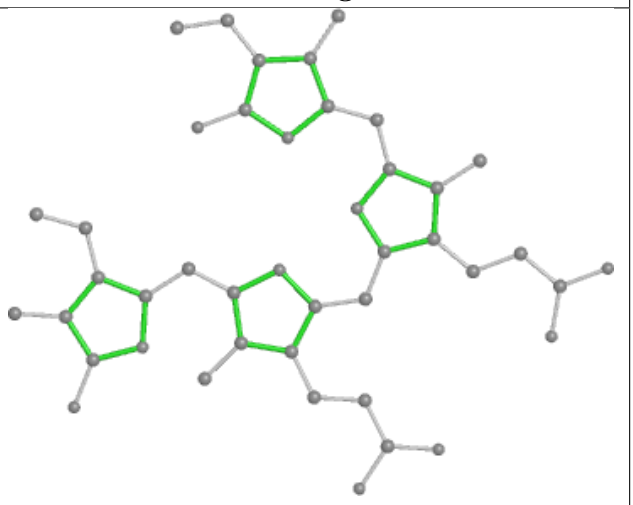
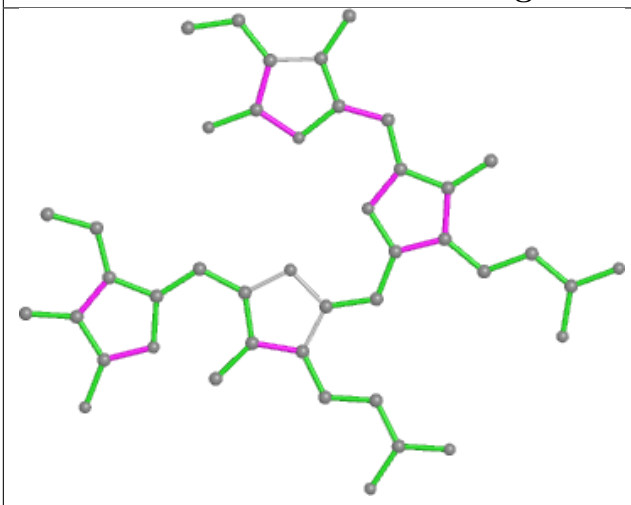


Rings

Ligand PUB E8 203



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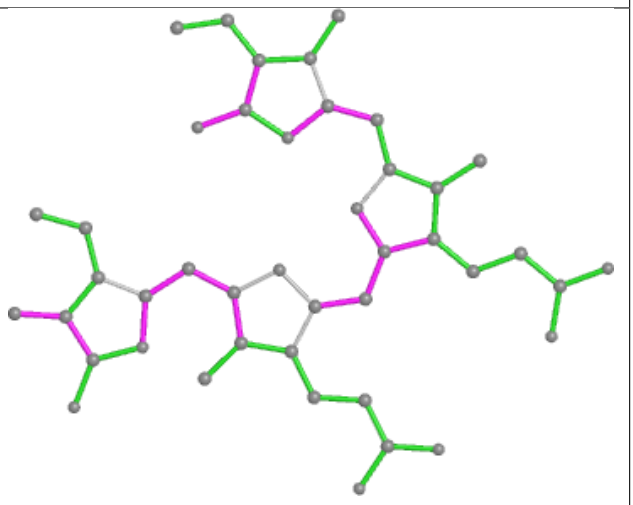

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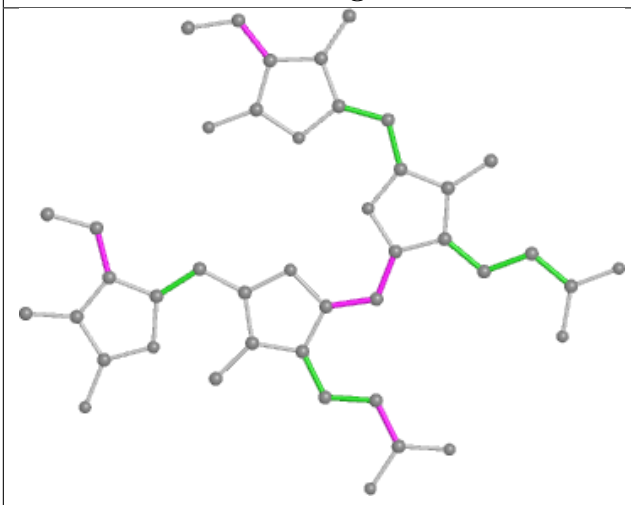

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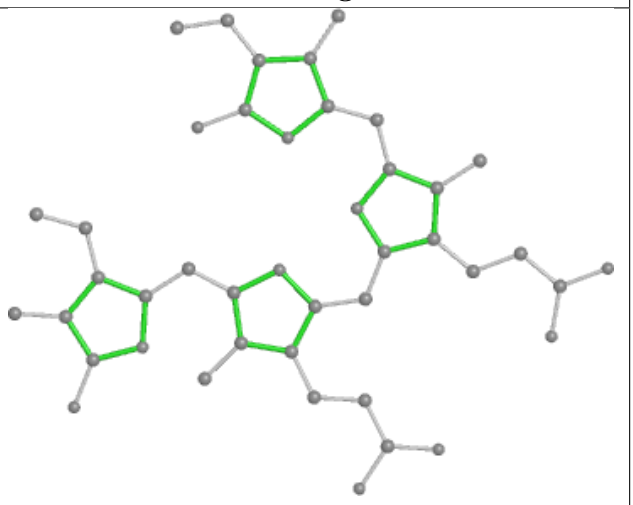
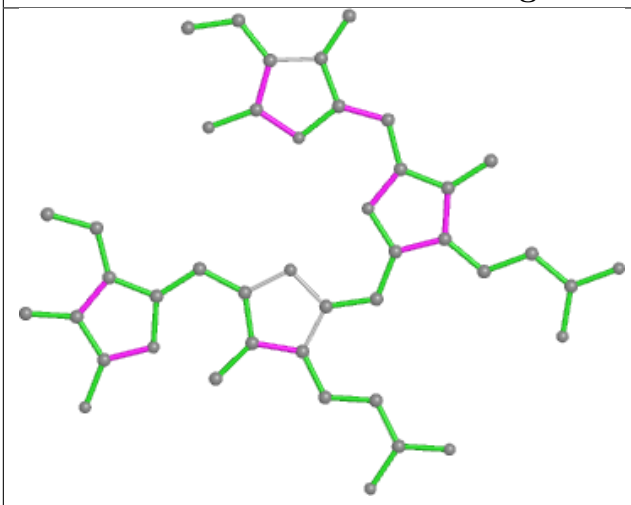


Rings

Ligand PUB r3 203



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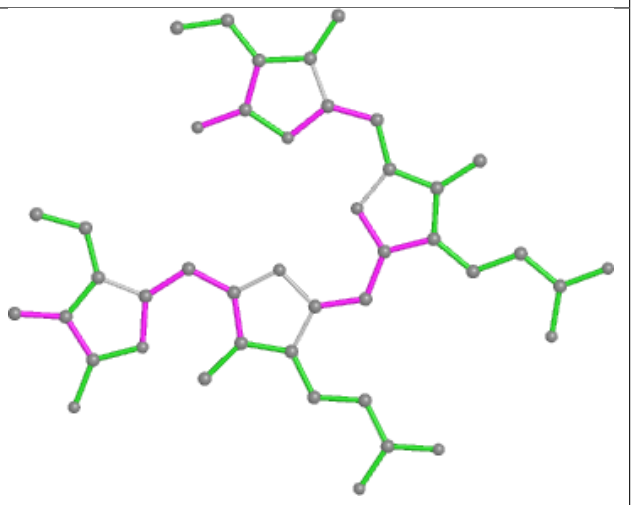

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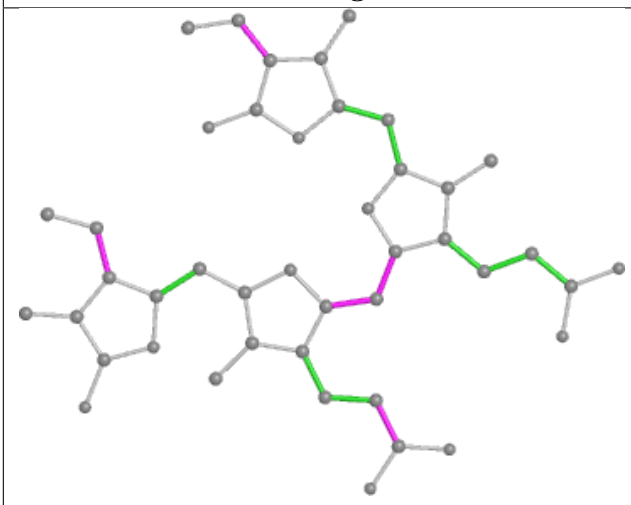

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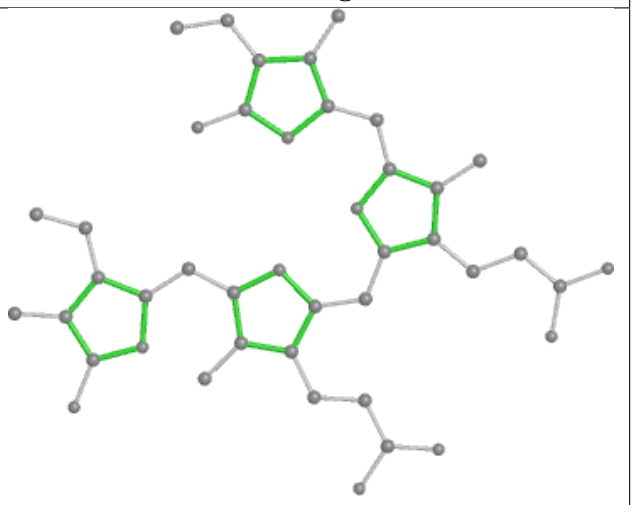
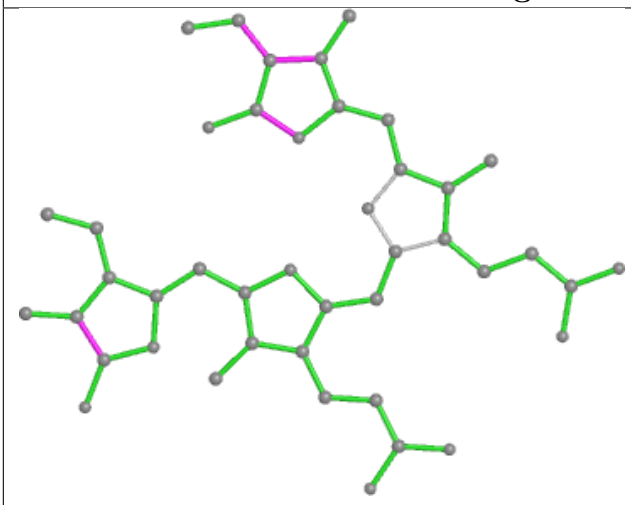


Rings

Ligand PEB m8 202



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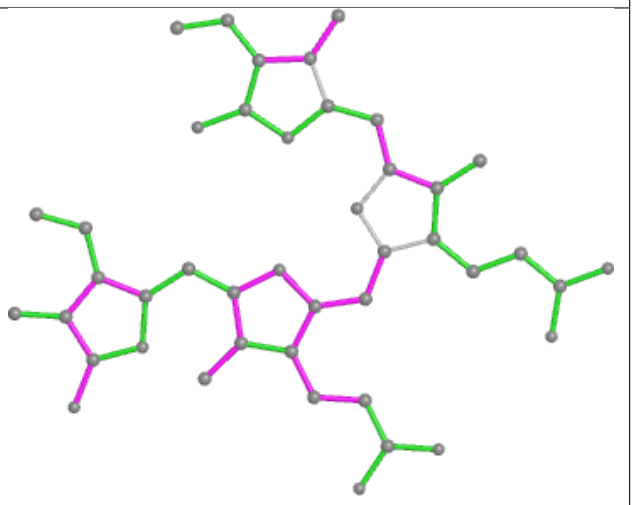

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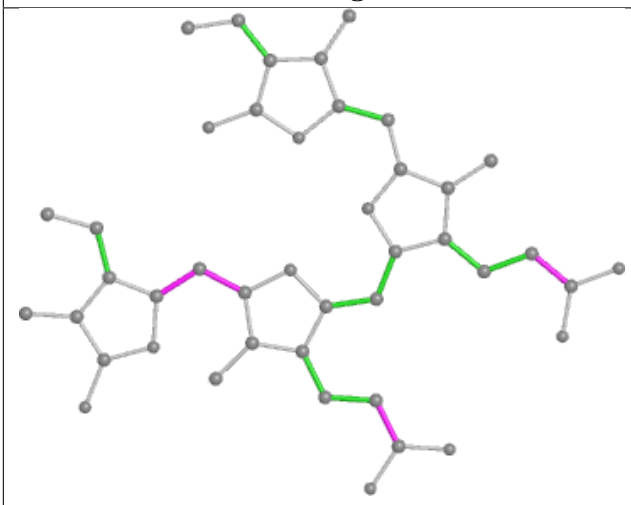

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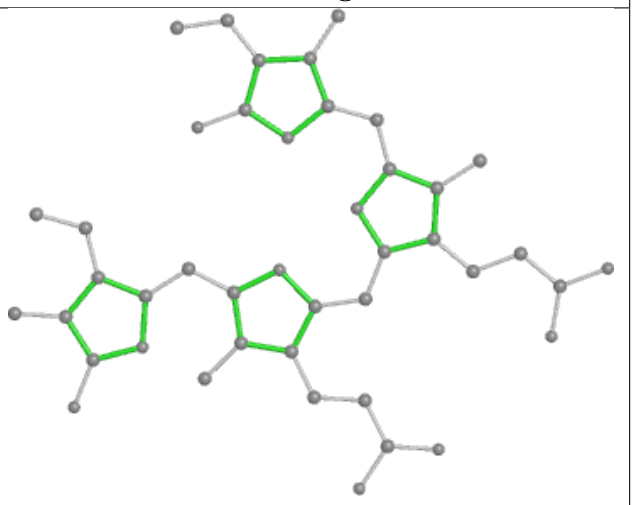

Rings

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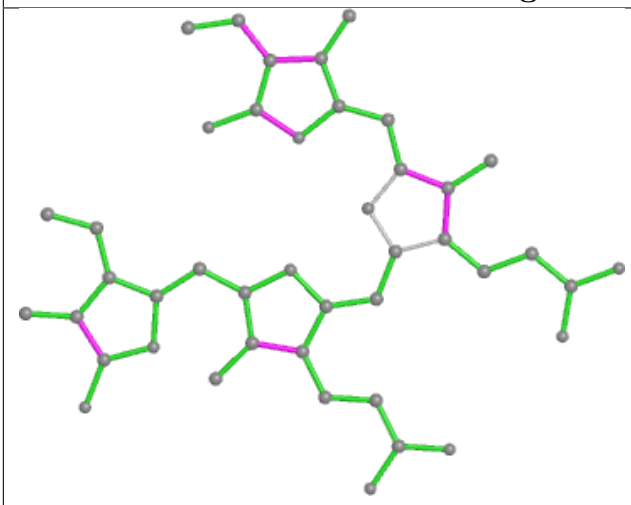

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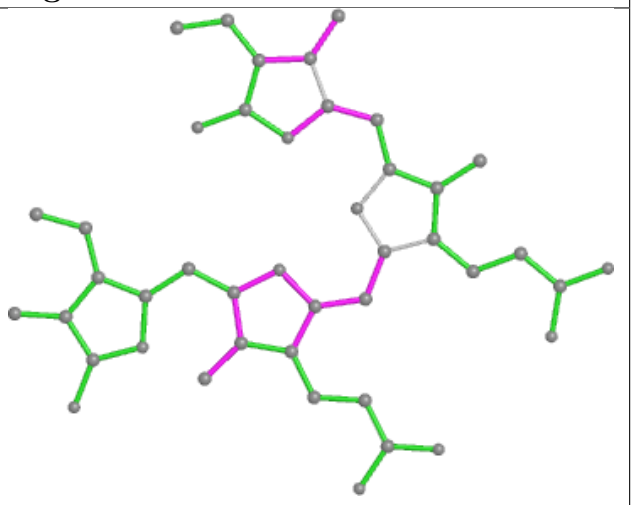

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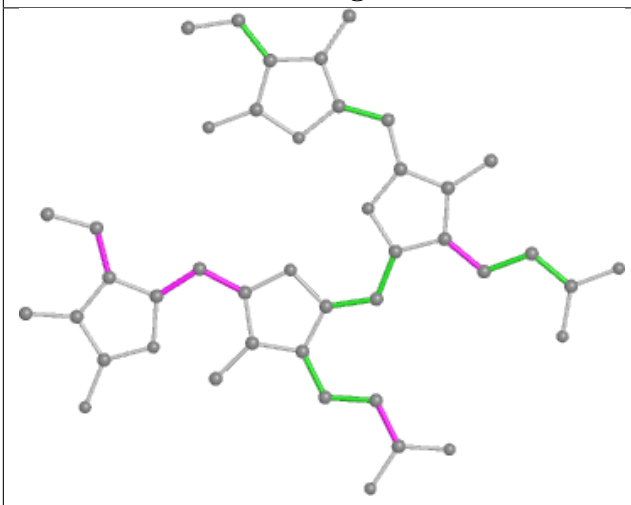

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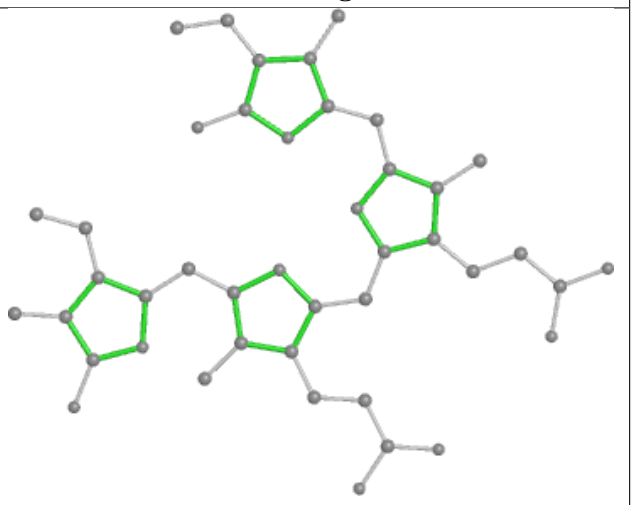
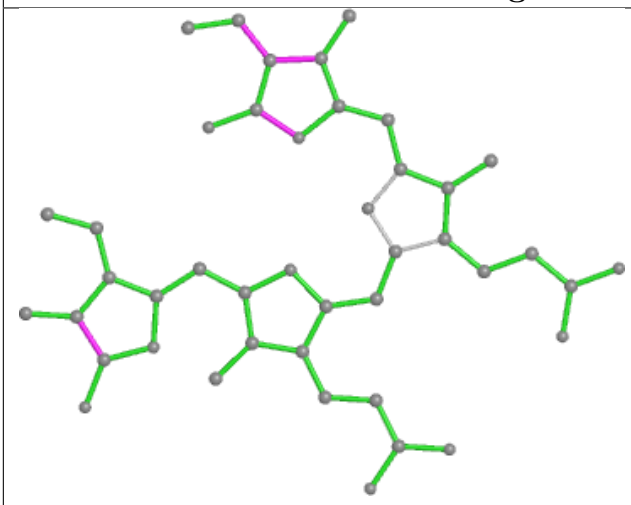


Rings

Ligand PEB cT 1002



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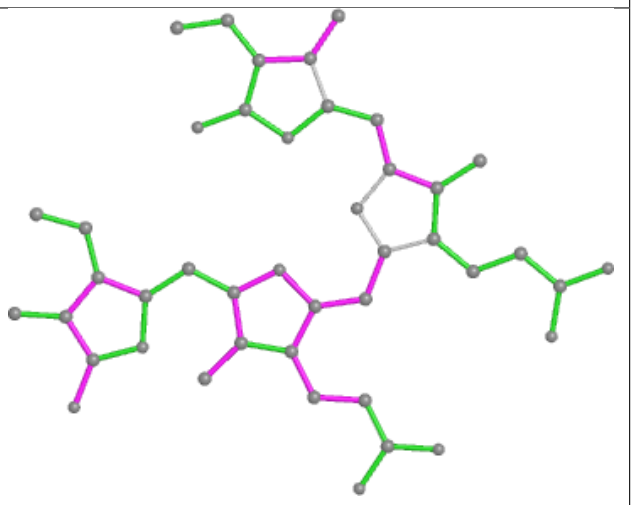
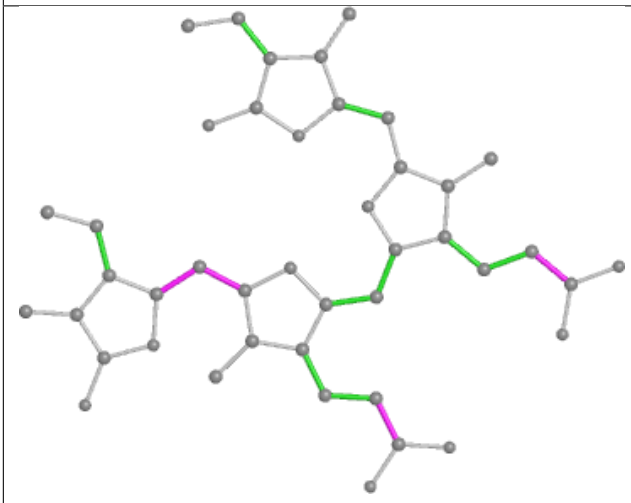


Bond angles



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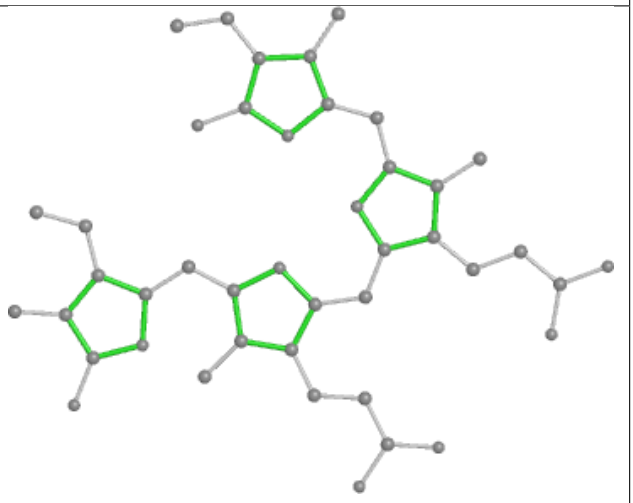
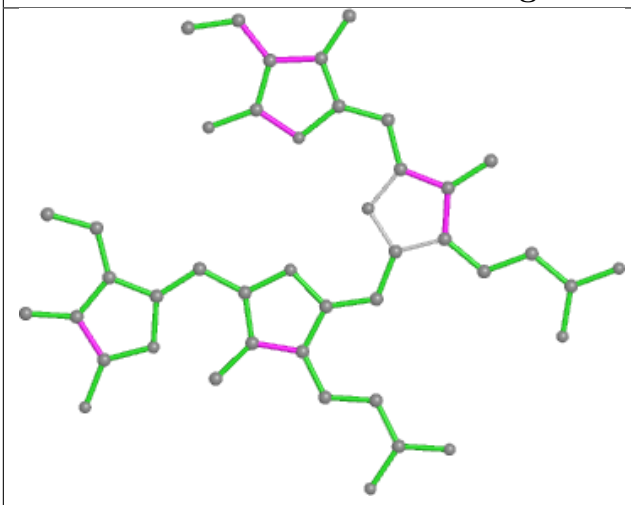


Rings

Ligand PEB J7 201



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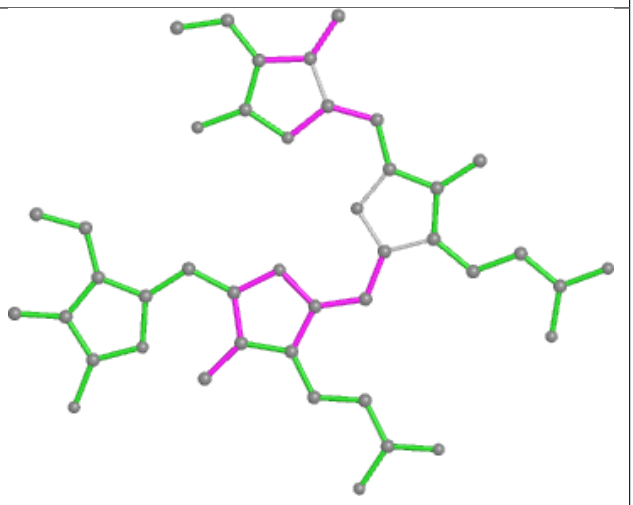

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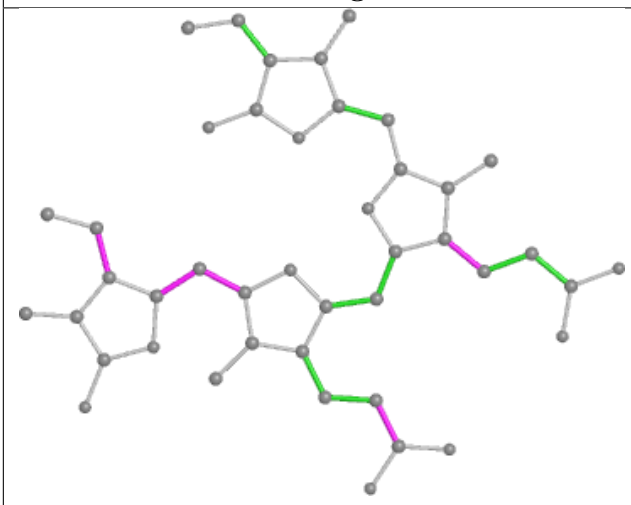

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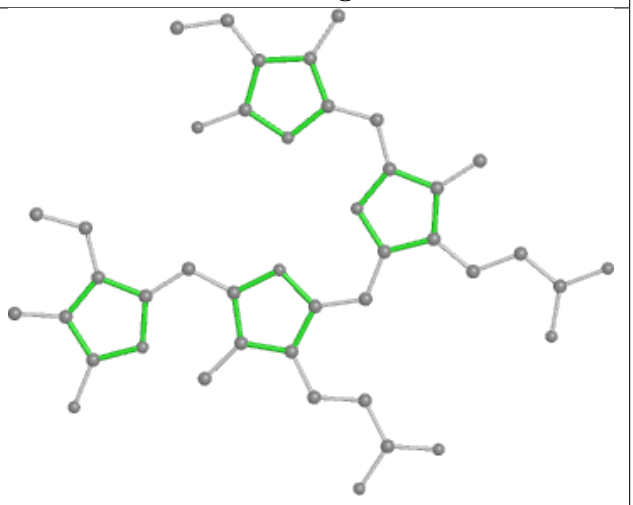

Rings

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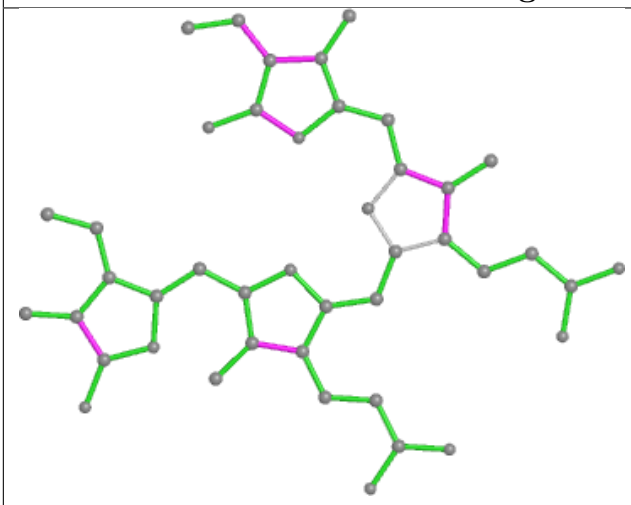

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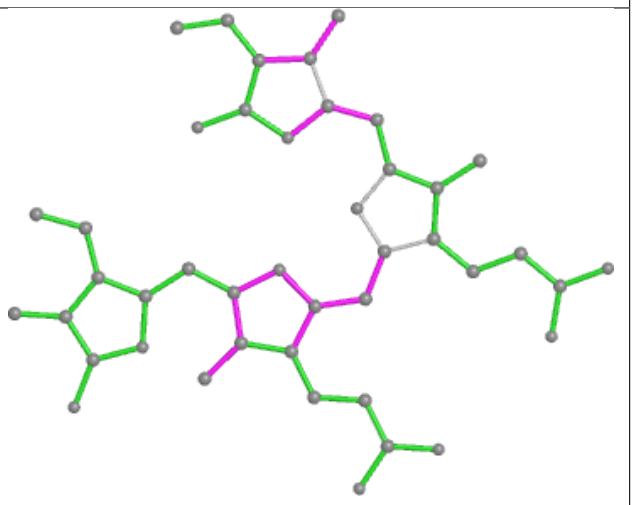

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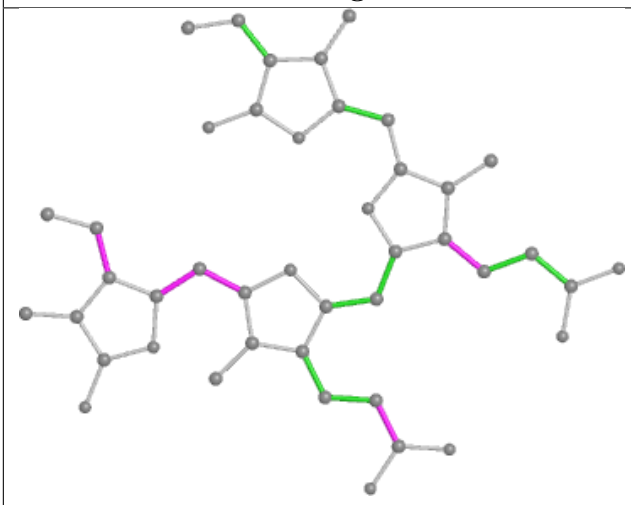

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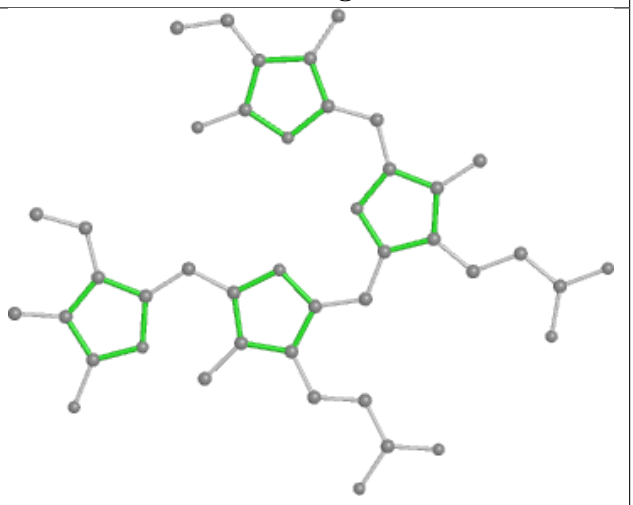
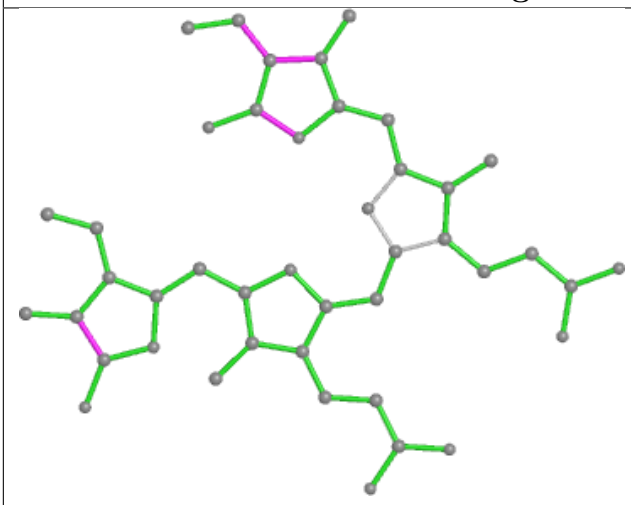


Rings

Ligand PEB ca 1001



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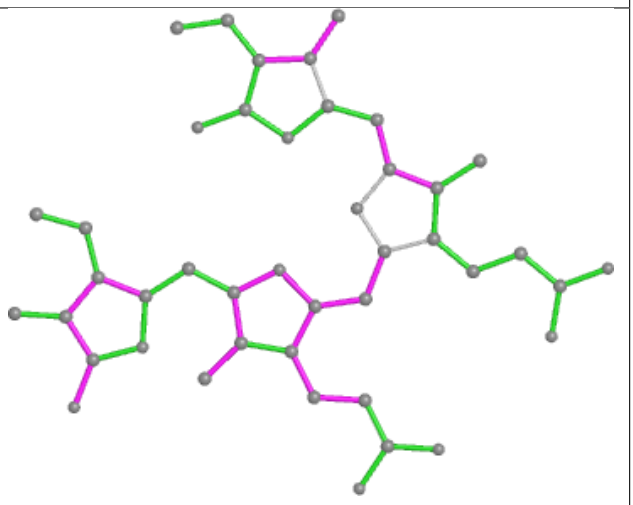

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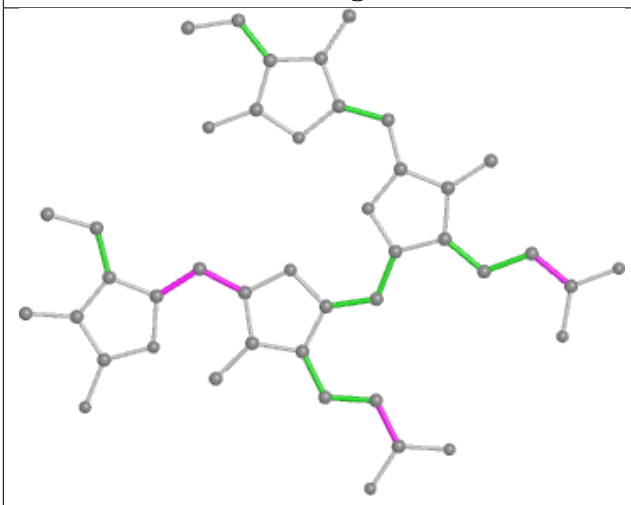

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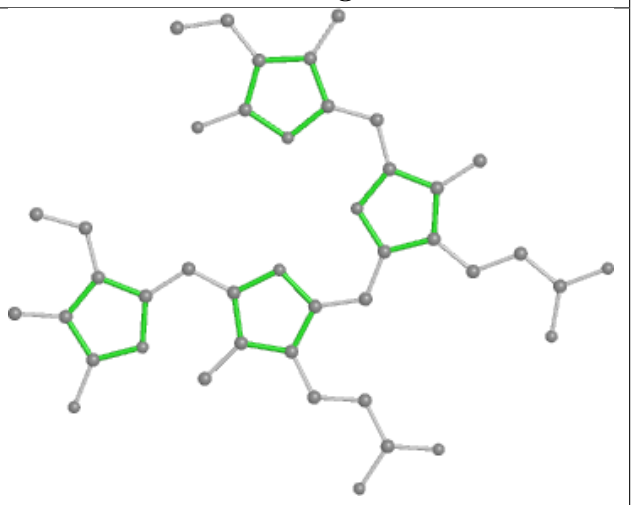
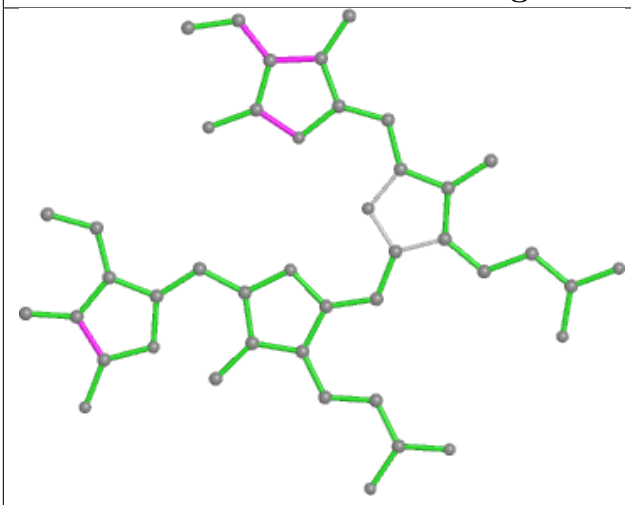


Rings

Ligand PEB 34 1007



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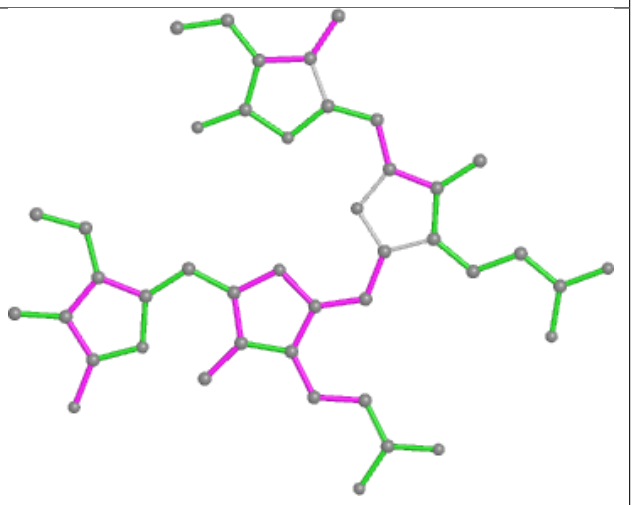

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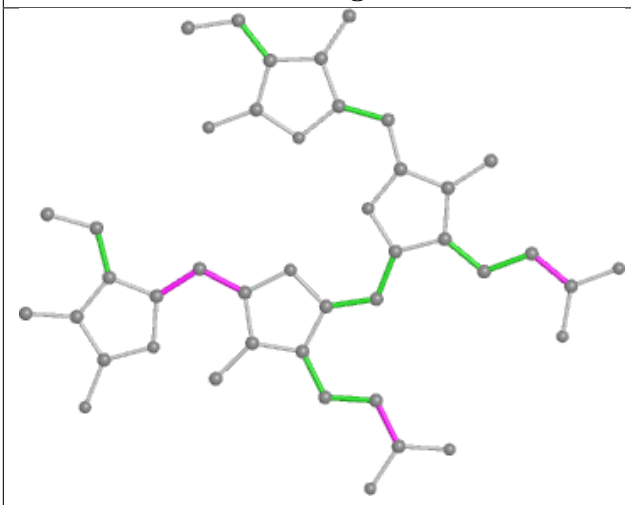

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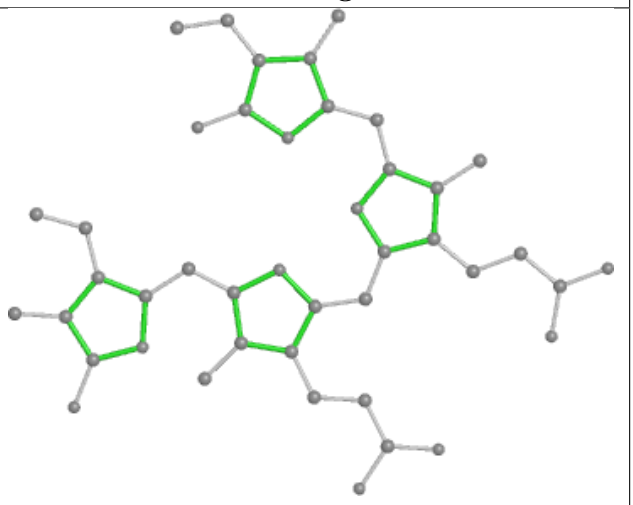
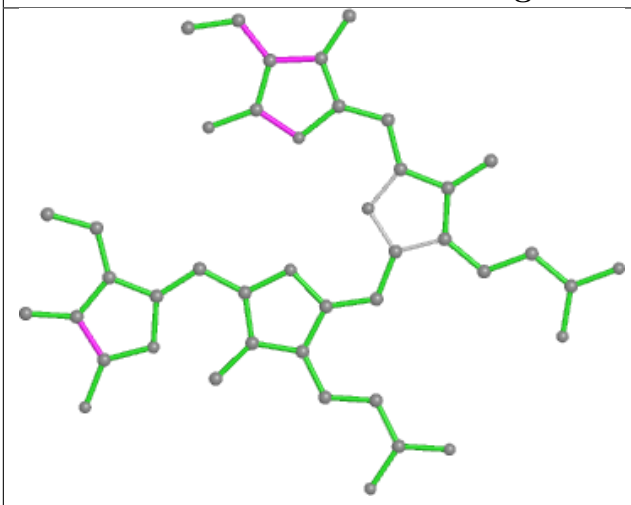


Rings

Ligand PEB dQ 201



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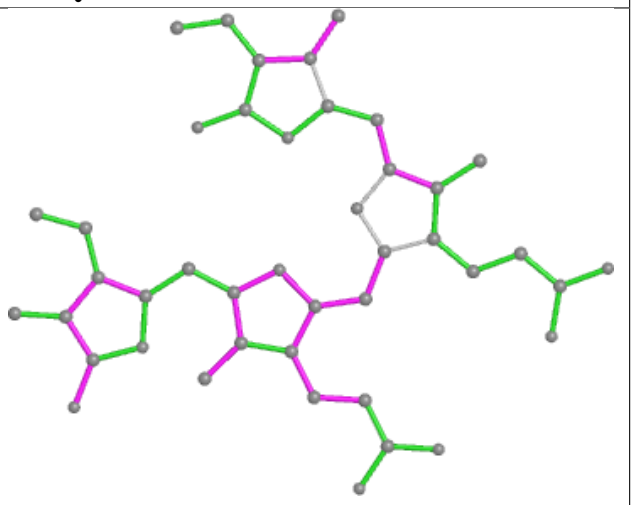
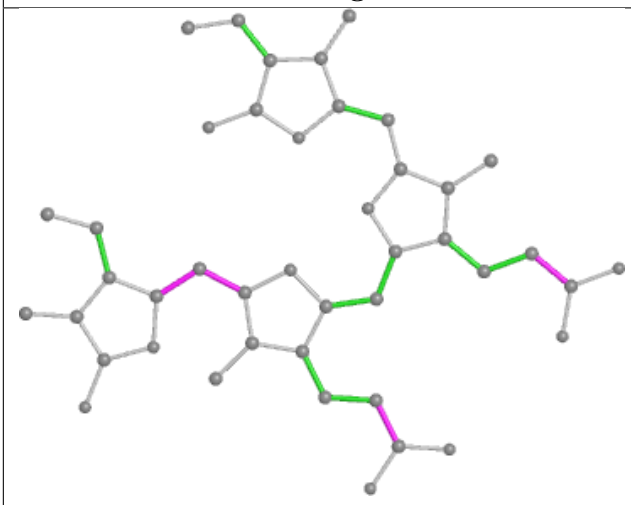


Bond angles



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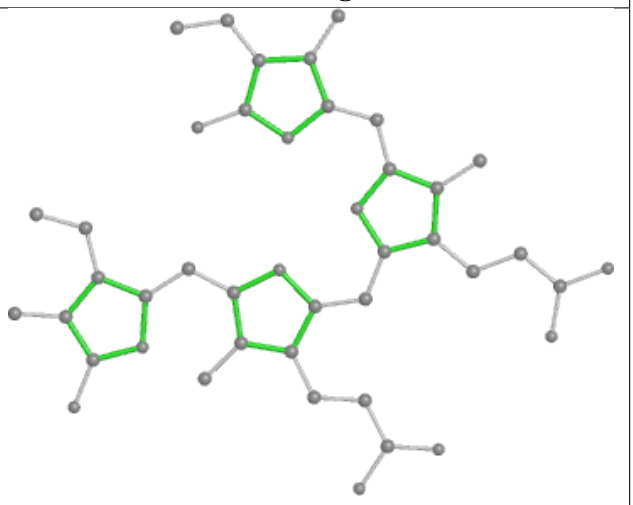
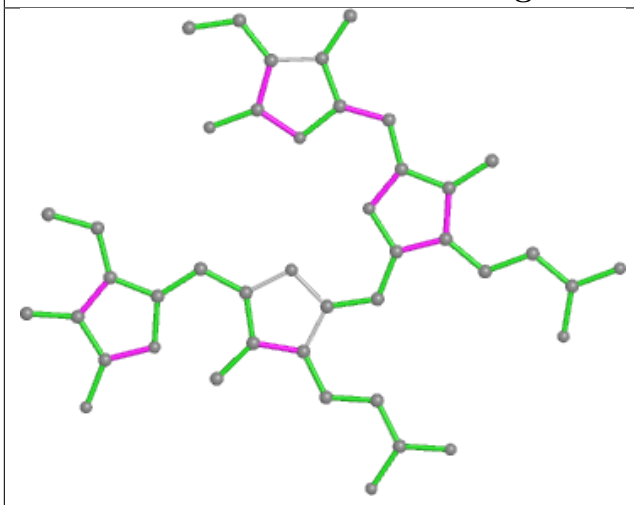
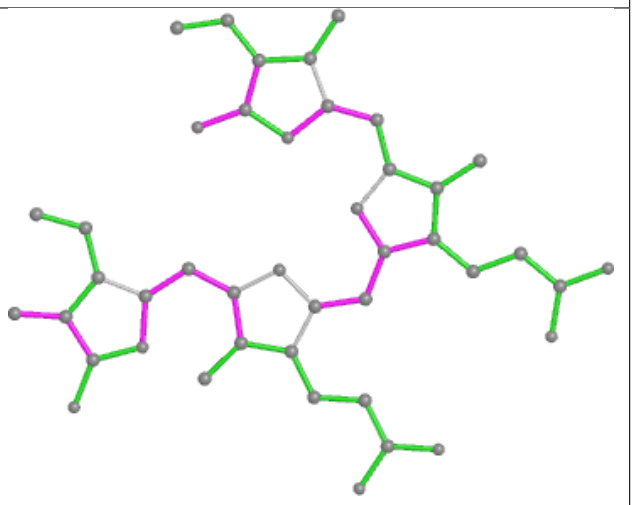


Rings

Ligand PUB C2 305



Bond lengths



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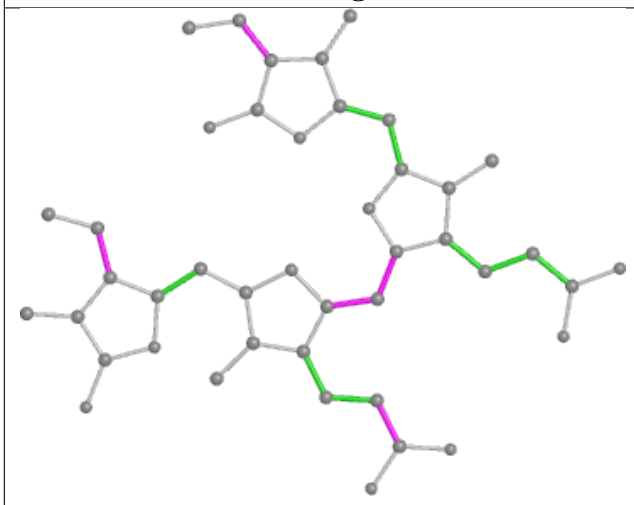
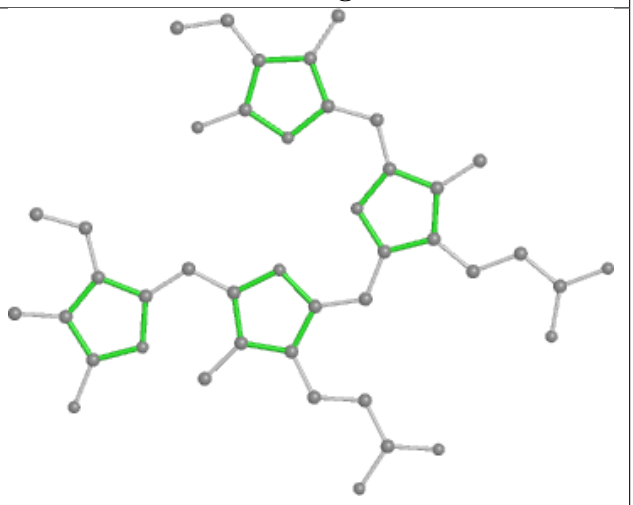
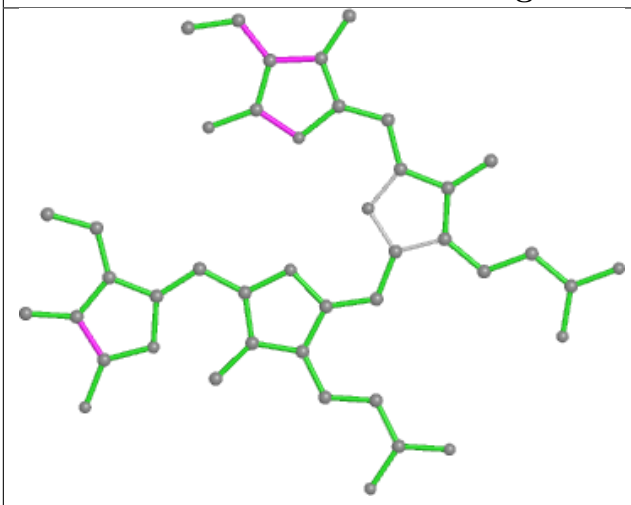


Torsions



Rings

Ligand PEB cK 201



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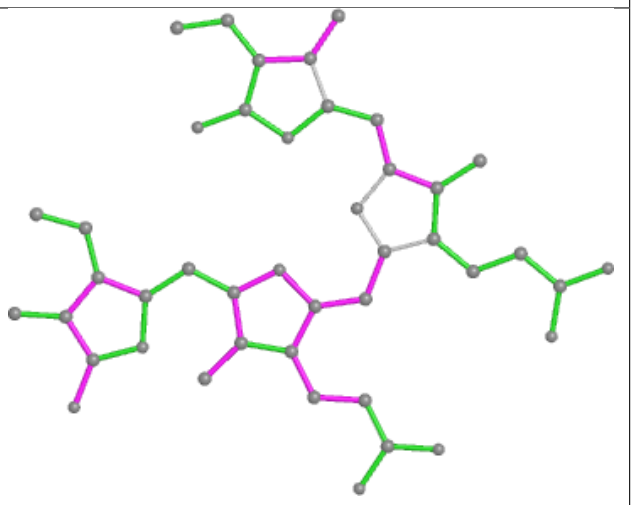

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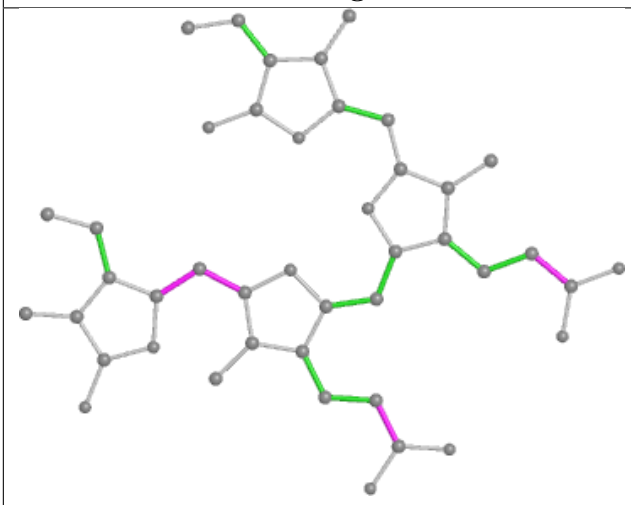

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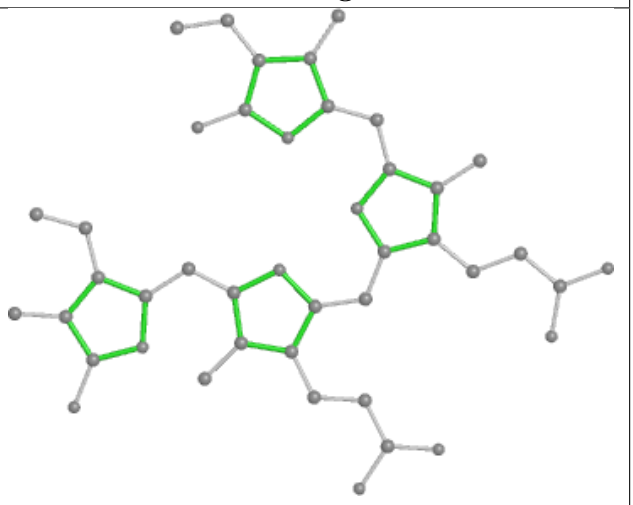
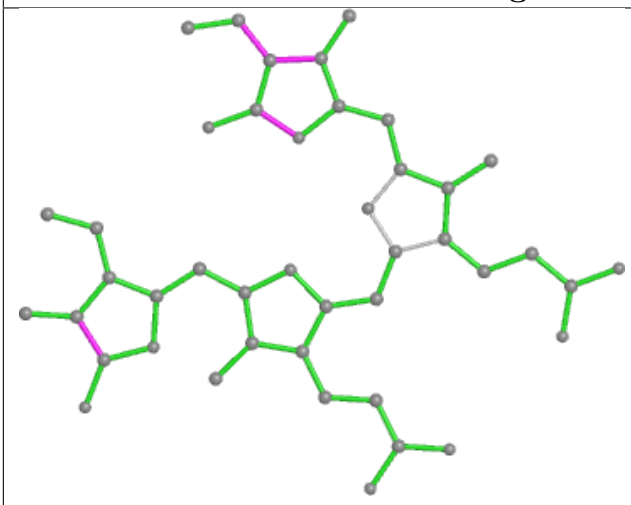


Rings

Ligand PEB dk 1002



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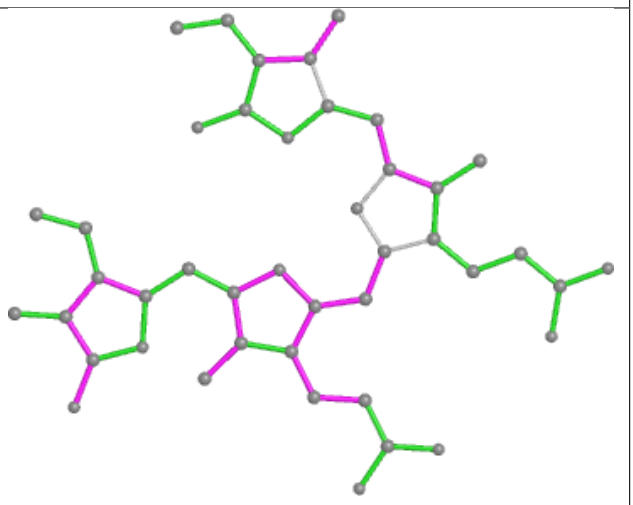

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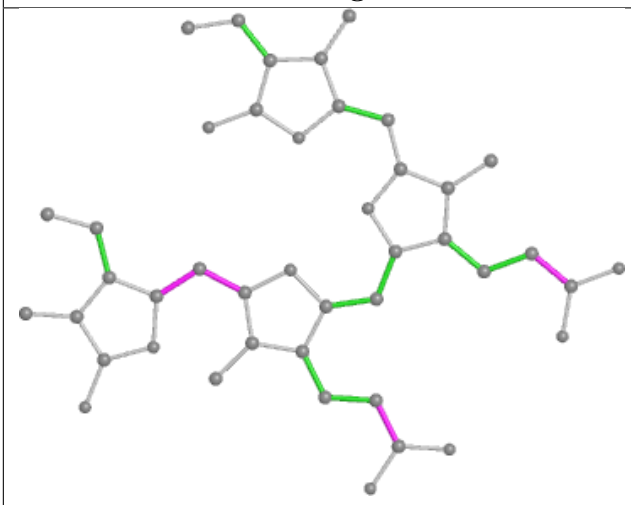

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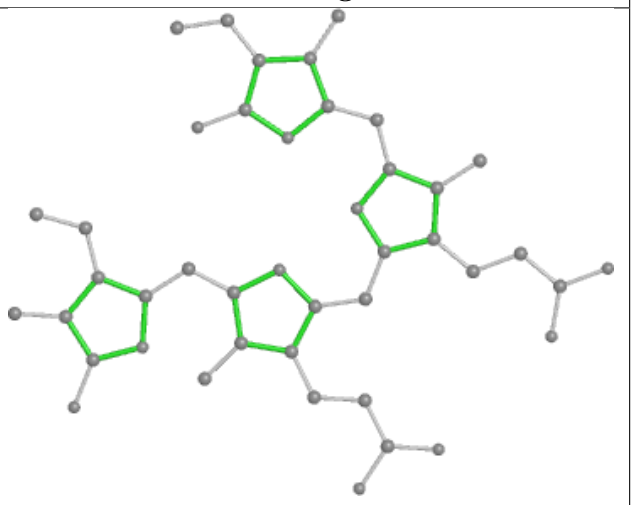
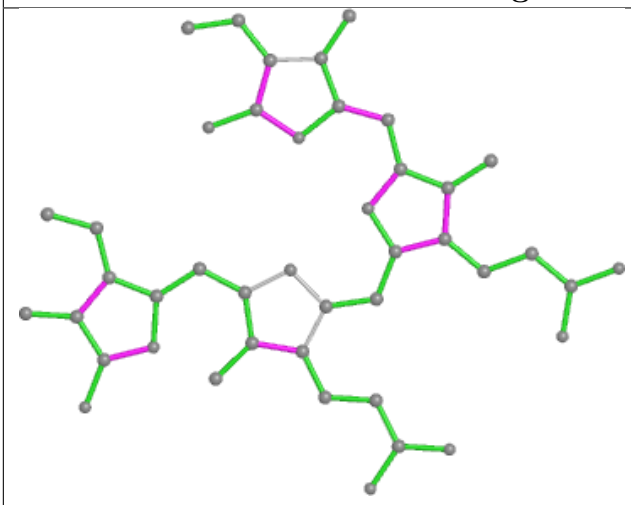


Rings

Ligand PUB bH 203



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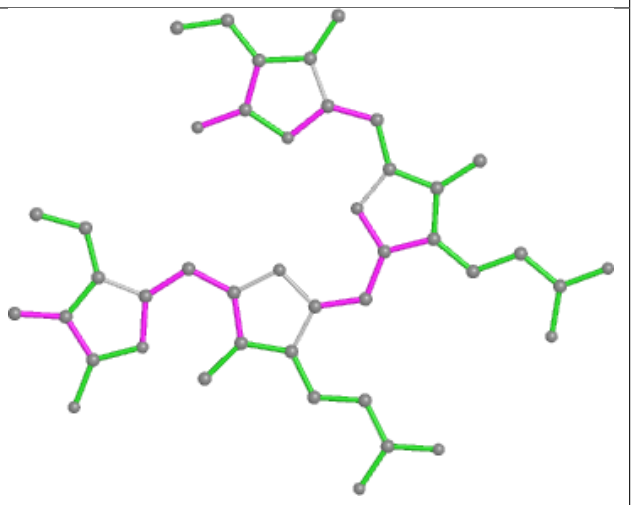

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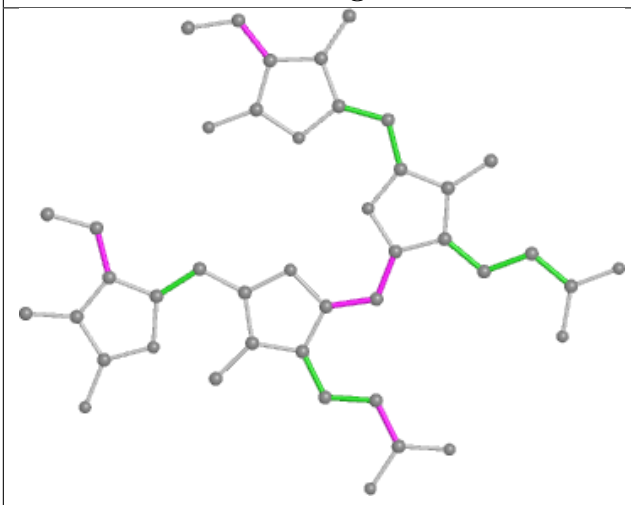

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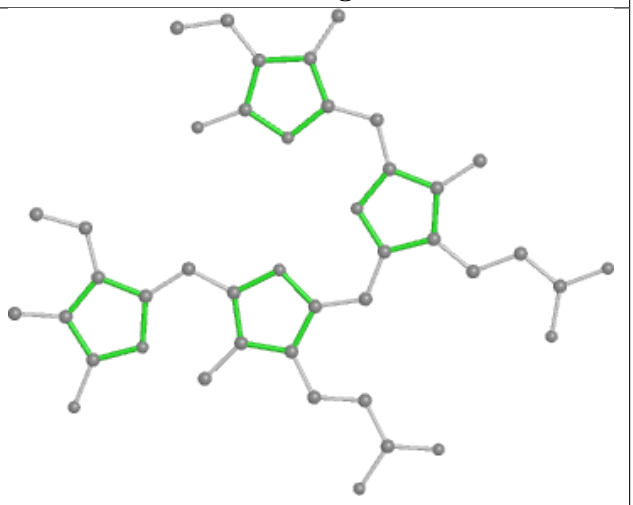

Rings

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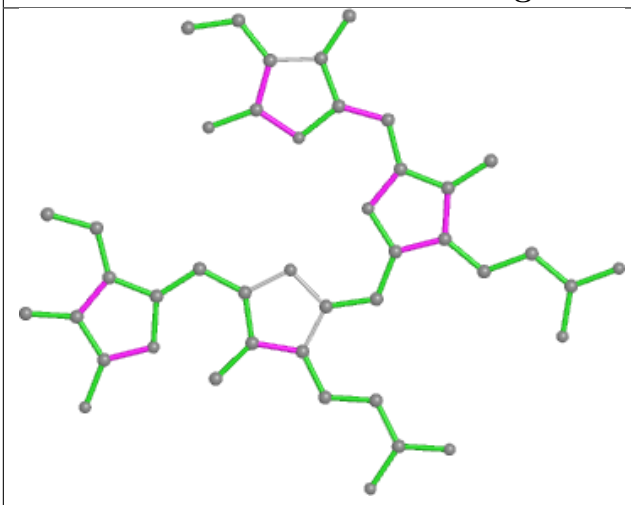

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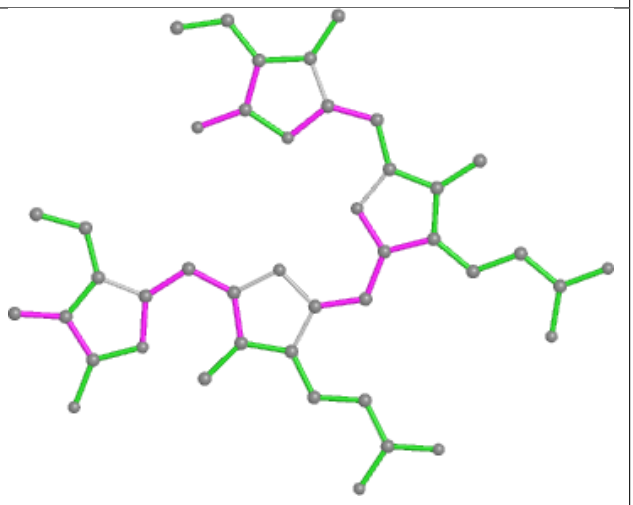

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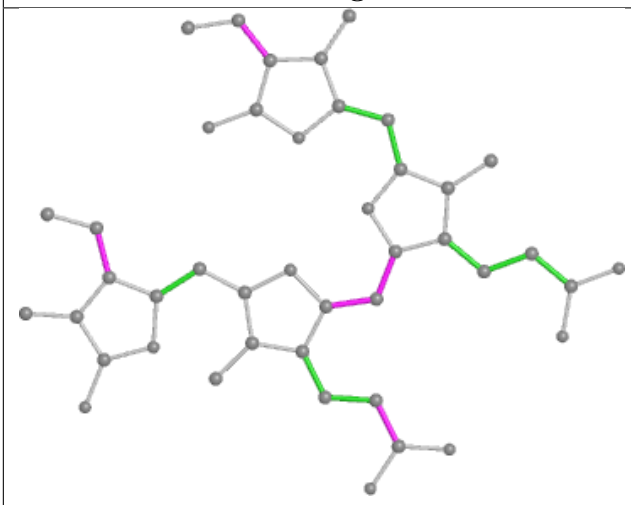

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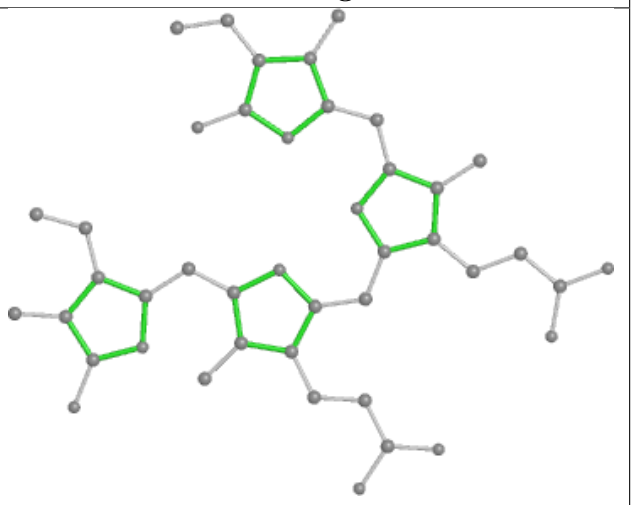
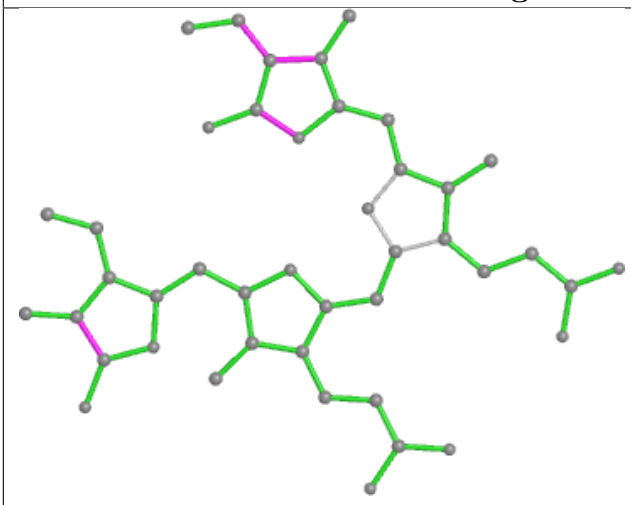


Rings

Ligand PEB a3 1001



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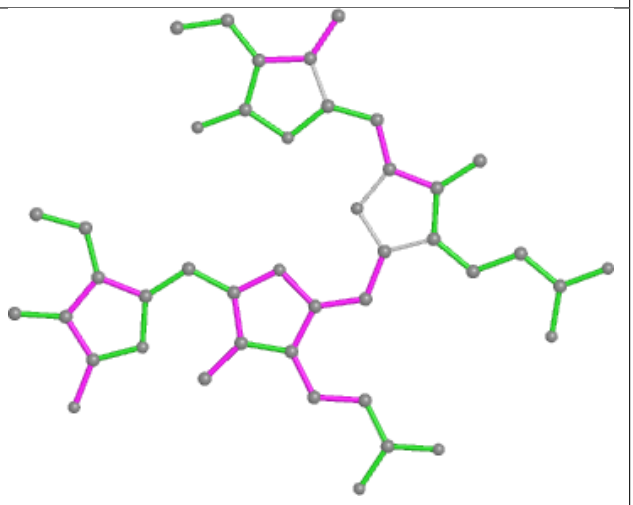

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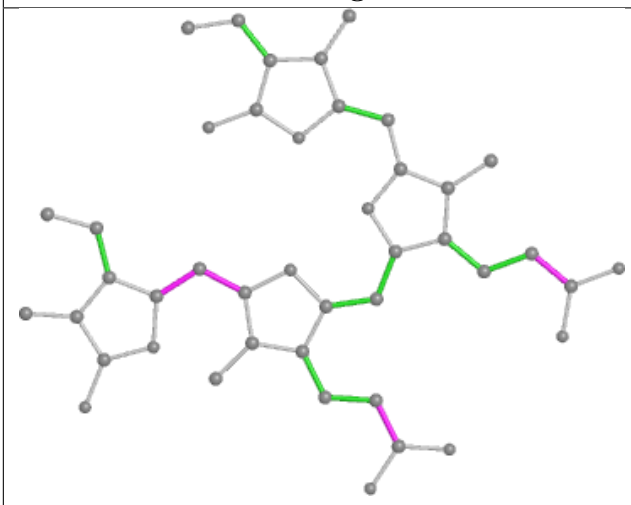

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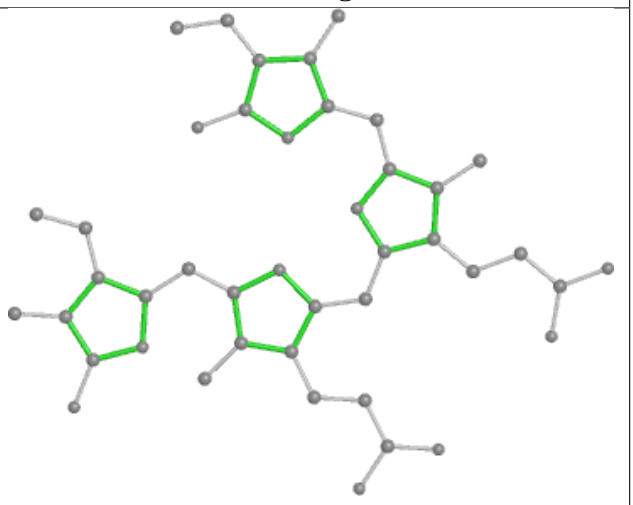

Rings

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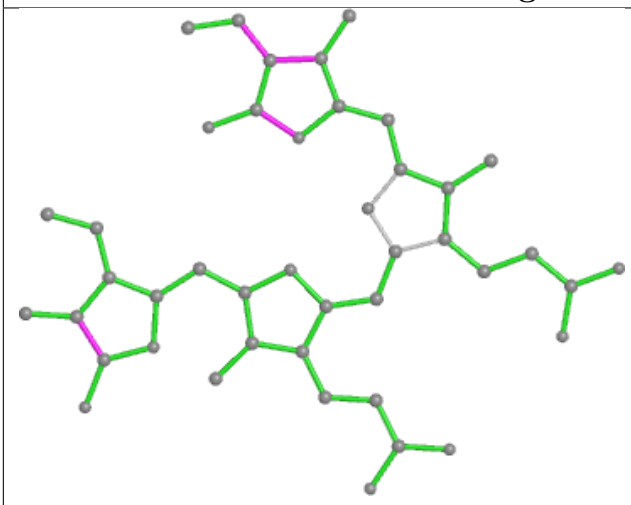

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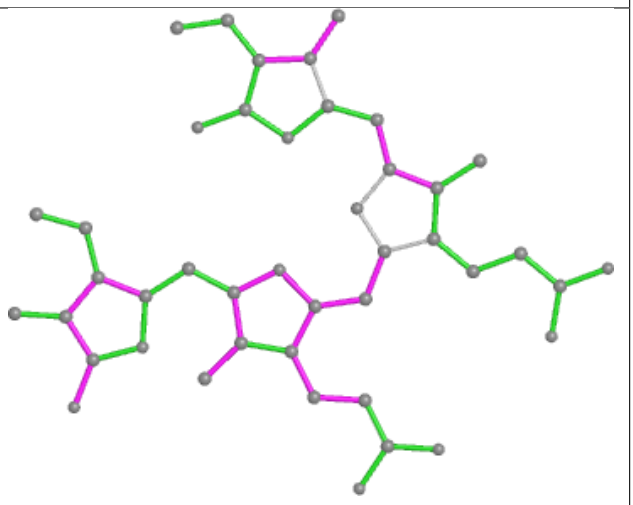

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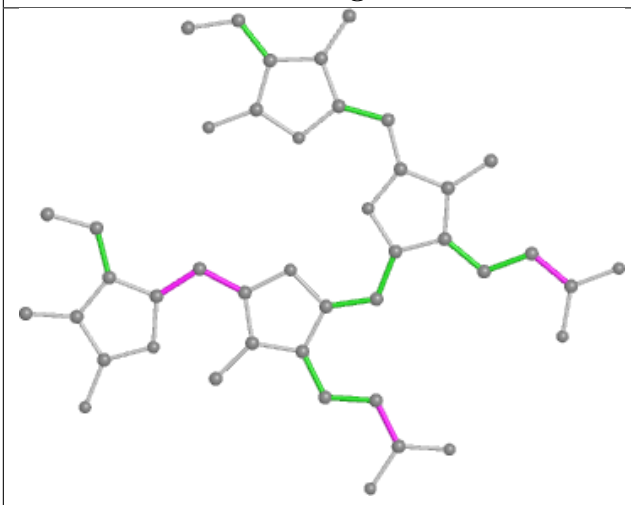

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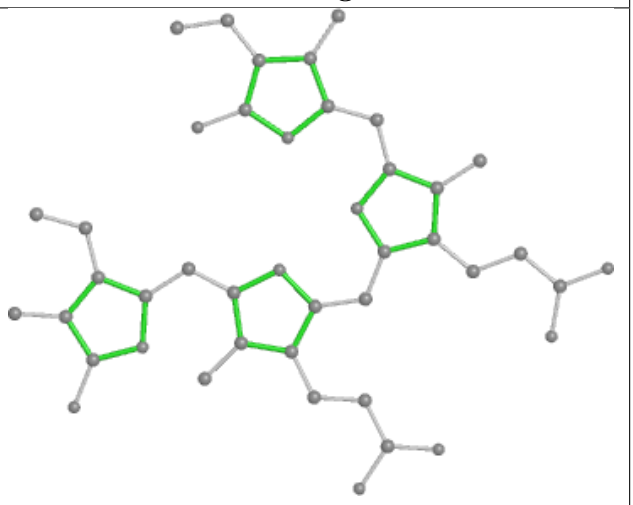
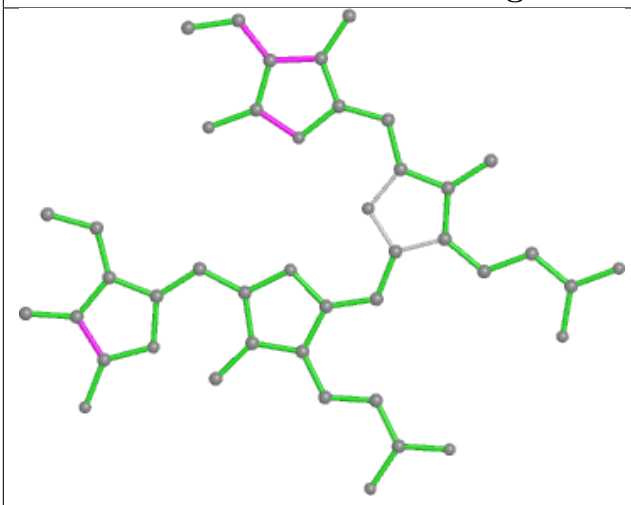


Rings

Ligand PEB A6 1001



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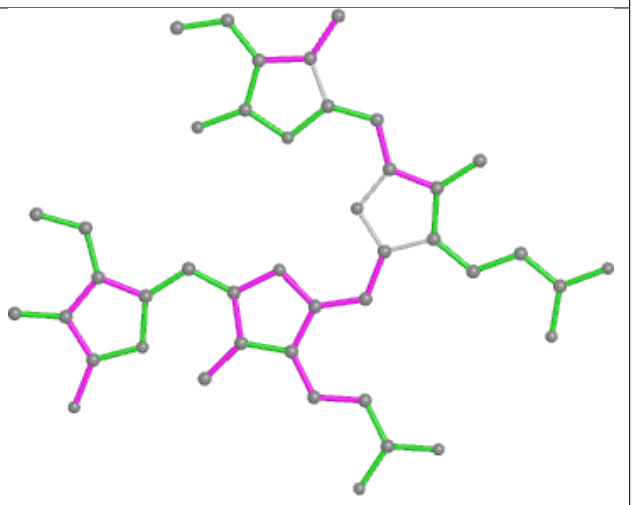

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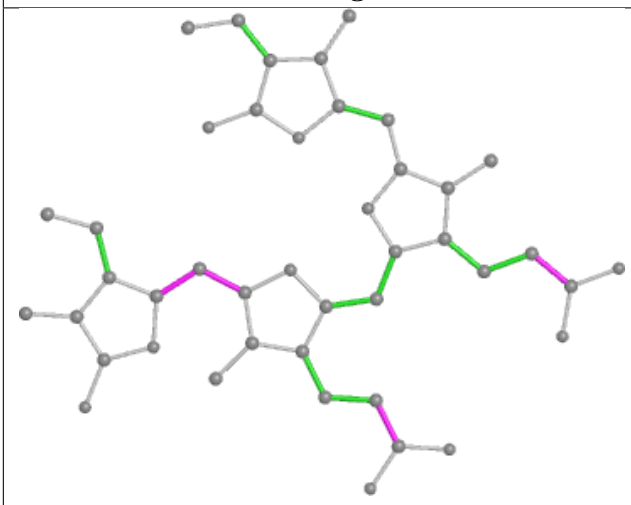

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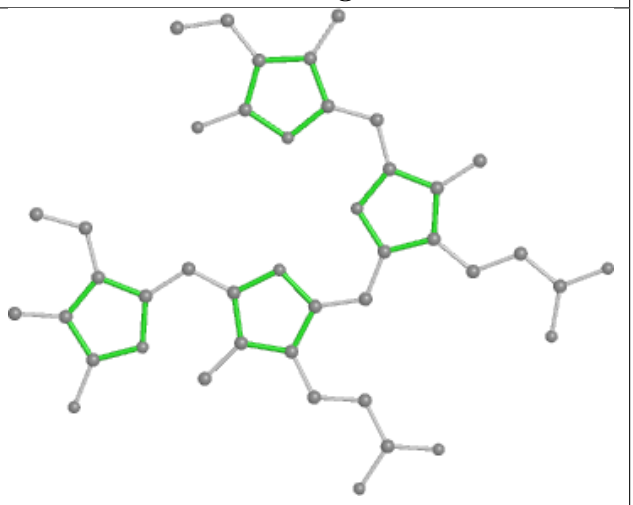
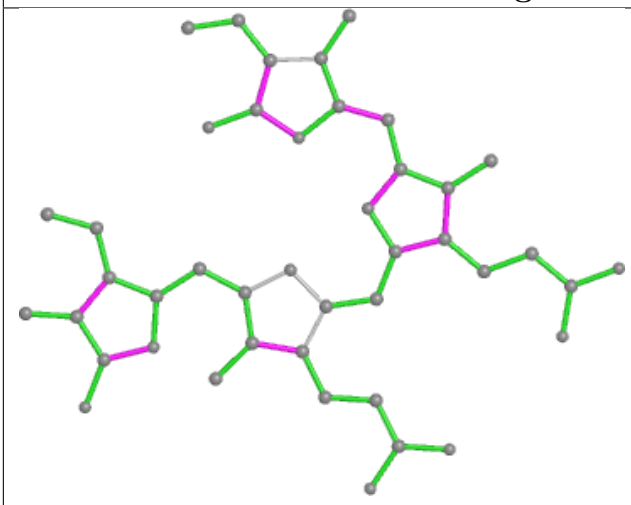


Rings

Ligand PUB aT 203



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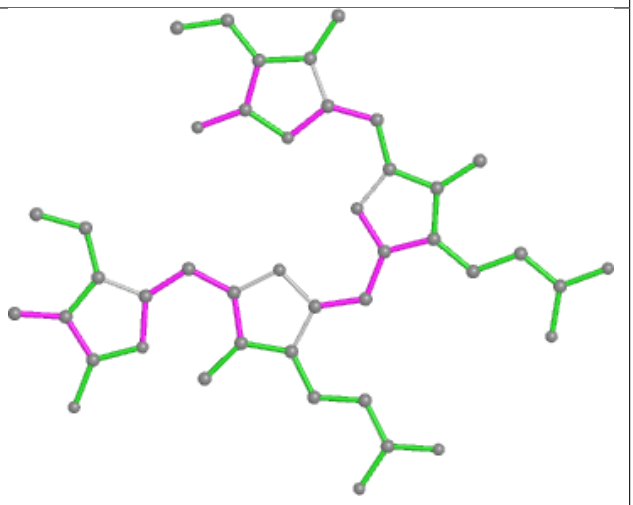

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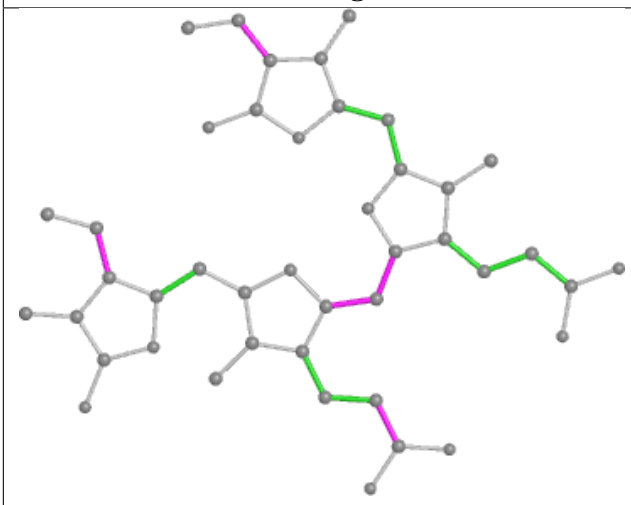

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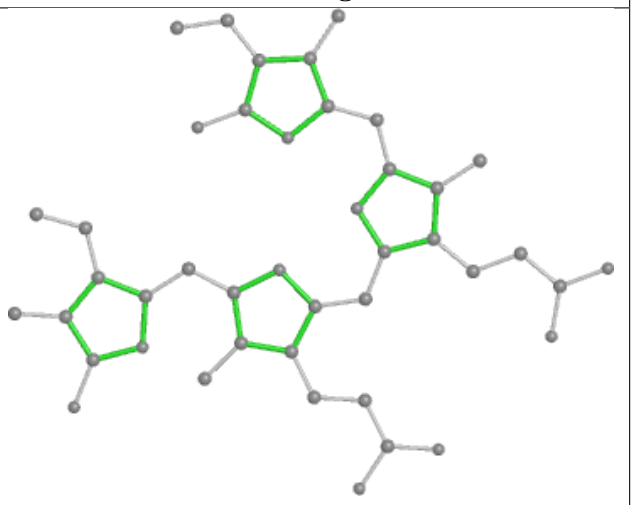
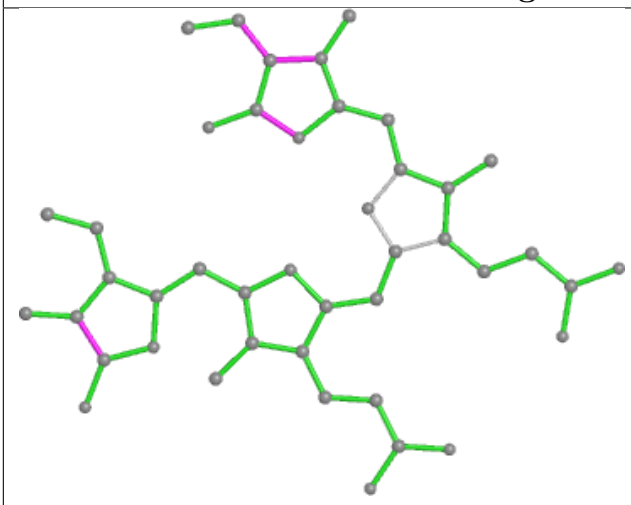


Rings

Ligand PEB dx 404



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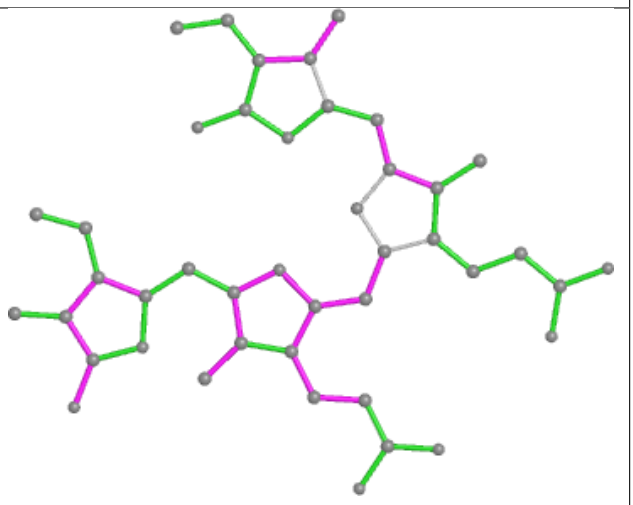

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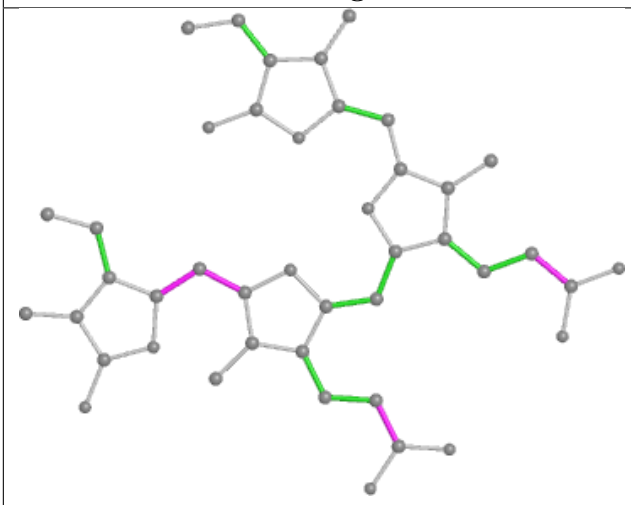

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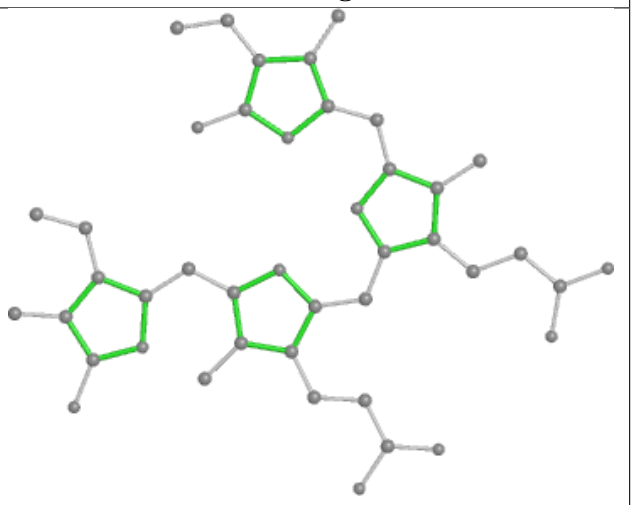
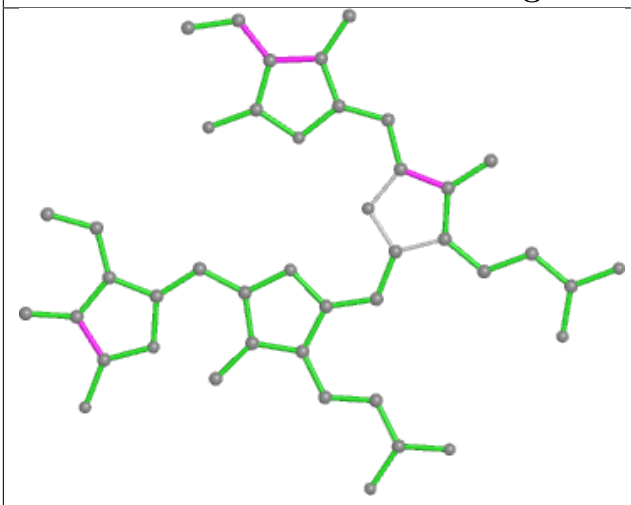


Rings

Ligand PEB f5 201



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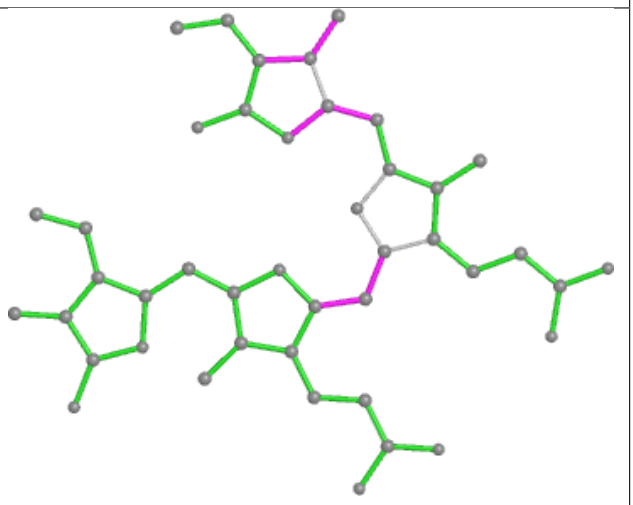

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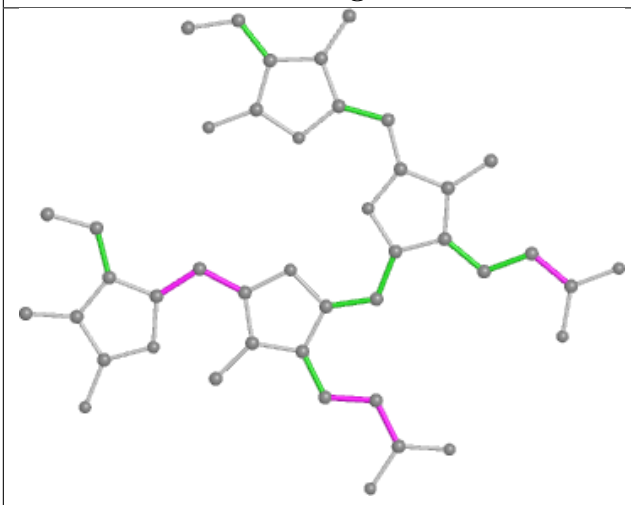

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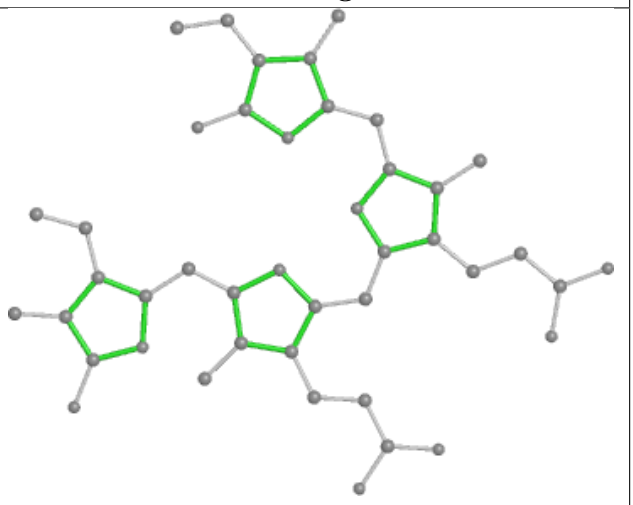
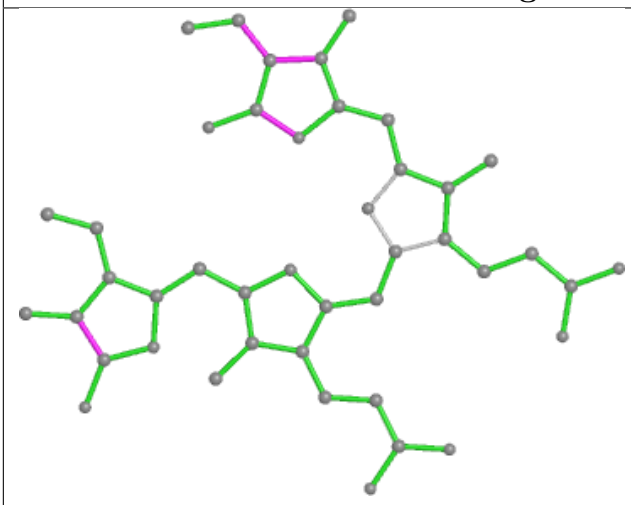


Rings

Ligand PEB k4 201



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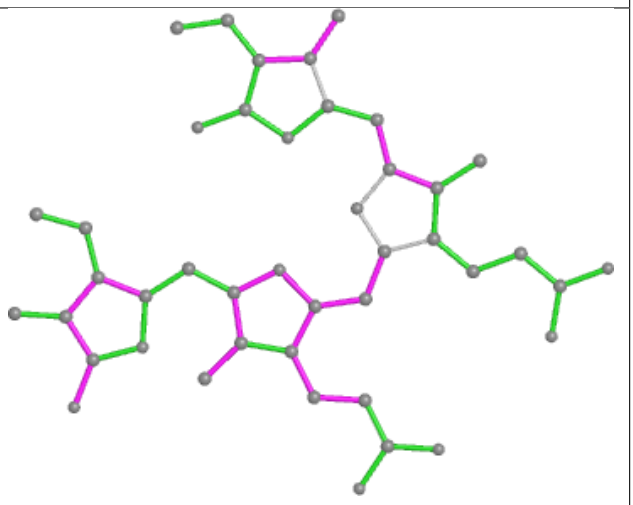

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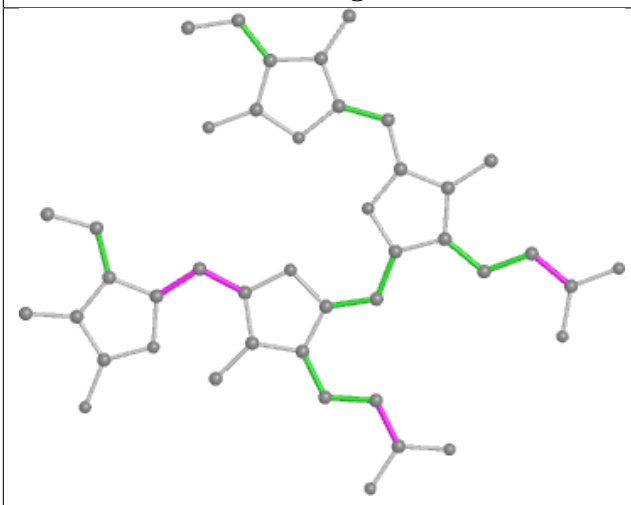

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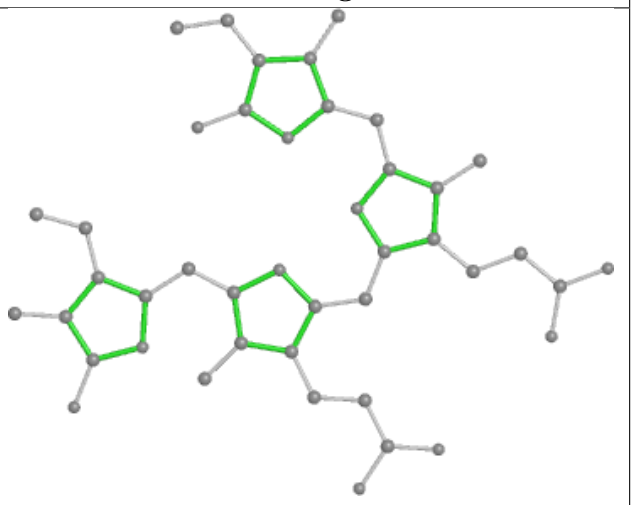
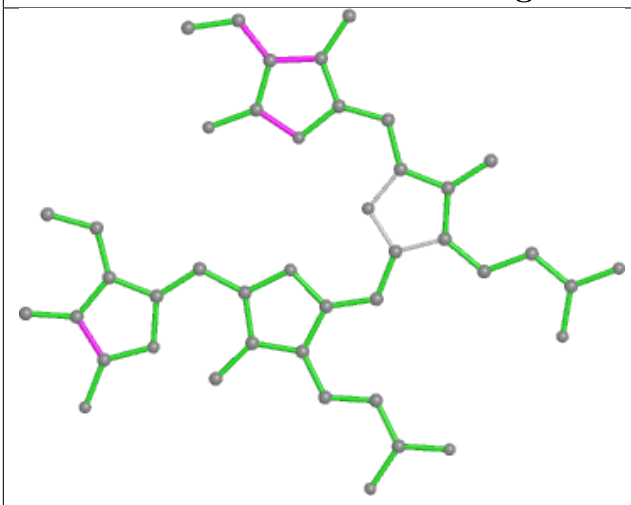


Rings

Ligand PEB O9 201



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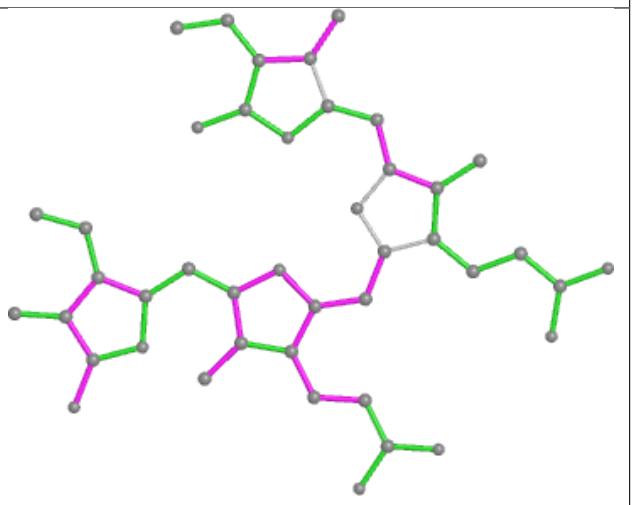

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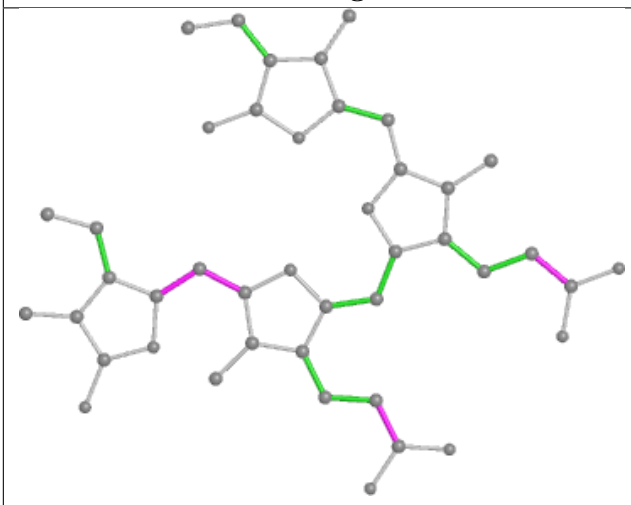

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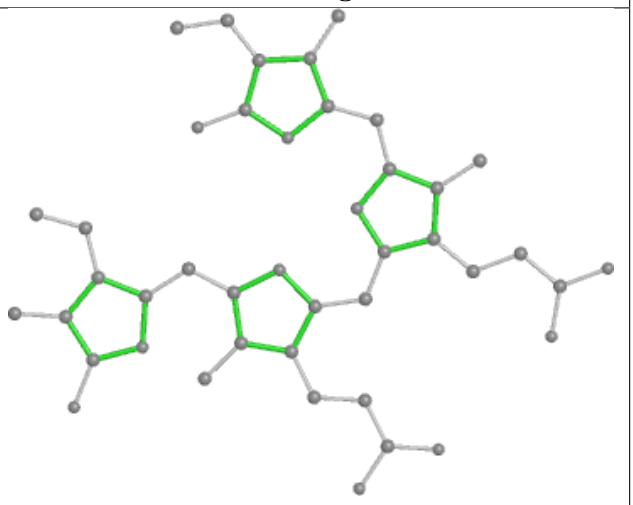
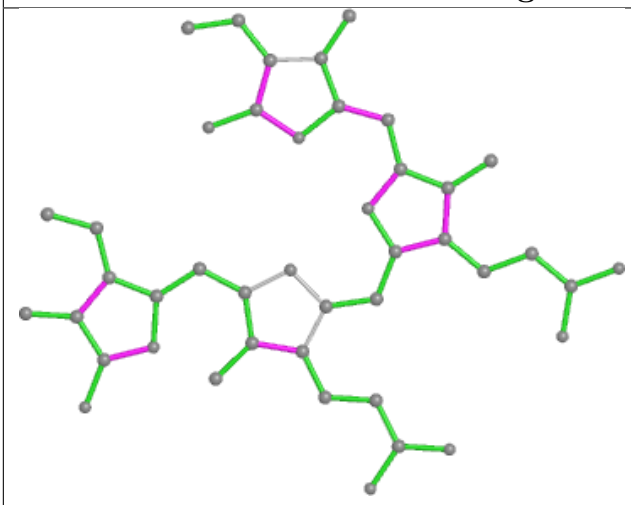


Rings

Ligand PUB v4 203



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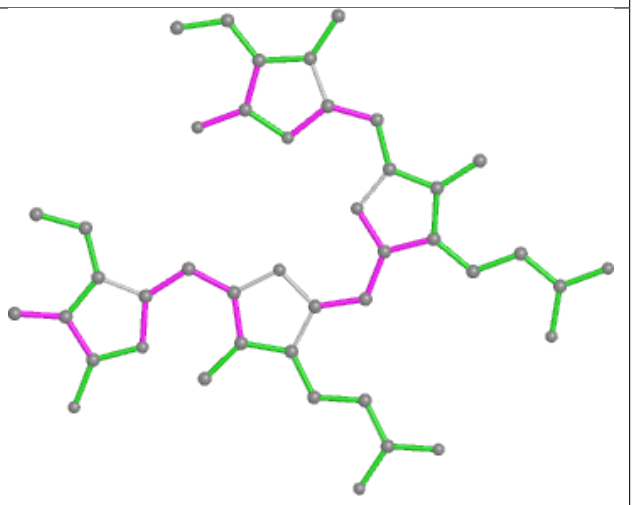
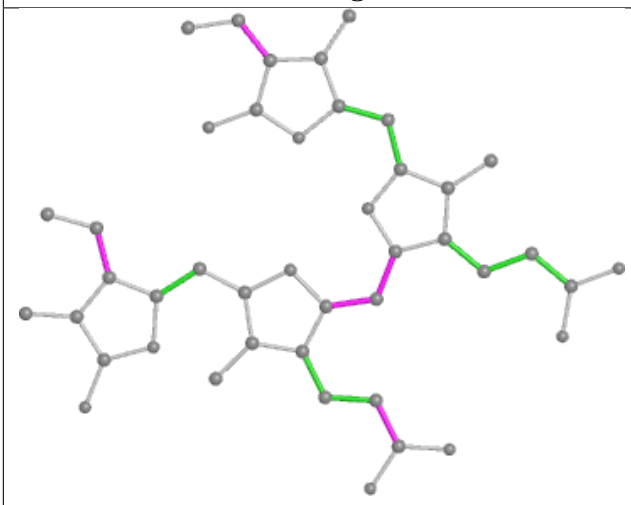
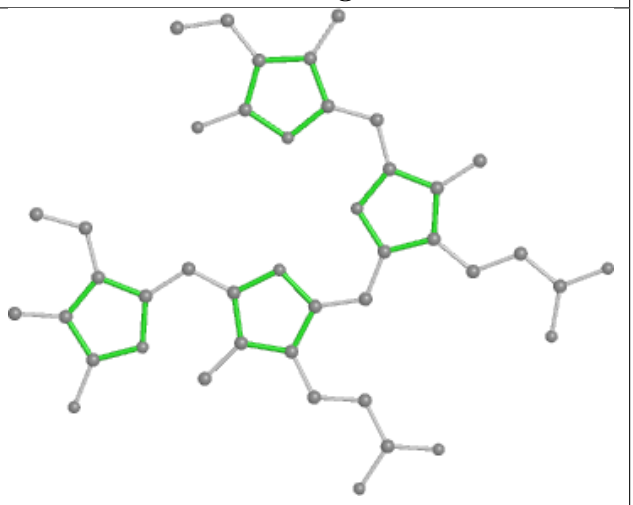


Bond angles

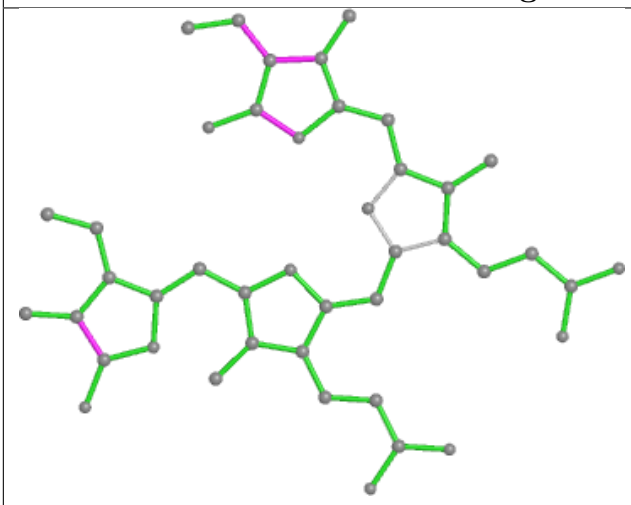


Torsions



Rings

Ligand PEB o5 201



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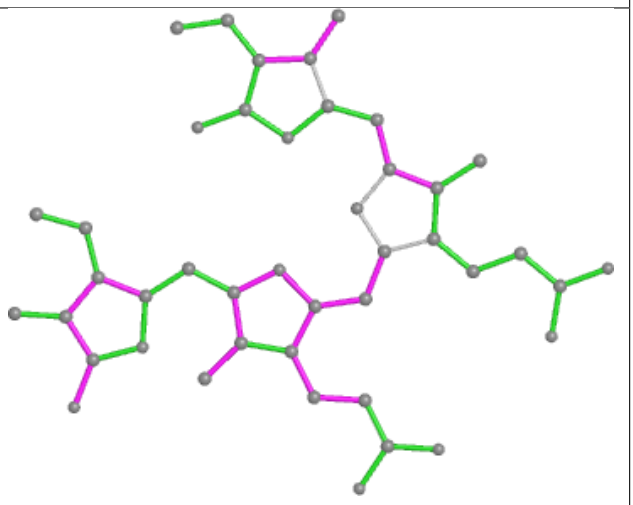

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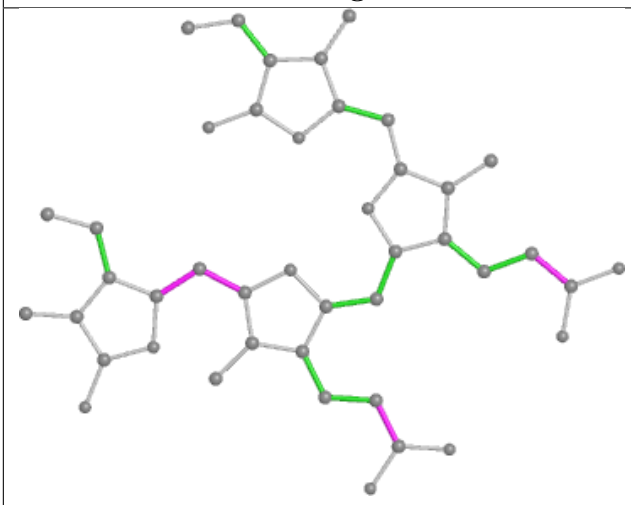

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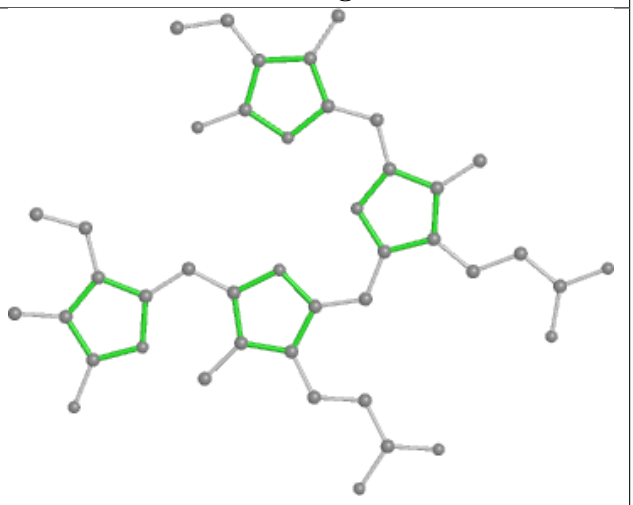
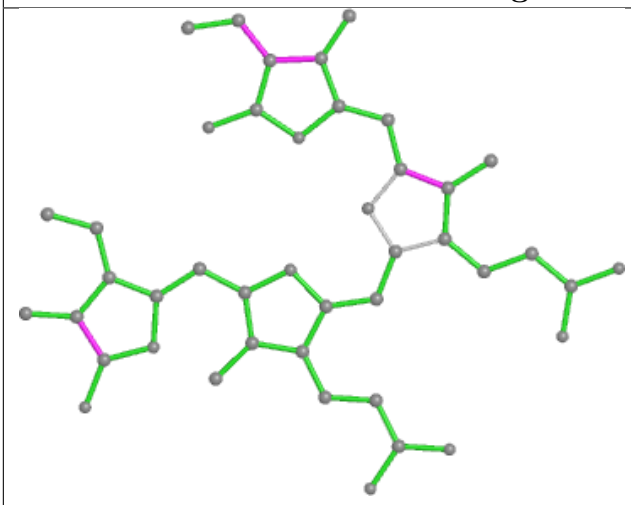


Rings

Ligand PEB iB 1002



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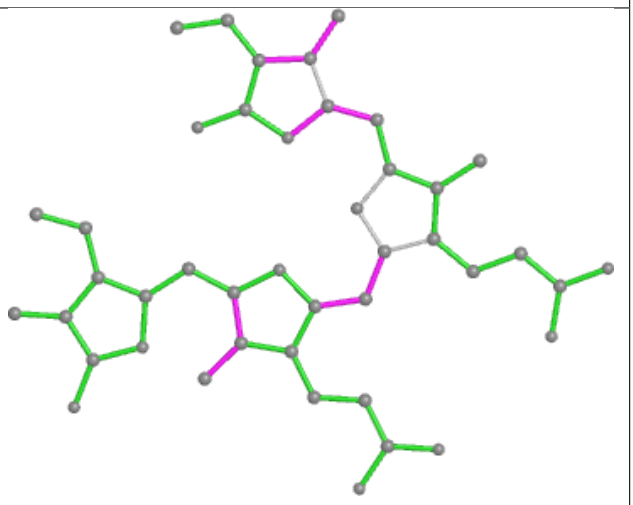

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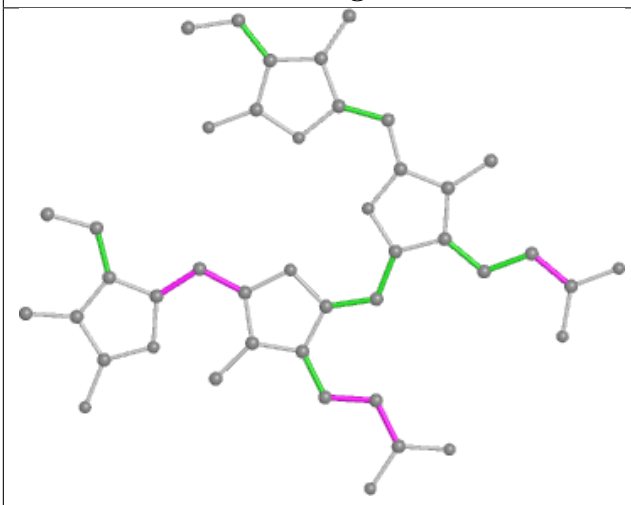

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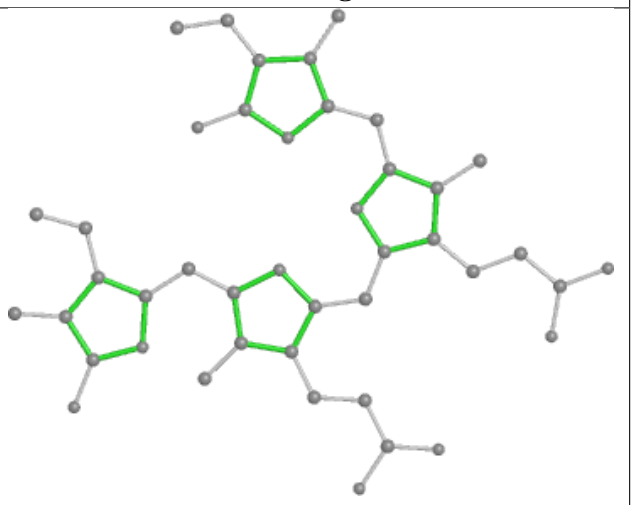

Rings

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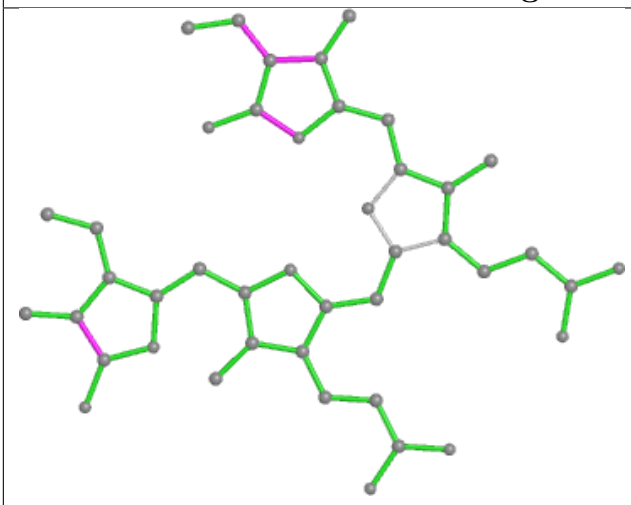

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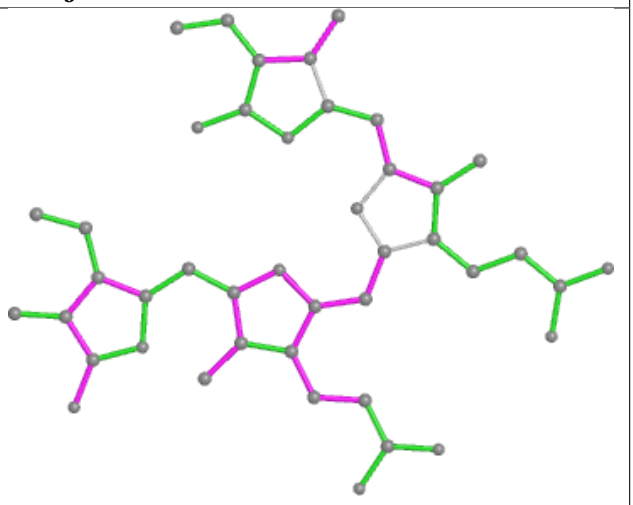

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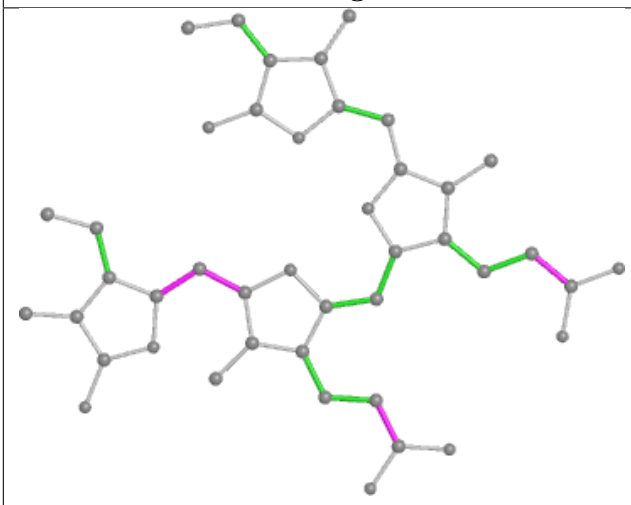

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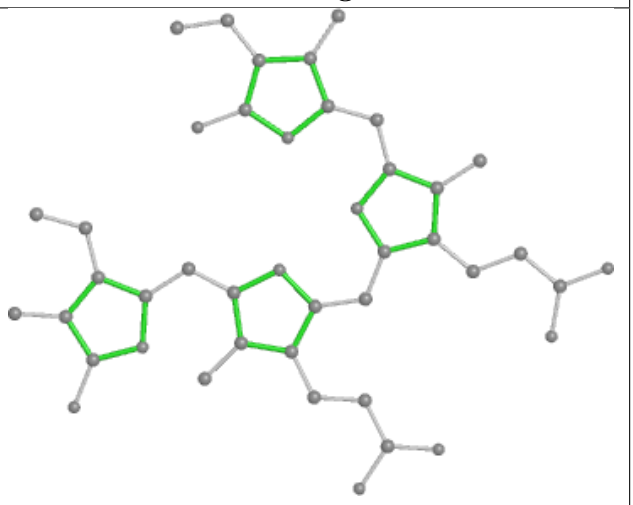
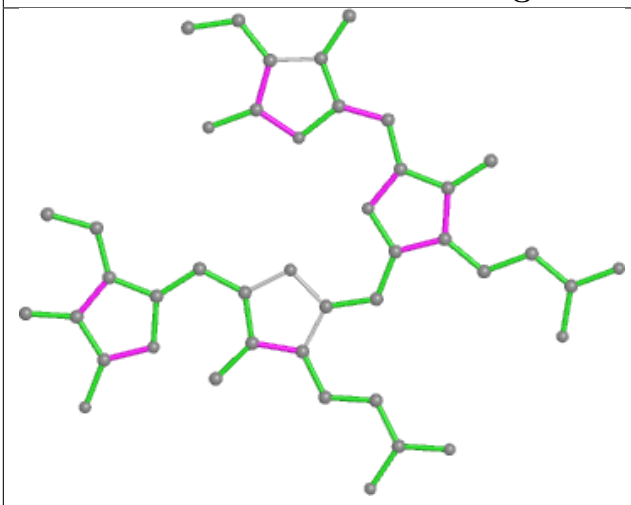


Rings

Ligand PUB R9 203



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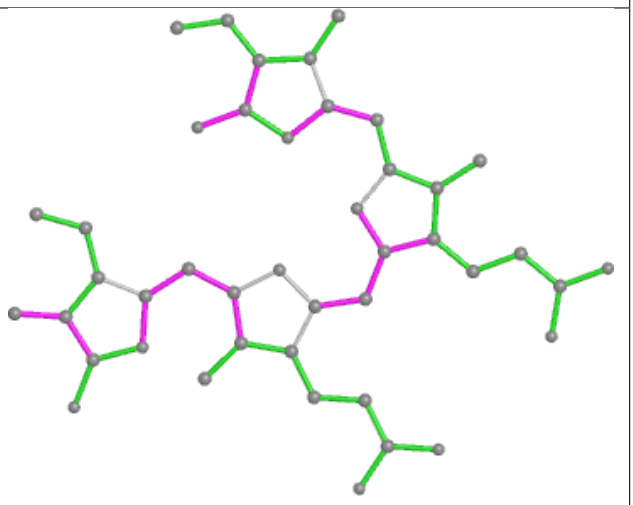

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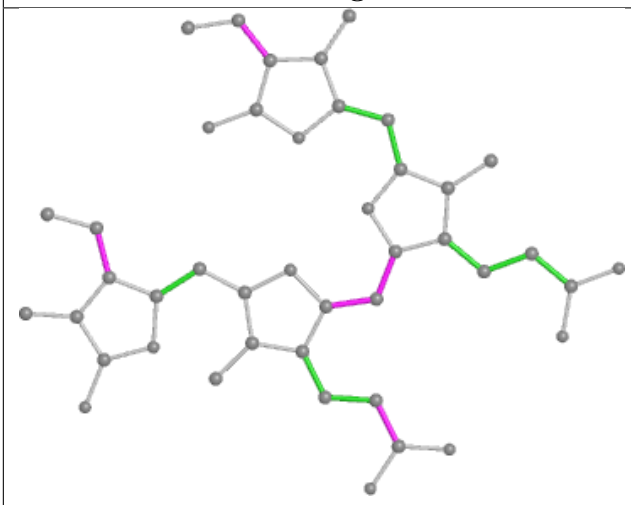

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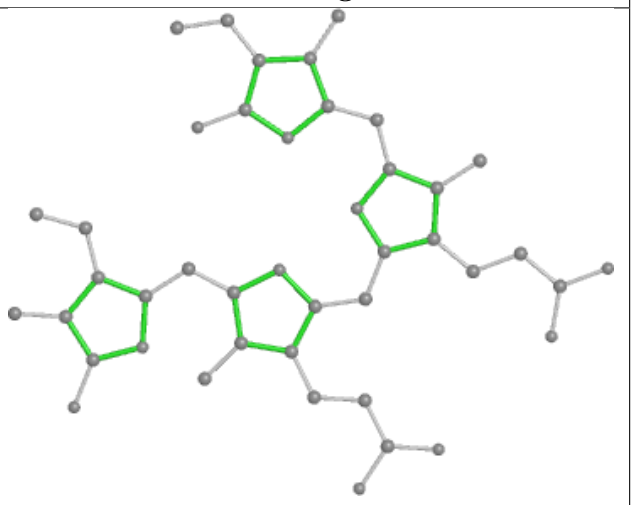
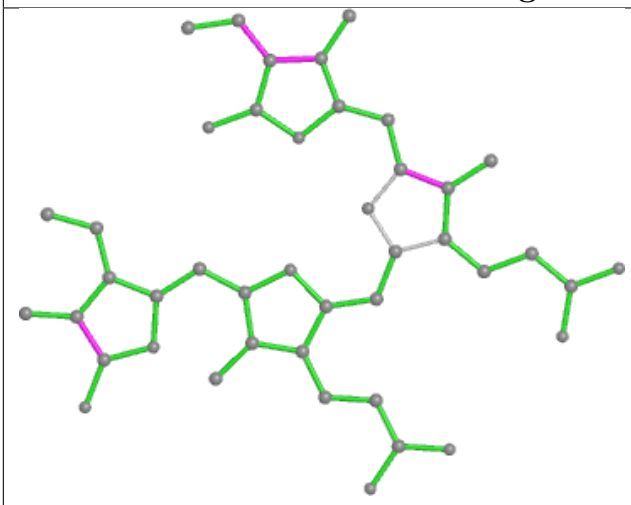


Rings

Ligand PEB dg 202



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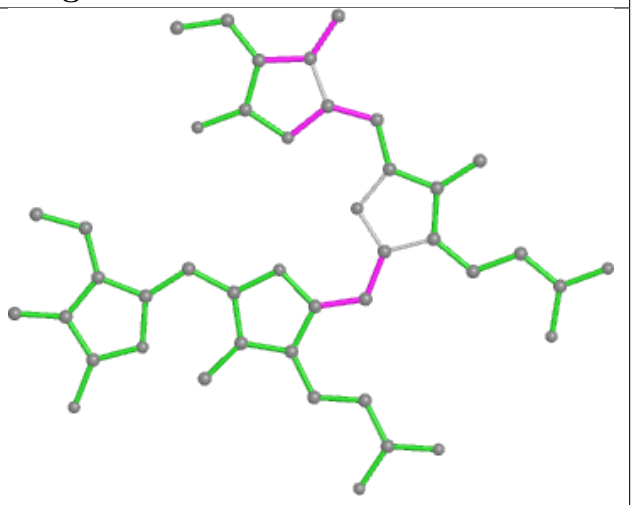

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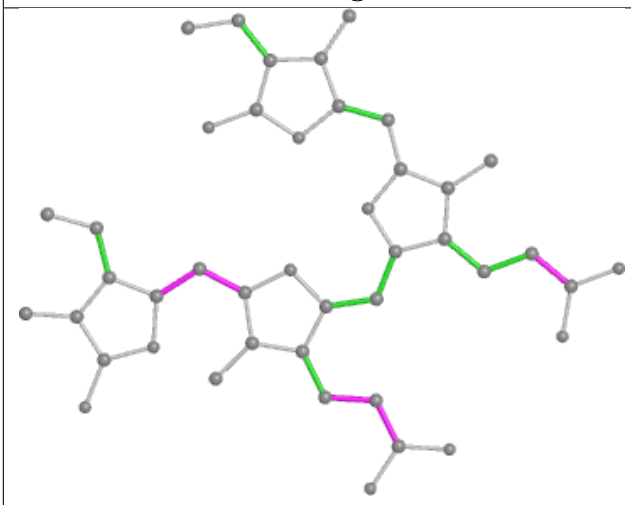

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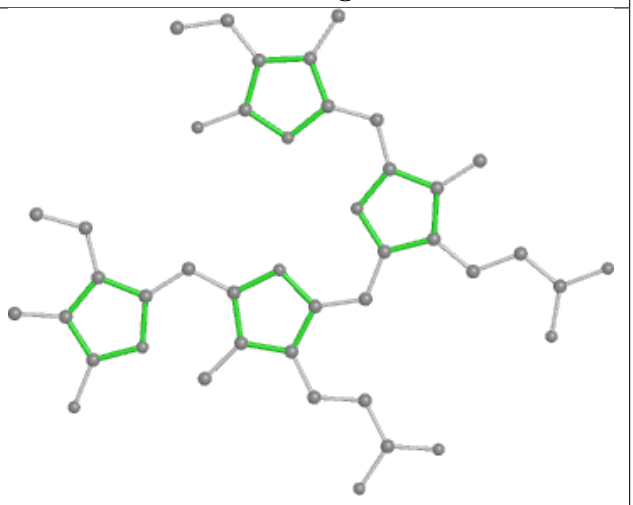

Rings

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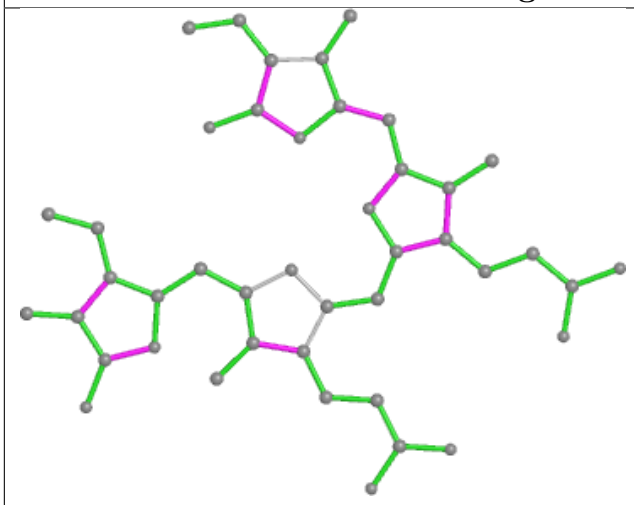

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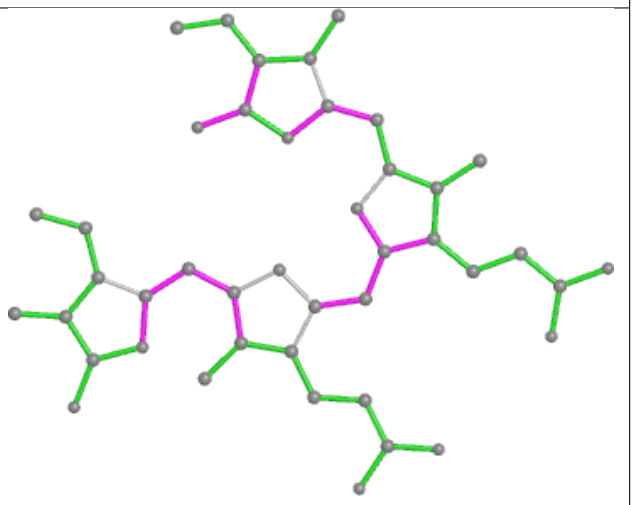

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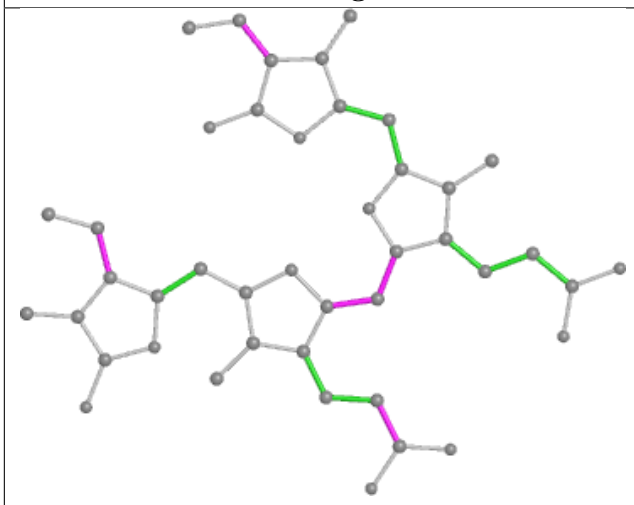

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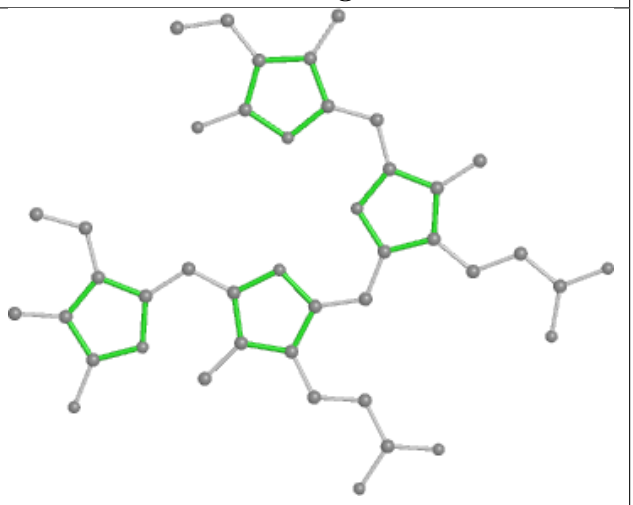

Rings

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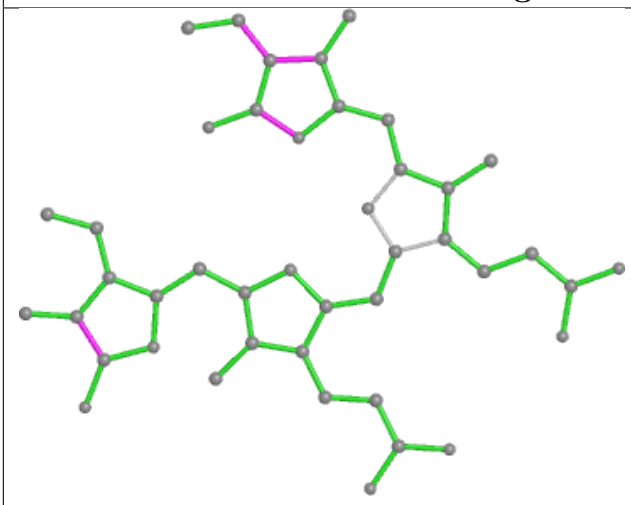

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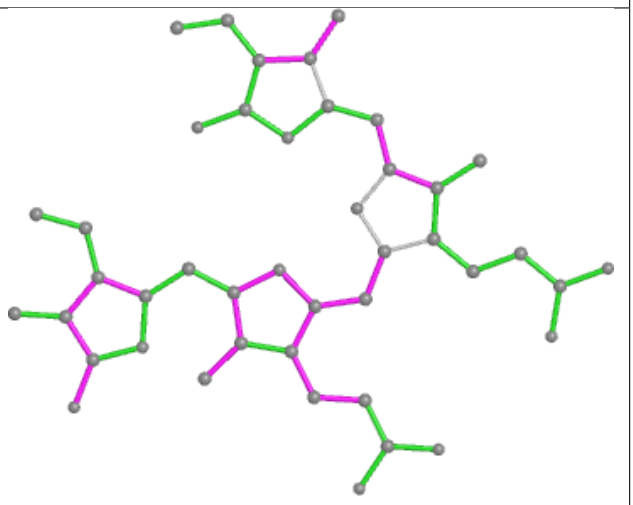

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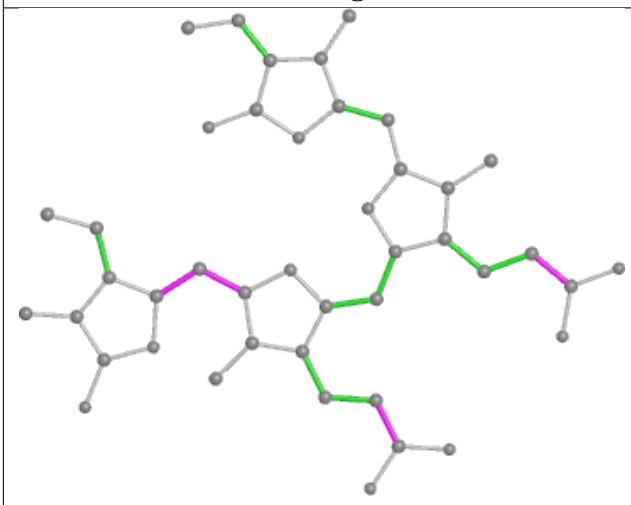

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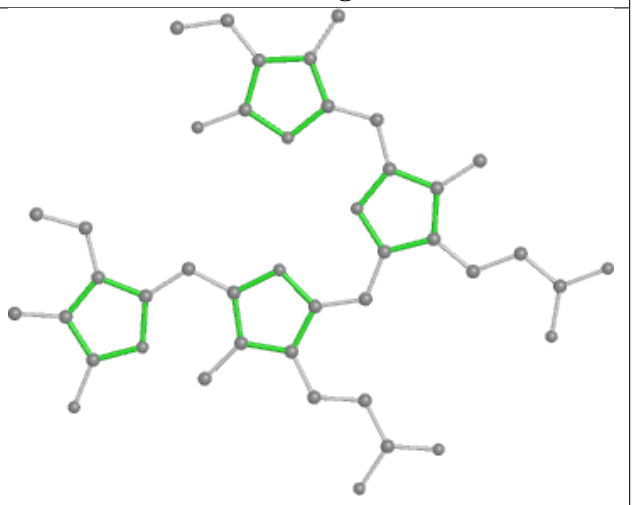
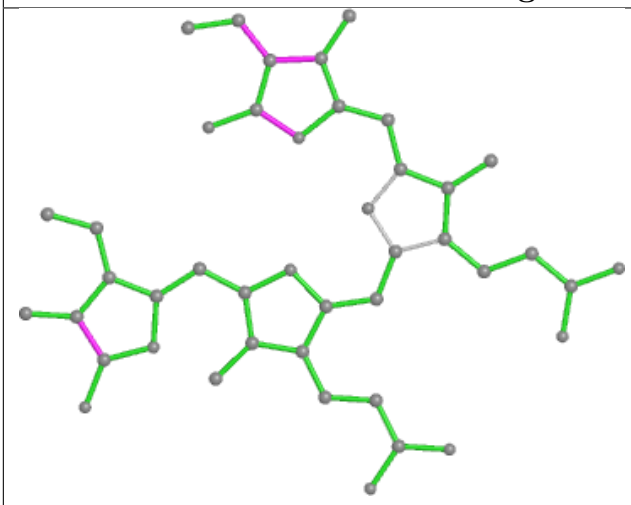


Rings

Ligand PEB L4 201



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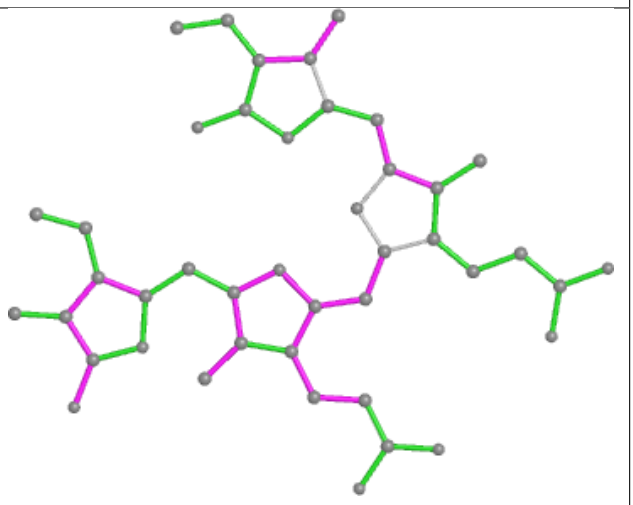

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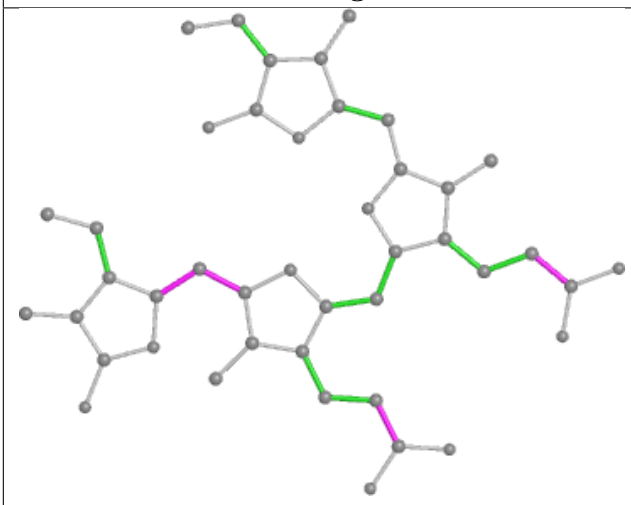

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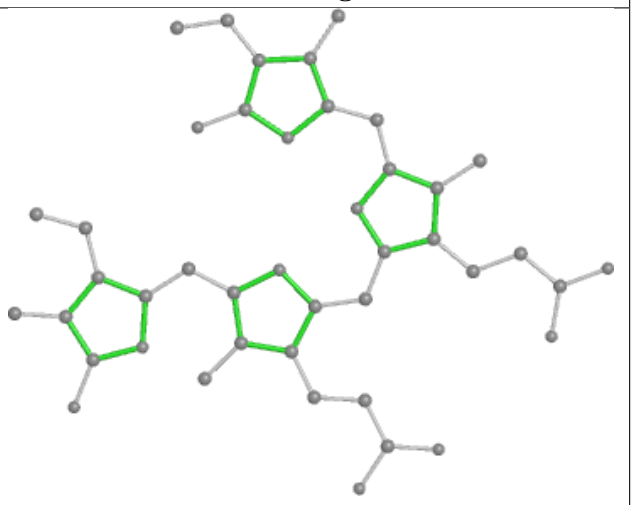
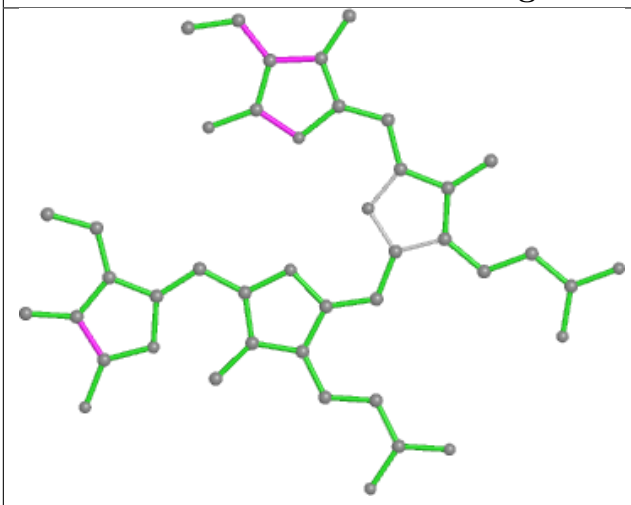


Rings

Ligand PEB dx 403



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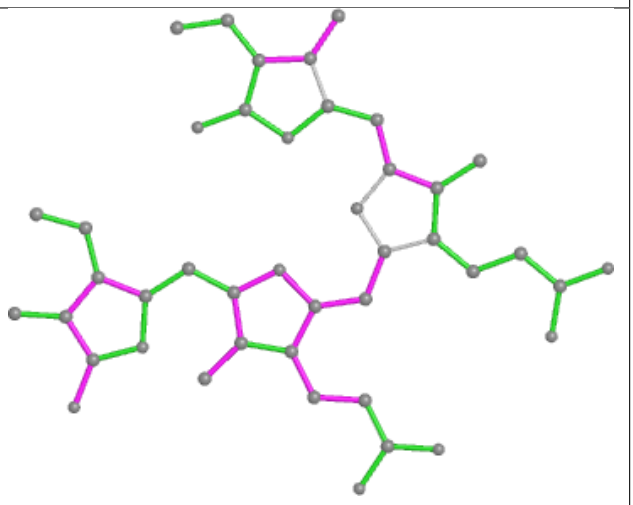

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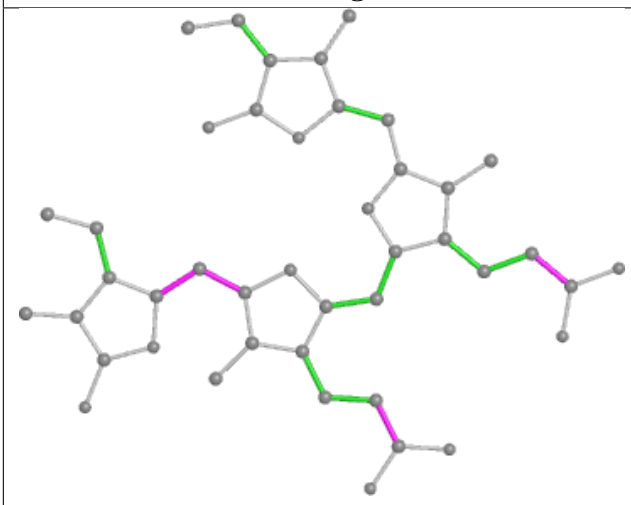

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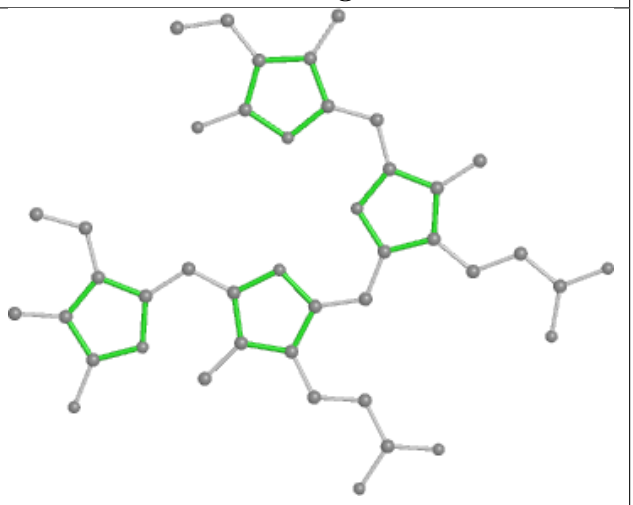

Rings

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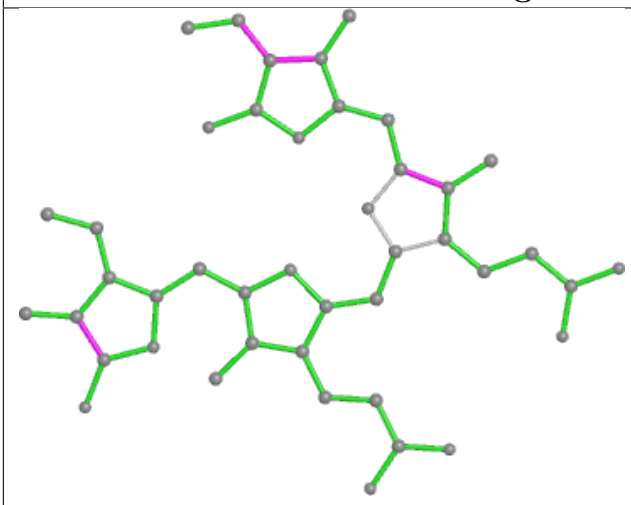

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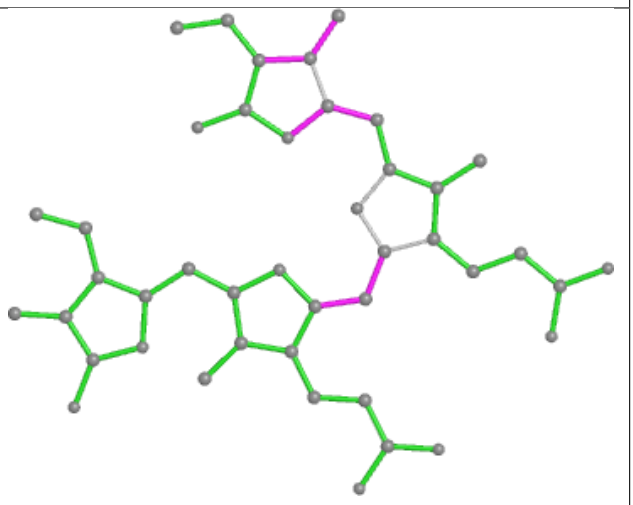

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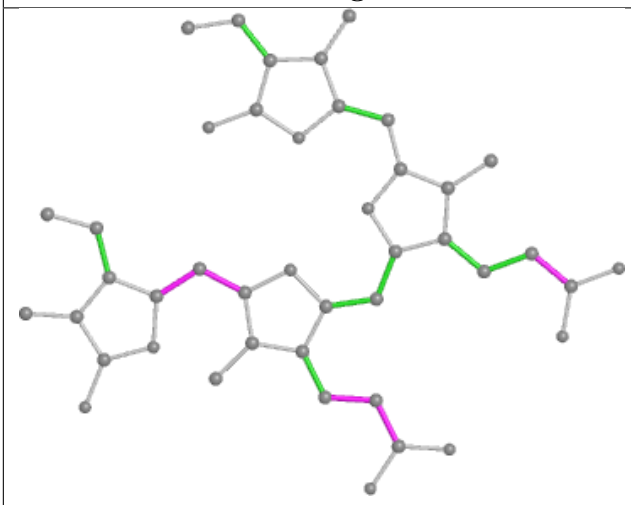

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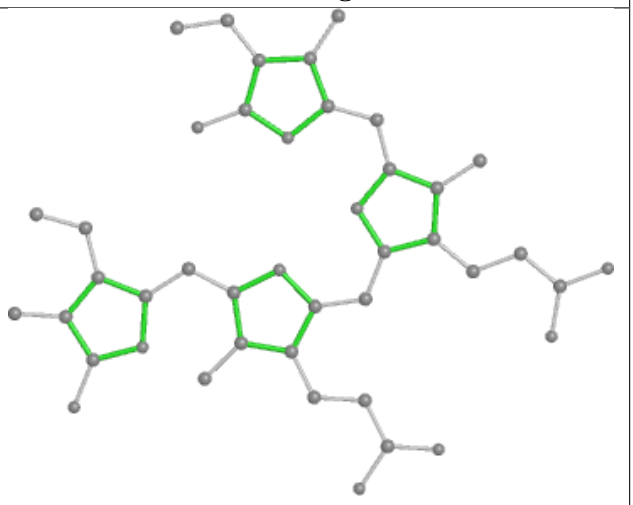
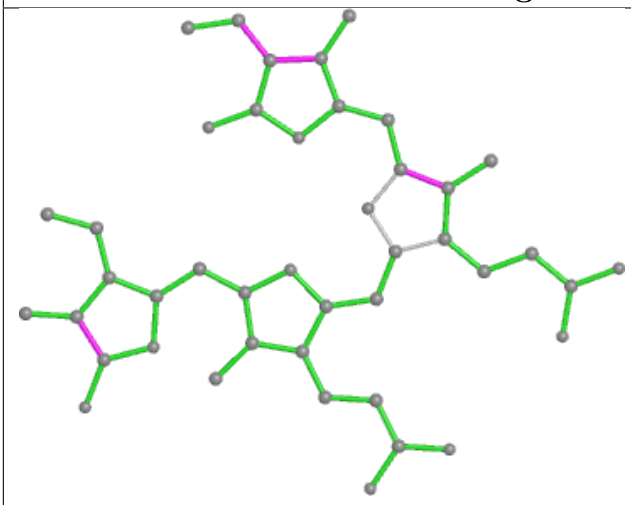


Rings

Ligand PEB A7 201



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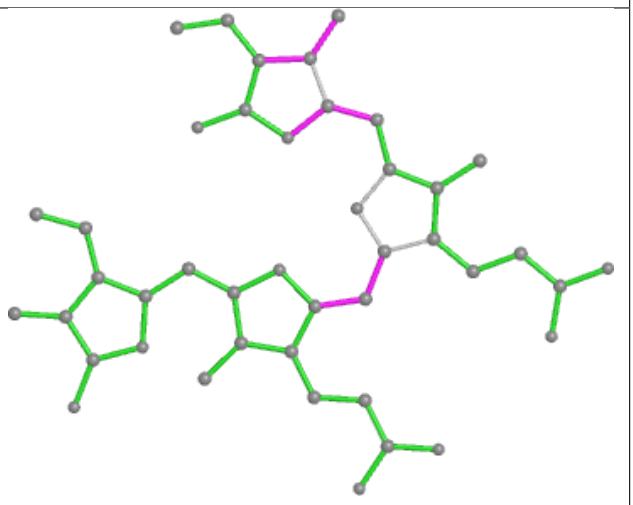

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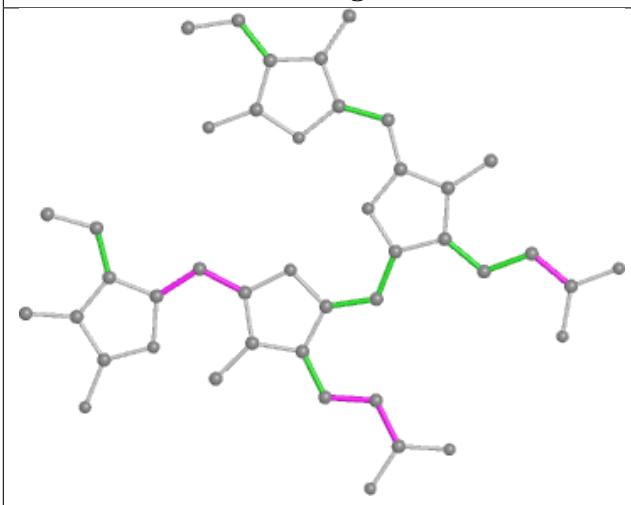

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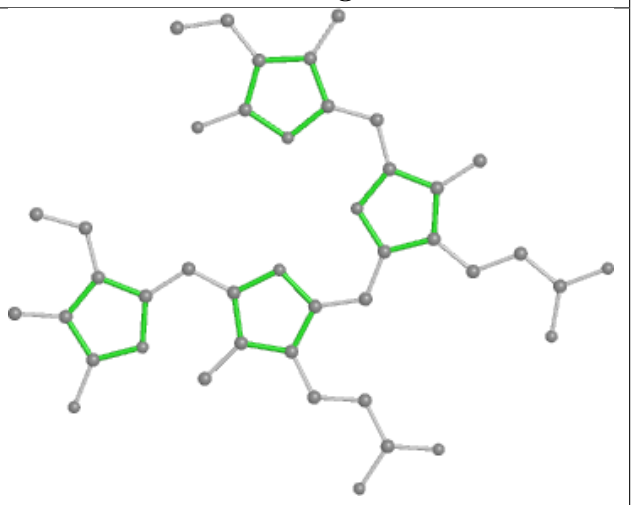

Rings

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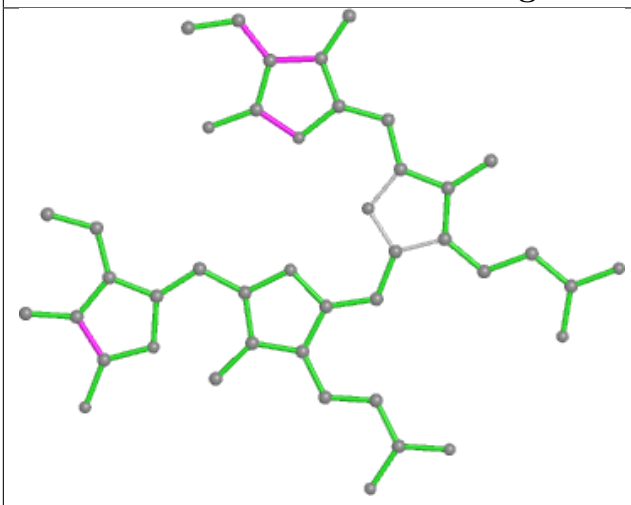

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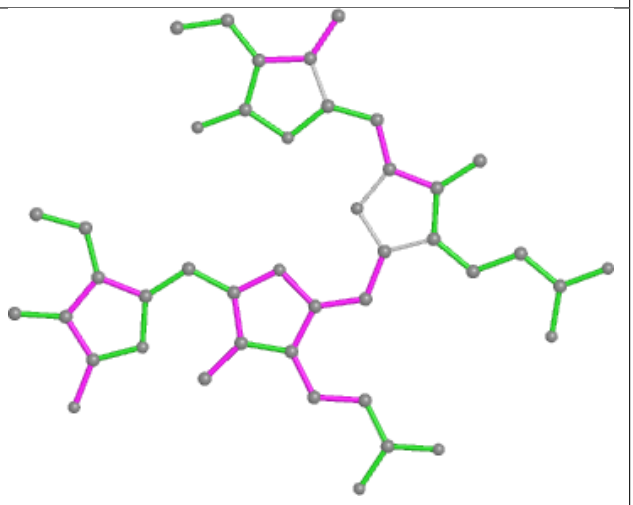

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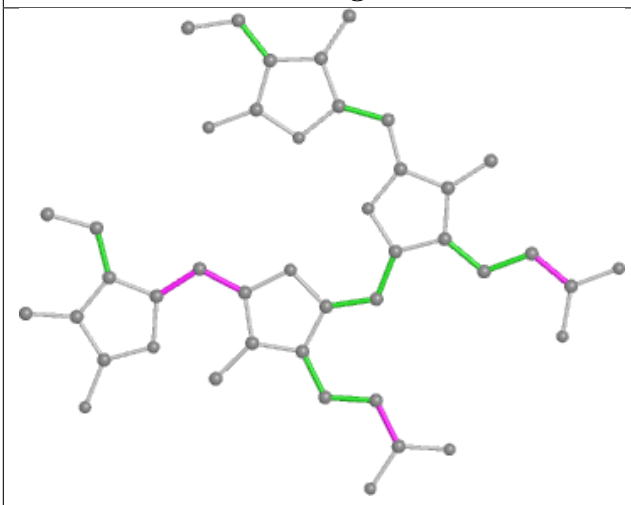

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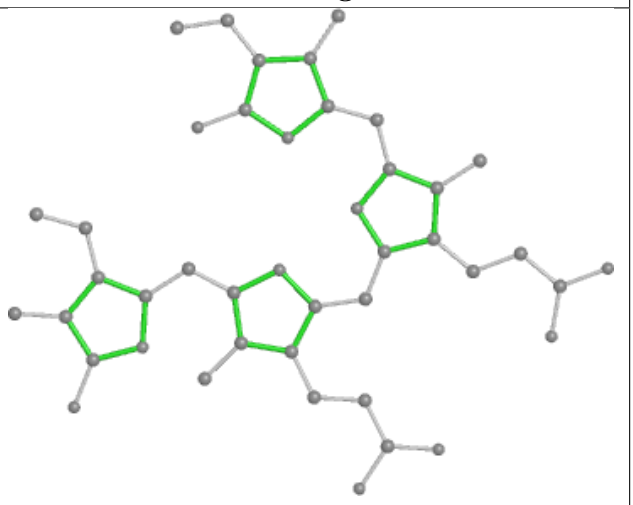
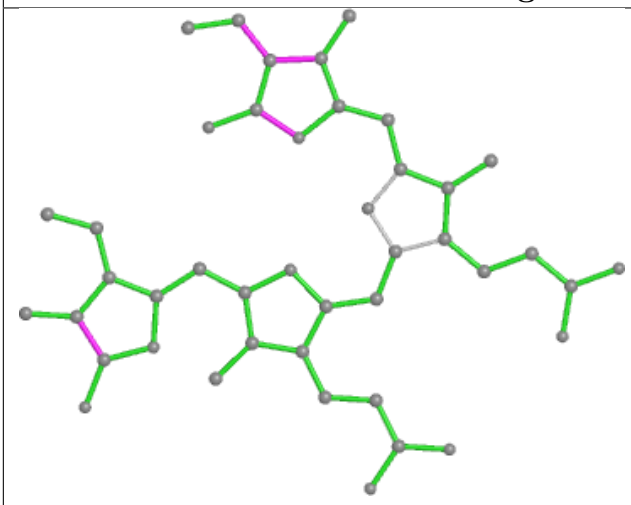


Rings

Ligand PEB Z2 201



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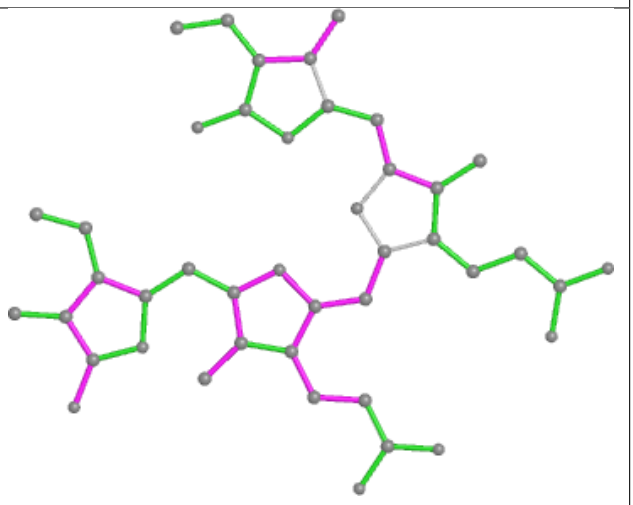
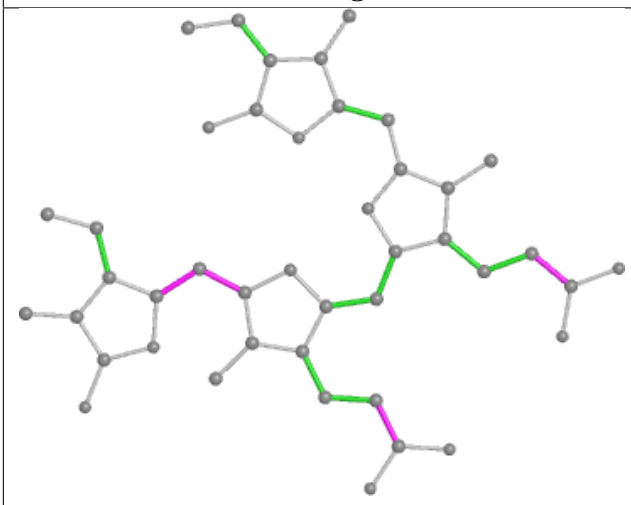
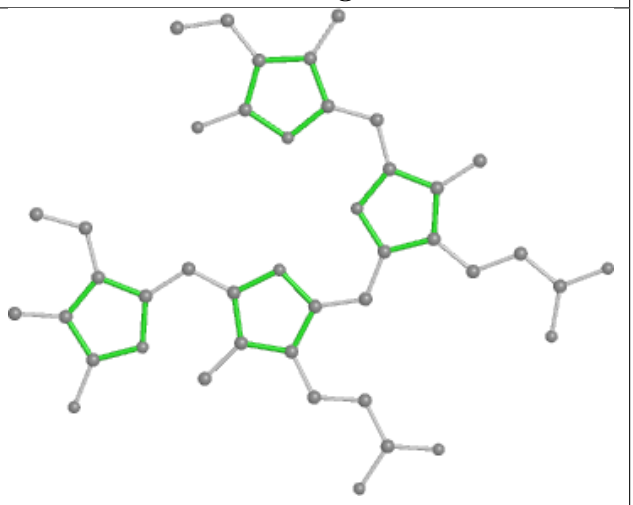


Bond angles

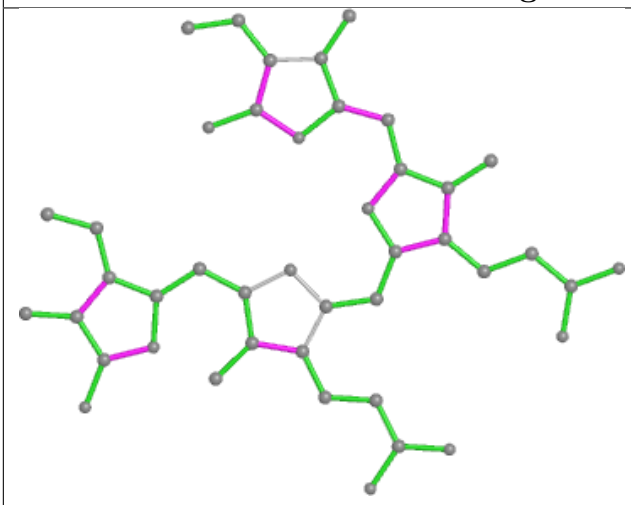


Torsions



Rings

Ligand PUB s7 203



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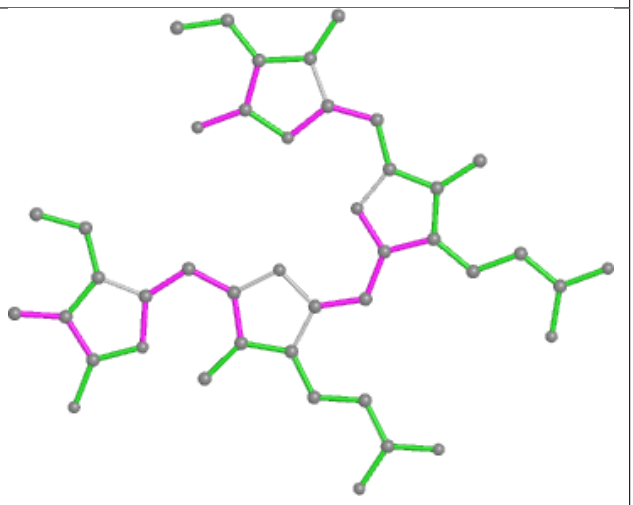
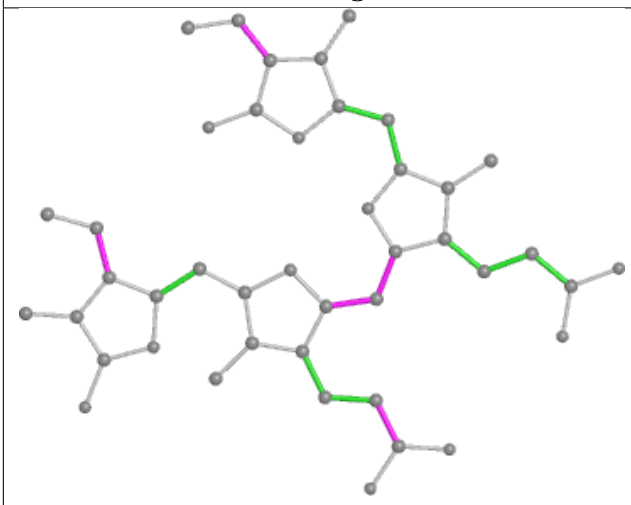
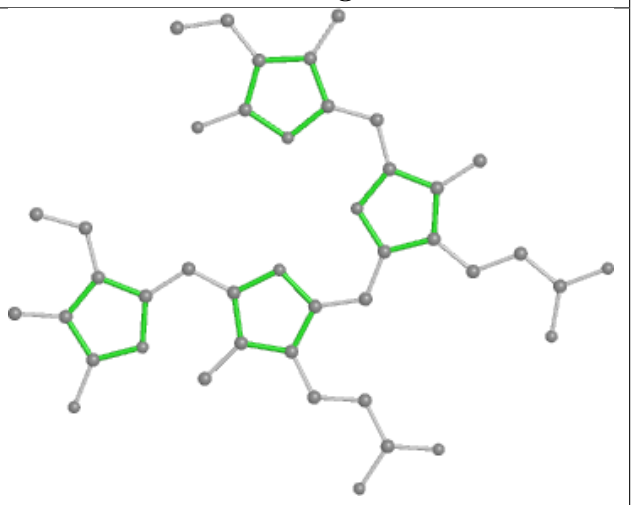


Bond angles

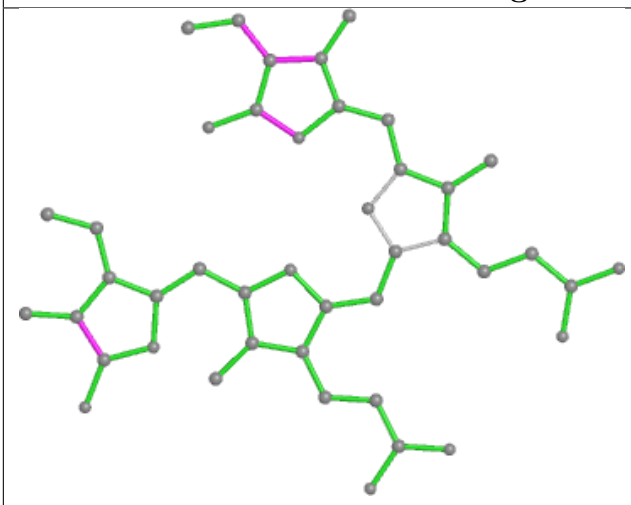


Torsions



Rings

Ligand PEB W2 201



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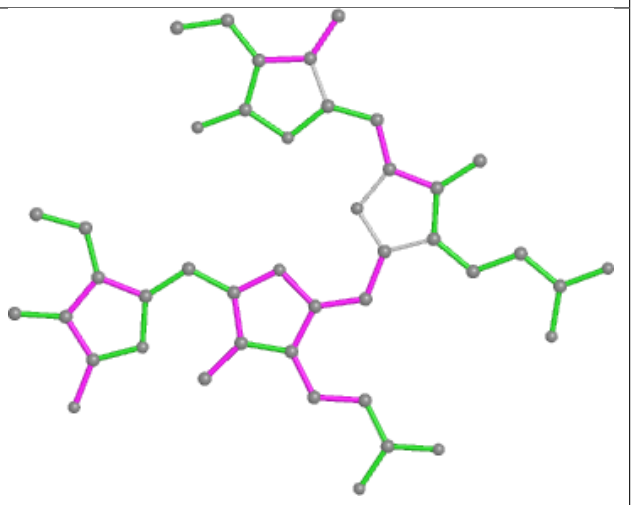

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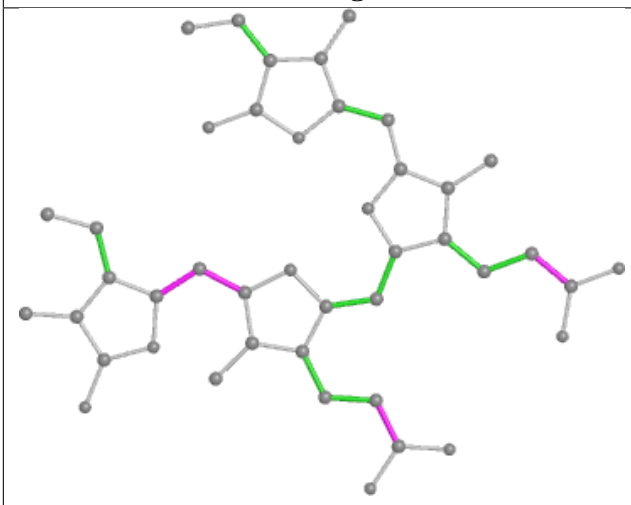

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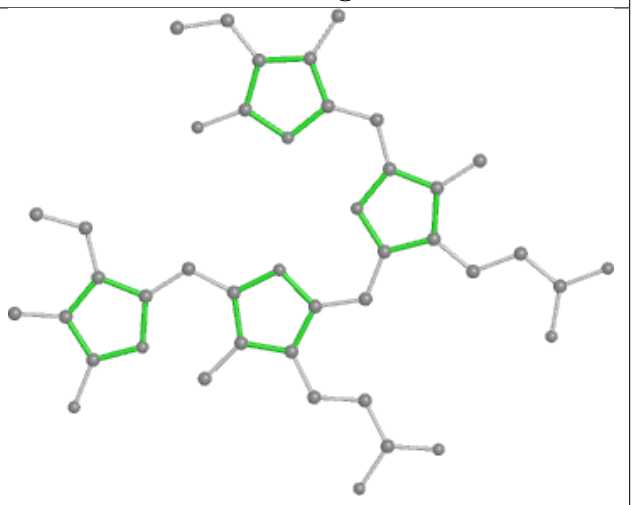
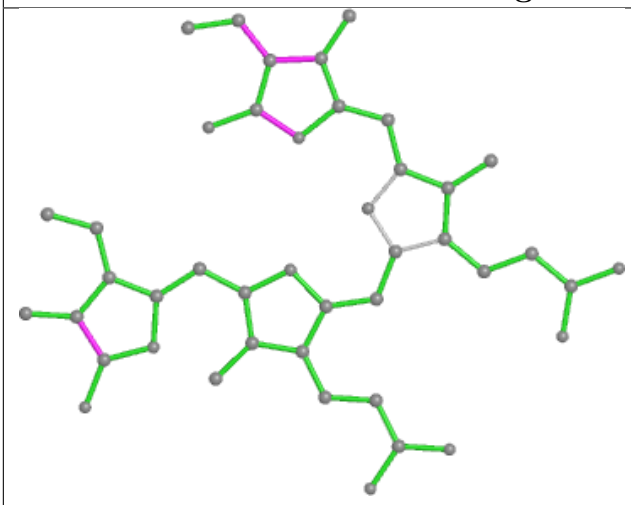


Rings

Ligand PEB aH 202



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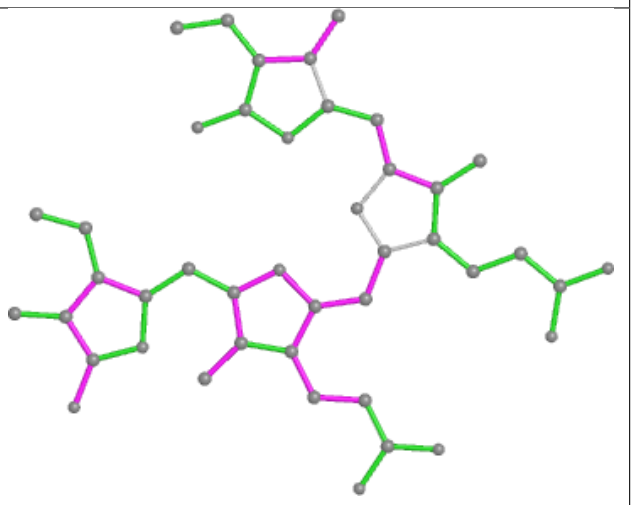
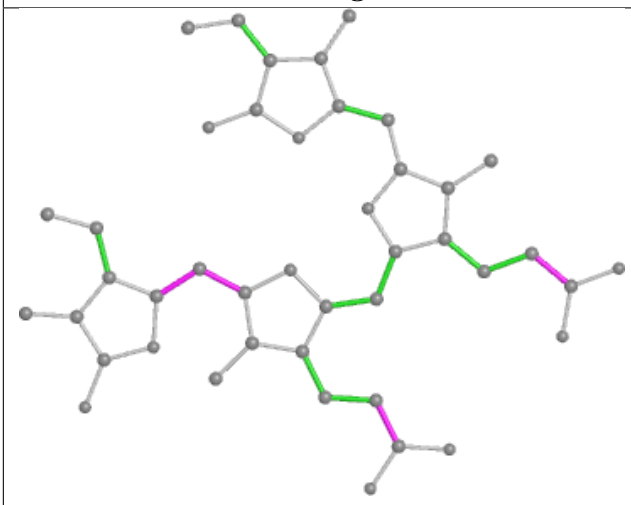


Bond angles



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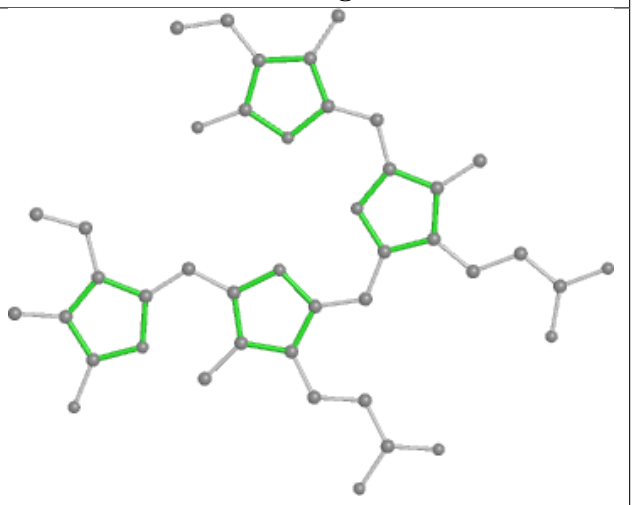
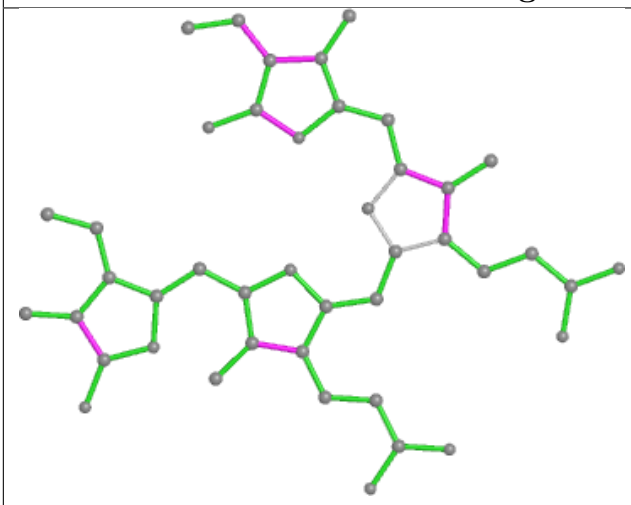


Rings

Ligand PEB n6 202



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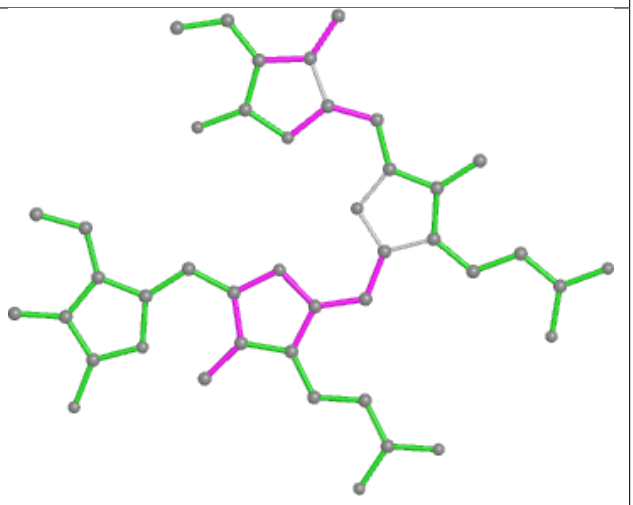

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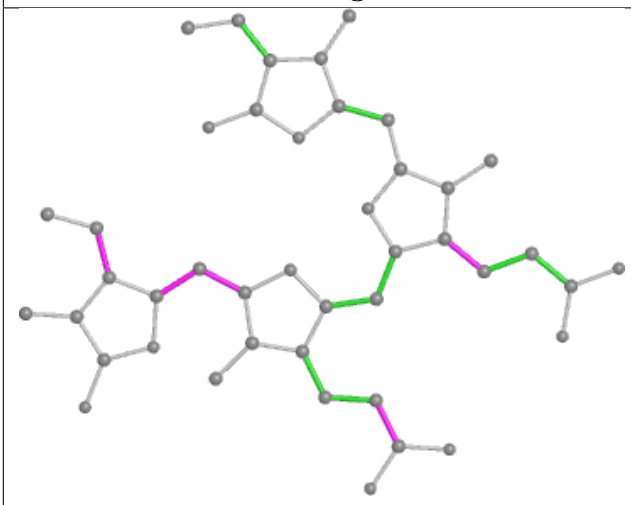

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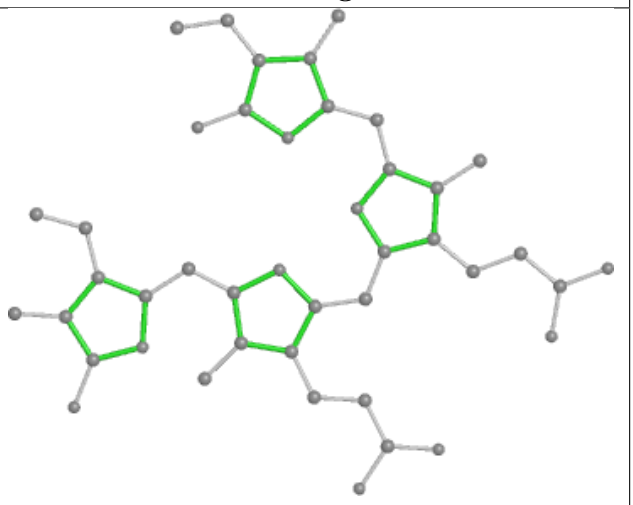
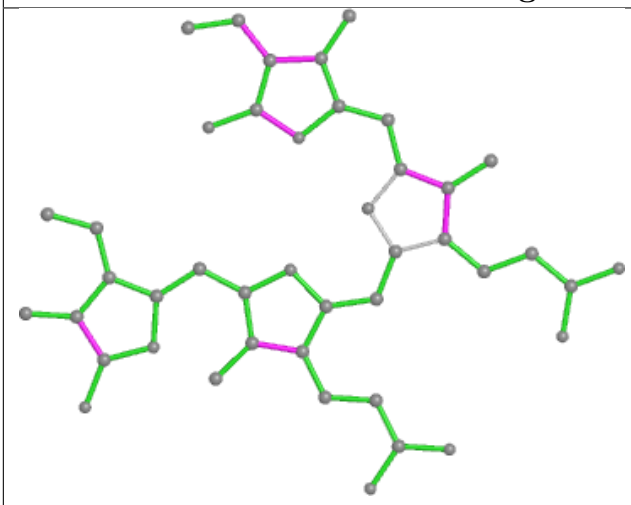


Rings

Ligand PEB p3 202



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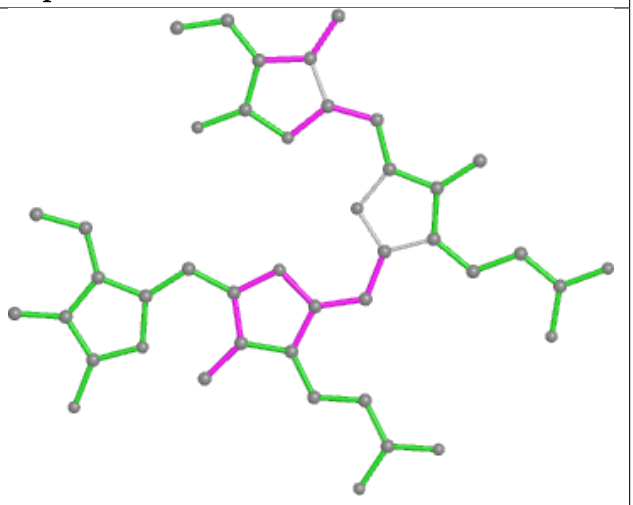

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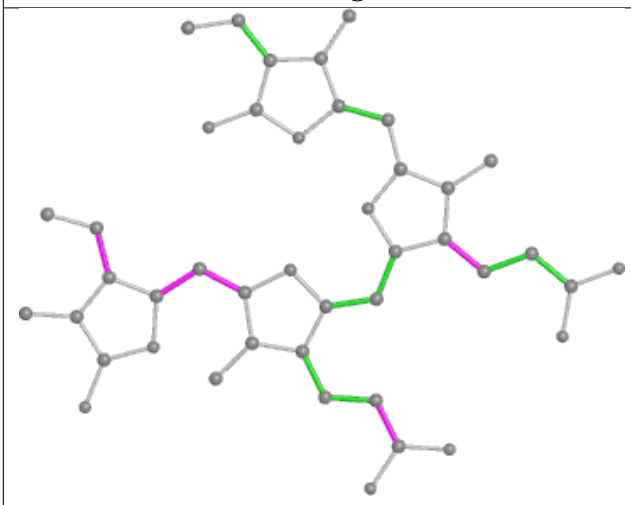

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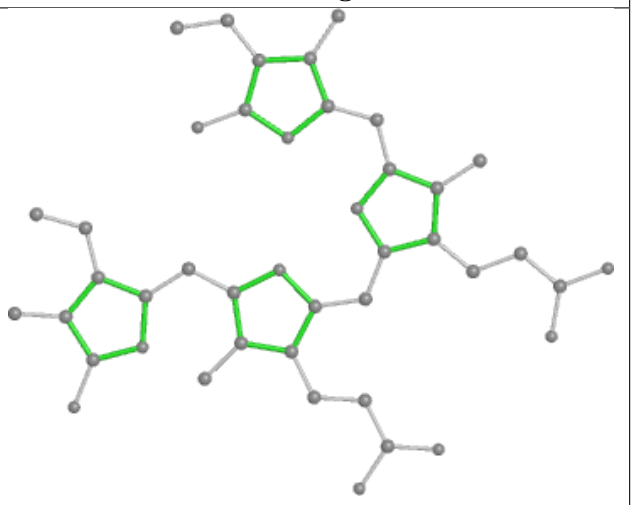
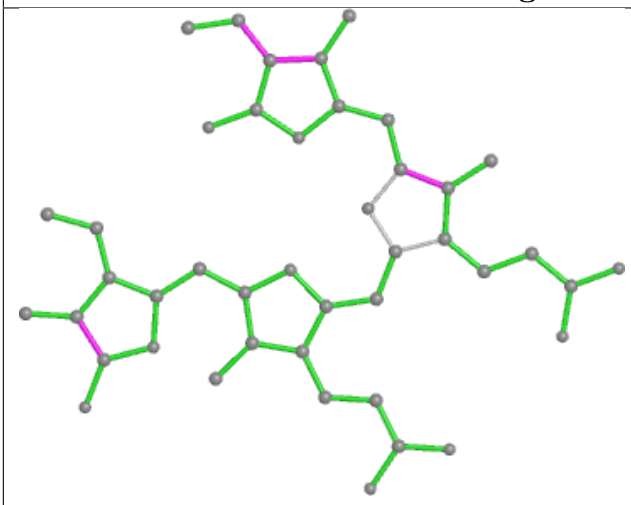


Rings

Ligand PEB n6 201



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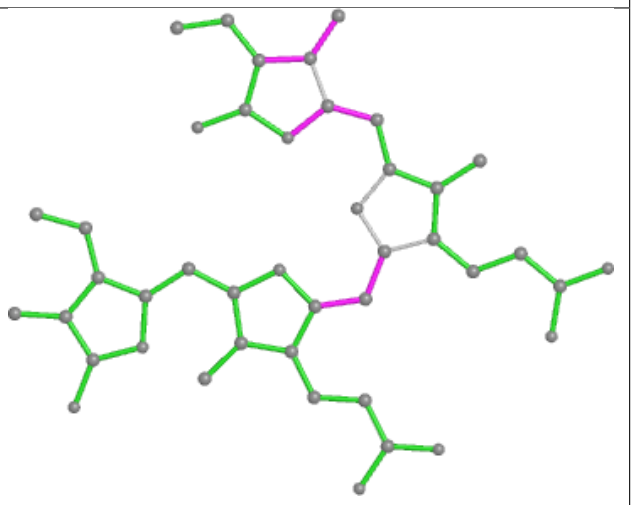

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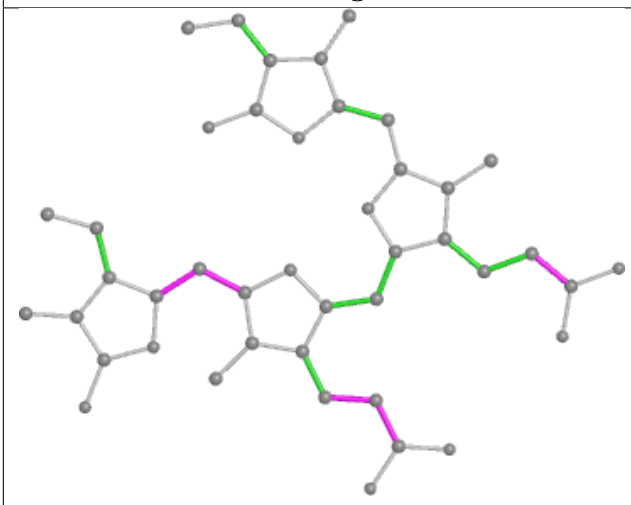

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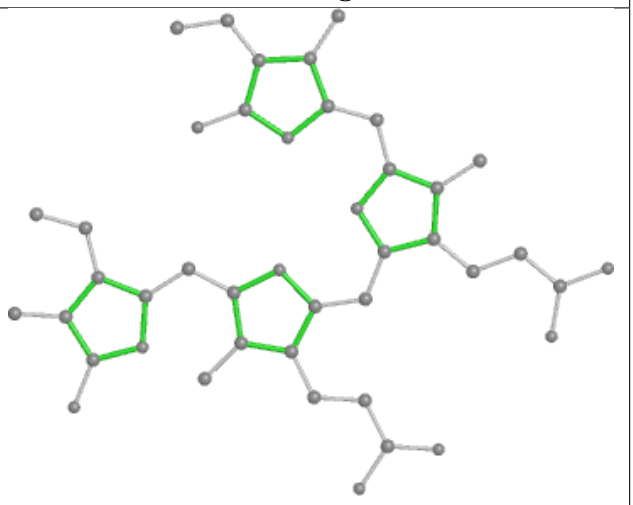
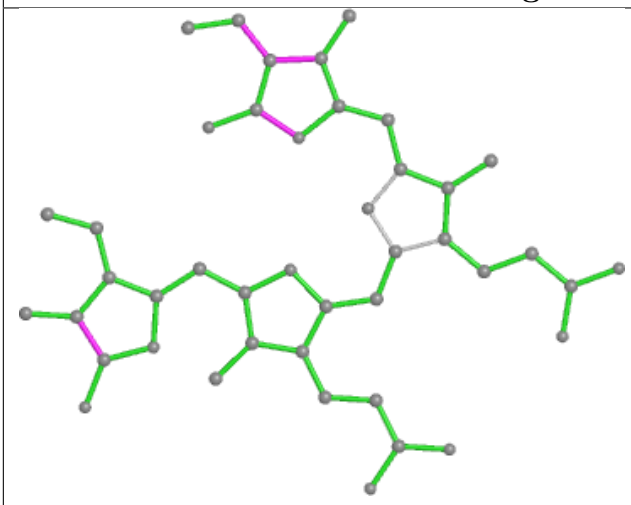


Rings

Ligand PEB dj 201



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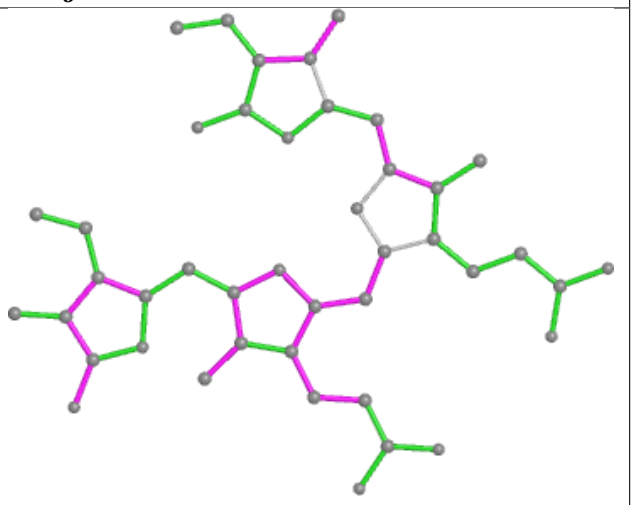

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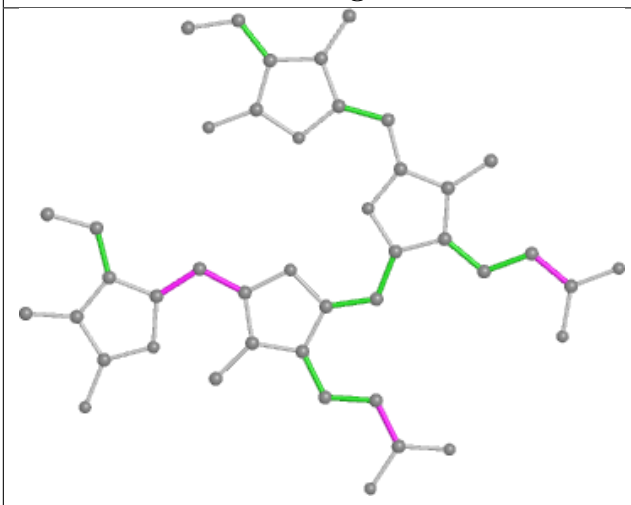

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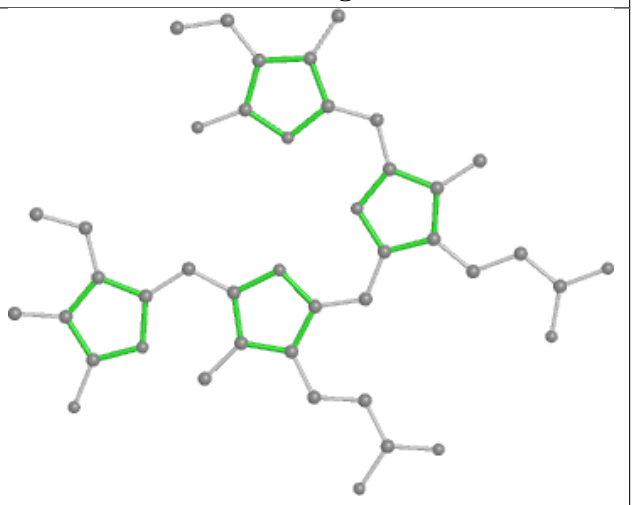
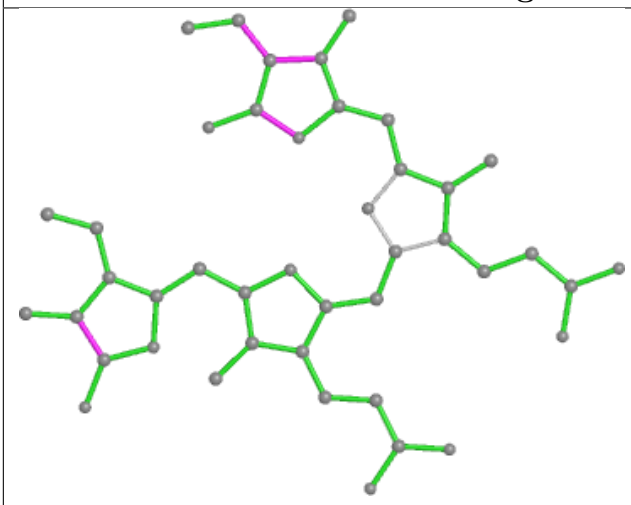


Rings

Ligand PEB bZ 301



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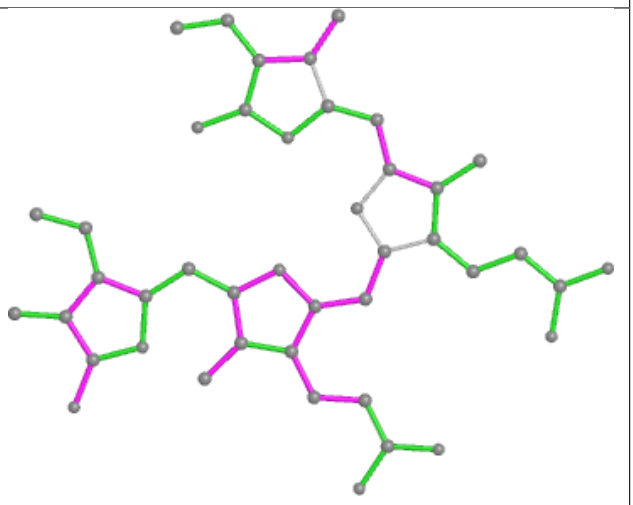

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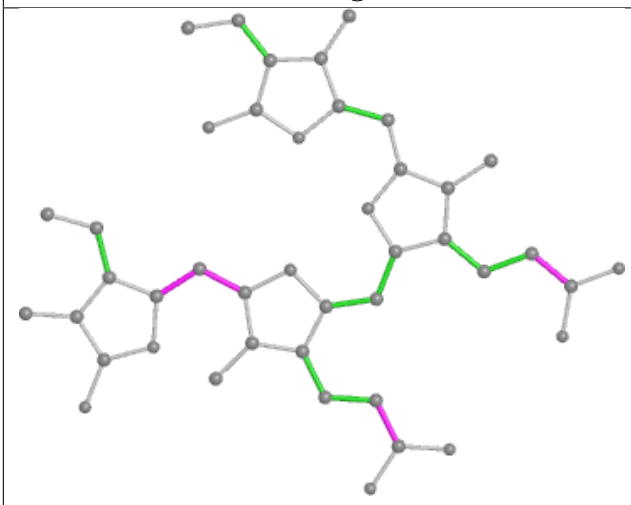

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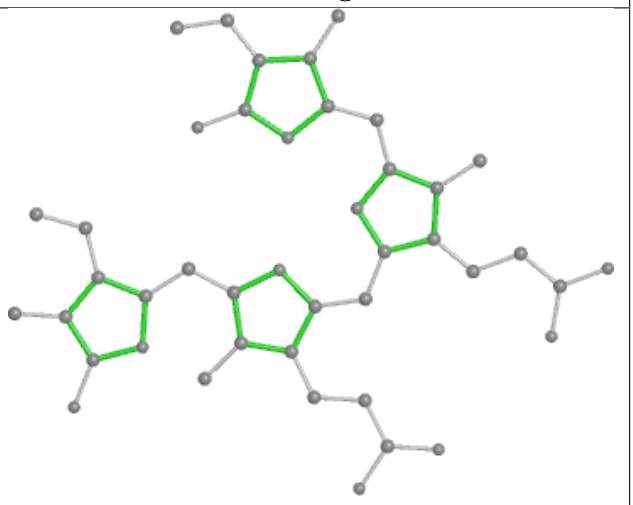
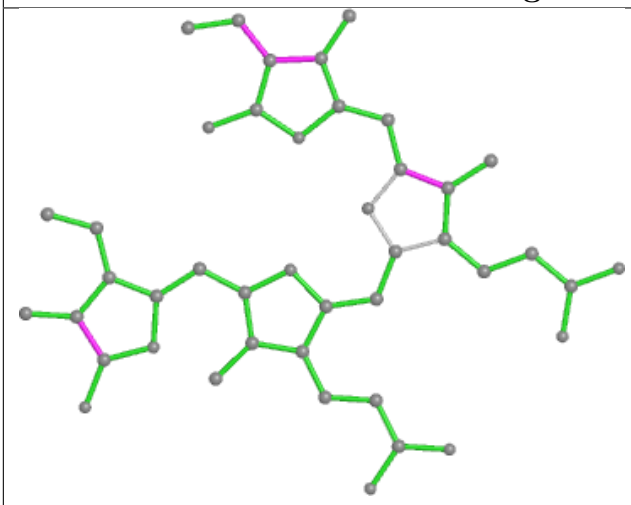


Rings

Ligand PEB lq 203



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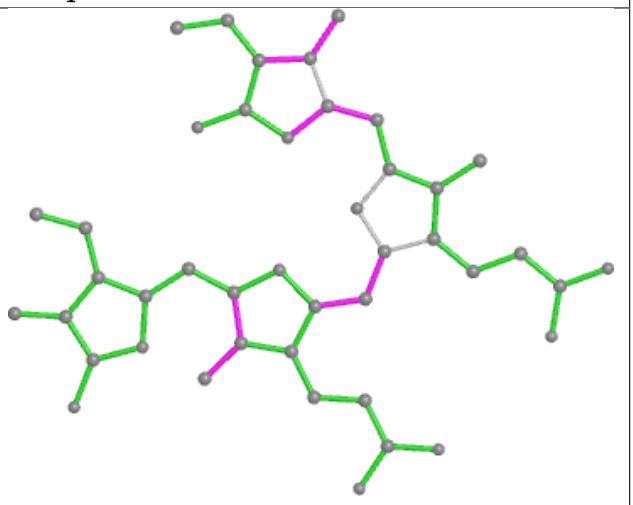

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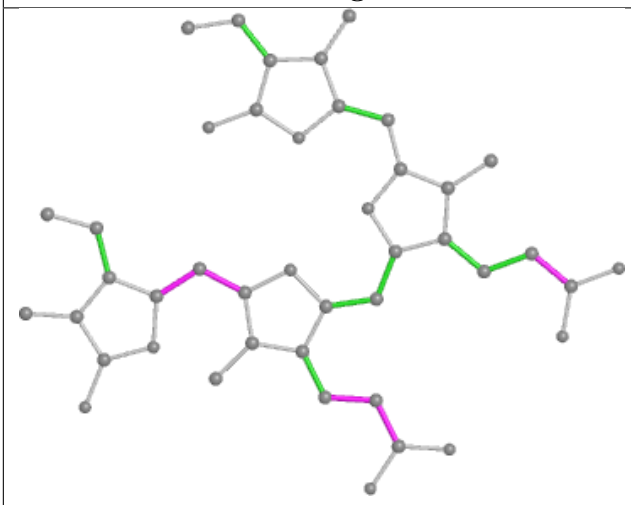

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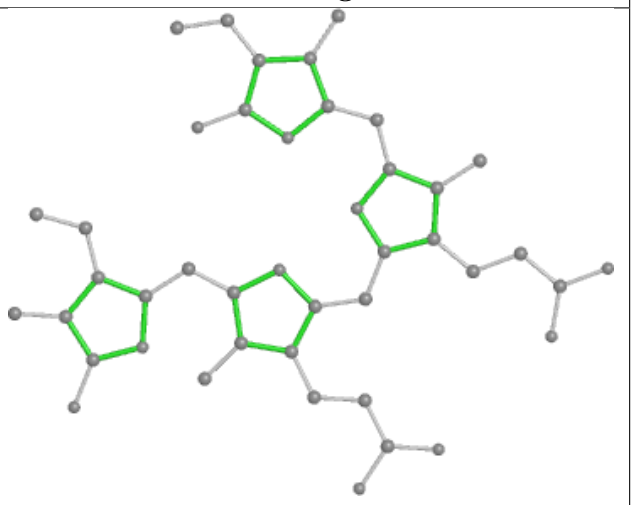
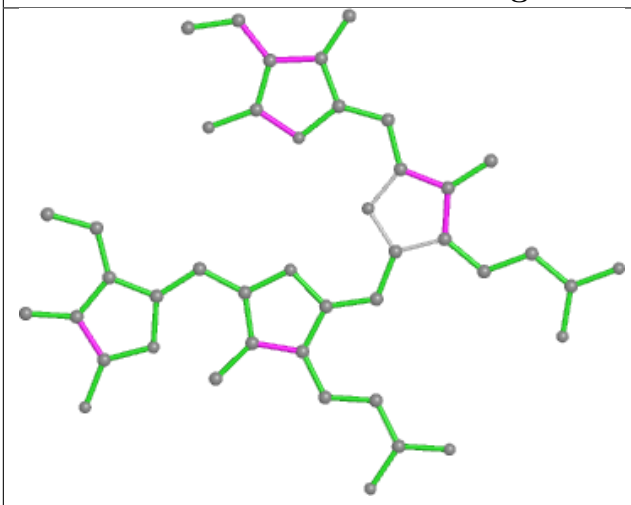


Rings

Ligand PEB iC 1002



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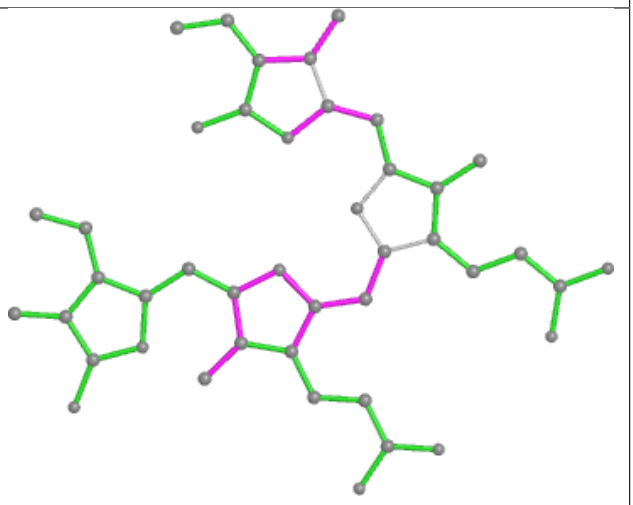

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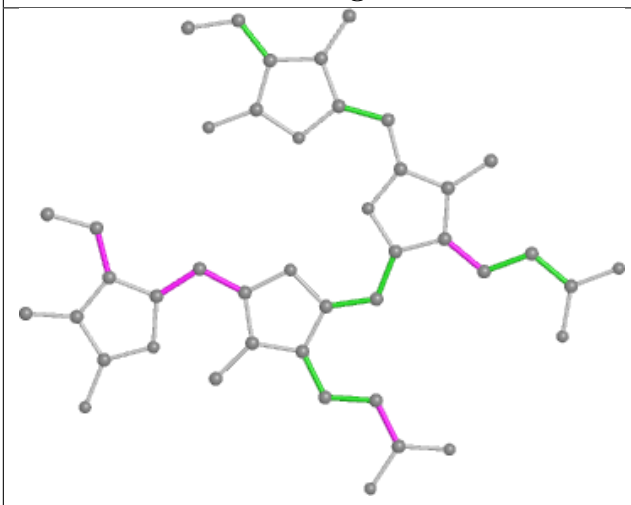

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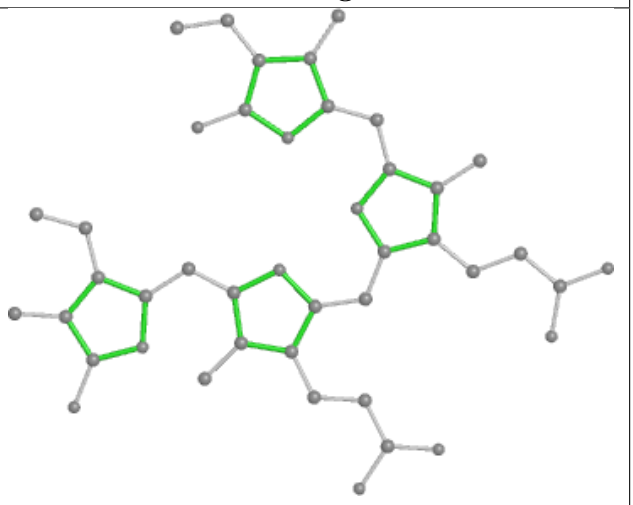
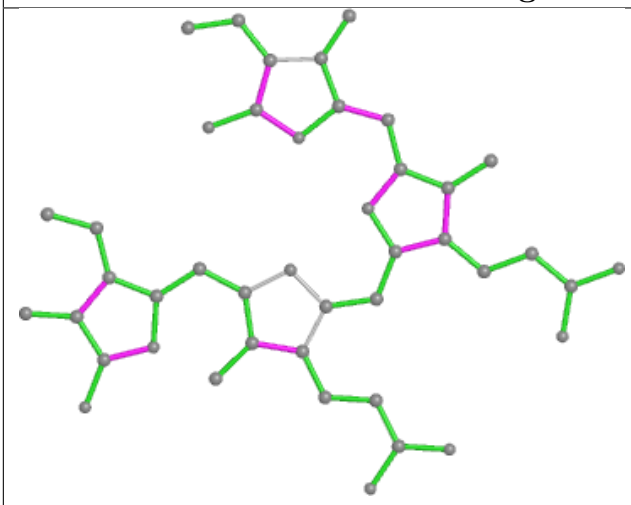


Rings

Ligand PUB z9 203



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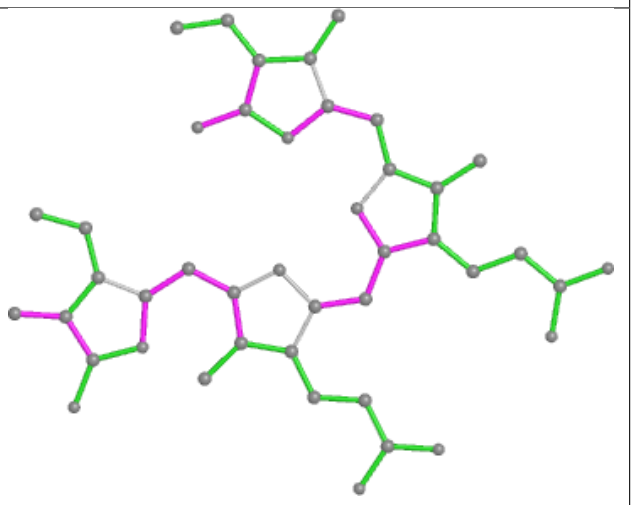

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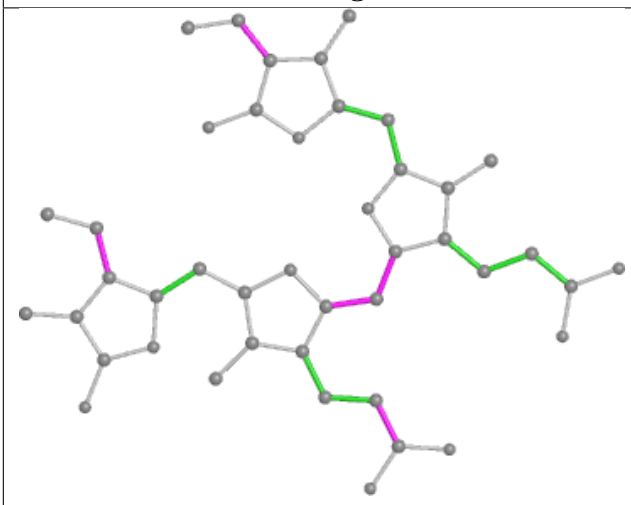

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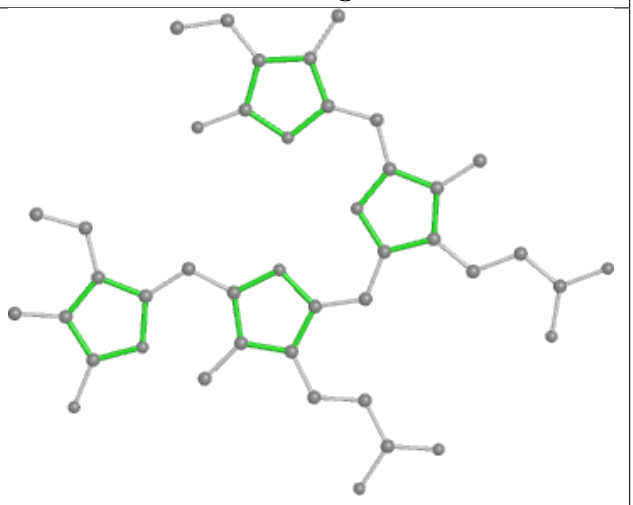
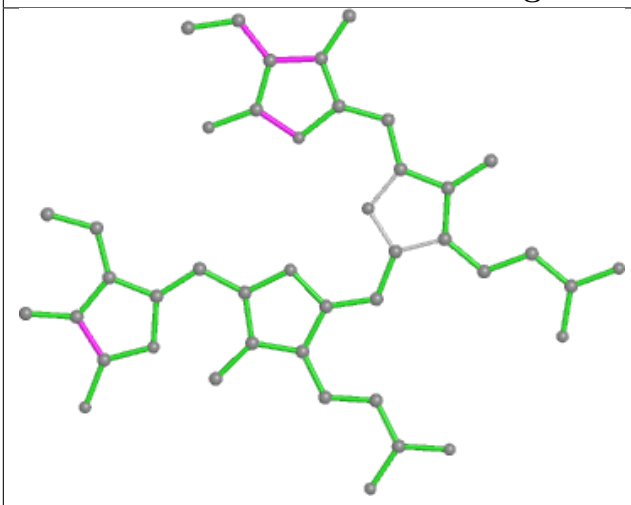


Rings

Ligand PEB i6 201



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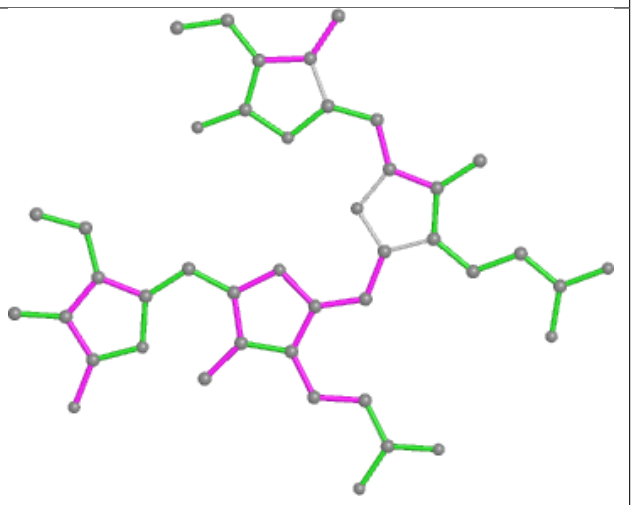

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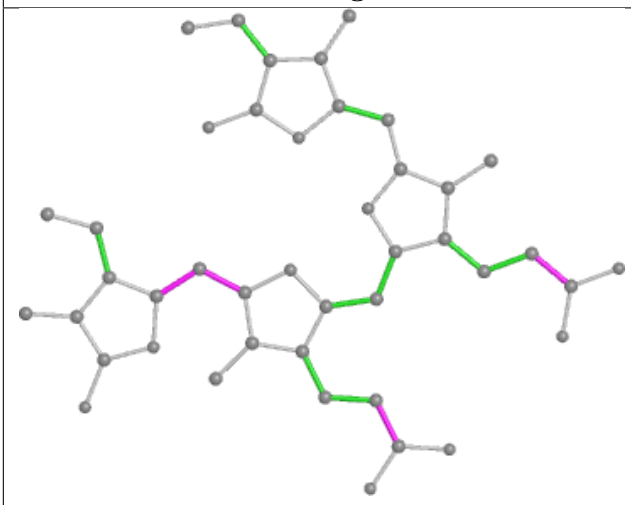

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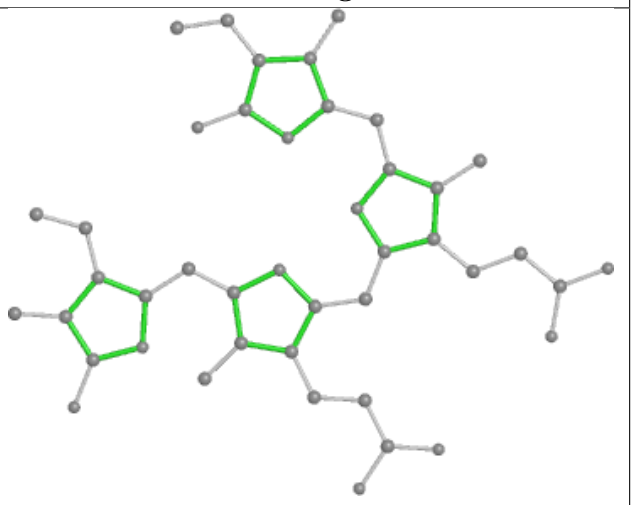
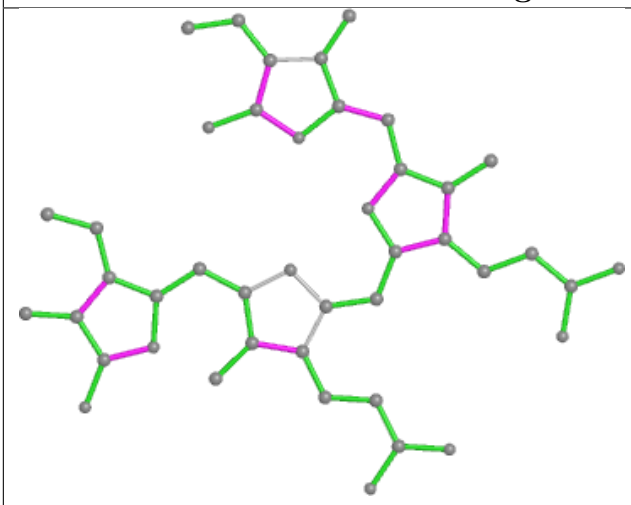


Rings

Ligand PUB P7 203



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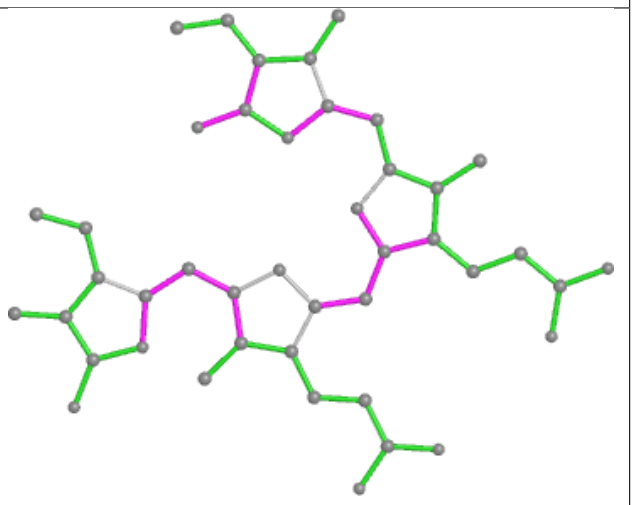

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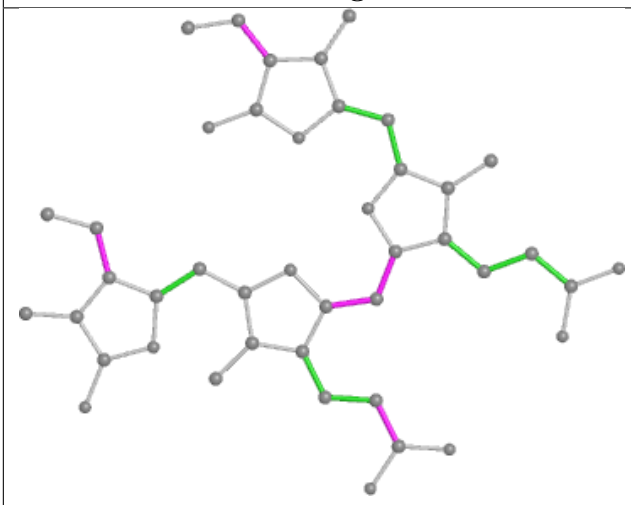

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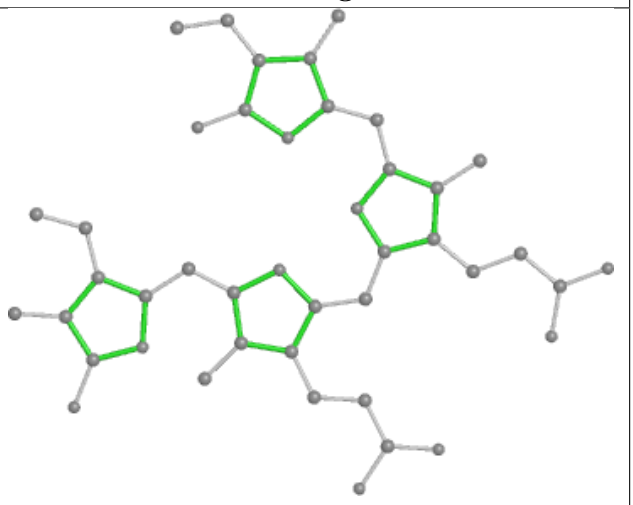
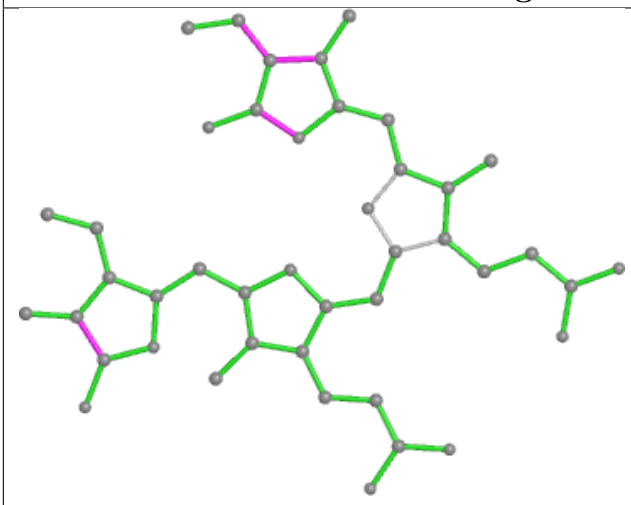


Rings

Ligand PEB U7 201



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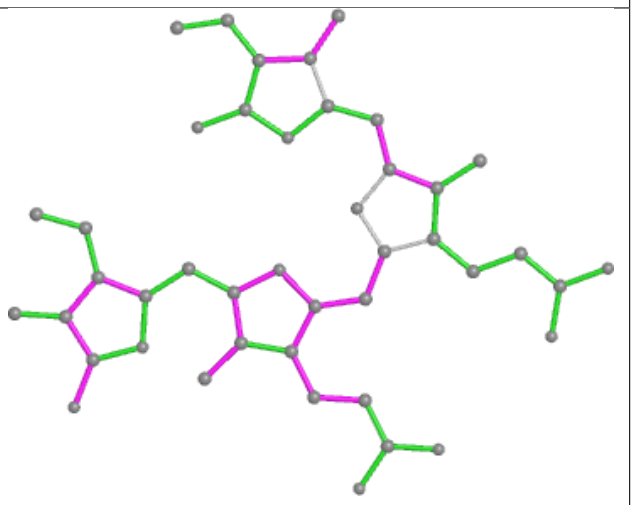

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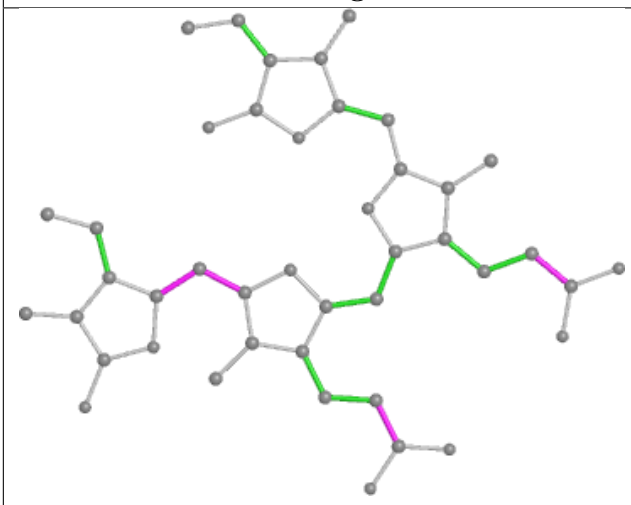
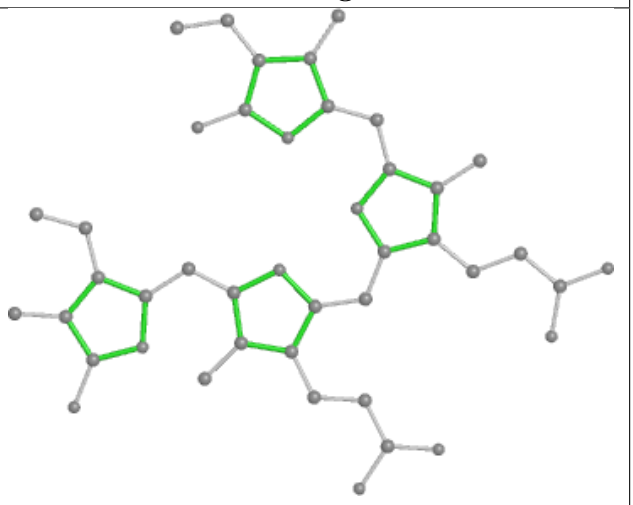
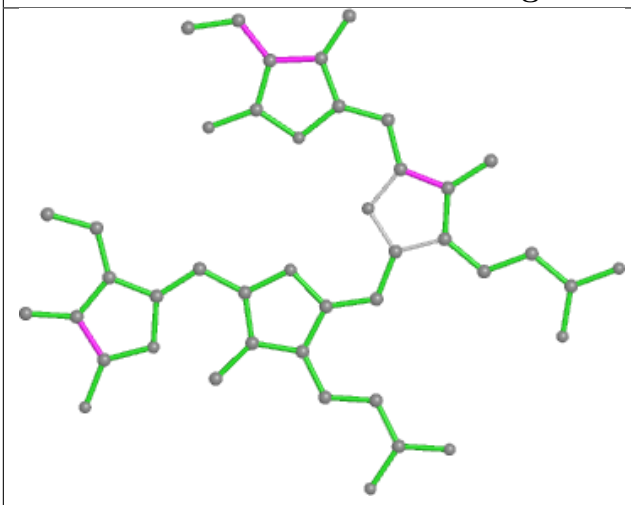


Torsions



Rings

Ligand PEB s4 202



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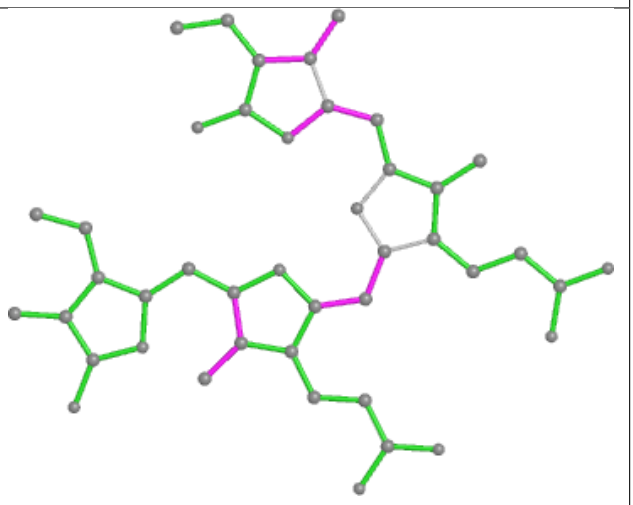

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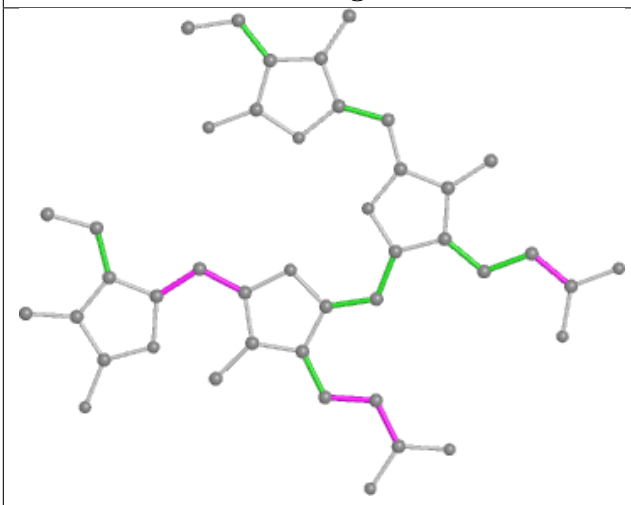

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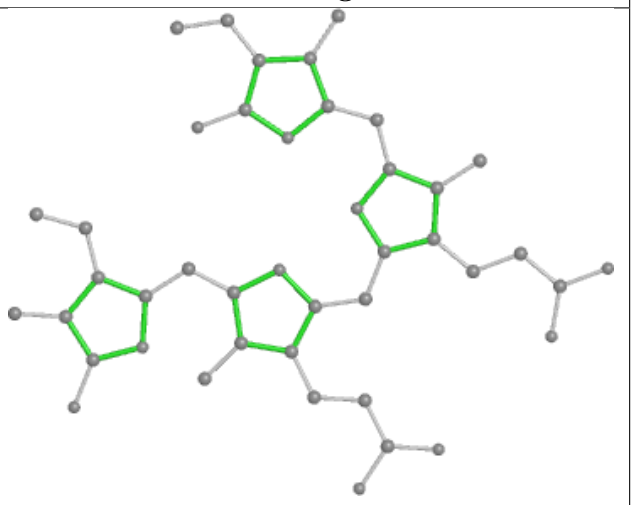
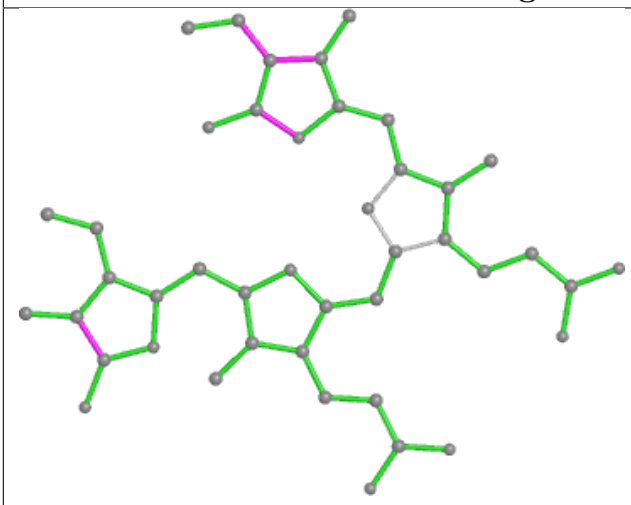


Rings

Ligand PEB b3 502



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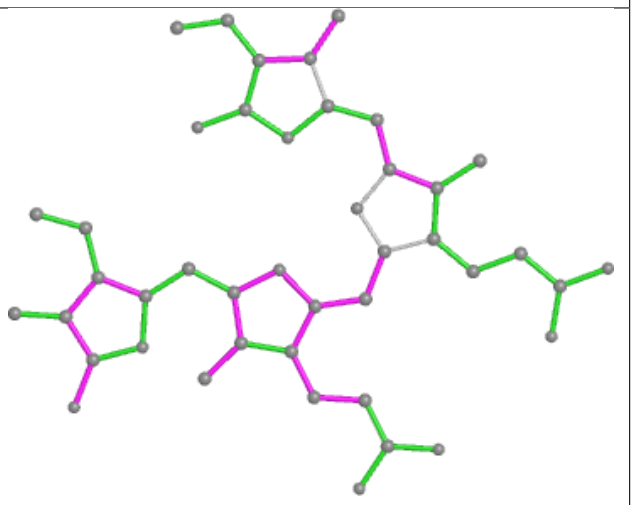

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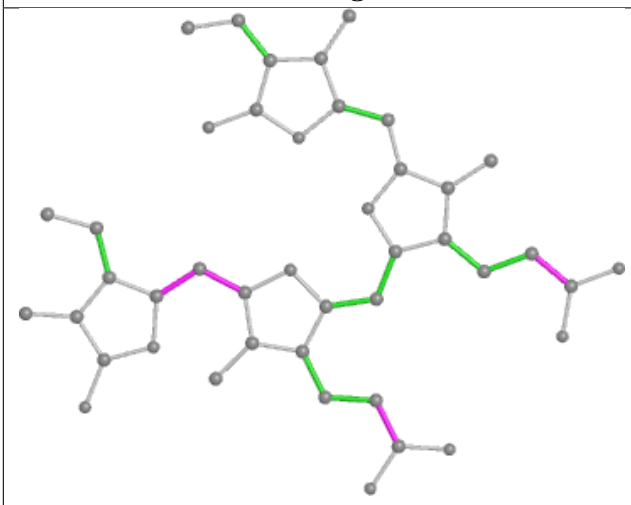

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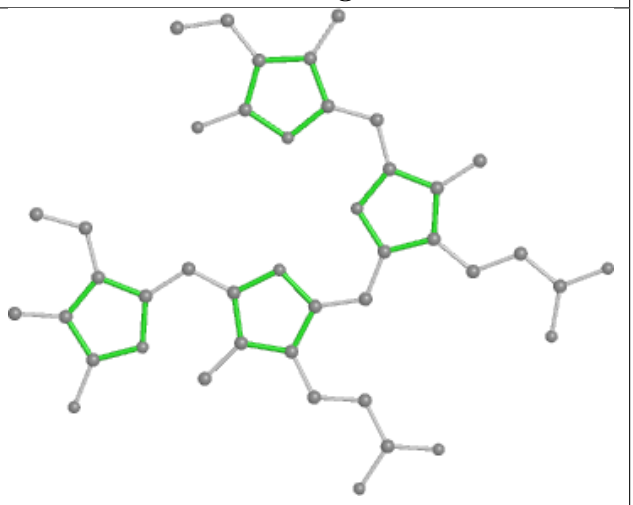
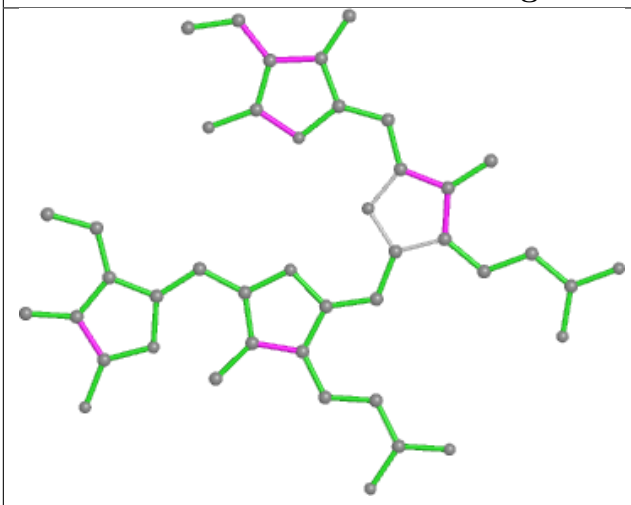


Rings

Ligand PEB ge 202



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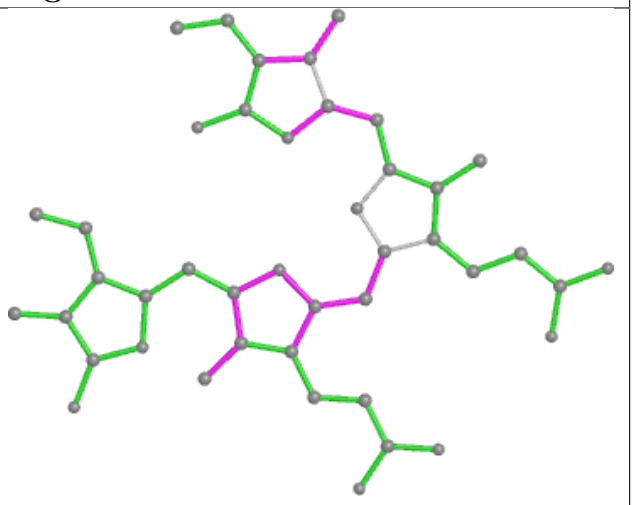

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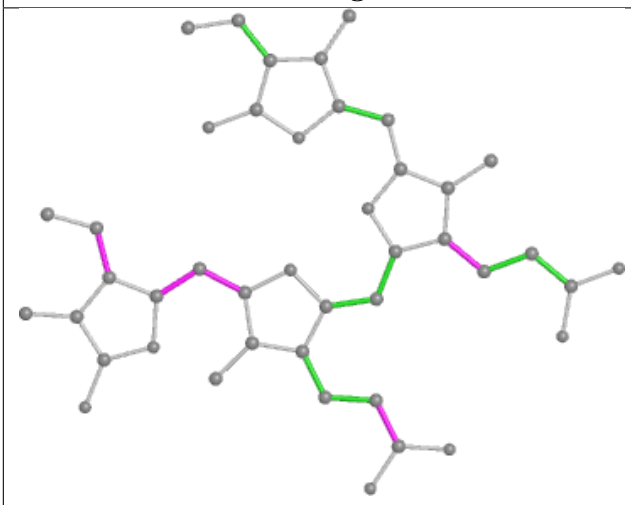

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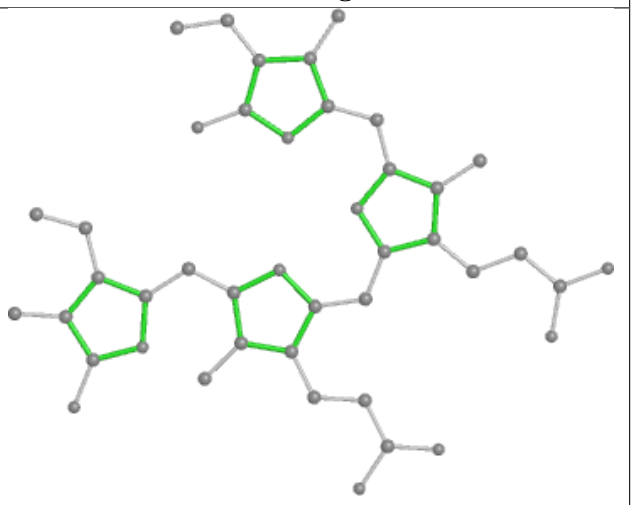
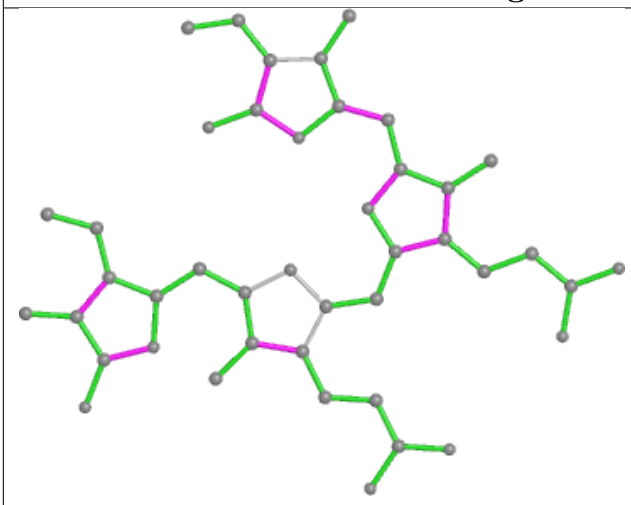


Rings

Ligand PUB jN 1003



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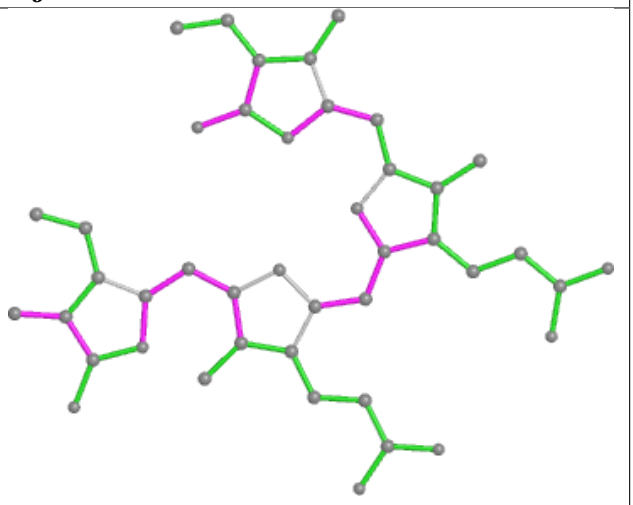

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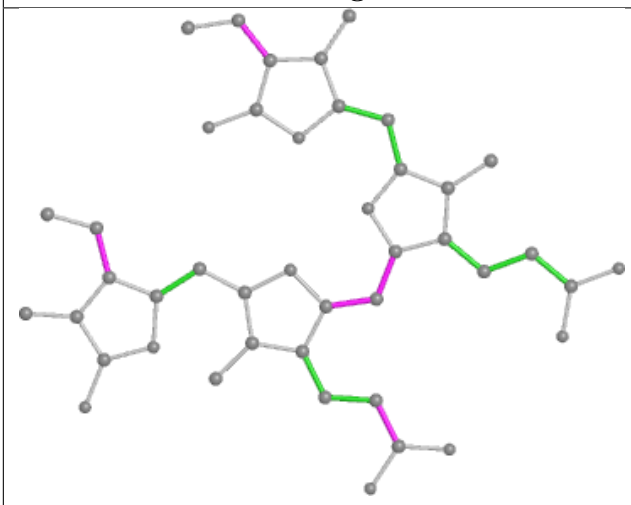

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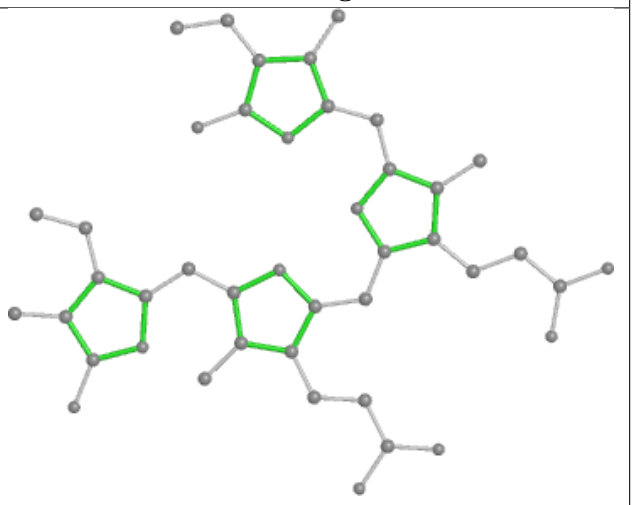
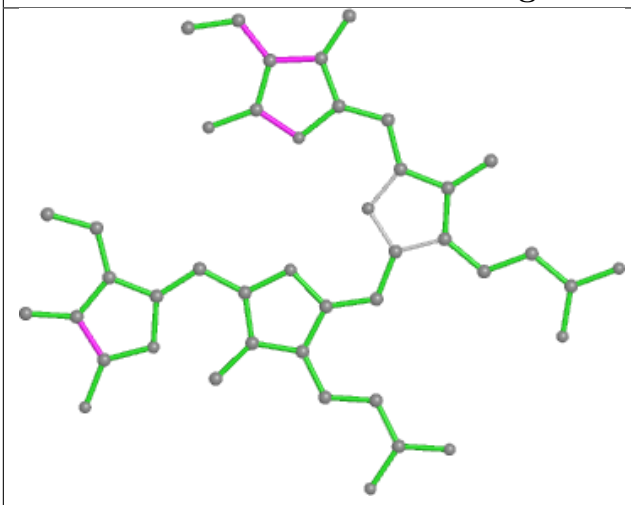


Rings

Ligand PEB p9 201



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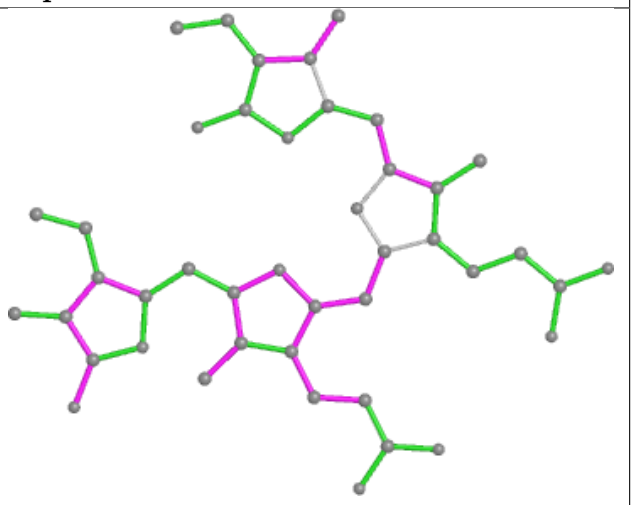

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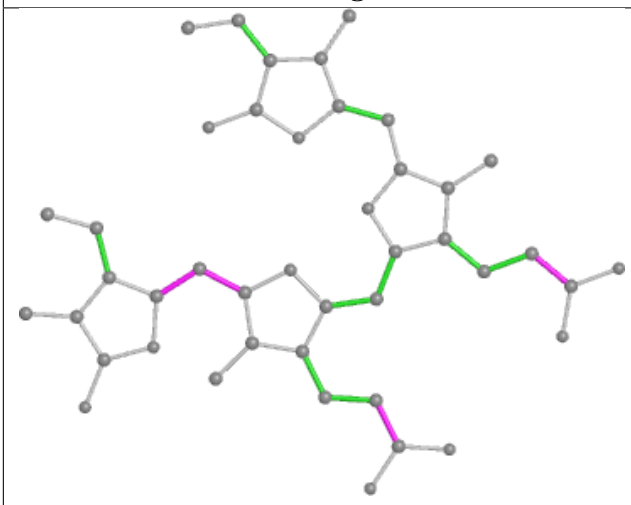

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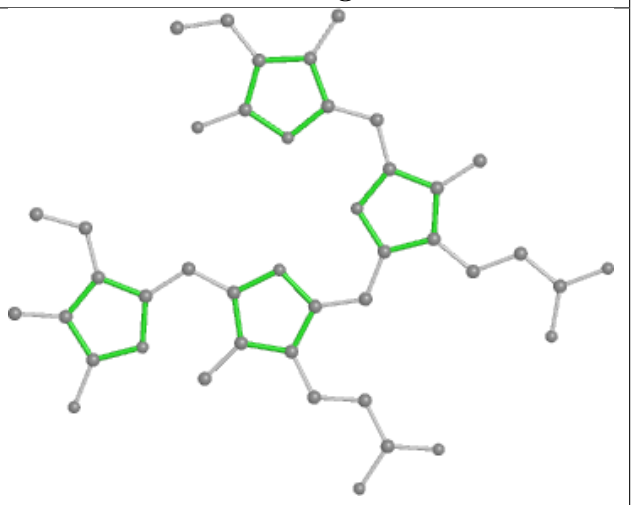
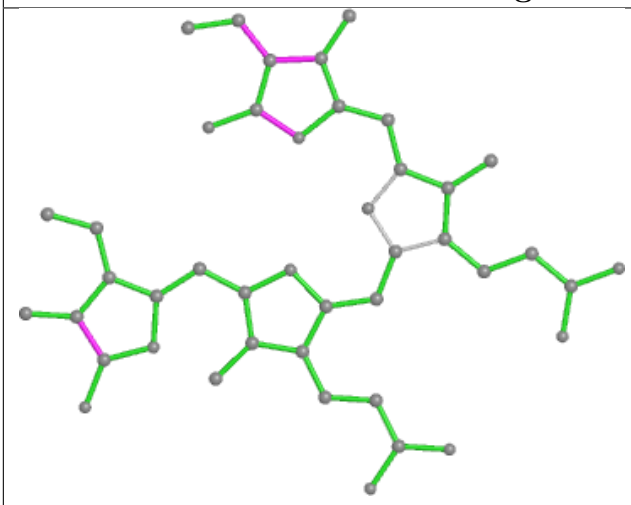


Rings

Ligand PEB H5 201



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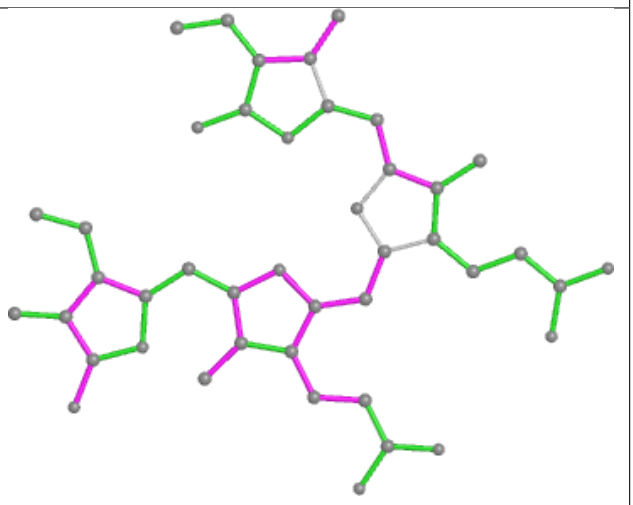

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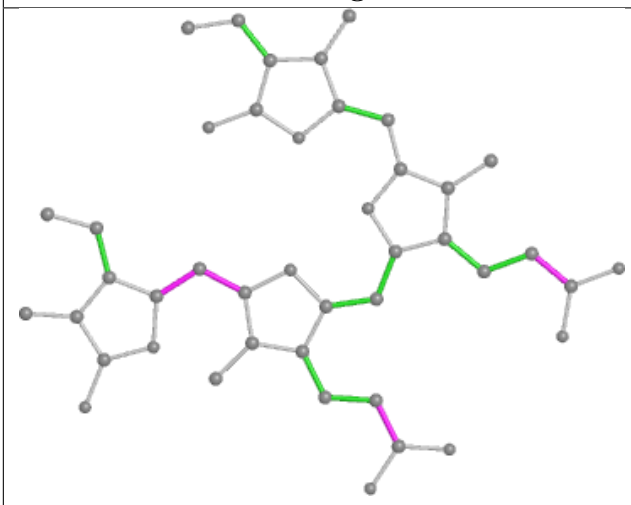

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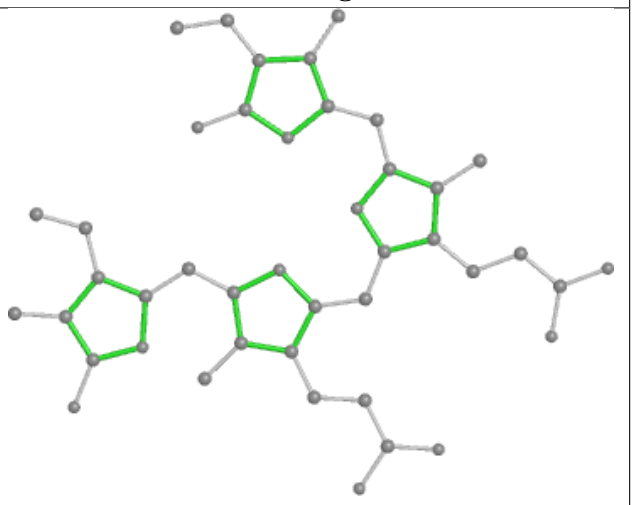
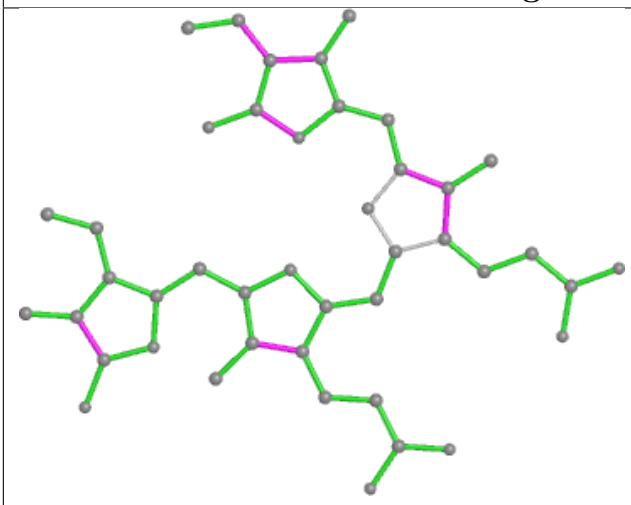


Rings

Ligand PEB lh 202



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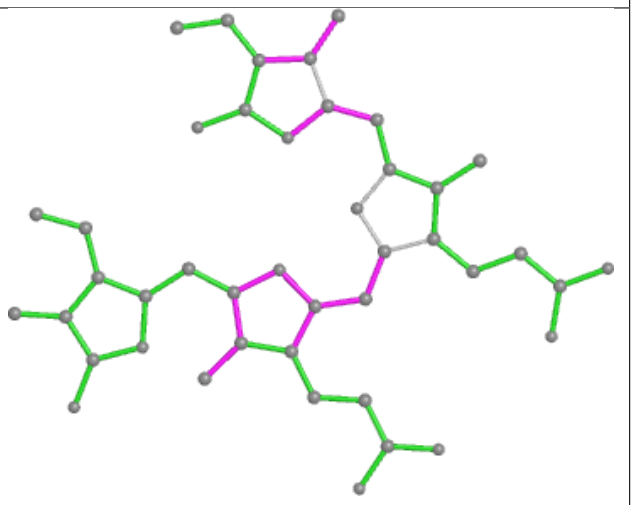

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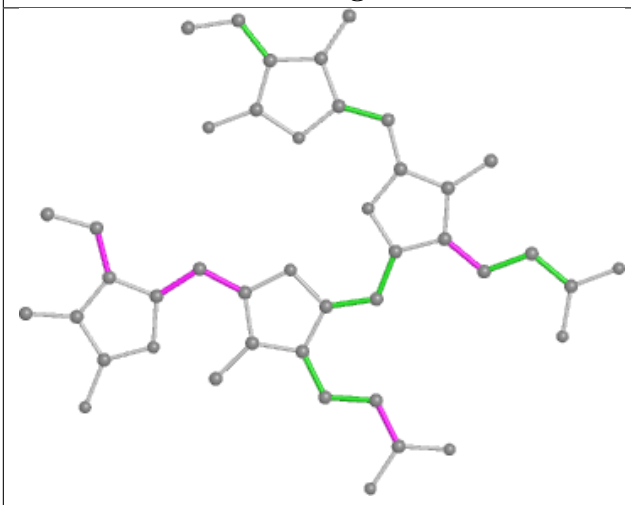

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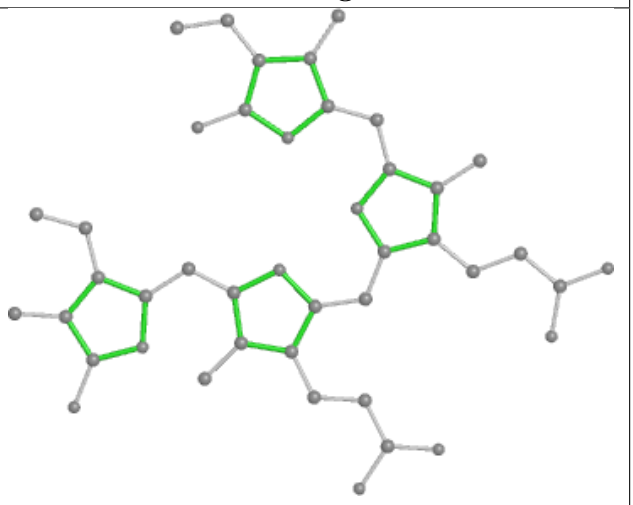

Rings

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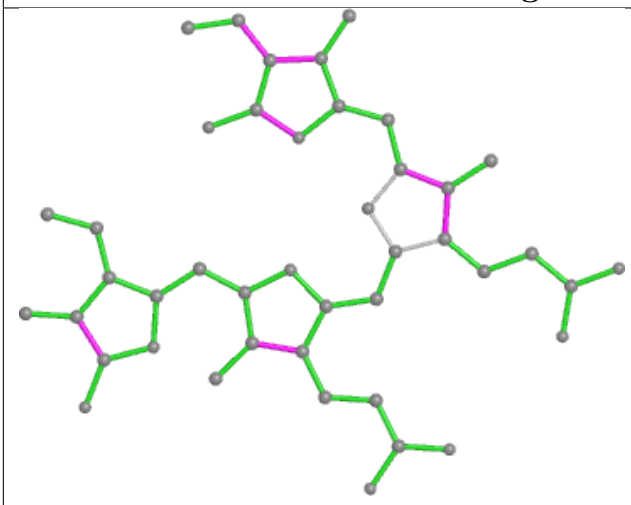

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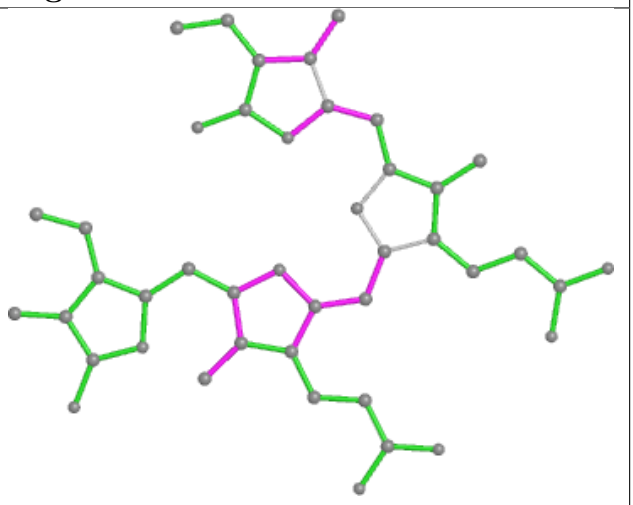

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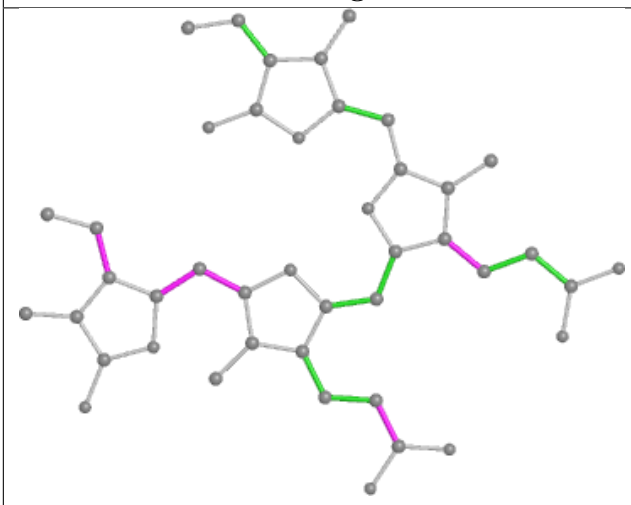

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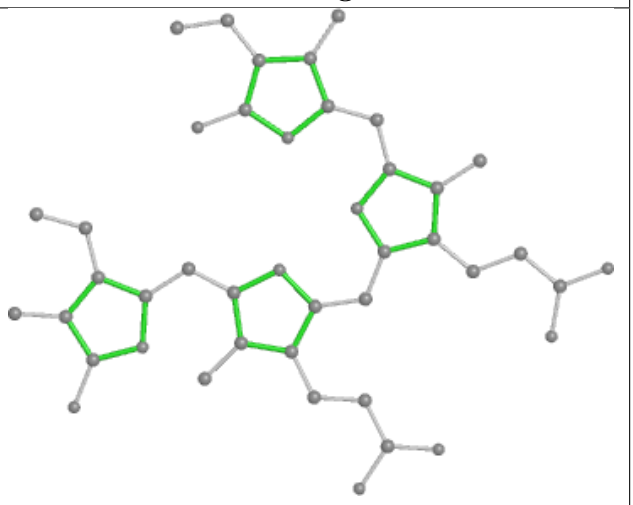
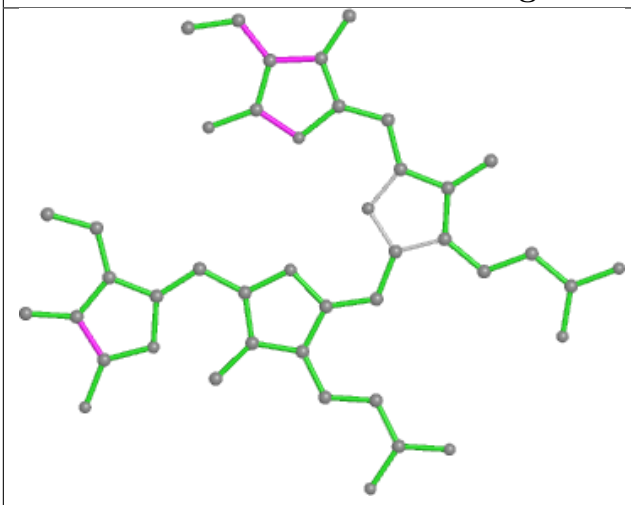


Rings

Ligand PEB ab 201



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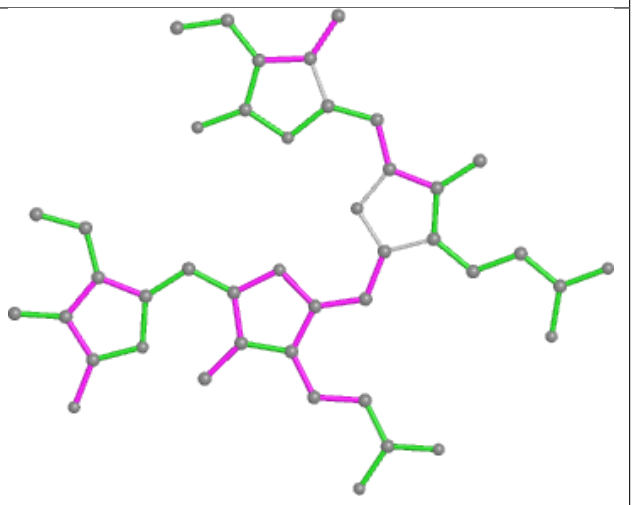

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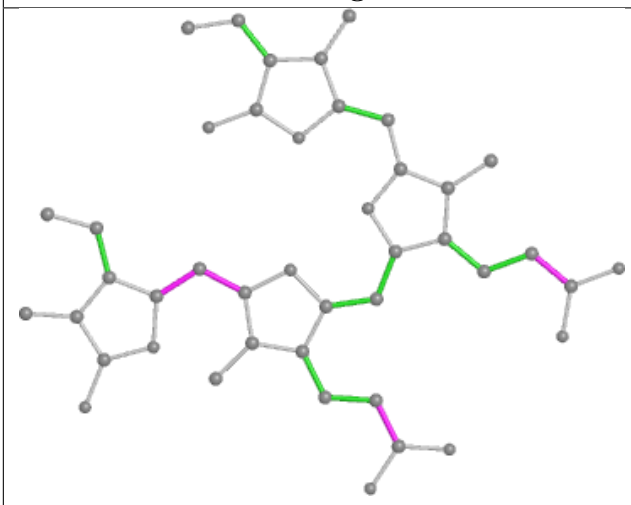

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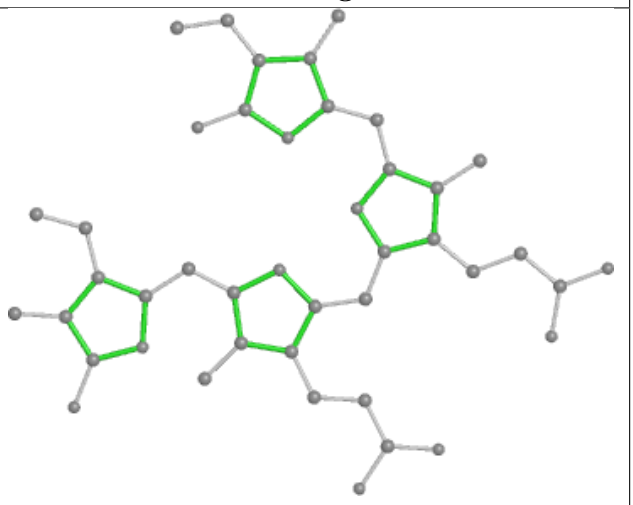

Rings

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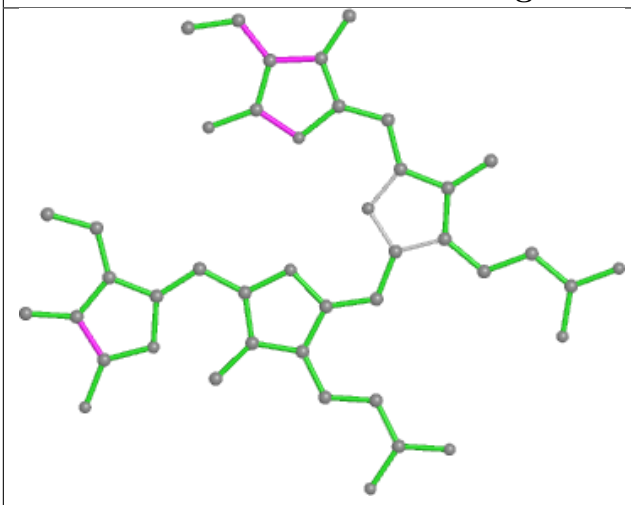

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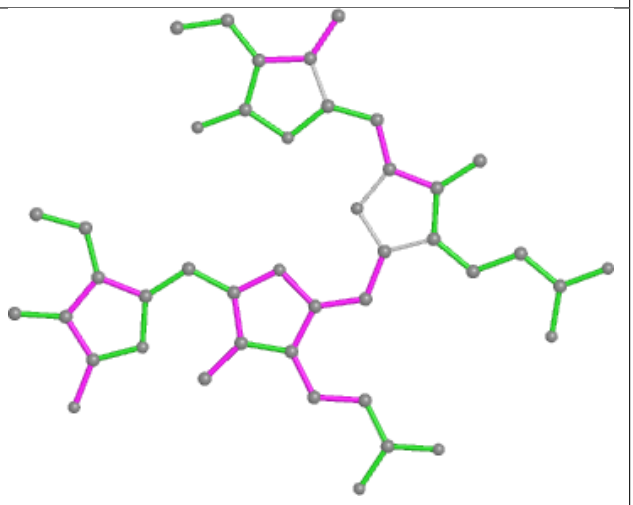

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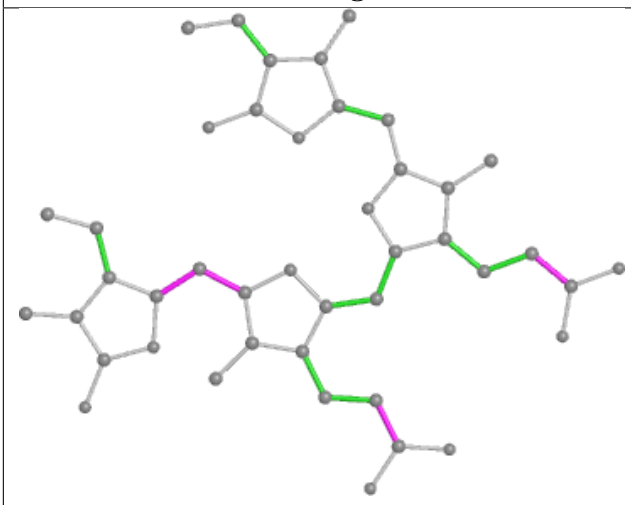

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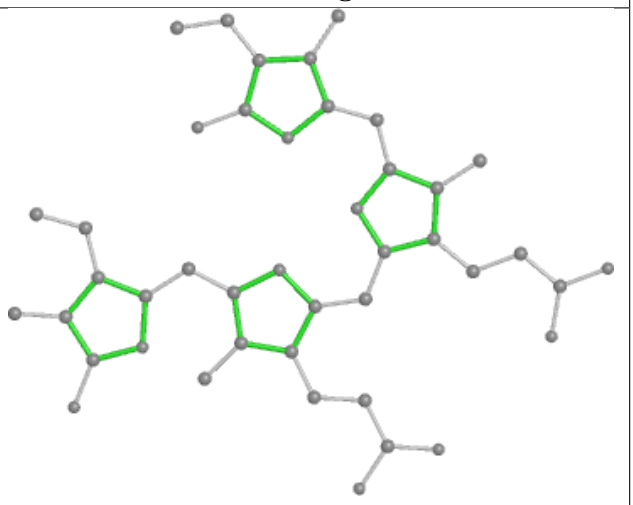
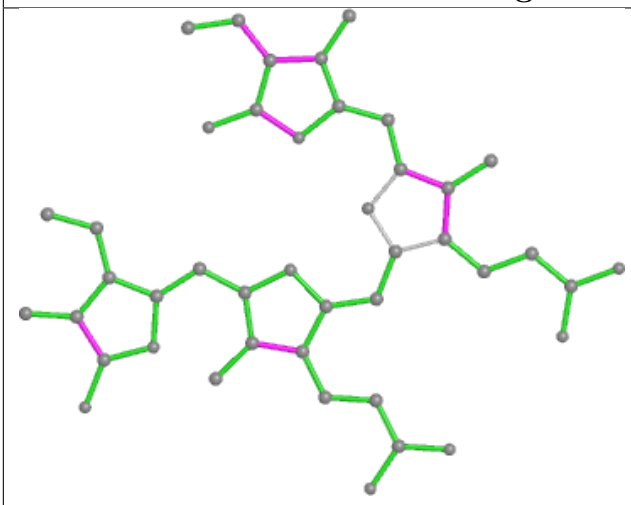


Rings

Ligand PEB A5 203



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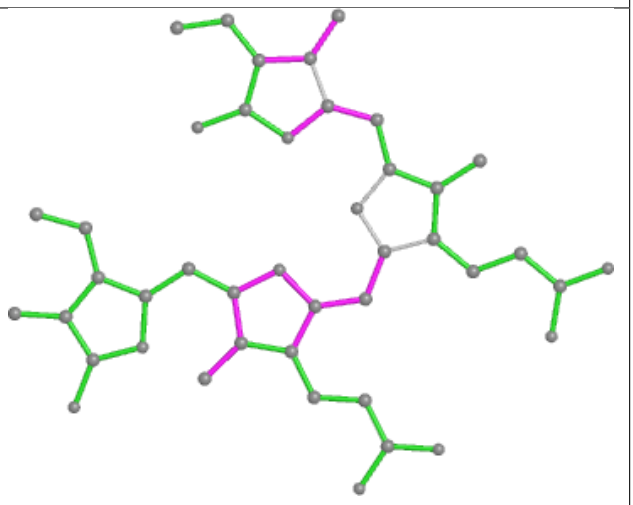

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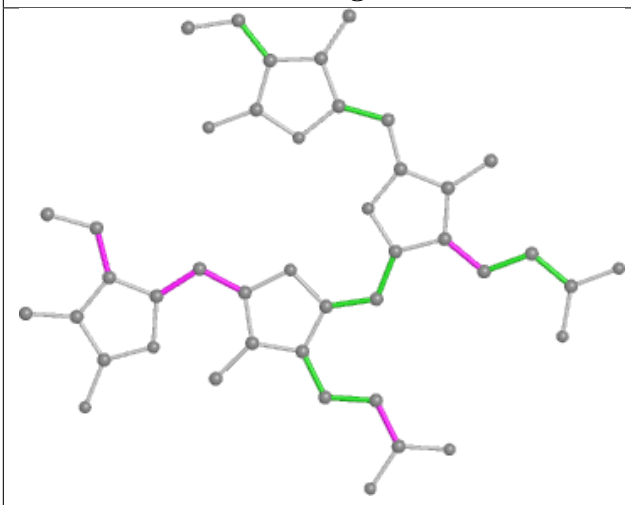

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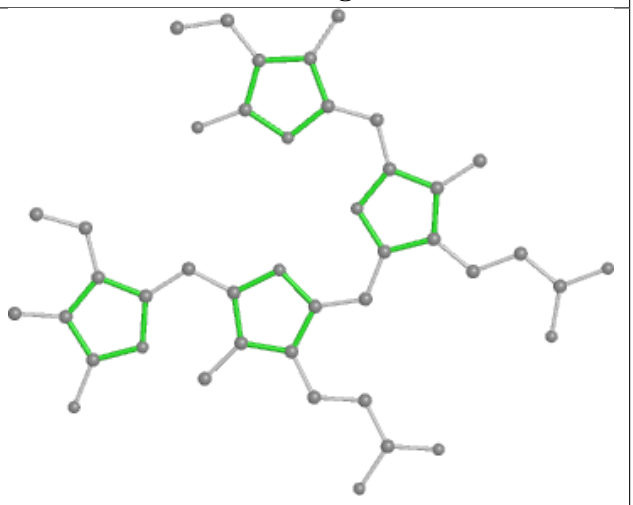
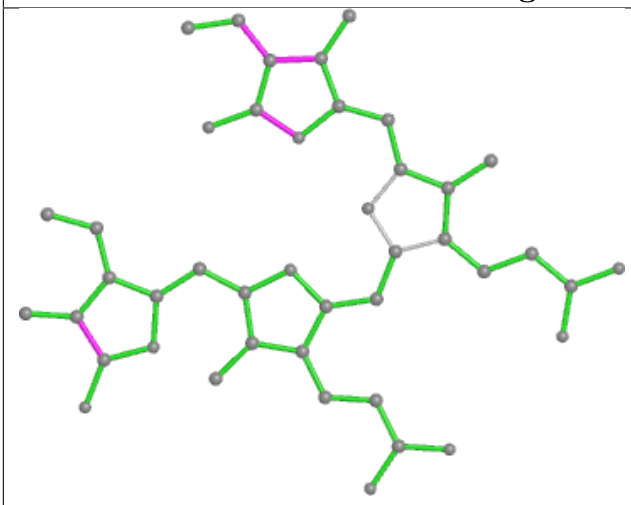


Rings

Ligand PEB u6 202



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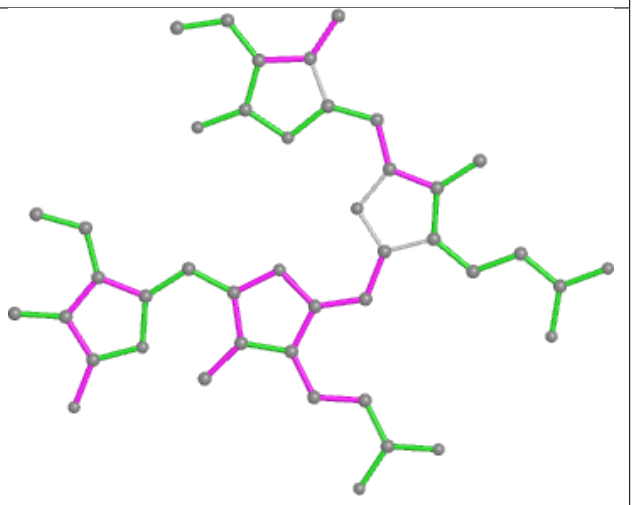

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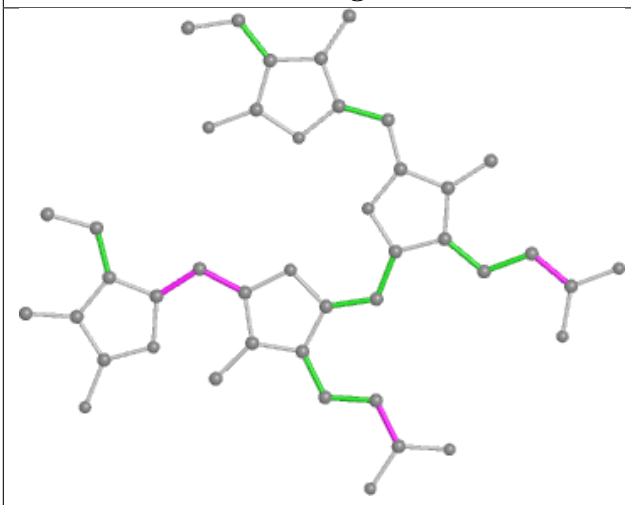

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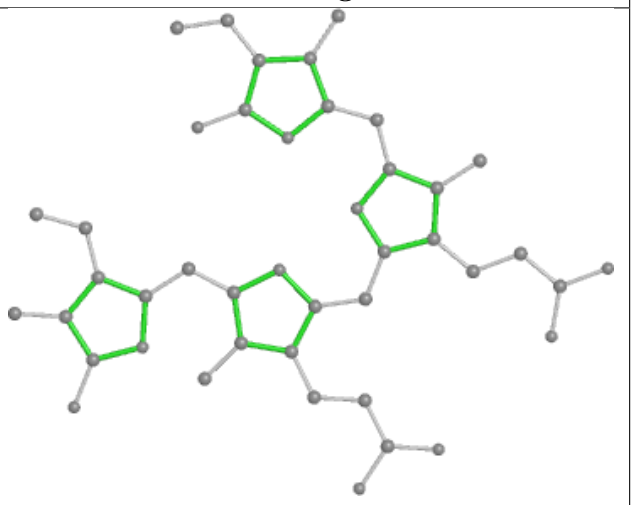
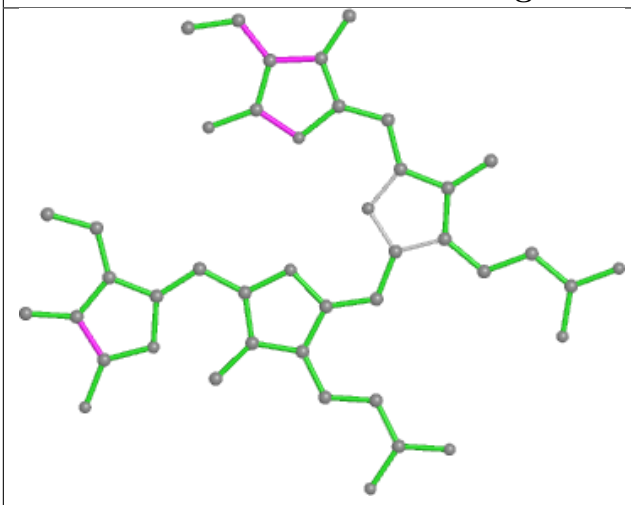


Rings

Ligand PEB D8 202



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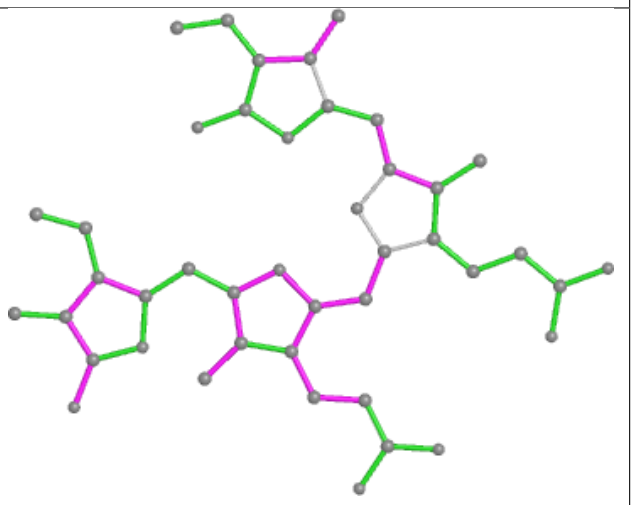

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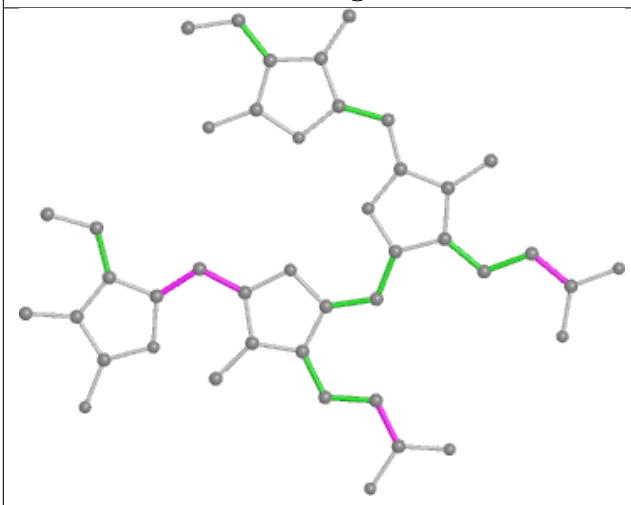
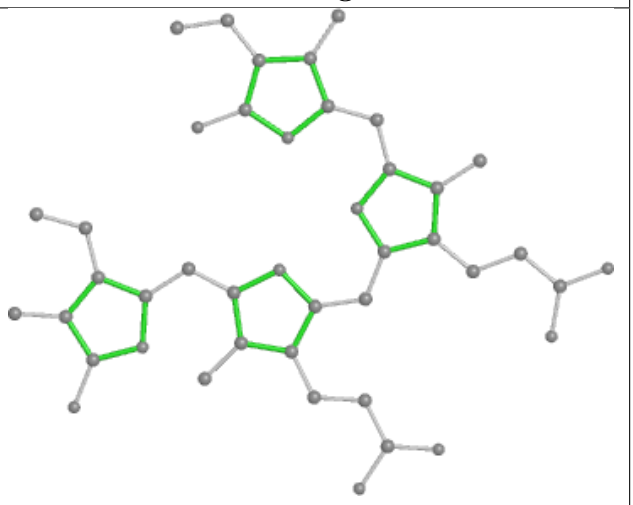
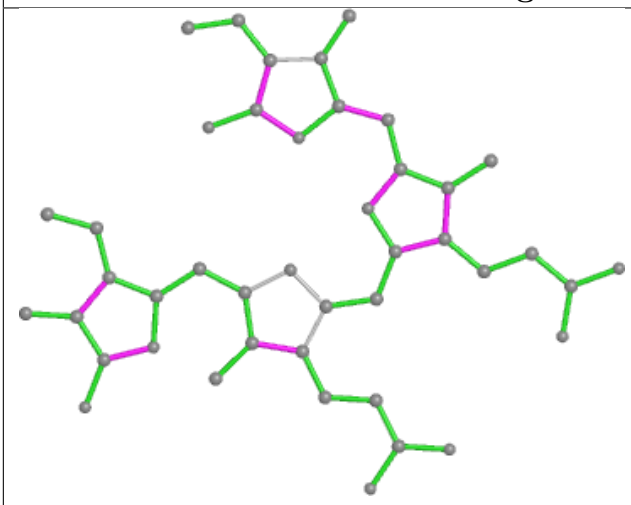


Torsions



Rings

Ligand PUB n8 202



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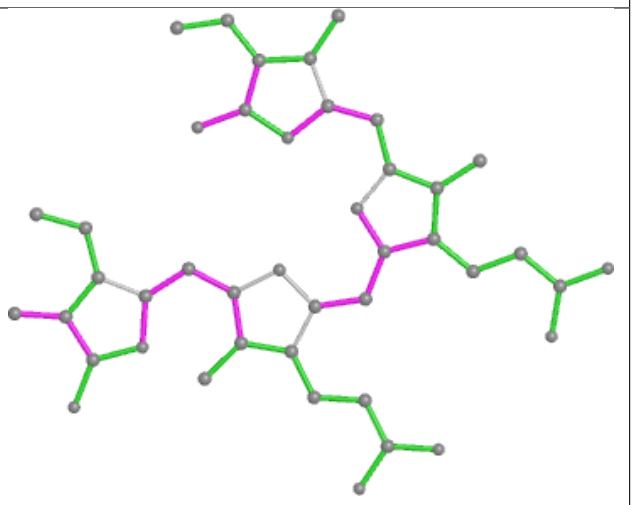

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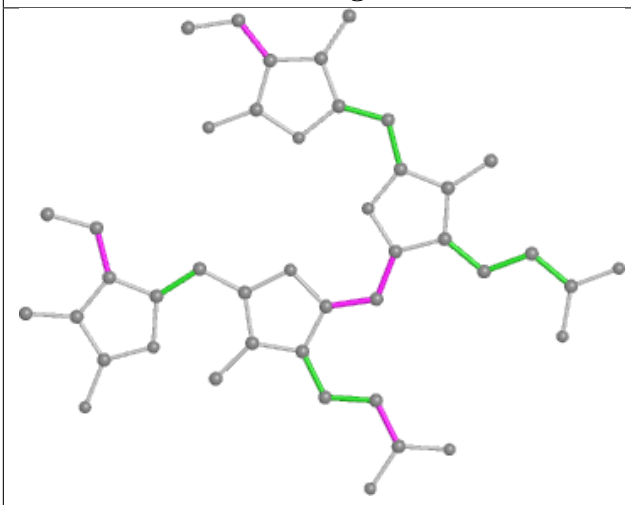

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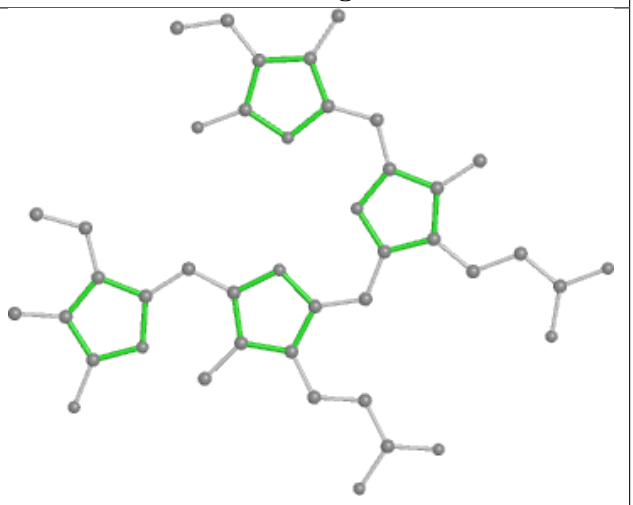
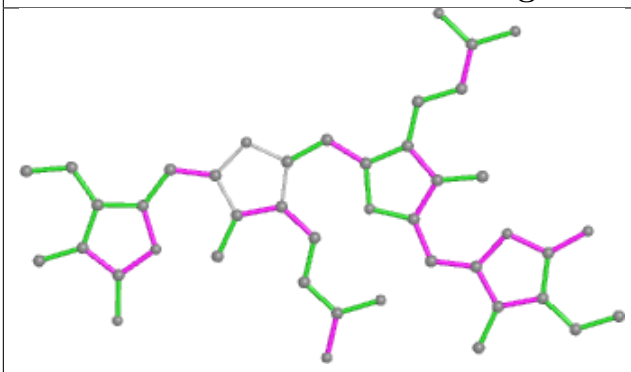


Rings

Ligand CYC c1 201



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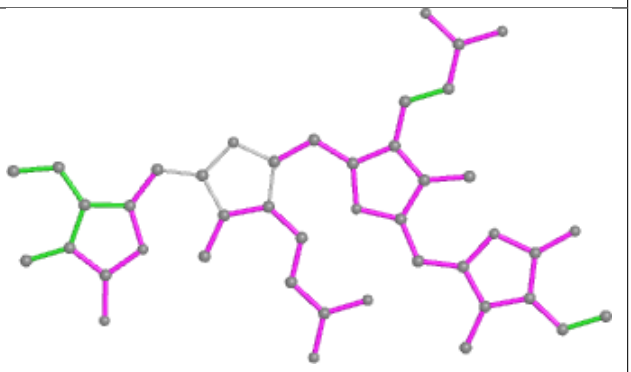

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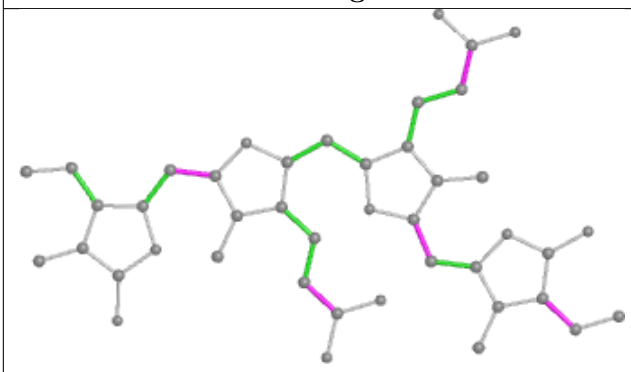

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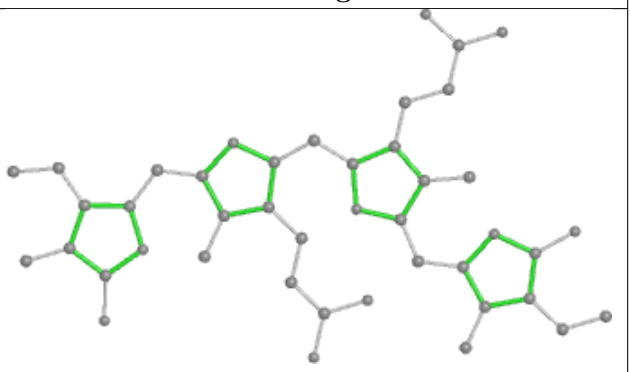
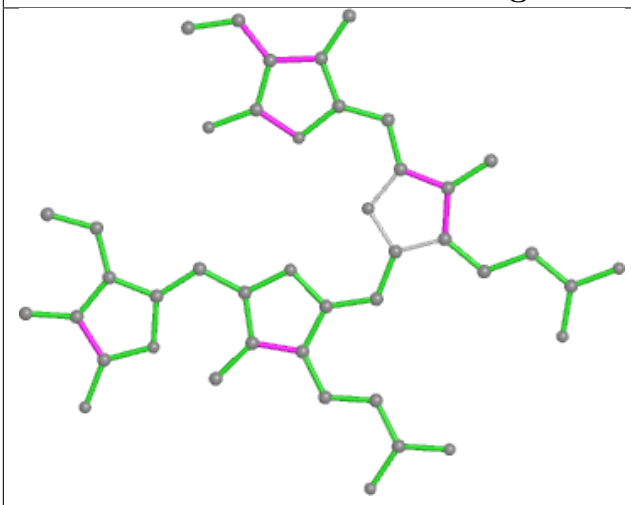


Rings

Ligand PEB jO 1002



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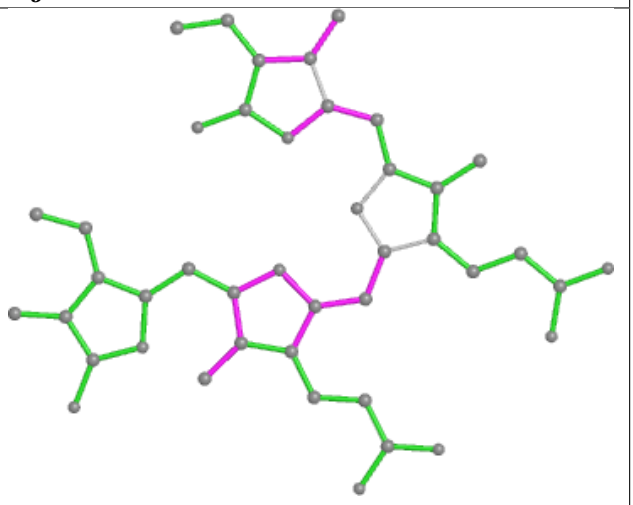

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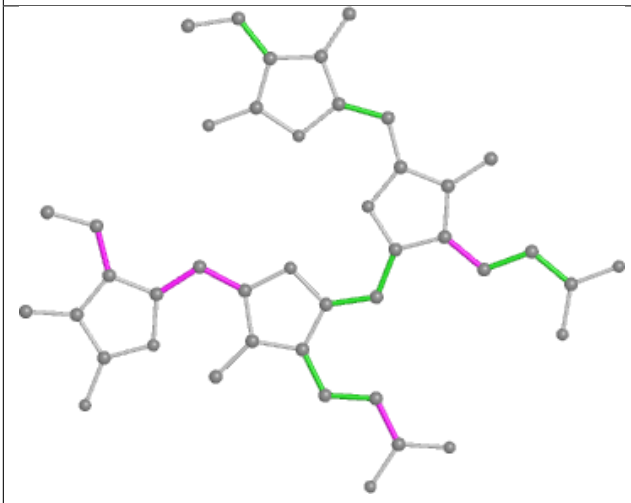

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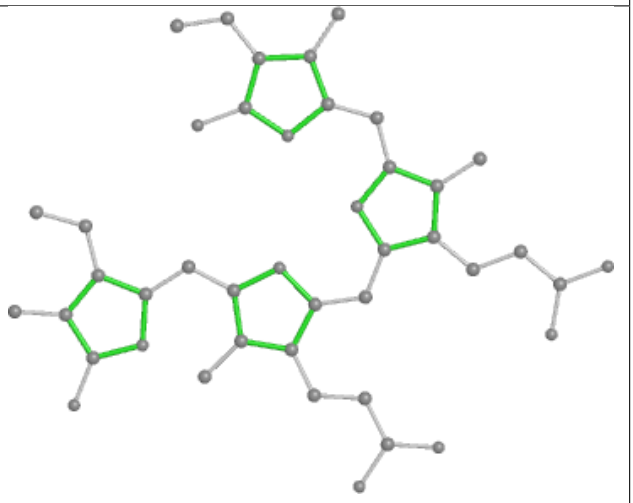
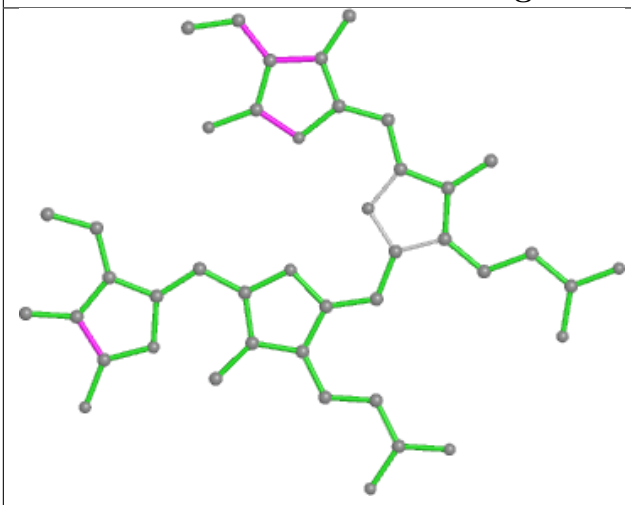


Rings

Ligand PEB G2 201



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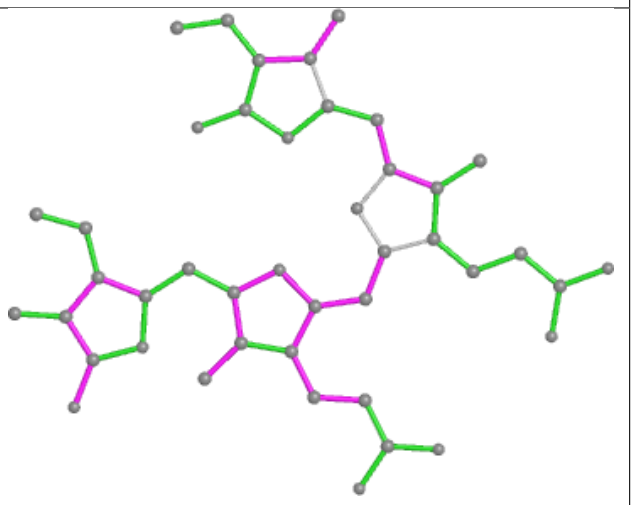

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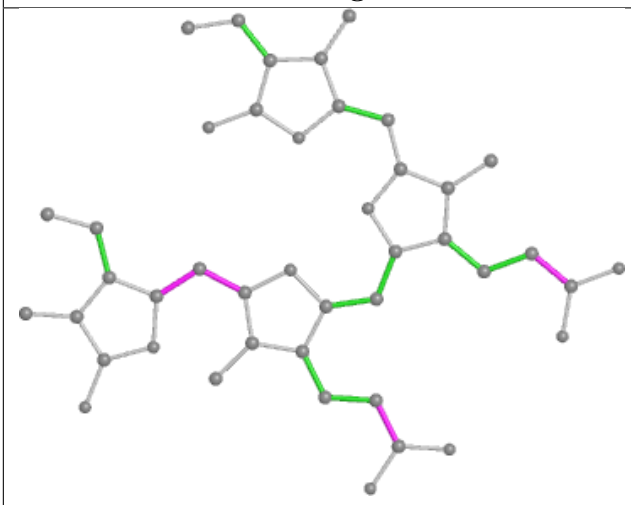

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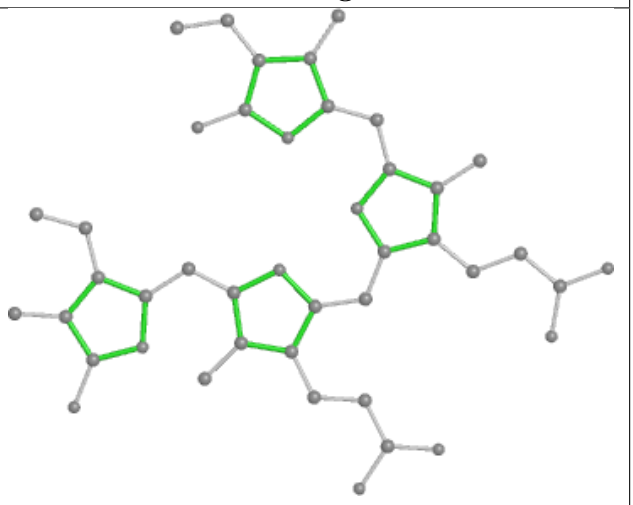
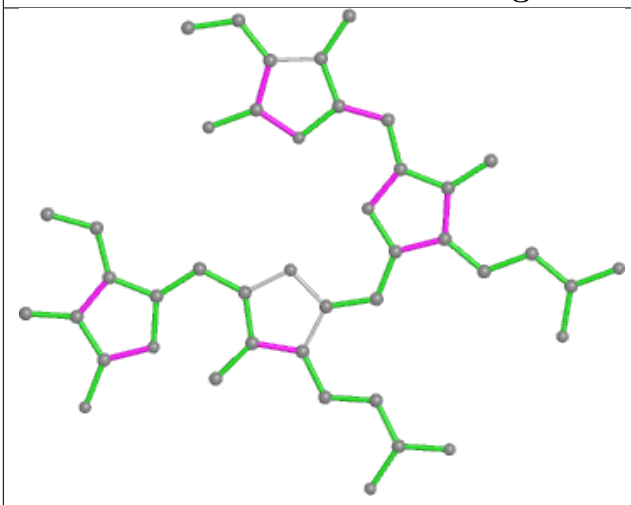


Rings

Ligand PUB hR 203



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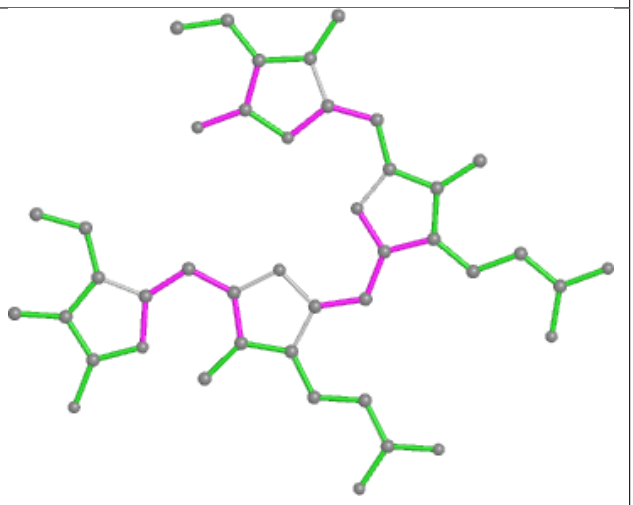

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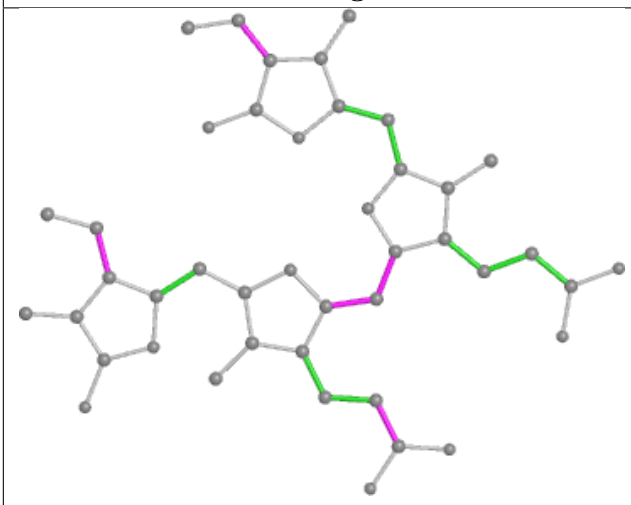

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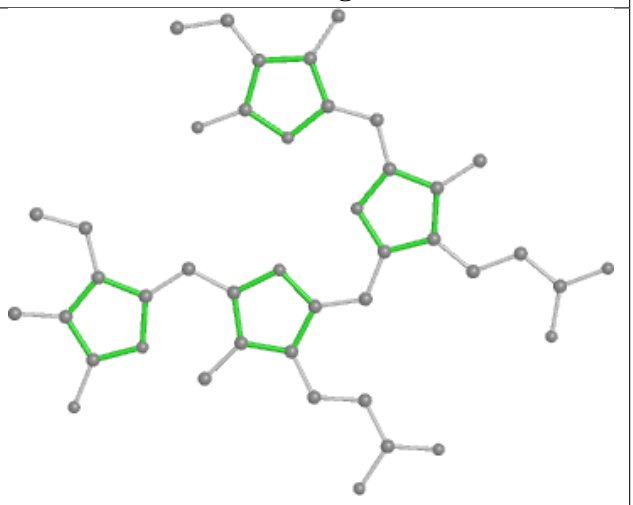

Rings

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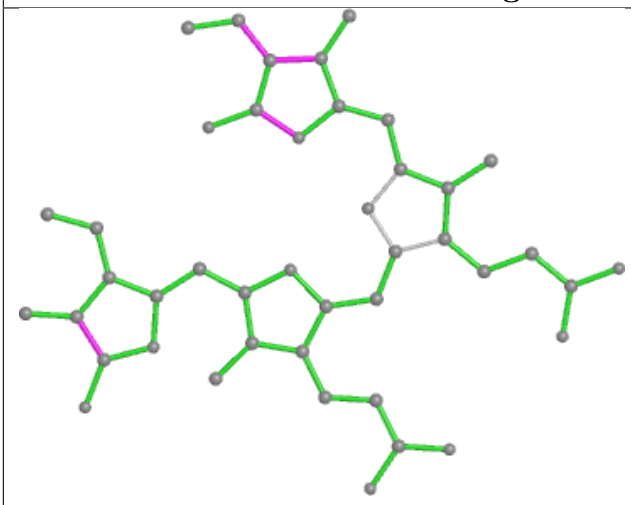

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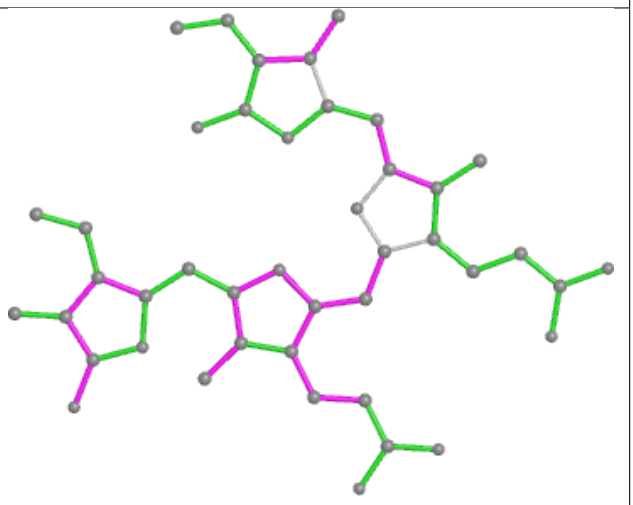

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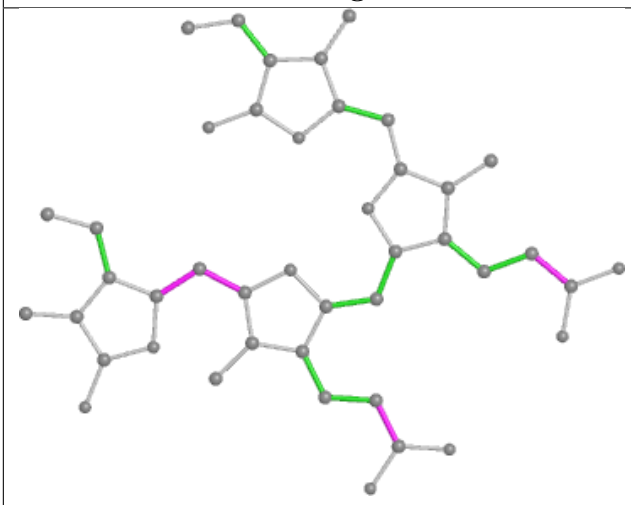

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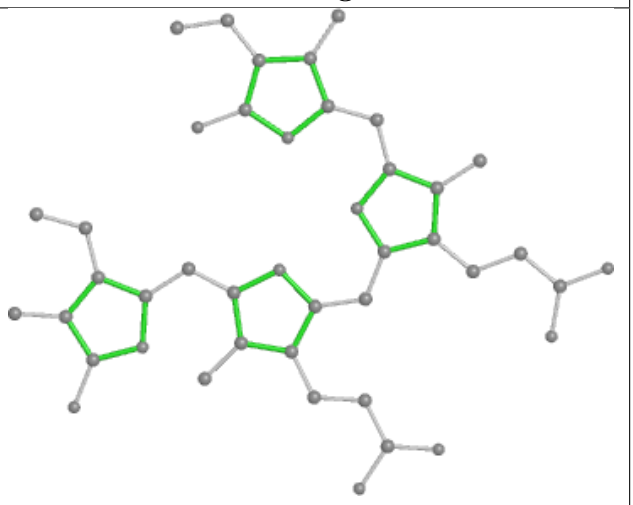

Rings

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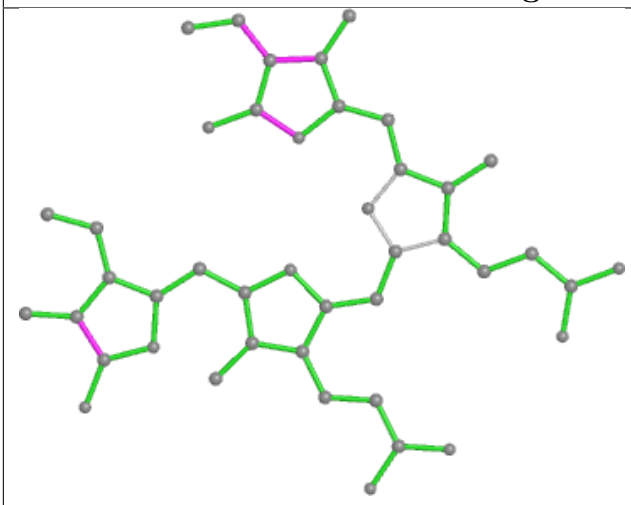

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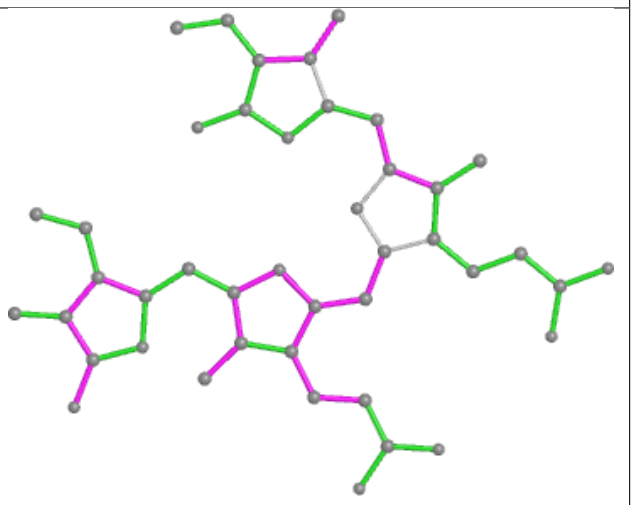

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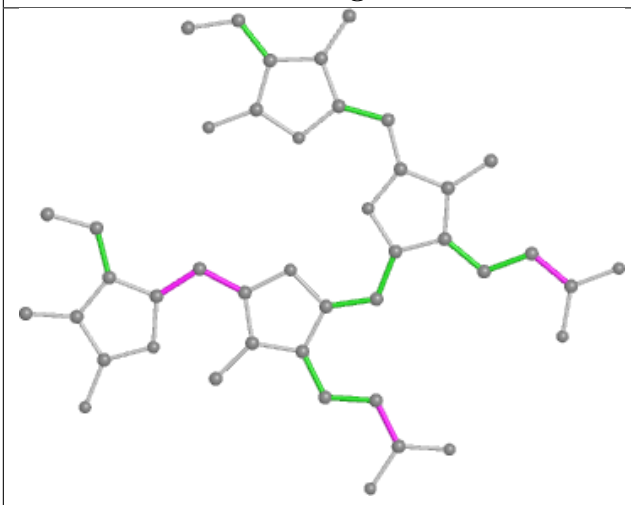

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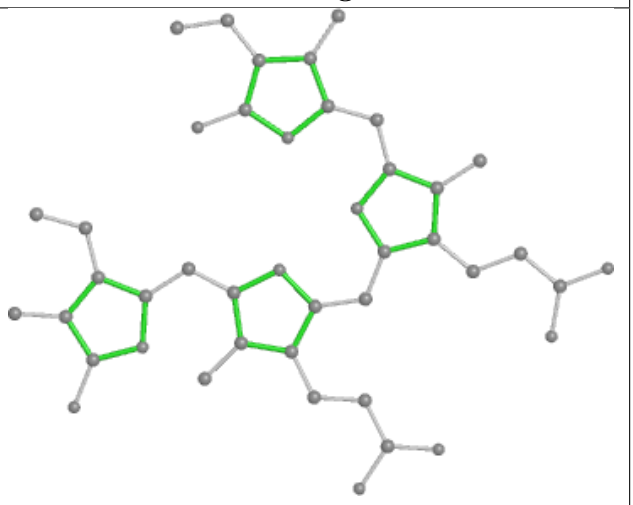

Rings

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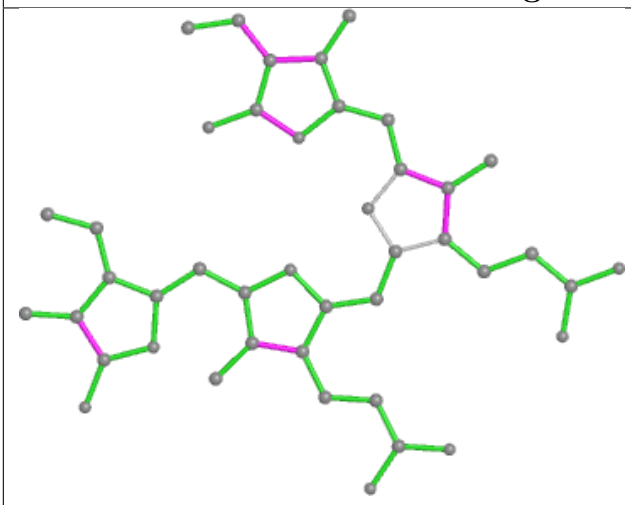

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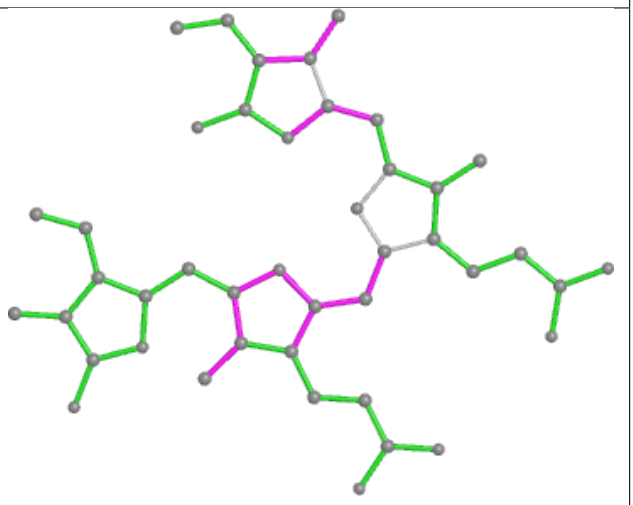

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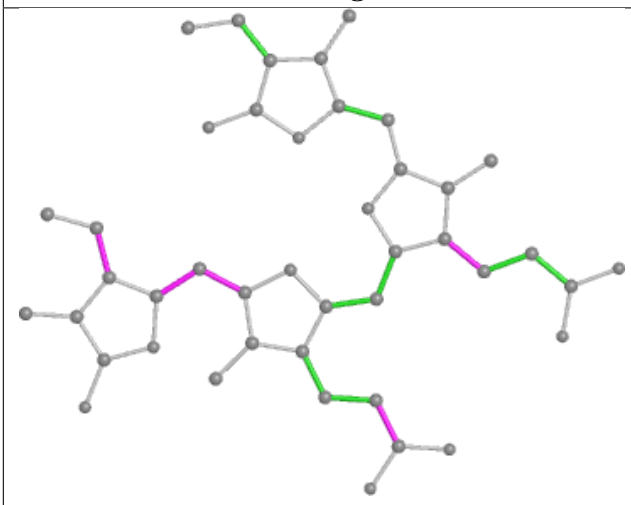

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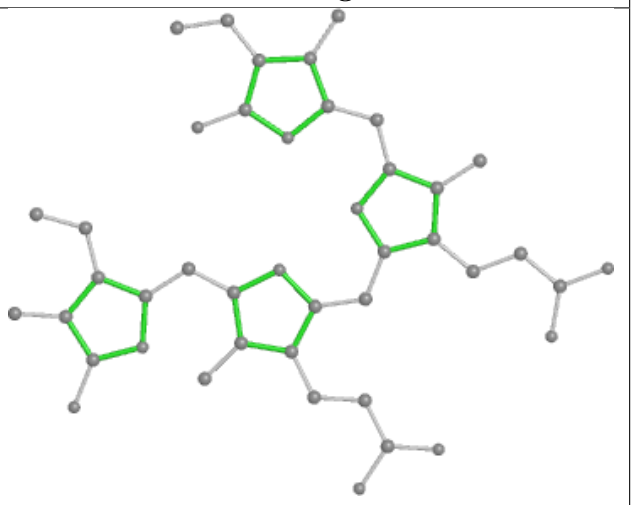

Rings

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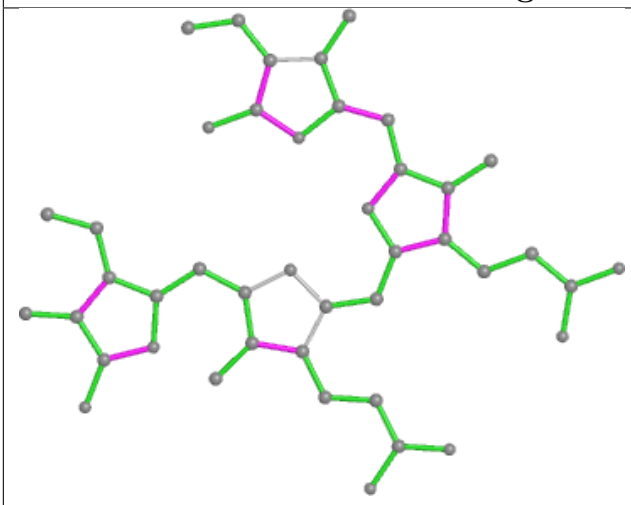

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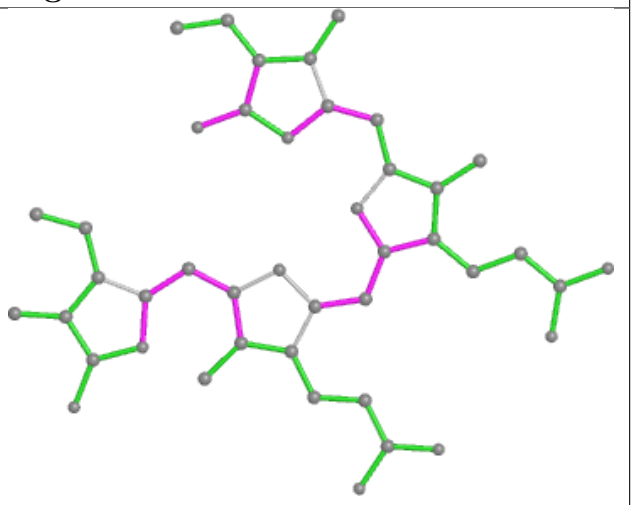

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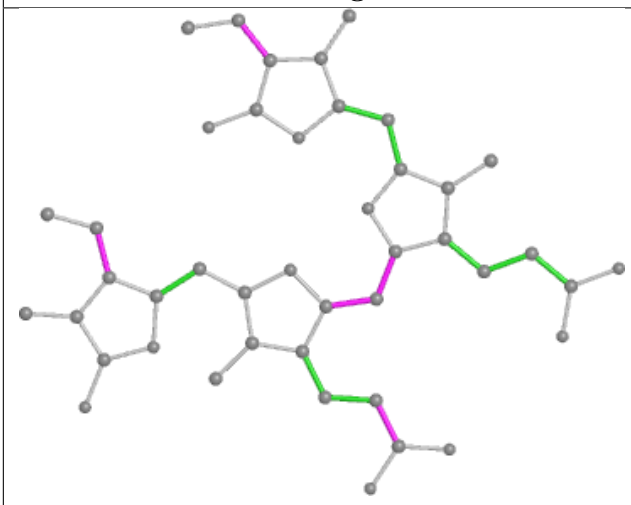

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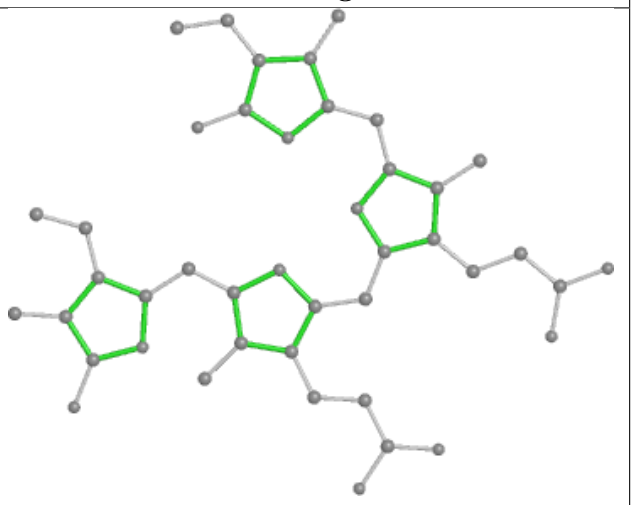
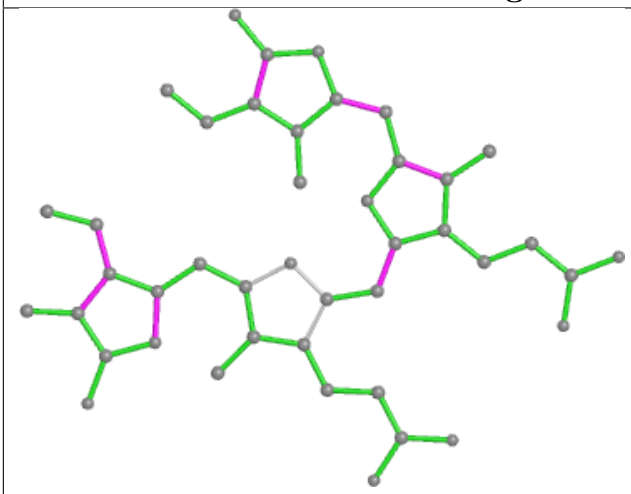


Rings

Ligand PVN Z9 1004



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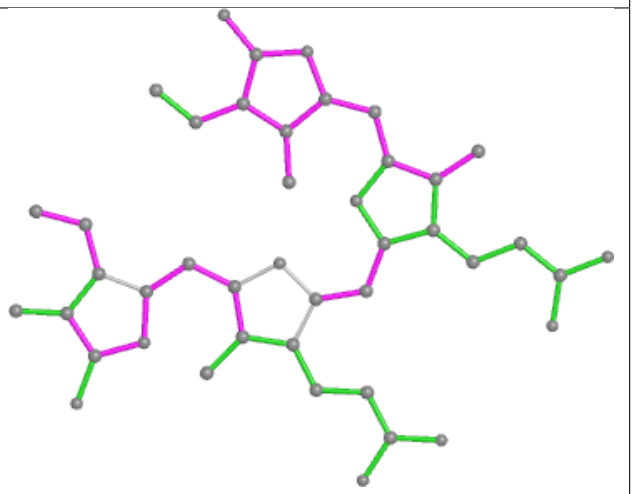

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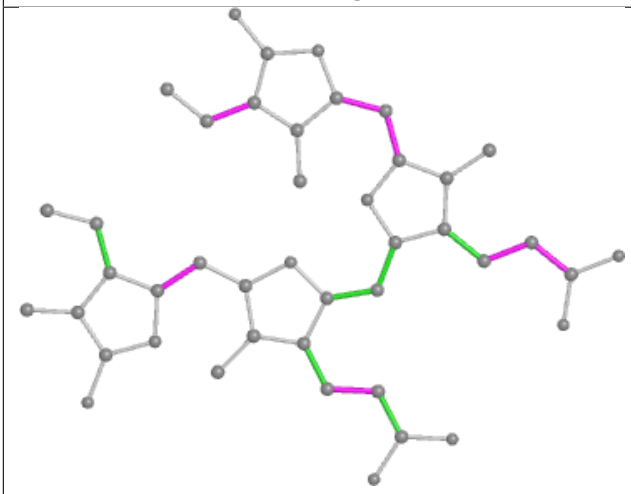

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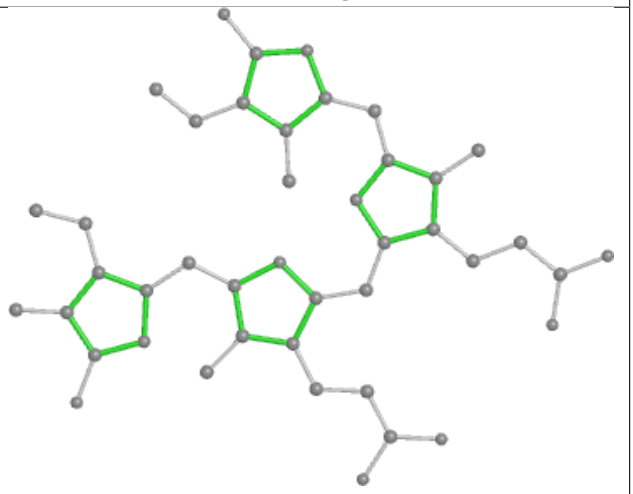

Rings

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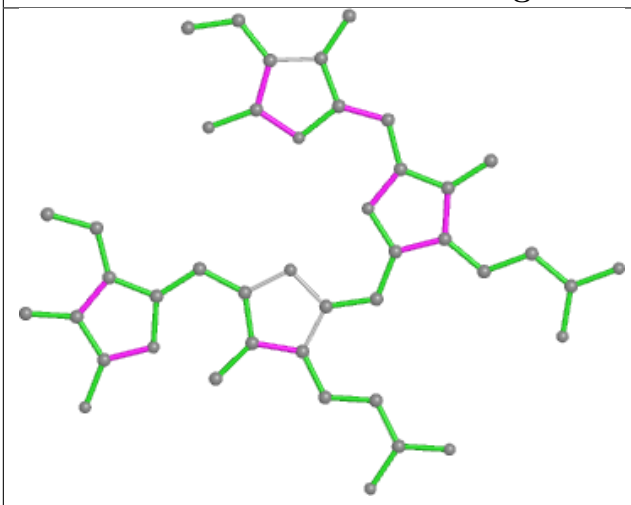

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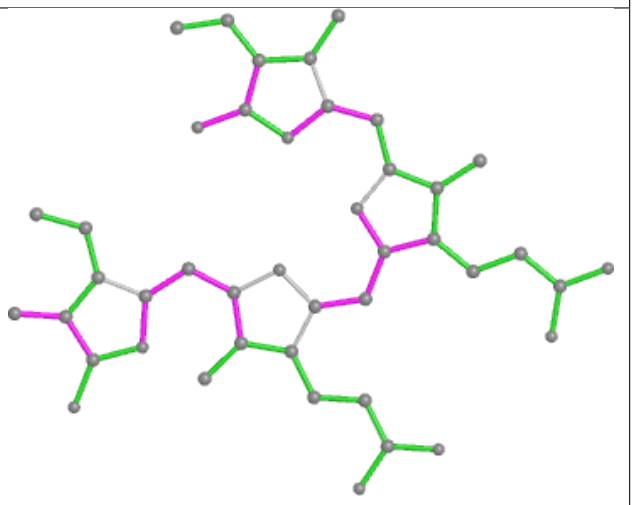

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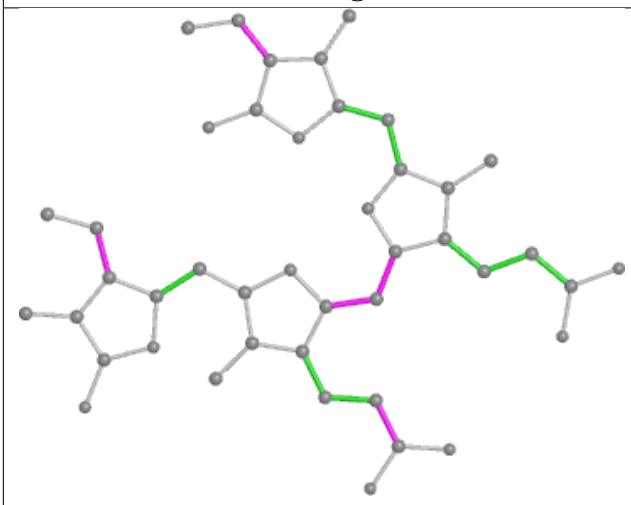

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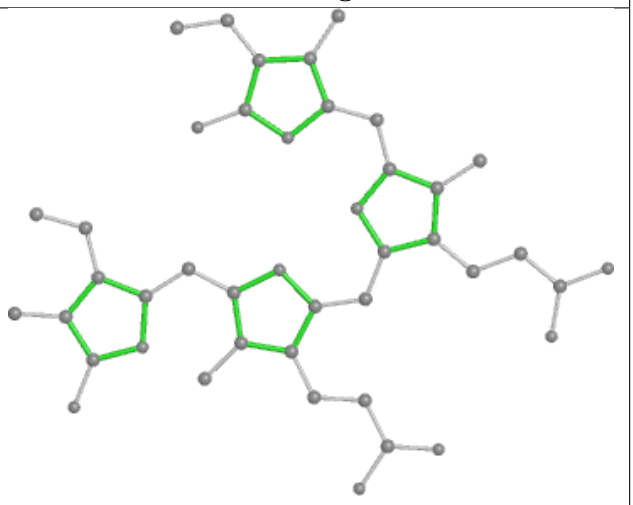
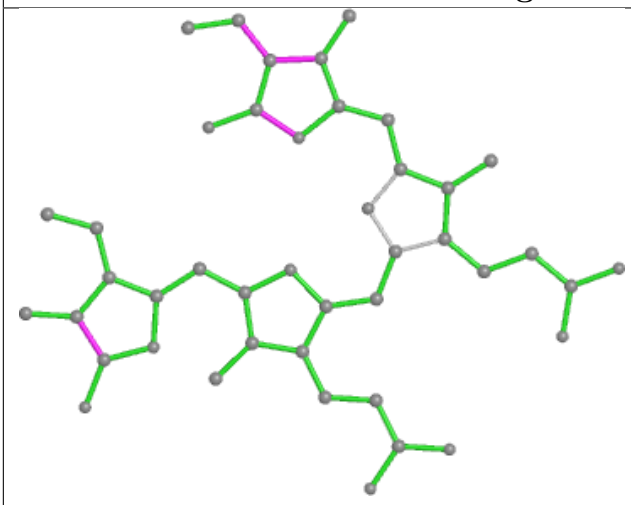


Rings

Ligand PEB B3 201



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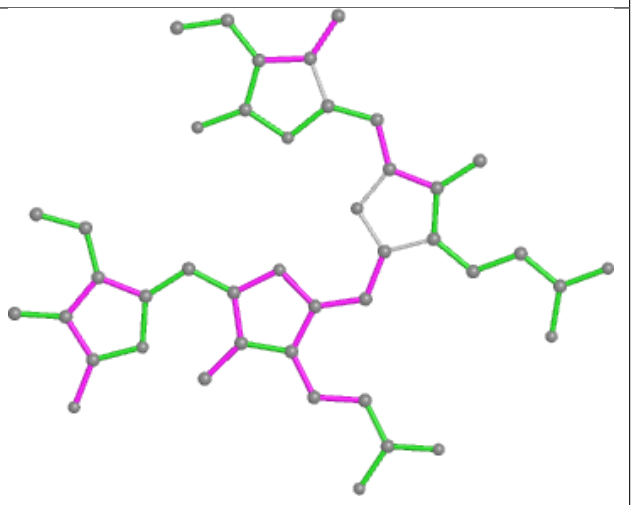

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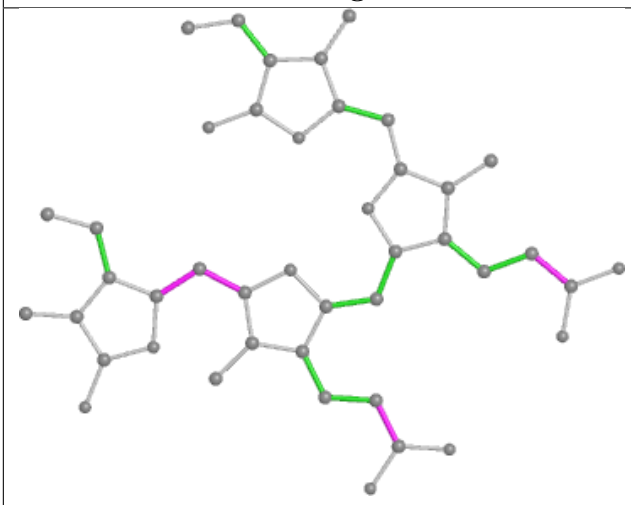

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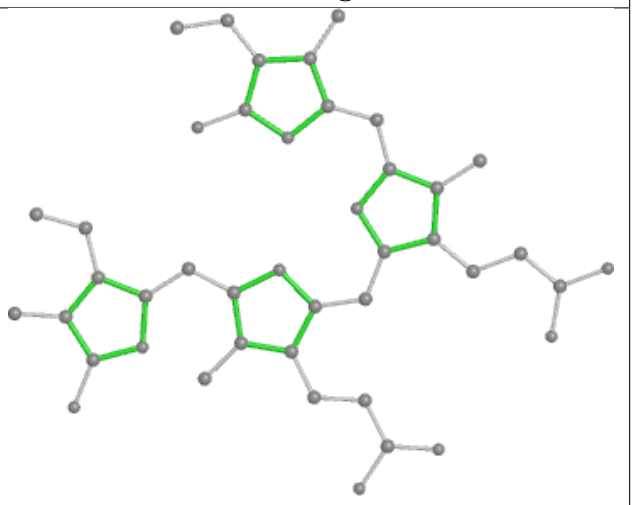
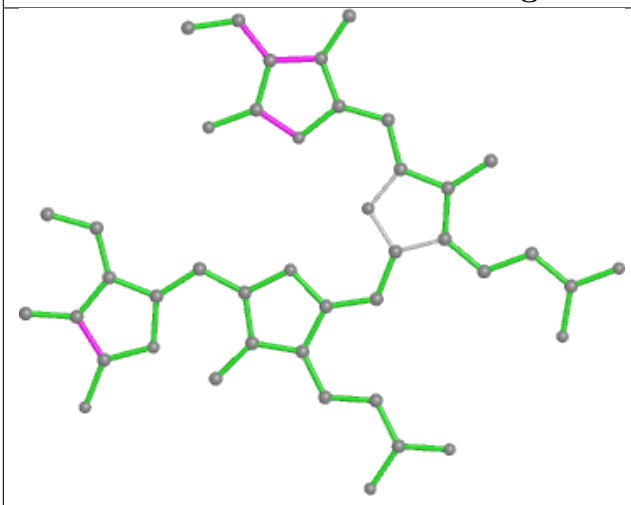


Rings

Ligand PEB eg 201



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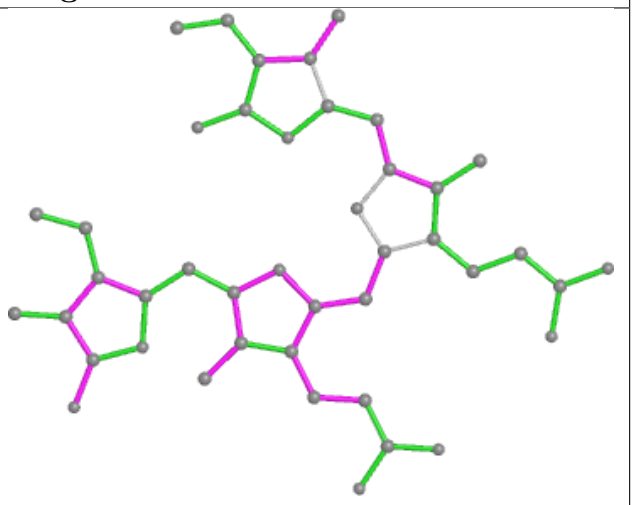
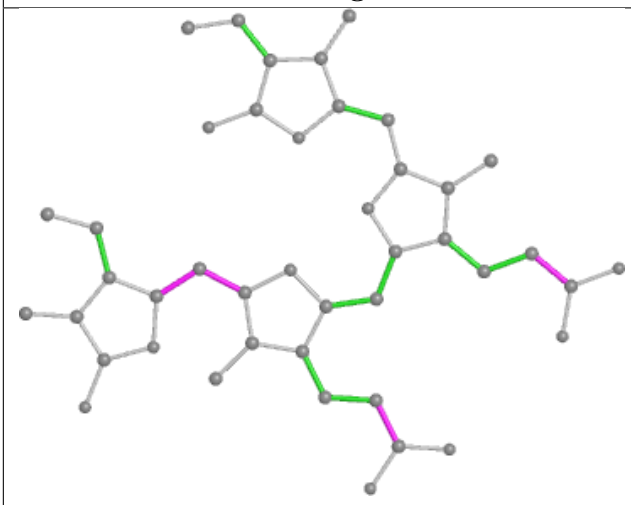
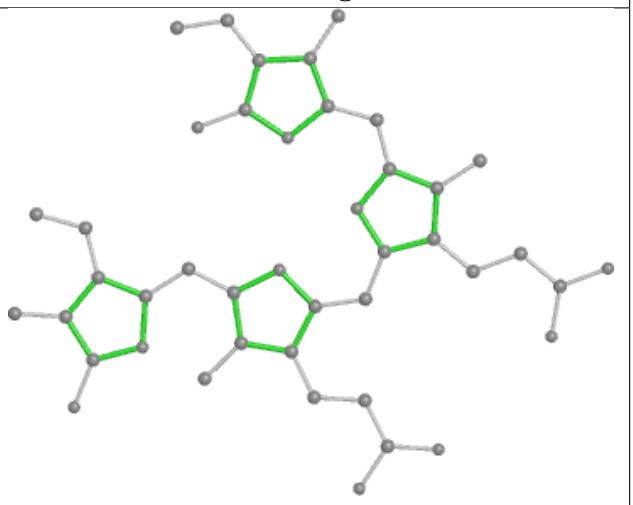


Bond angles

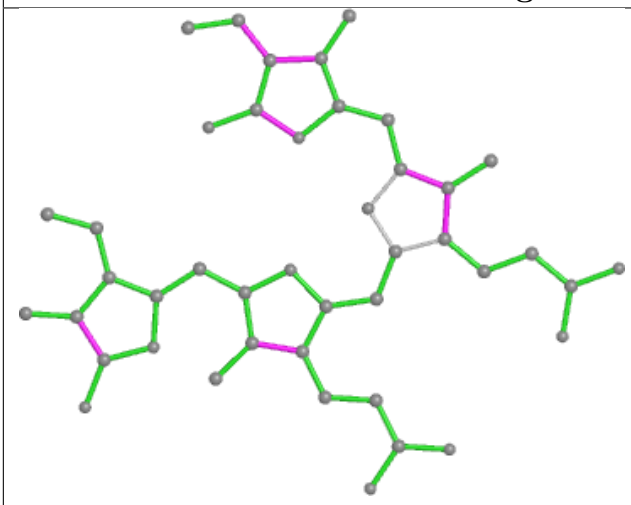


Torsions



Rings

Ligand PEB B7 201



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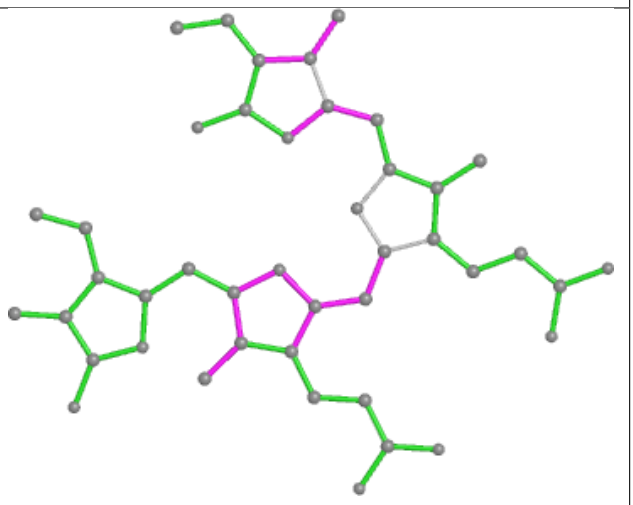

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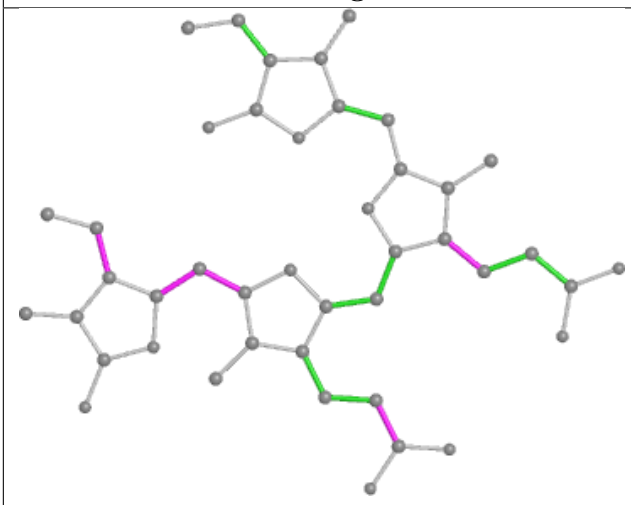

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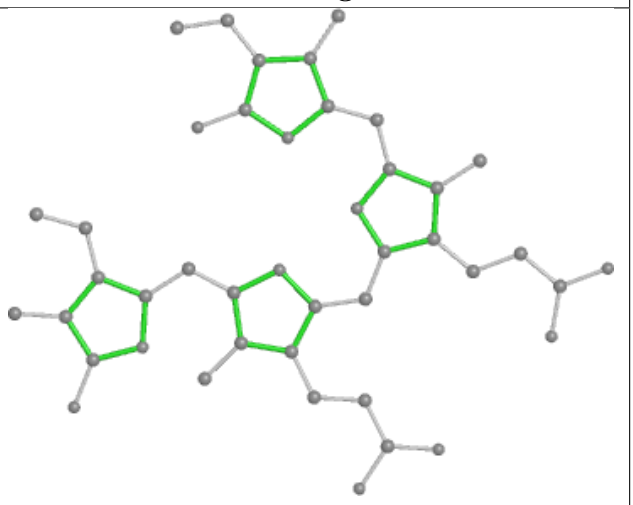
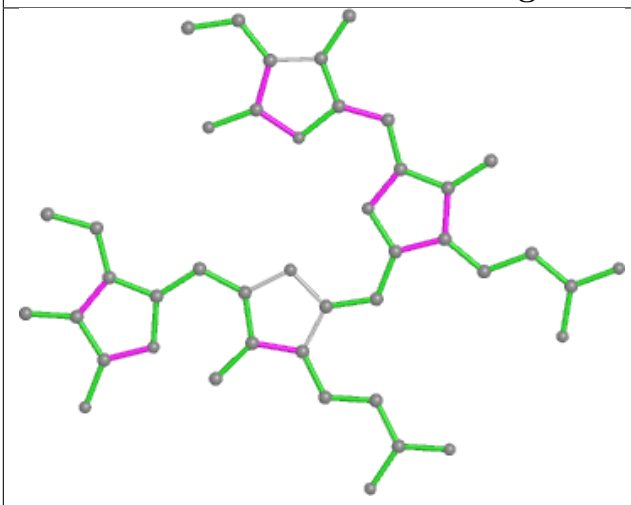


Rings

Ligand PUB br 203



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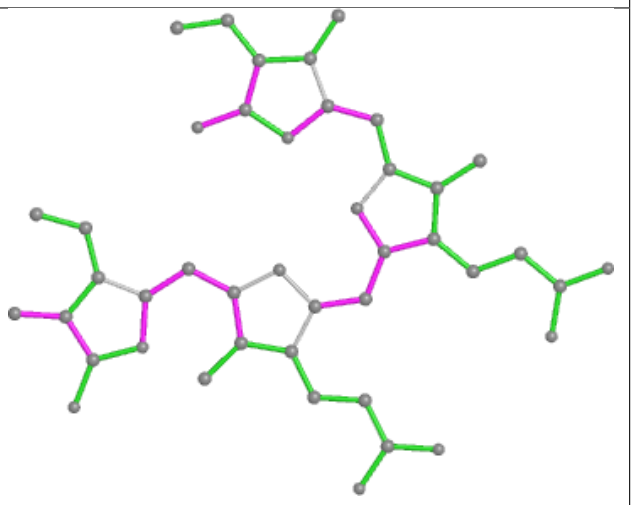

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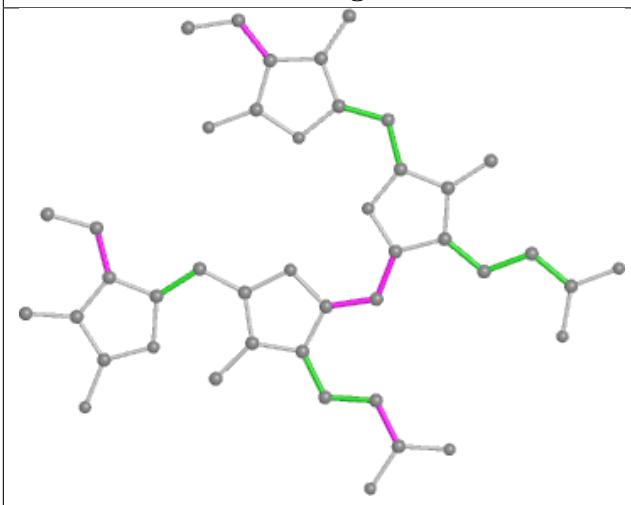

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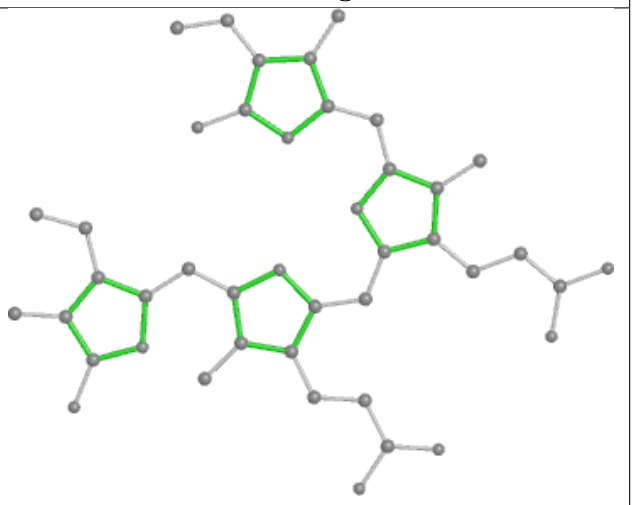
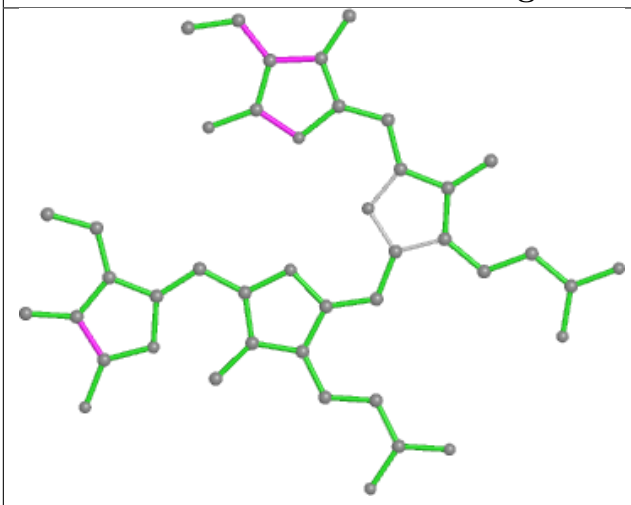


Rings

Ligand PEB Z3 201



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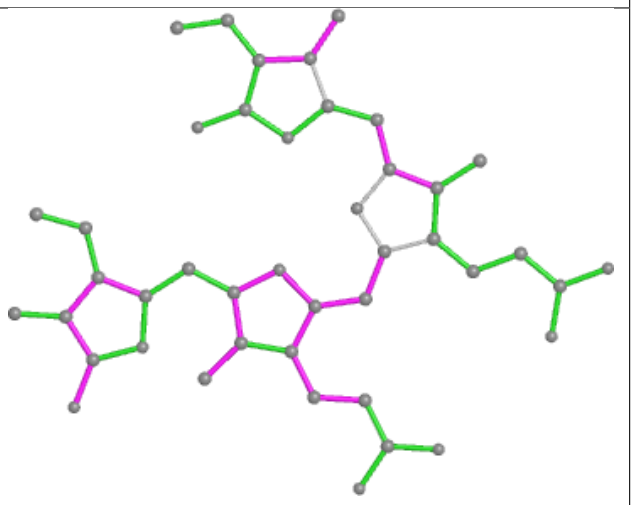

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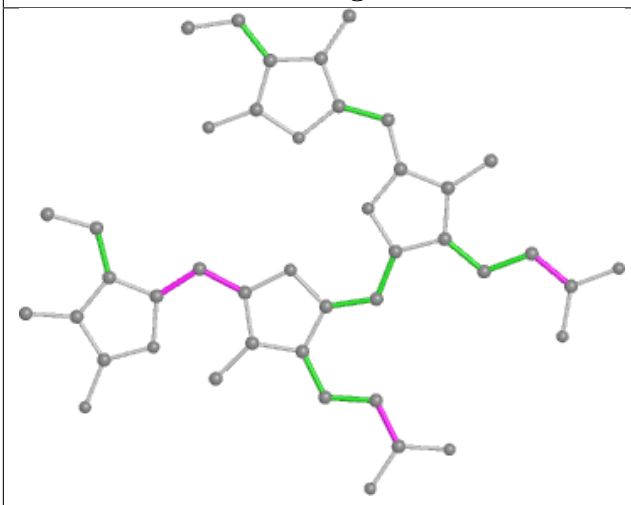

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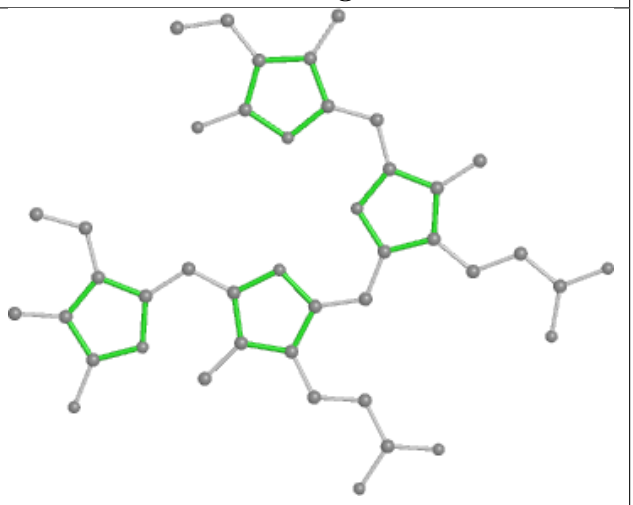
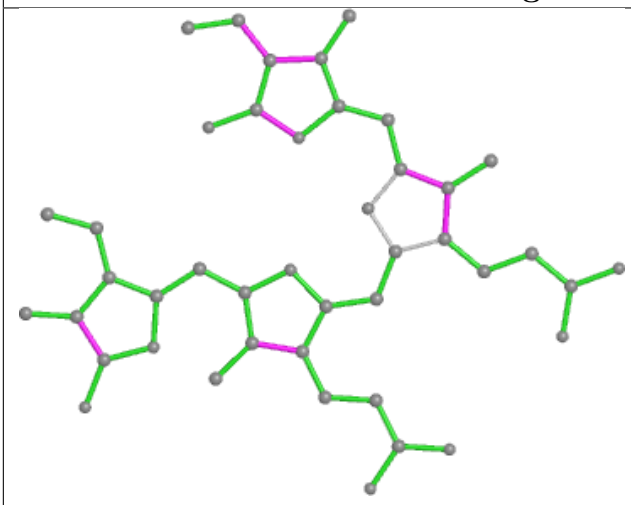


Rings

Ligand PEB dl 202



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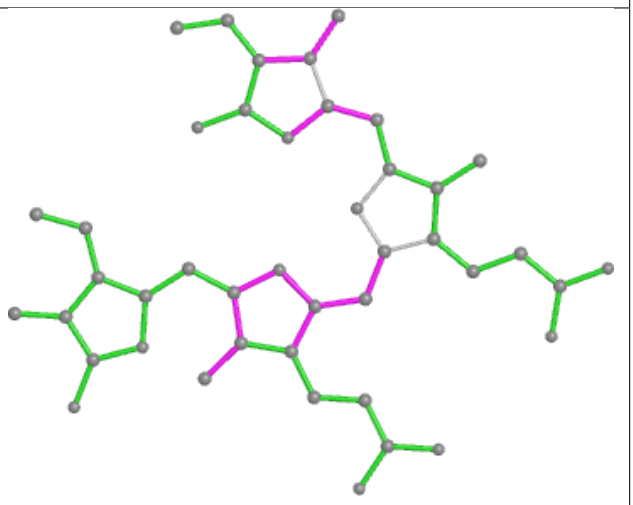

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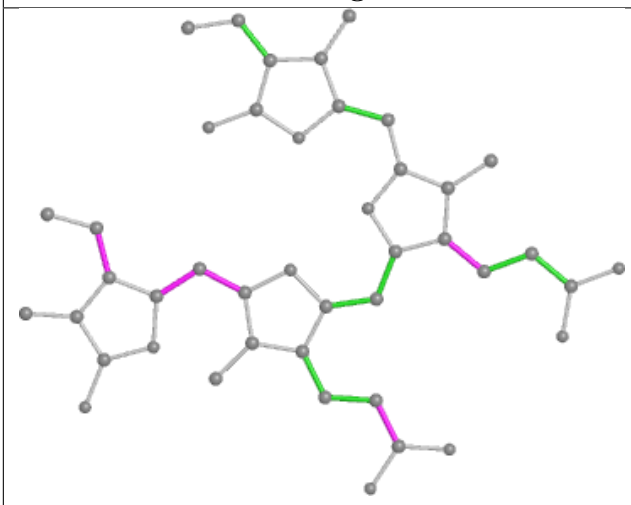

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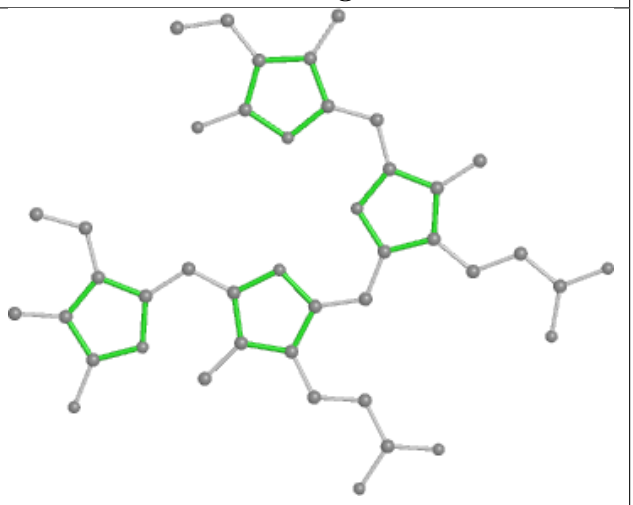
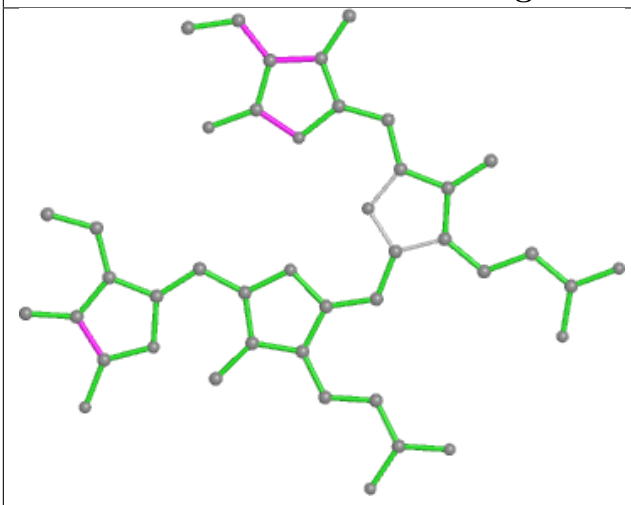


Rings

Ligand PEB D9 201



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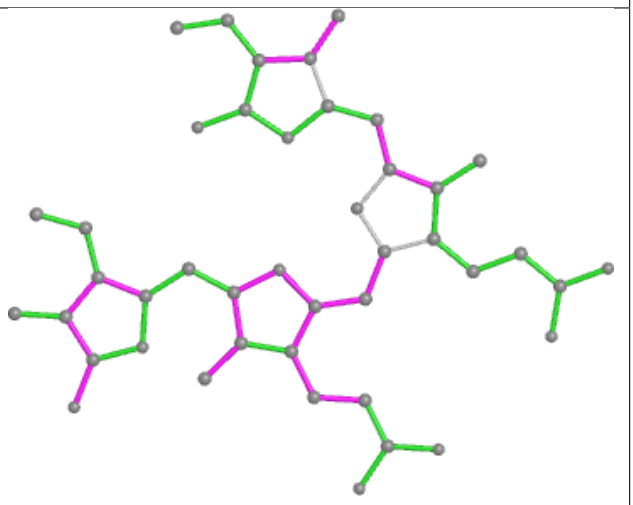

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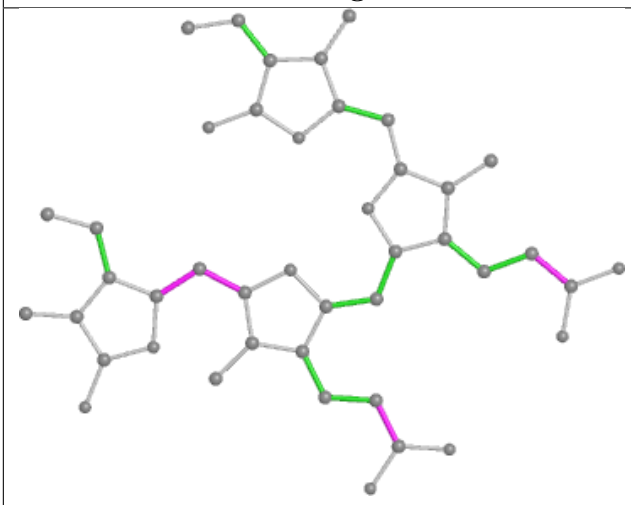

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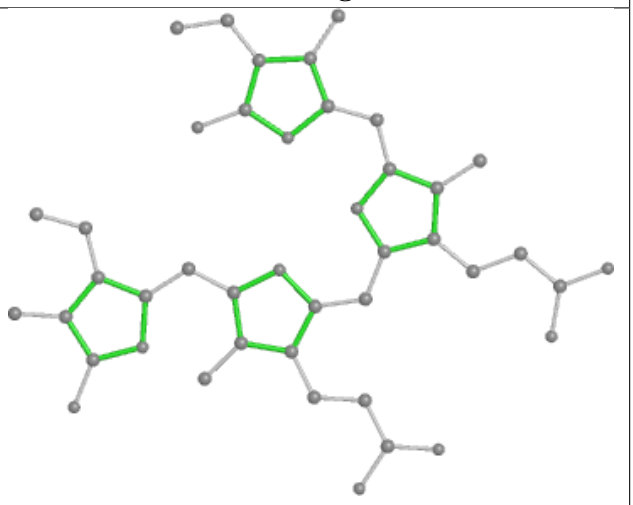
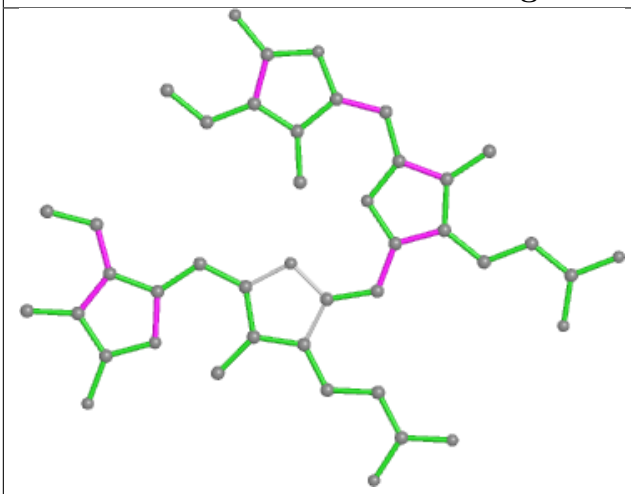


Rings

Ligand PVN ly 404



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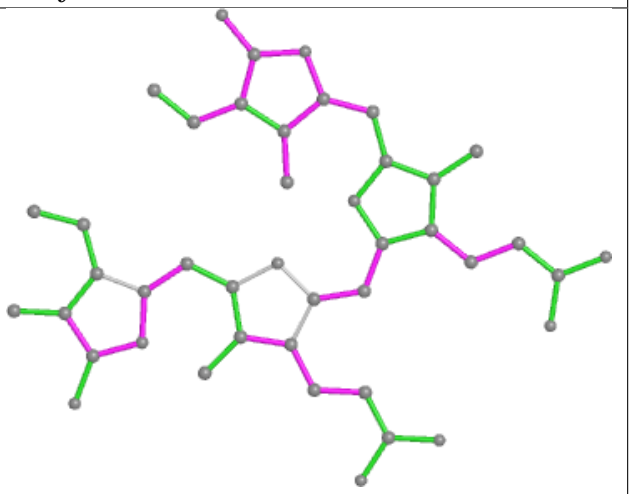

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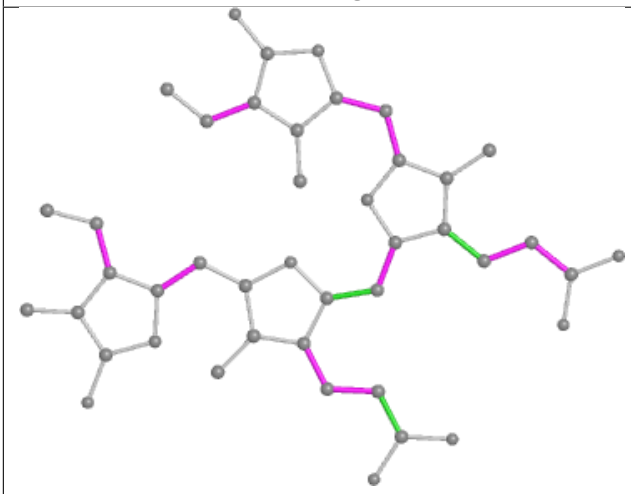

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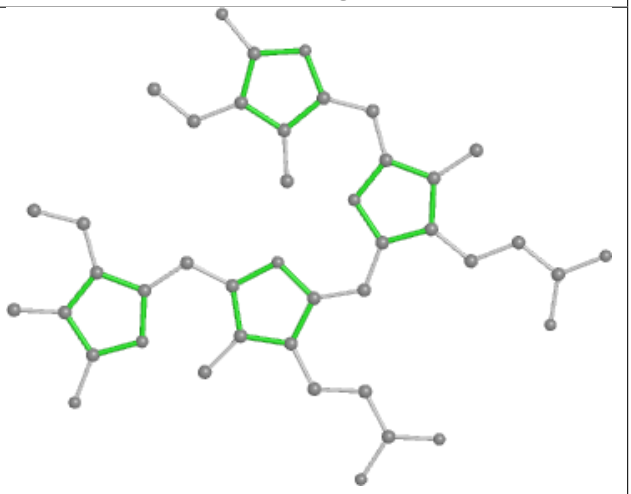
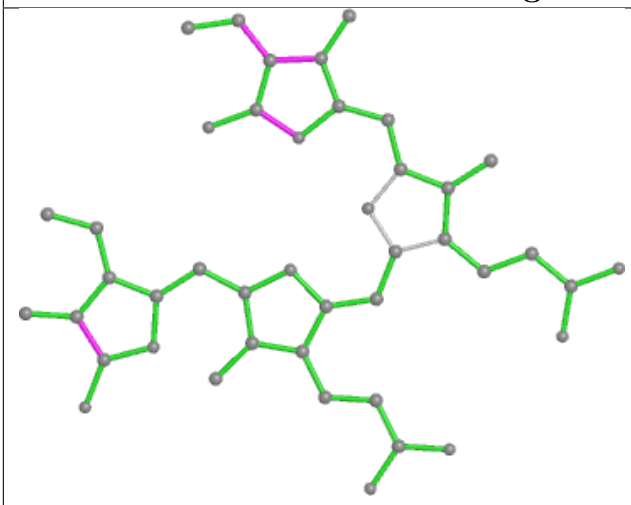


Rings

Ligand PEB lk 201



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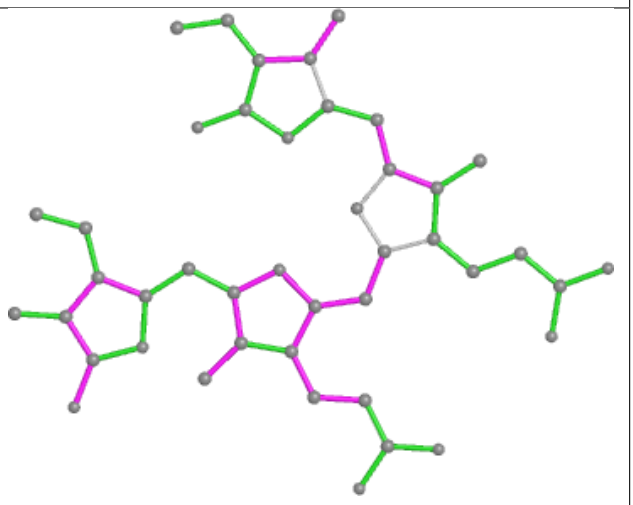

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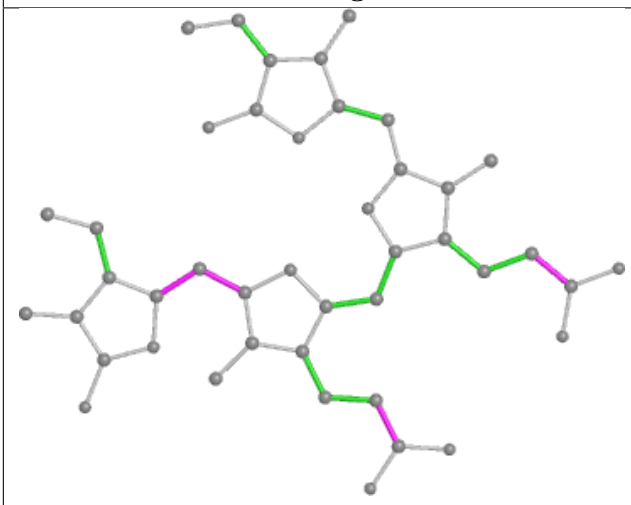

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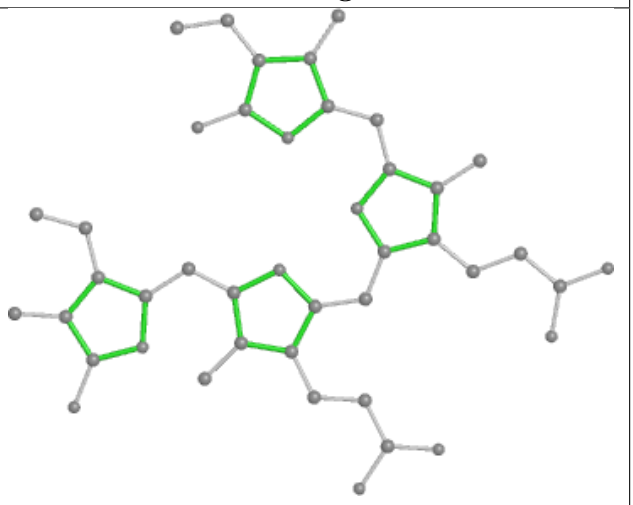

Rings

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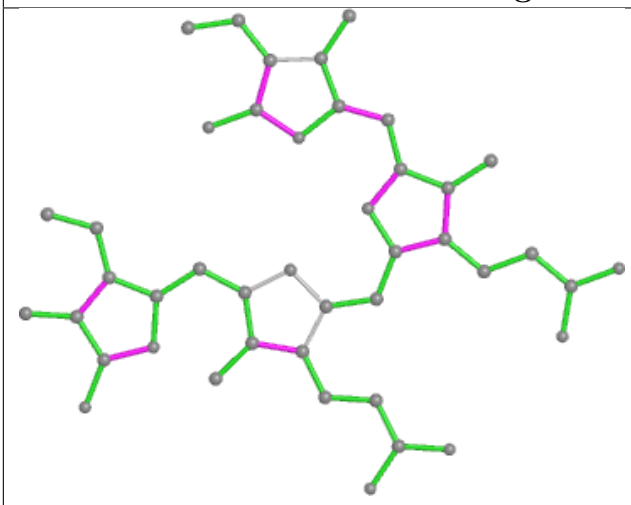

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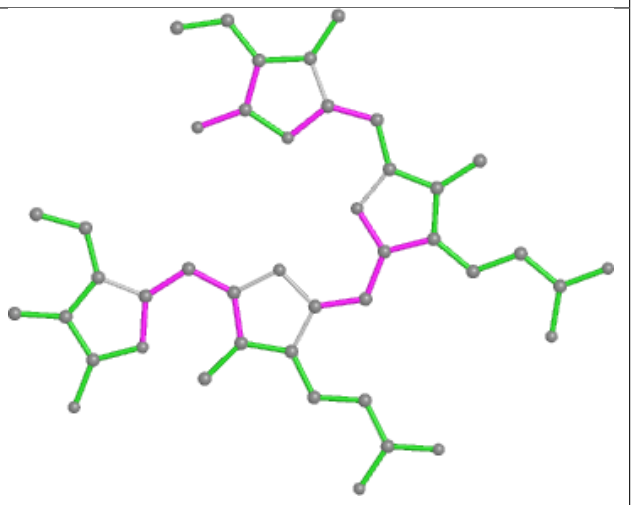

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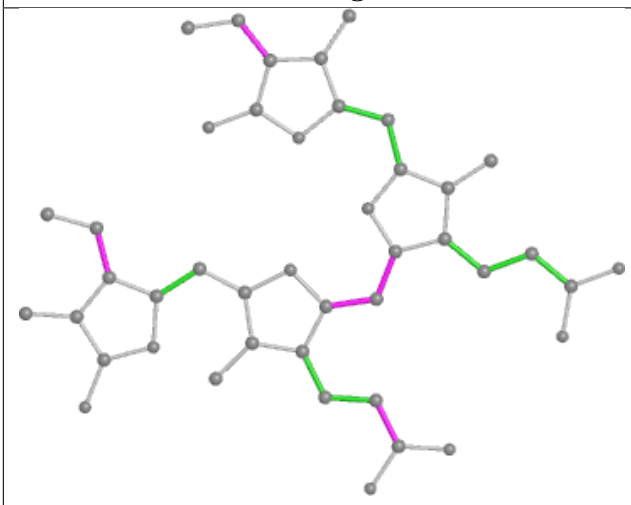

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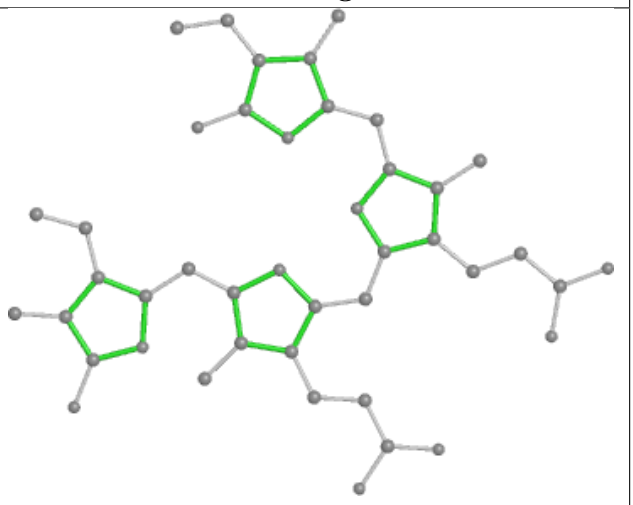

Rings

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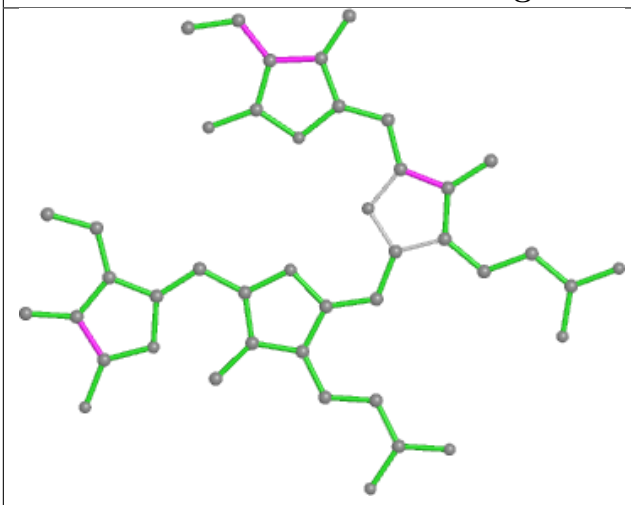

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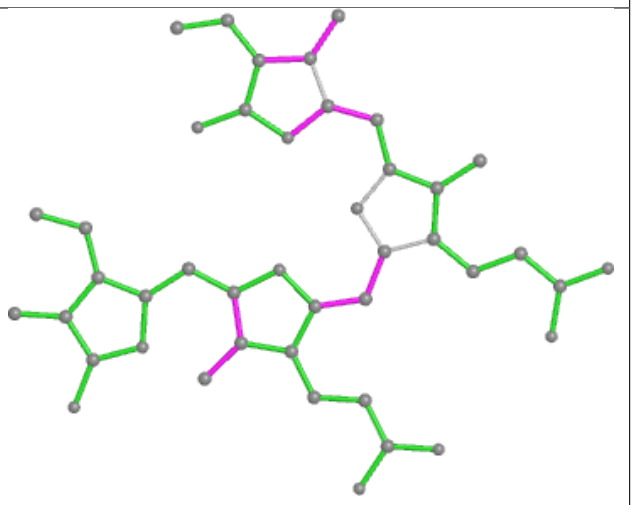

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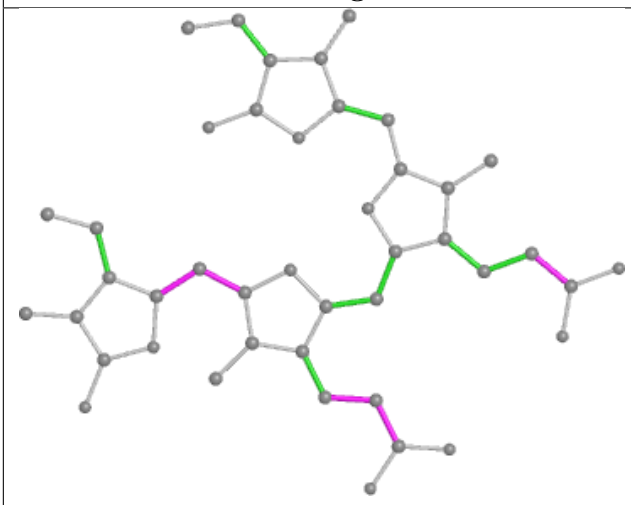

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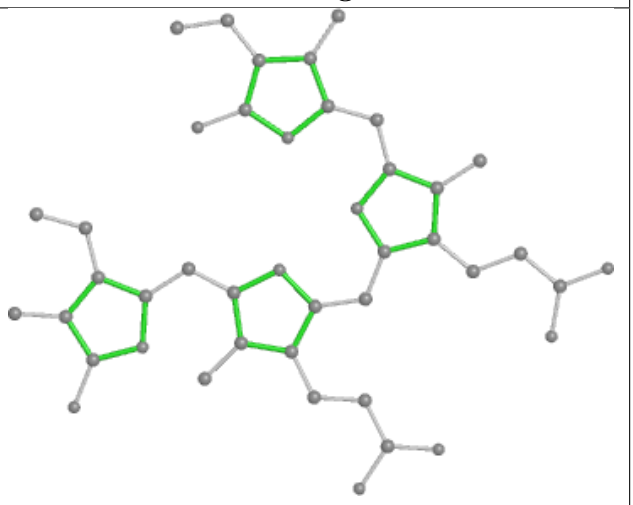

Rings

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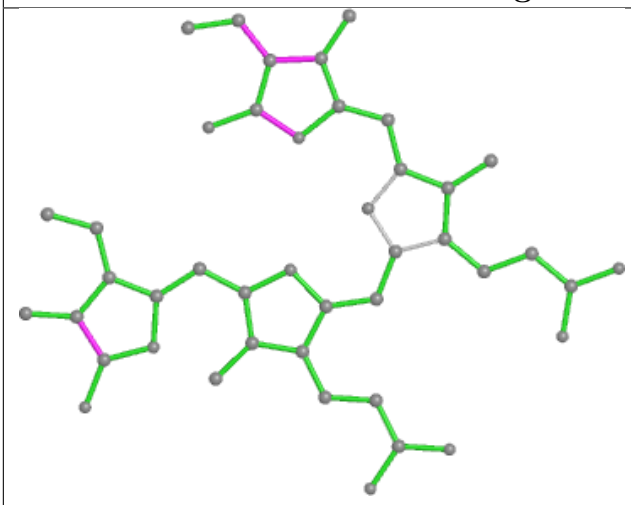

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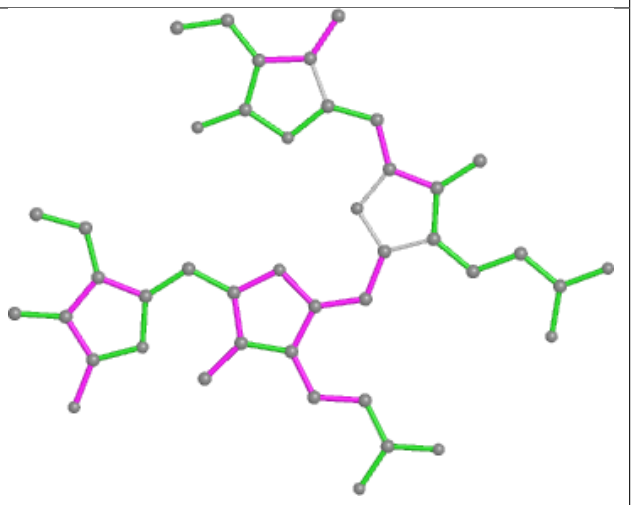

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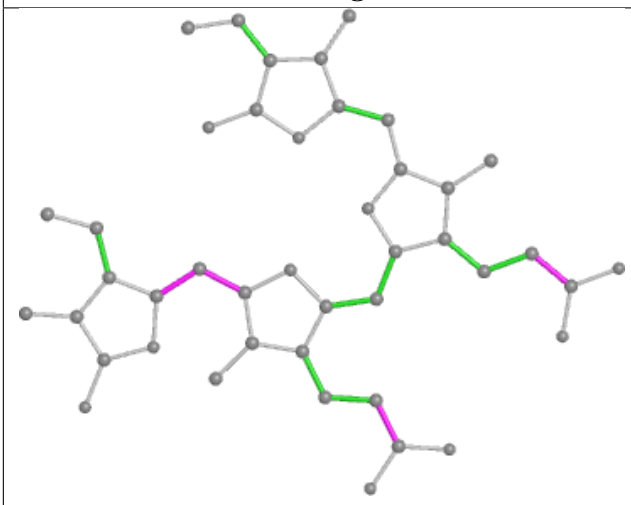

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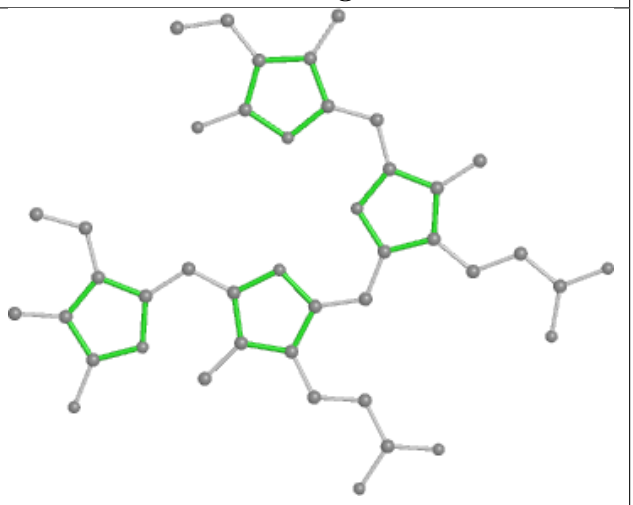

Rings

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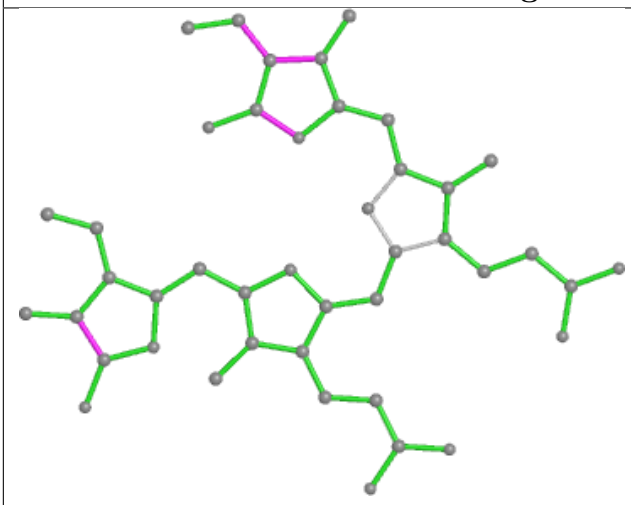

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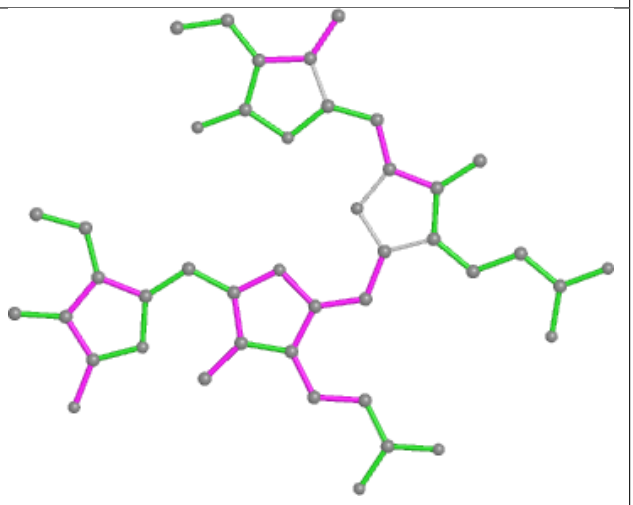

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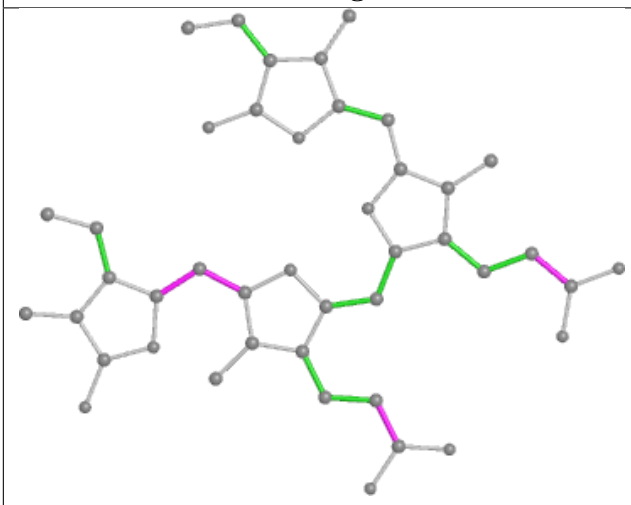

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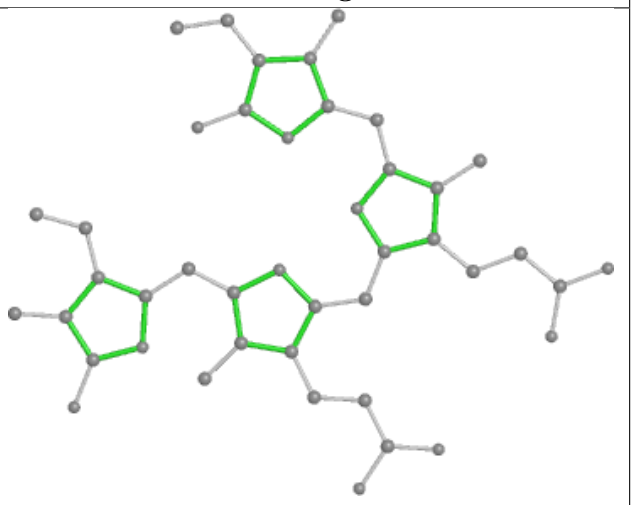
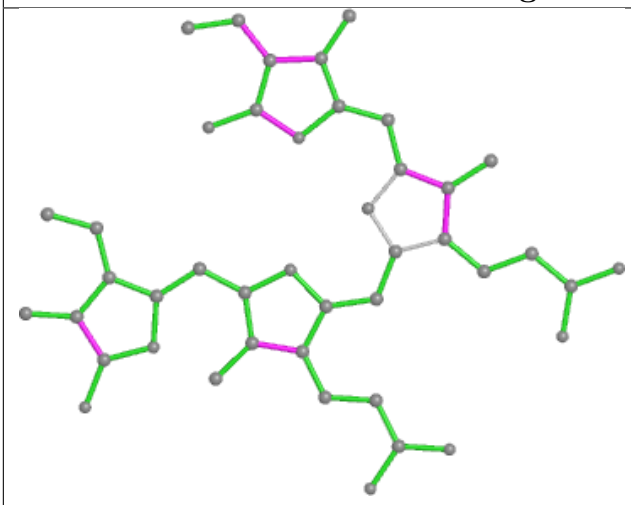


Rings

Ligand PEB v9 202



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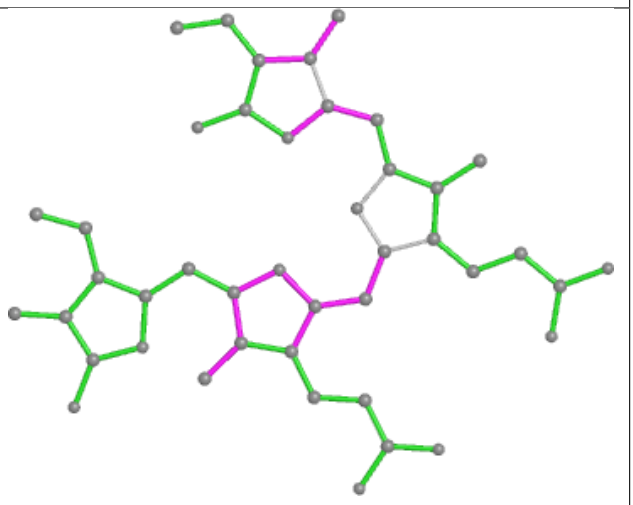

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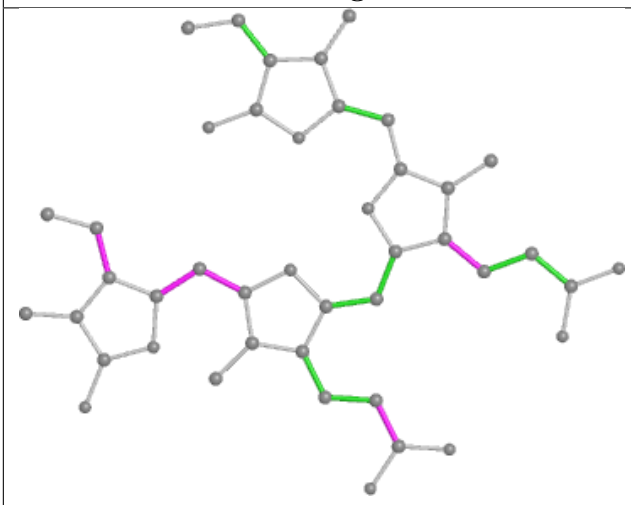

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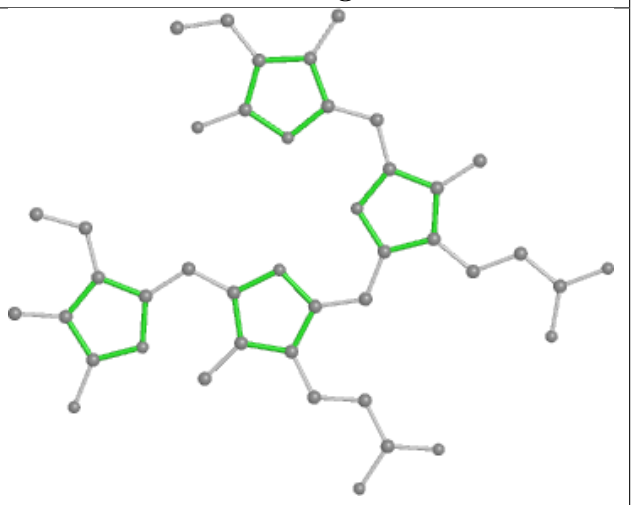
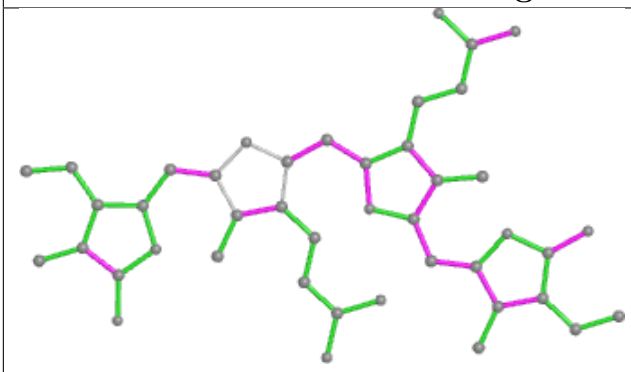


Rings

Ligand CYC L1 201



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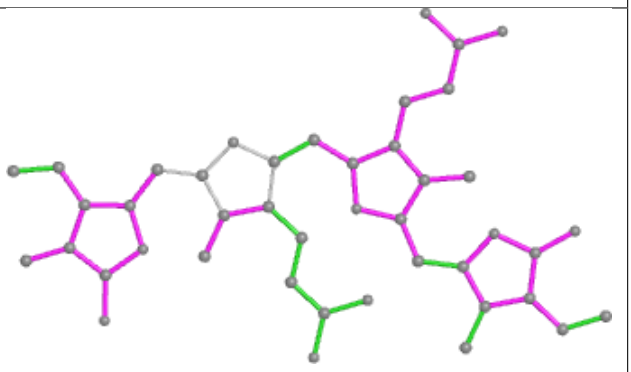
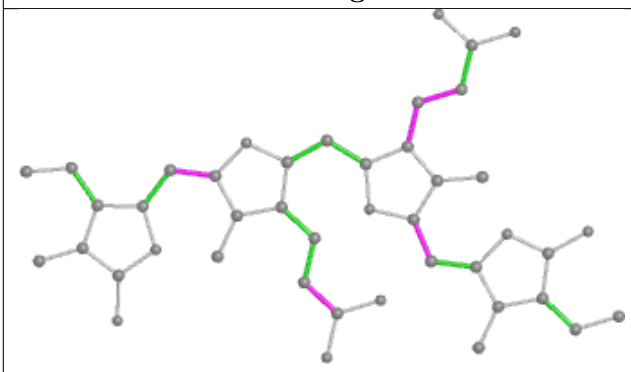


Bond angles



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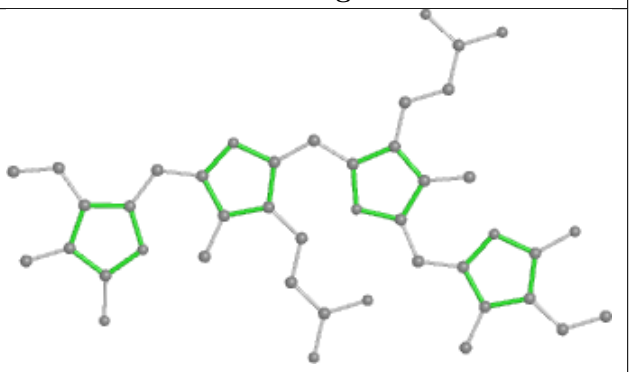
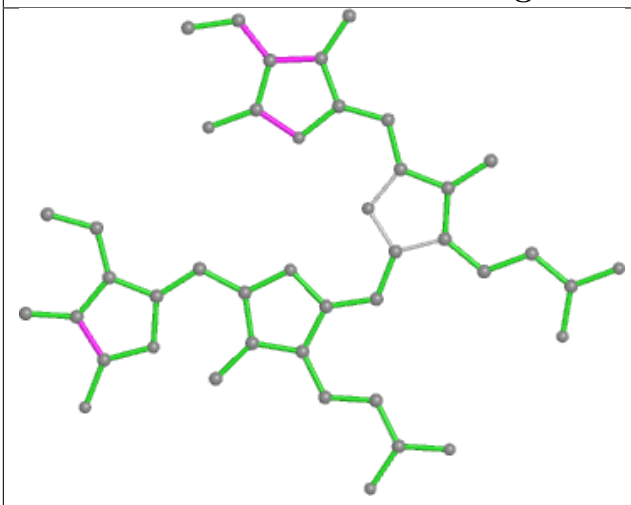
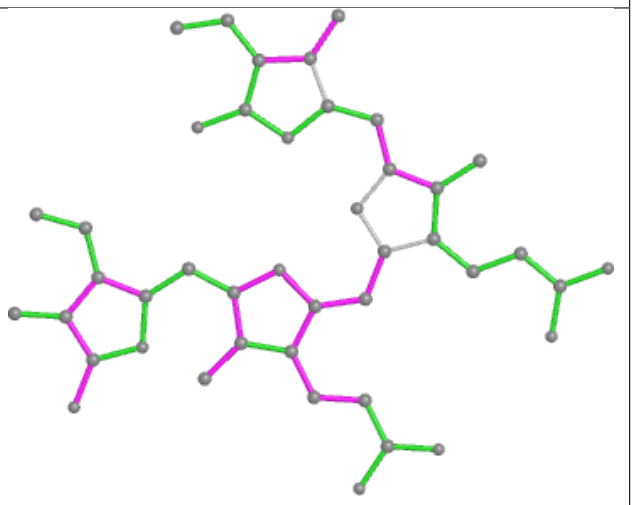


Rings

Ligand PEB H6 202



Bond lengths



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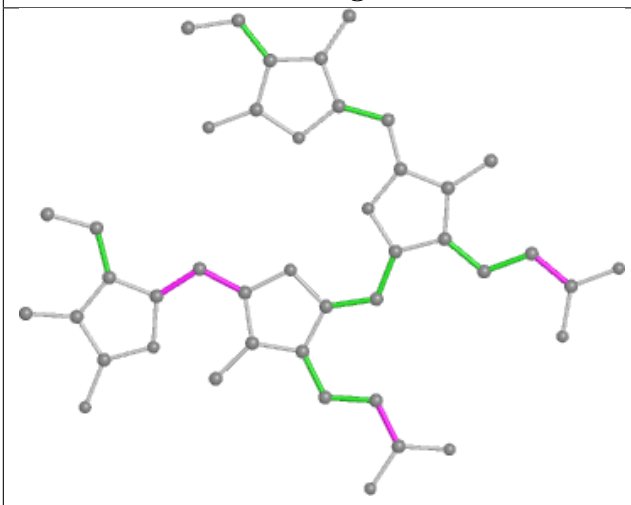
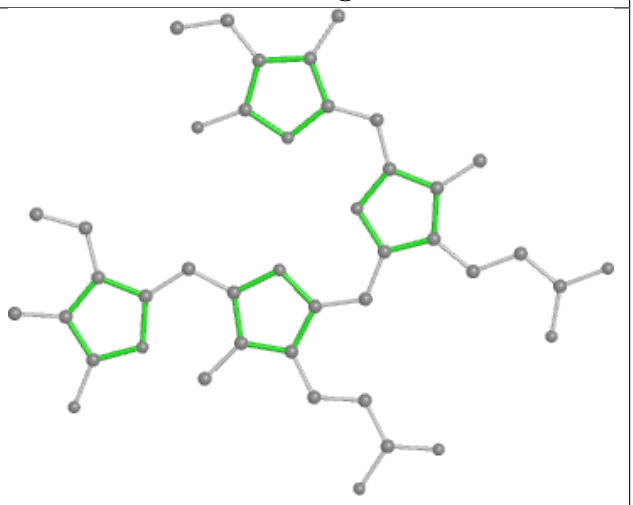
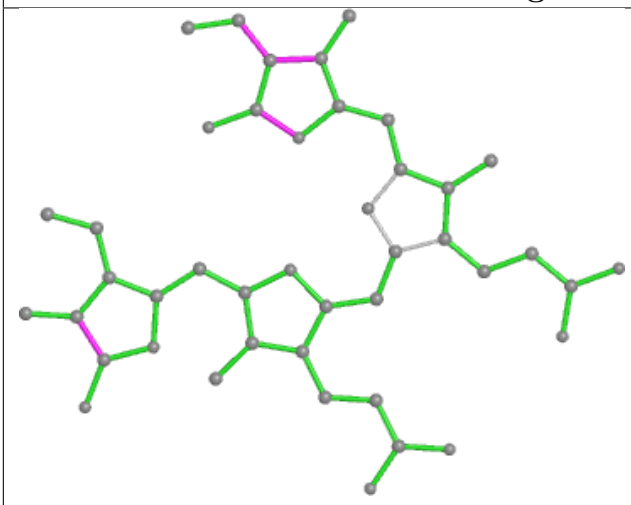


Torsions



Rings

Ligand PEB lf 201



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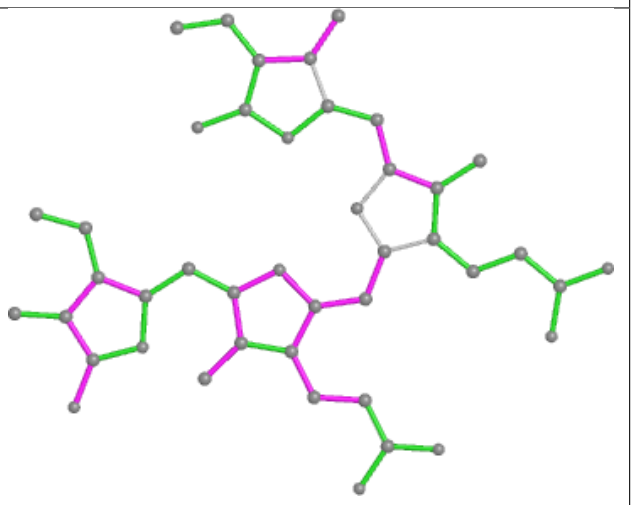

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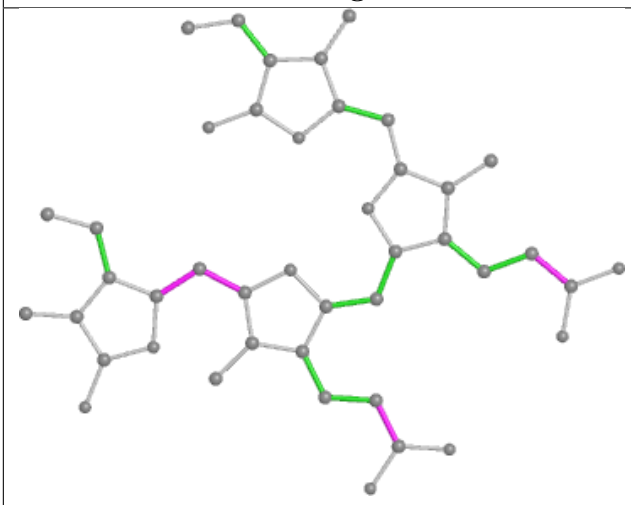

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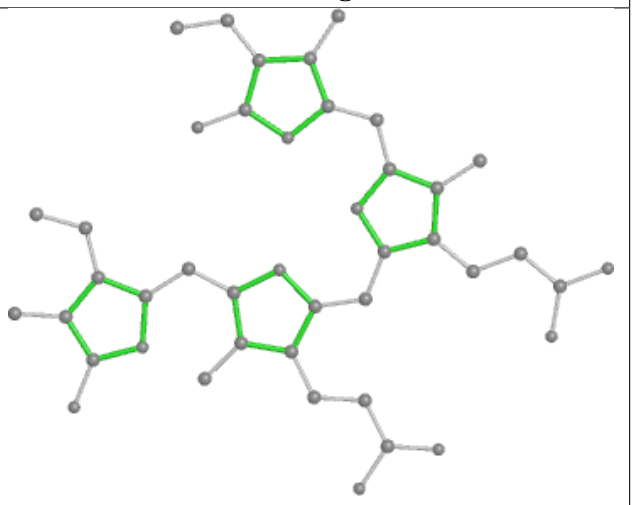
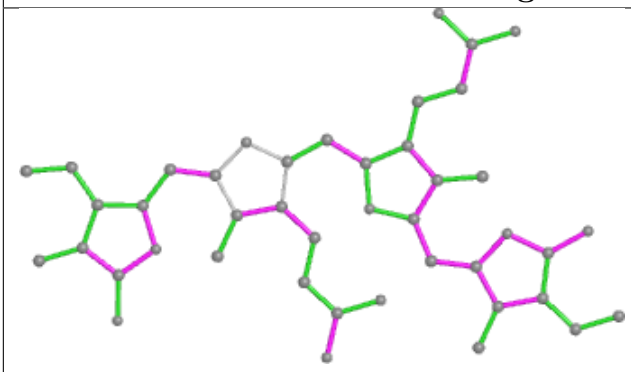


Rings

Ligand CYC a2 902



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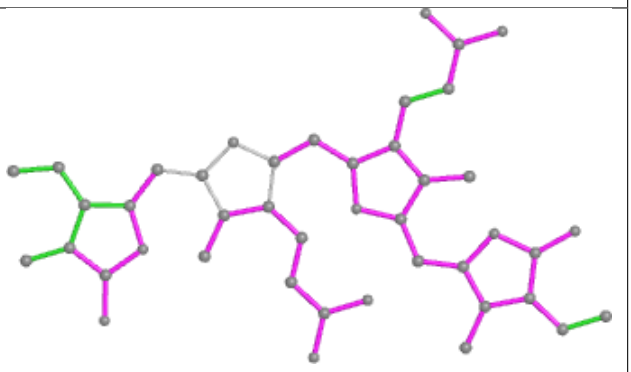

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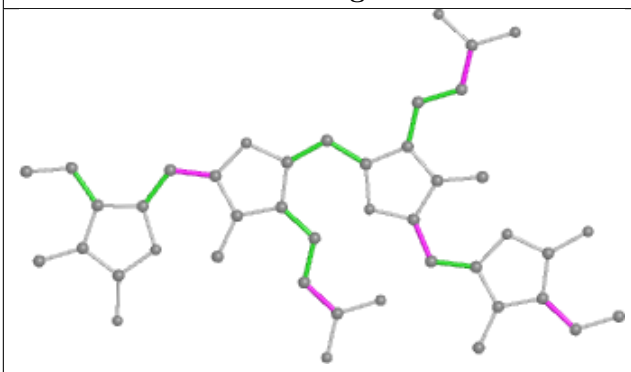

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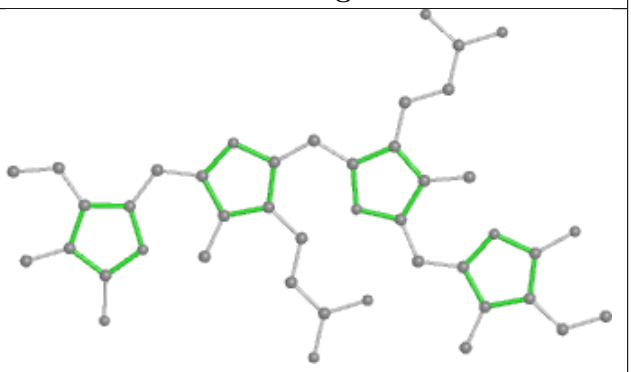
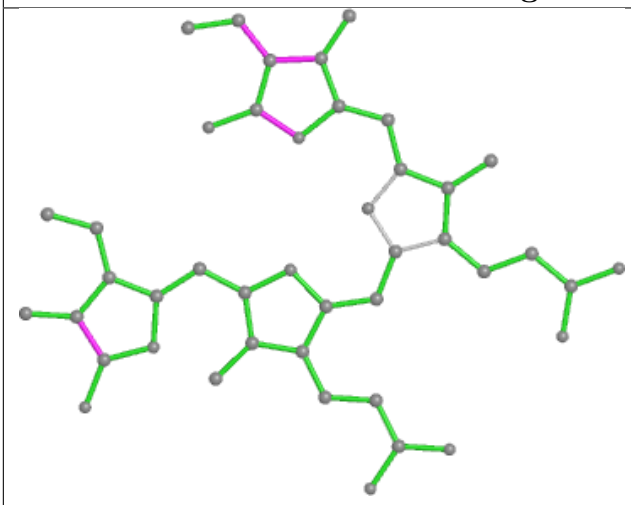


Rings

Ligand PEB e6 201



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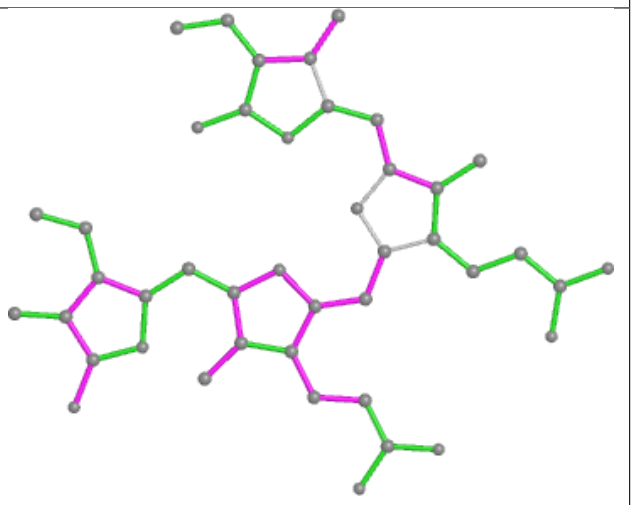

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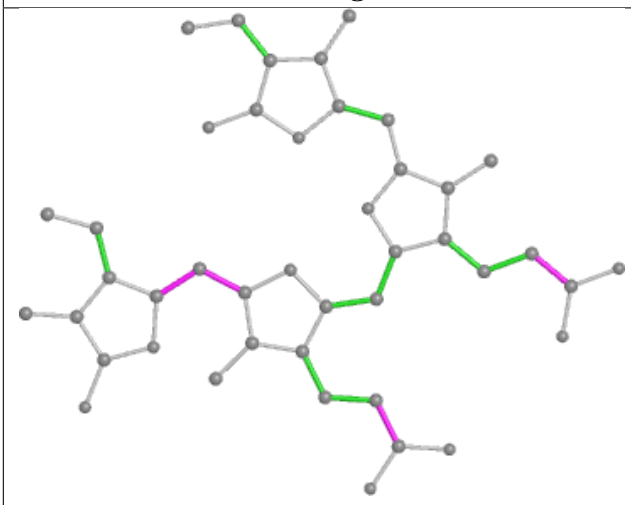

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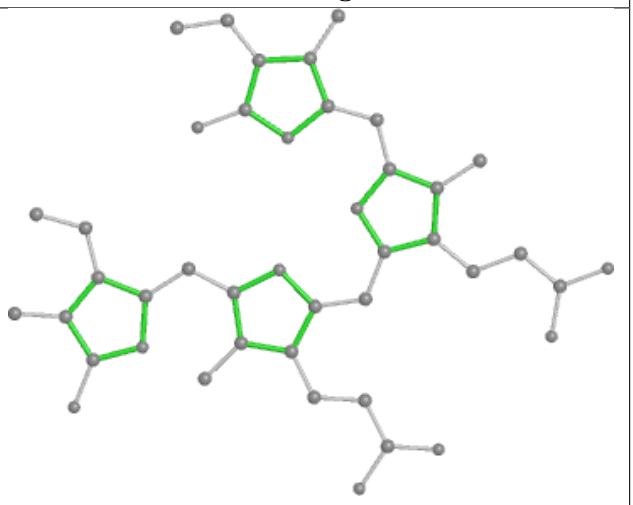
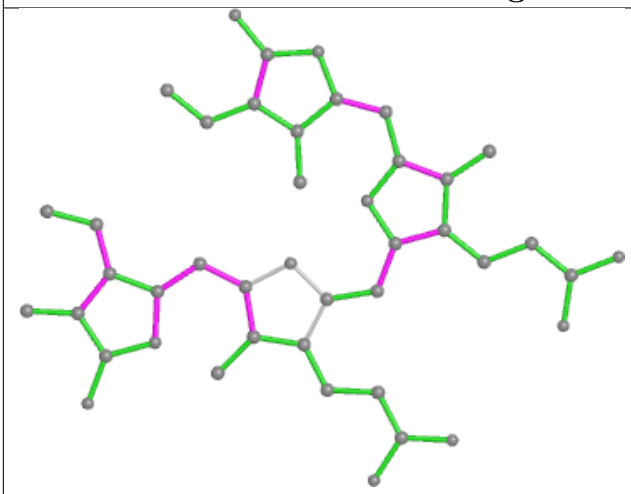


Rings

Ligand PVN 34 1004



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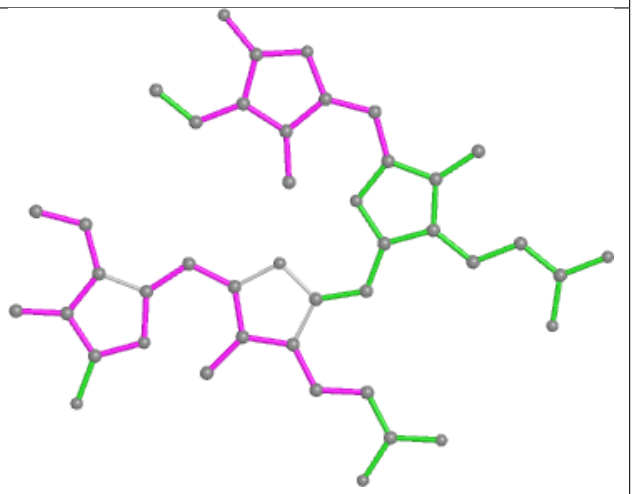

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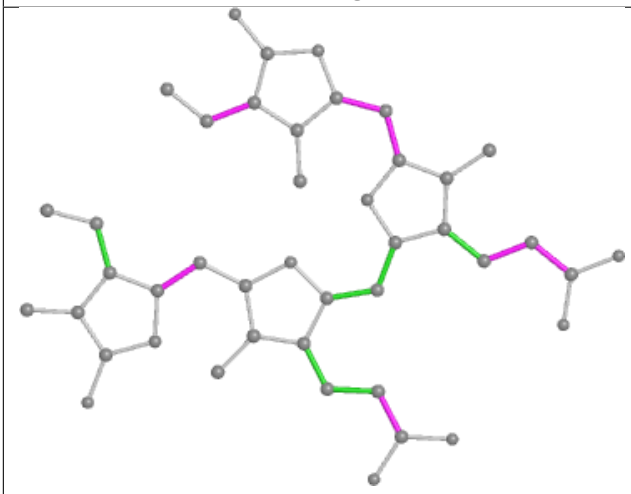

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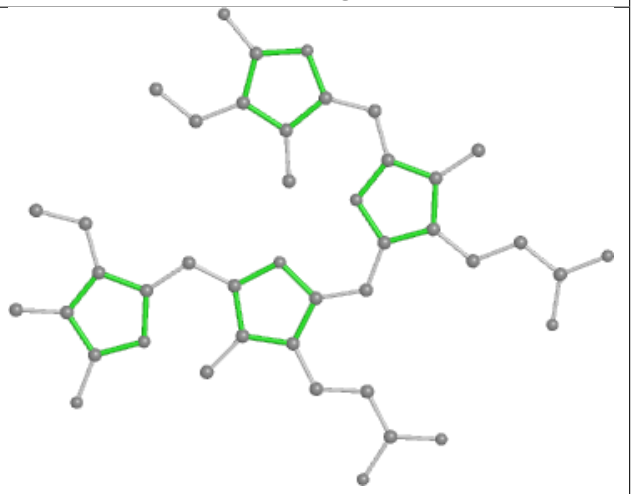
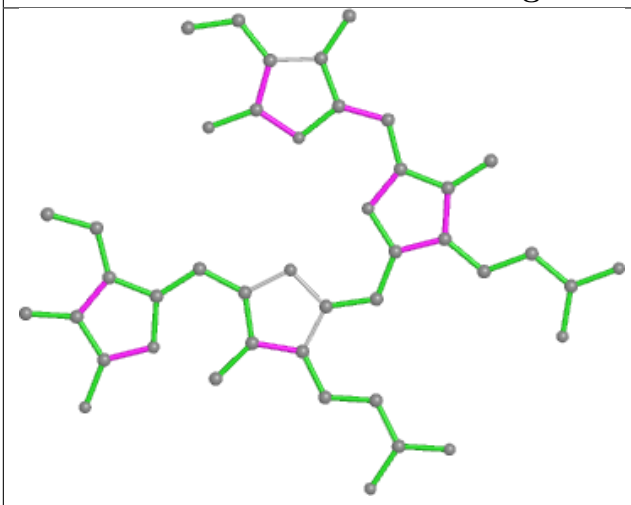


Rings

Ligand PUB lz 404



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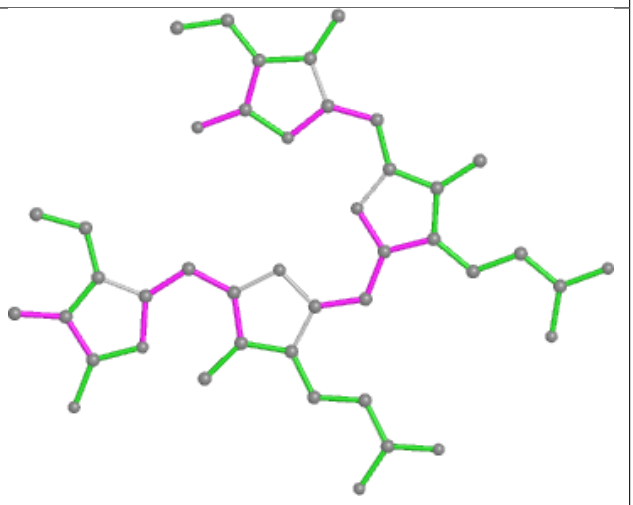

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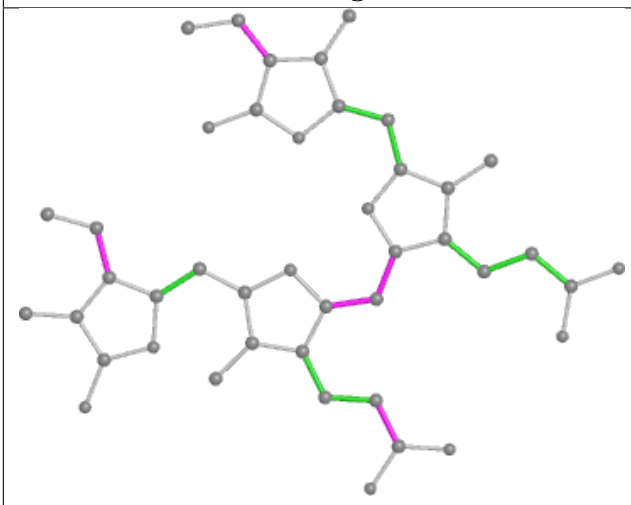

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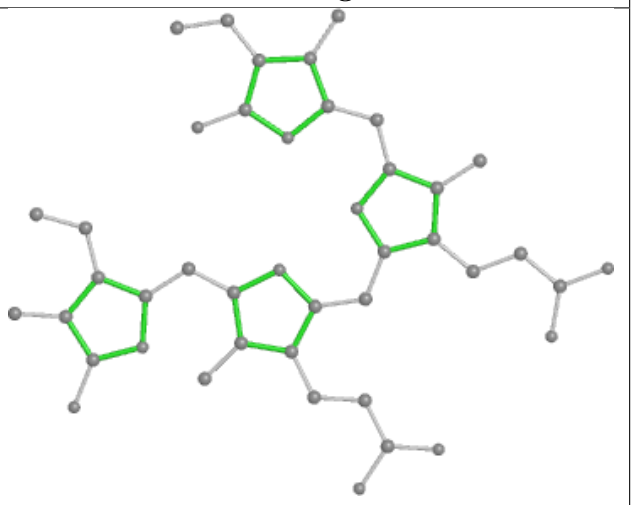
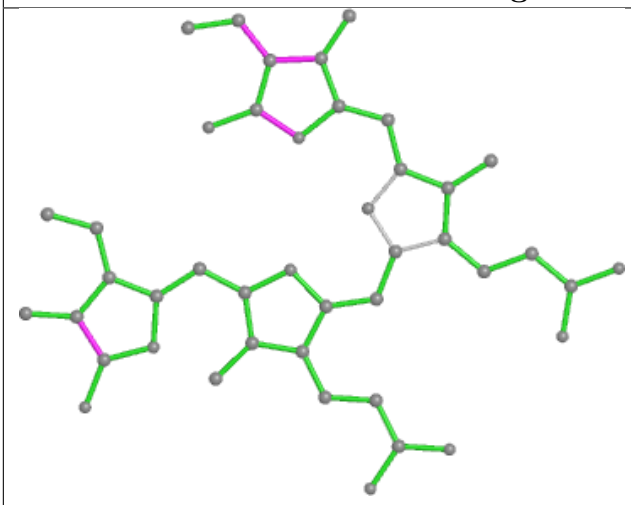


Rings

Ligand PEB q3 1001



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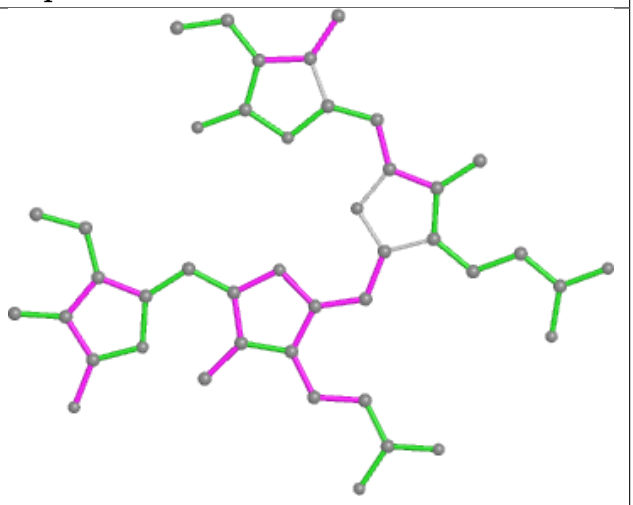

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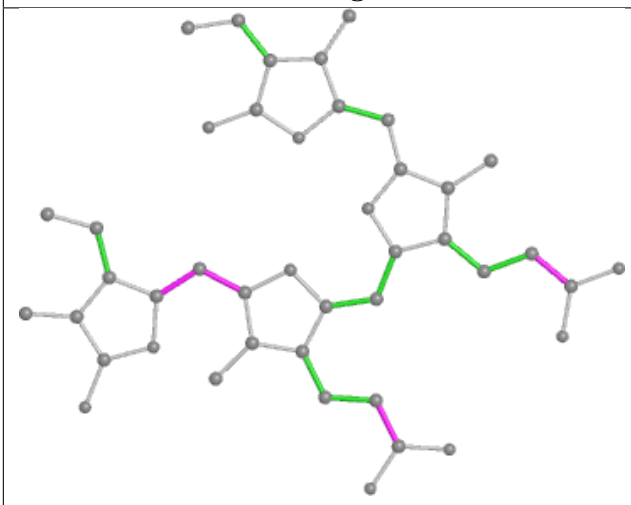

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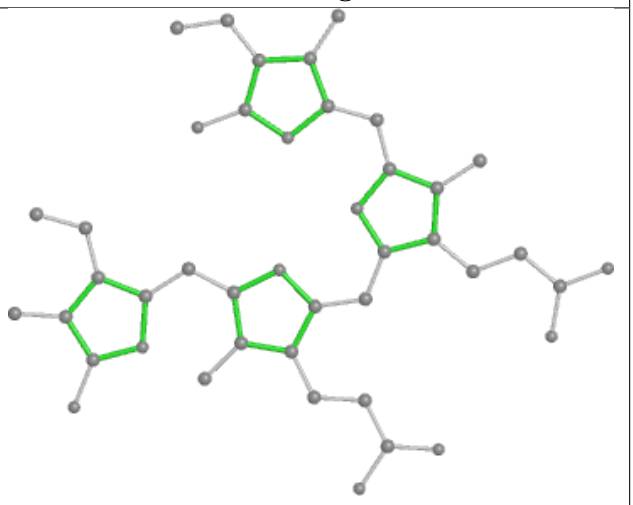

Rings

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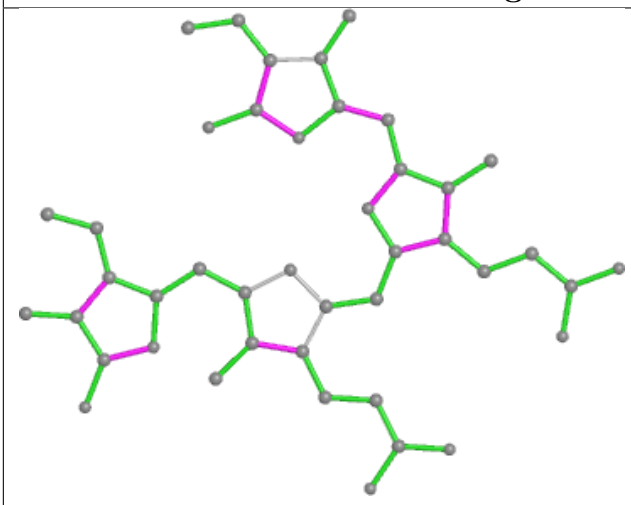

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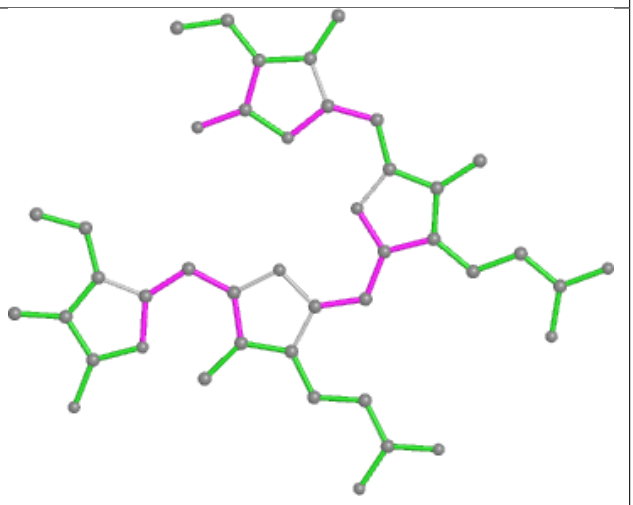

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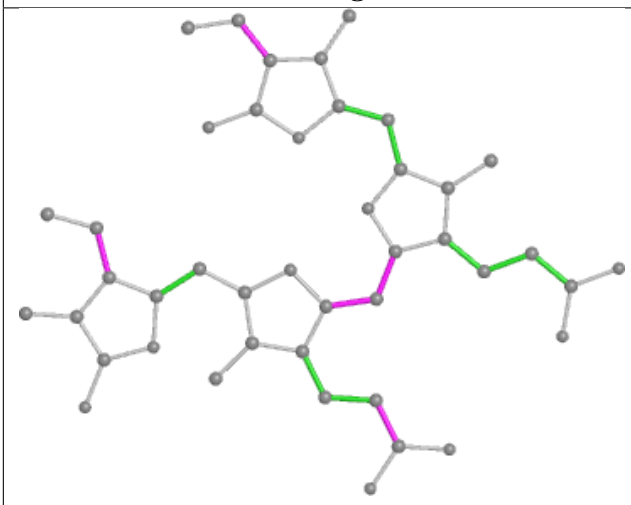

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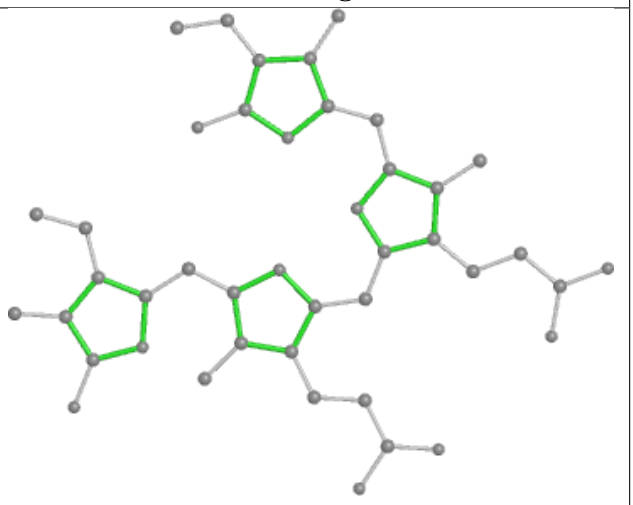
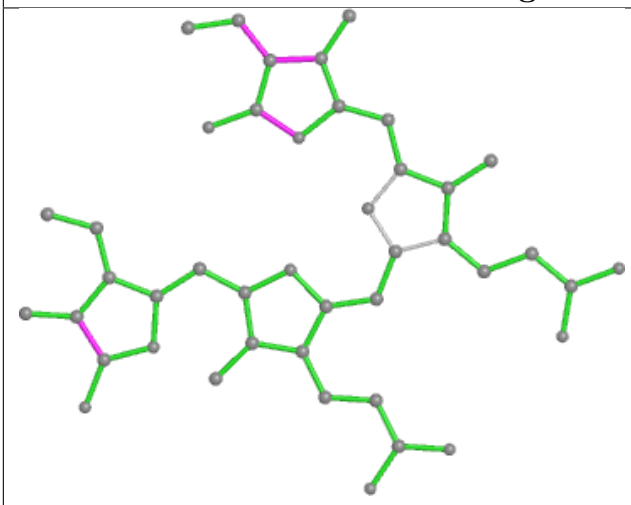


Rings

Ligand PEB d7 201



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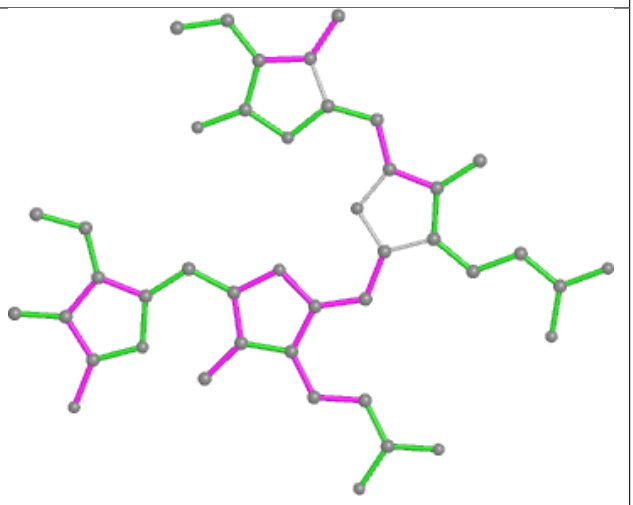

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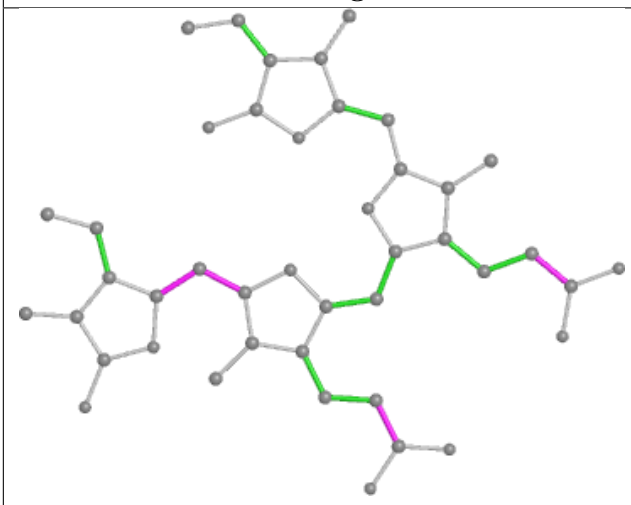

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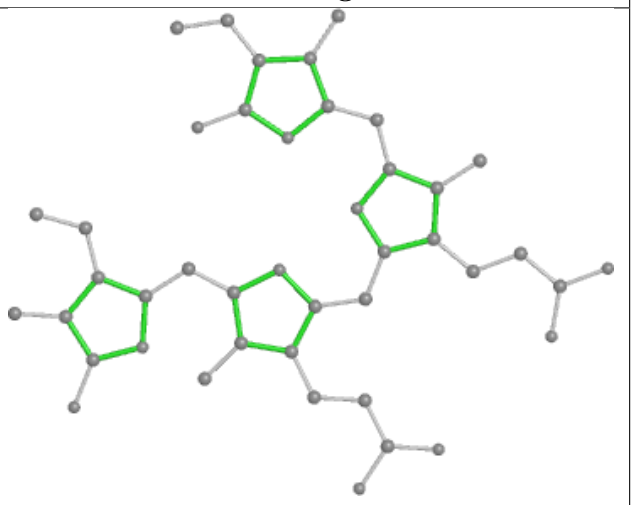
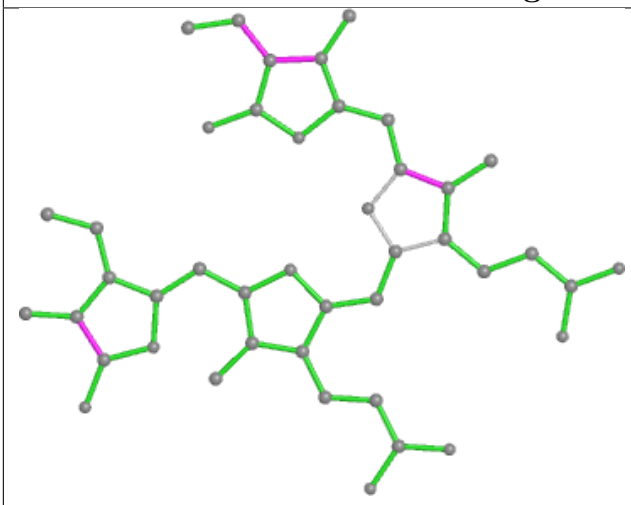


Rings

Ligand PEB f7 202



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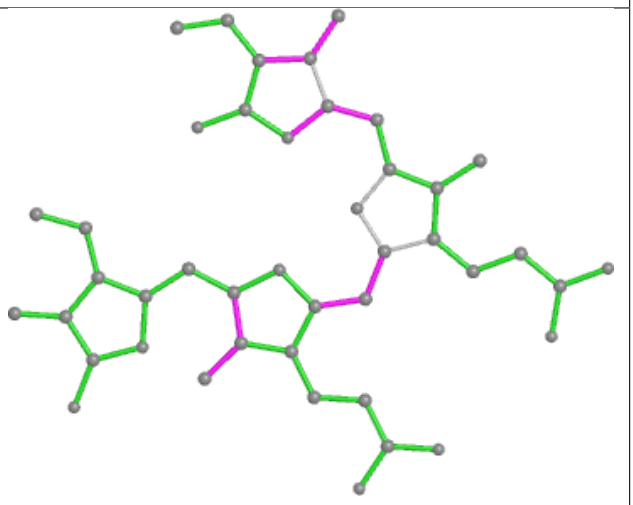

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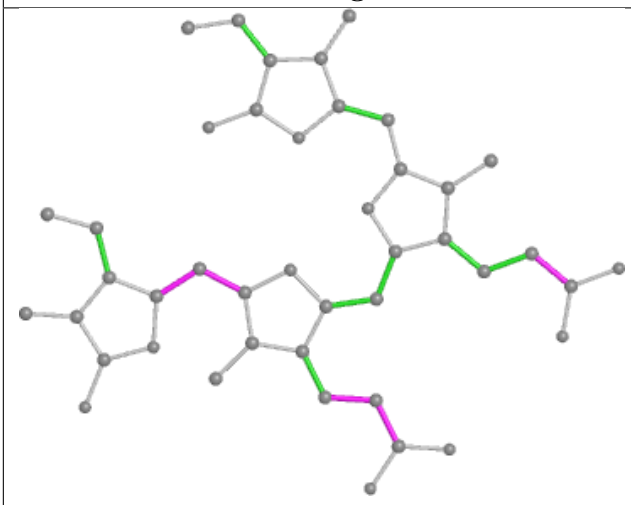

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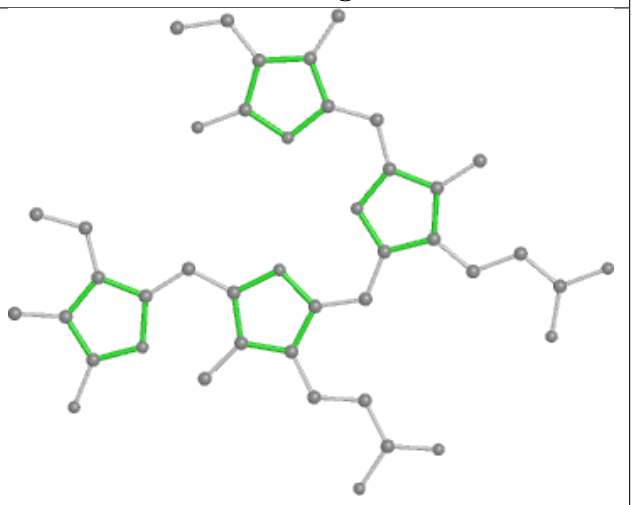
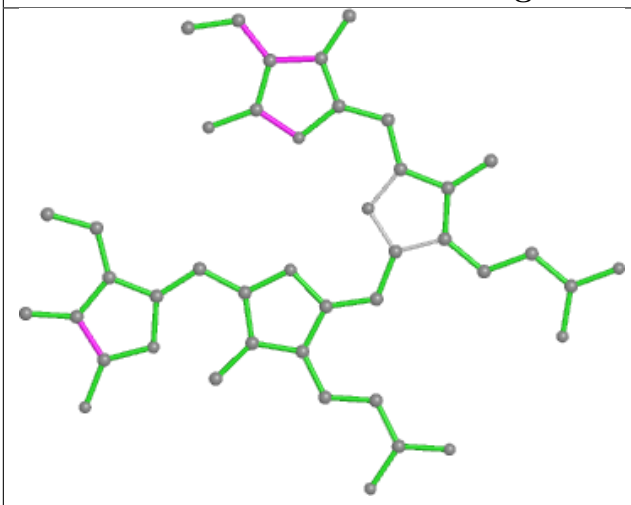


Rings

Ligand PEB H4 202



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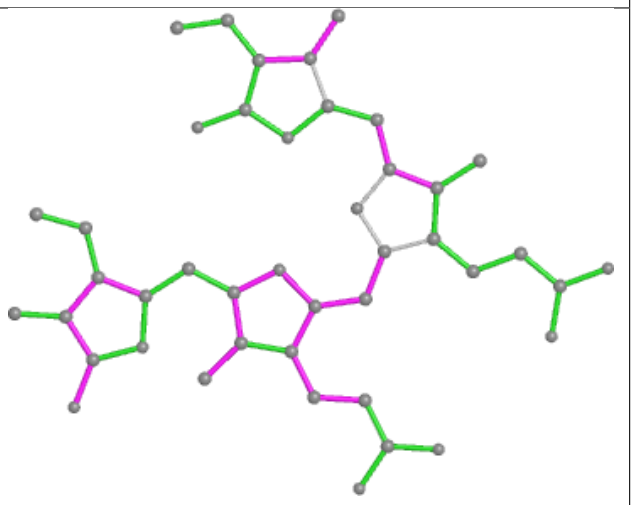

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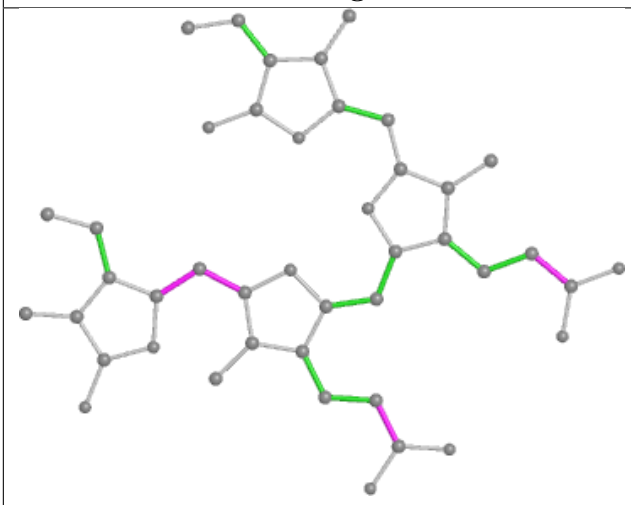

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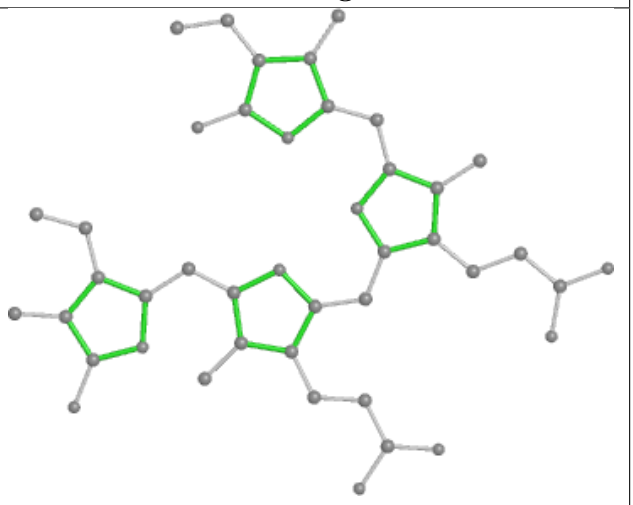
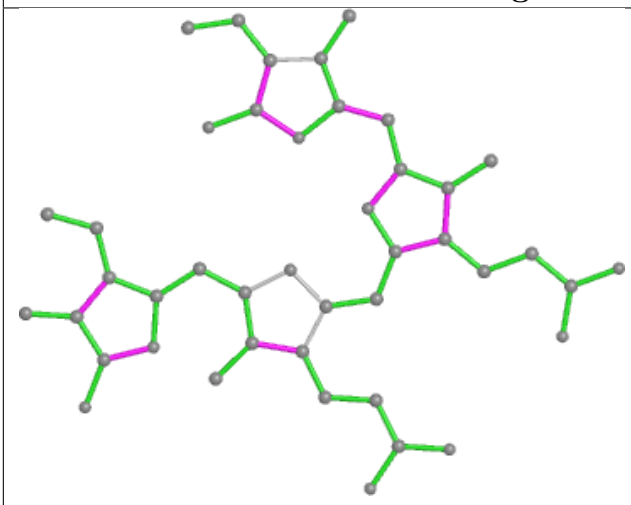


Rings

Ligand PUB dH 203



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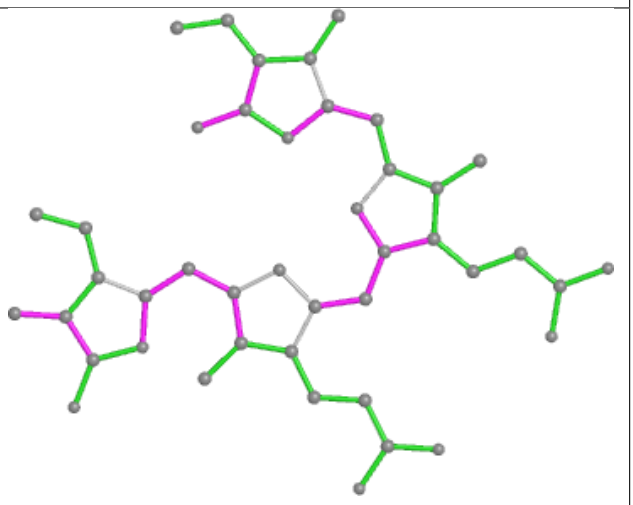

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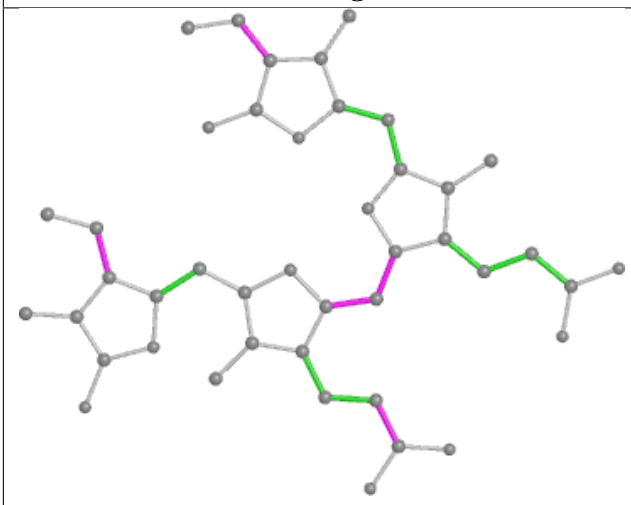

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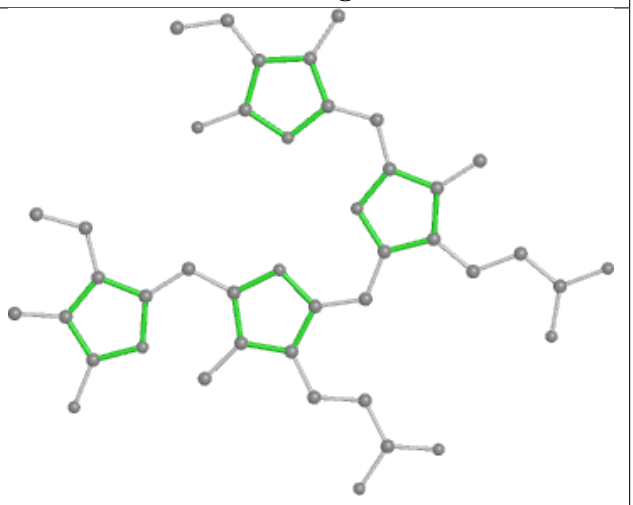
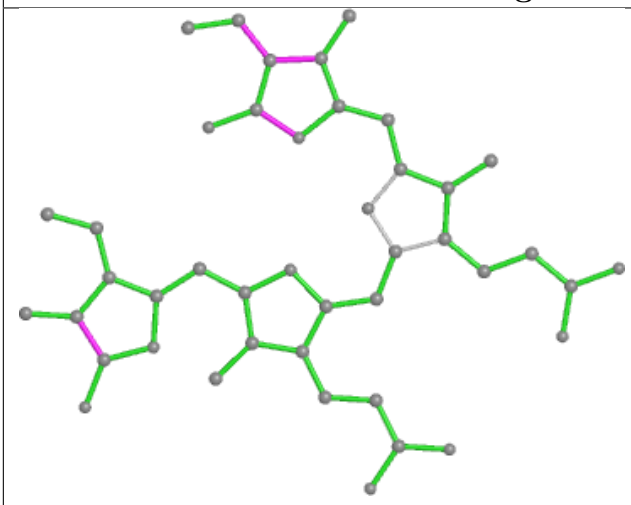


Rings

Ligand PEB U9 201



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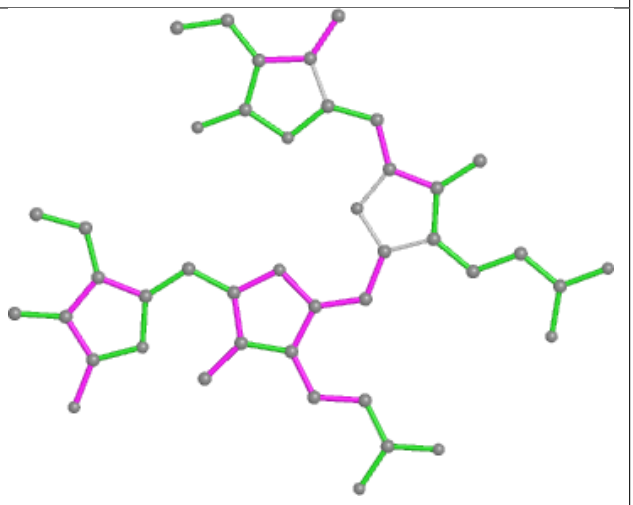

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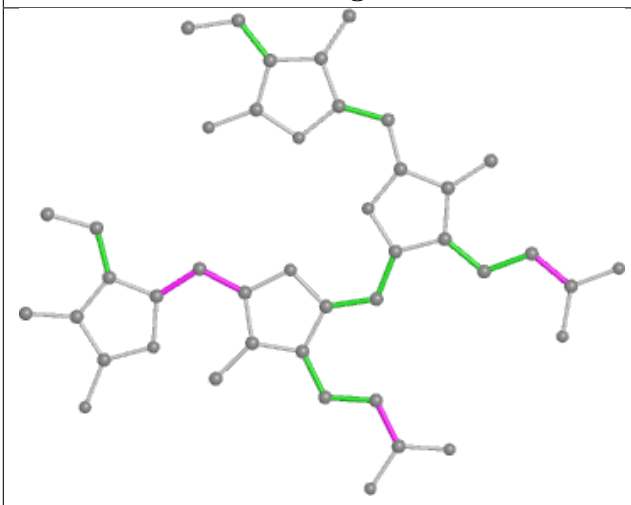

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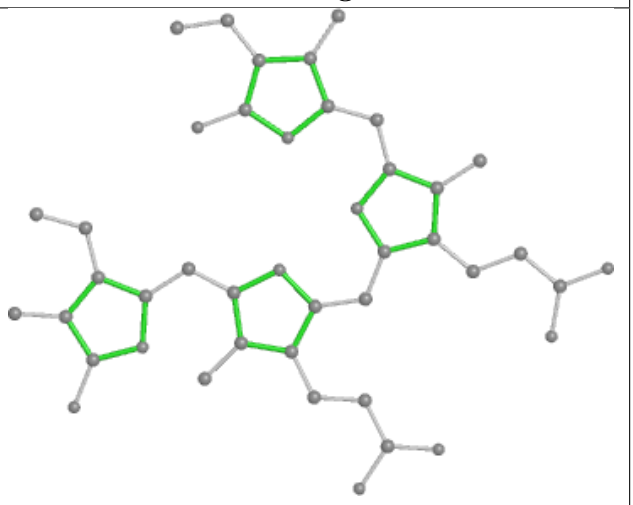
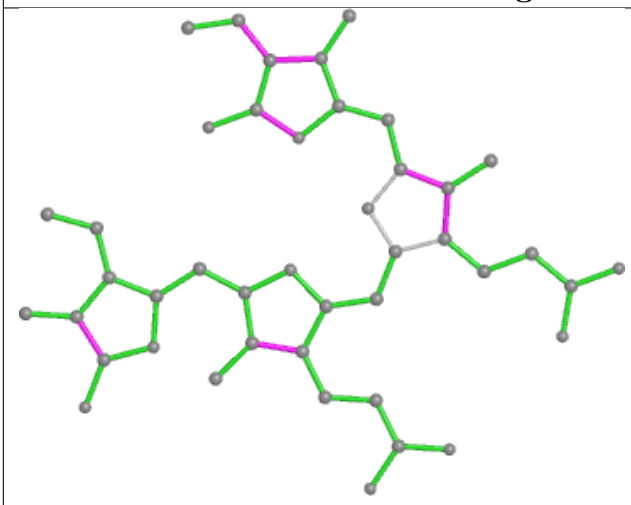


Rings

Ligand PEB V2 202



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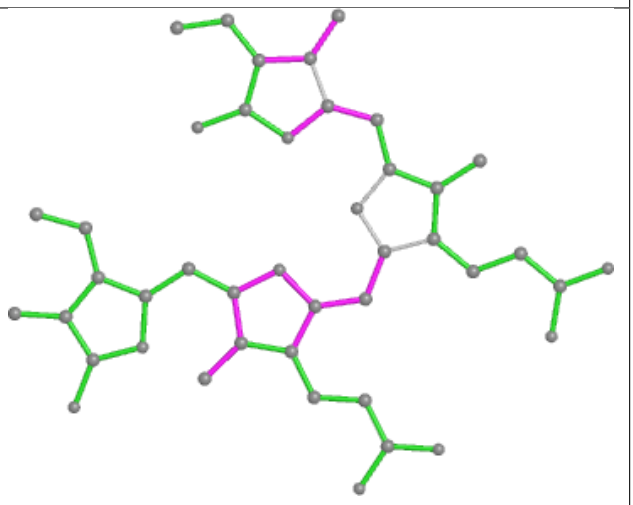
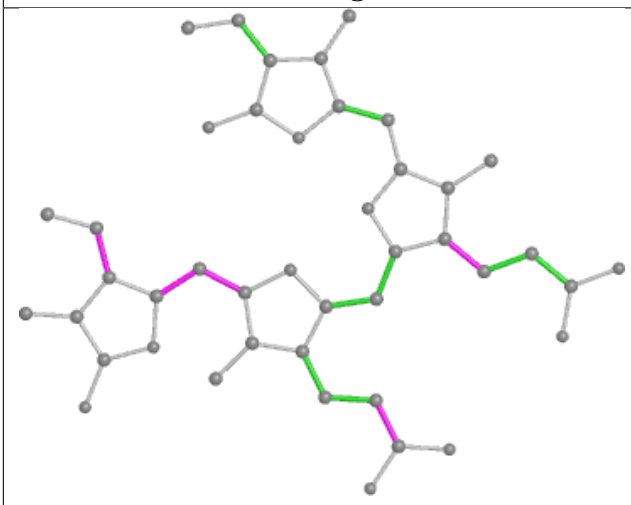
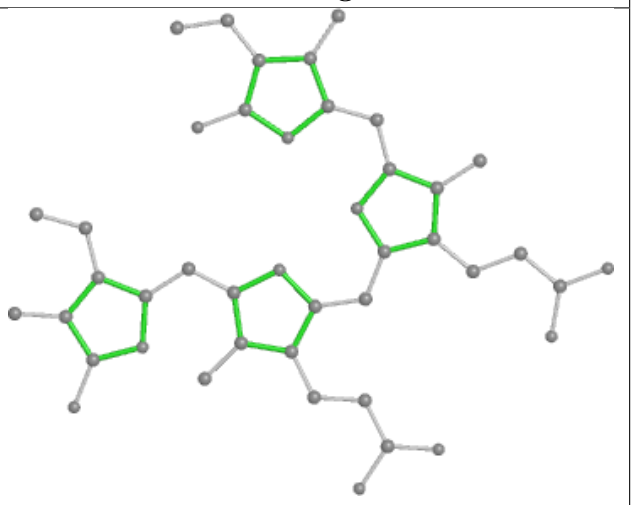


Bond angles

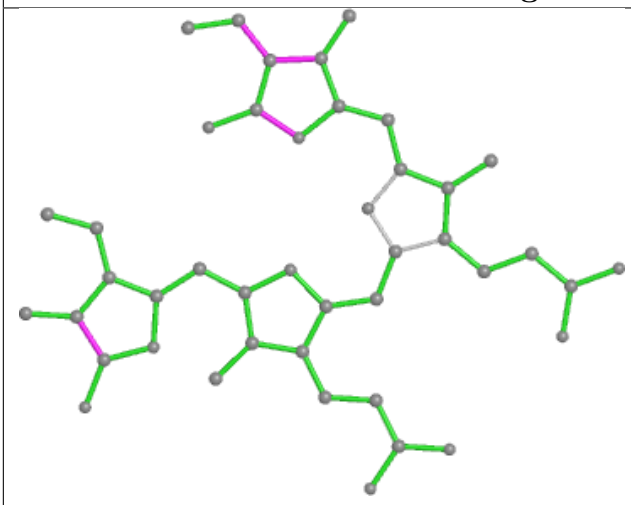


Torsions



Rings

Ligand PEB gz 303



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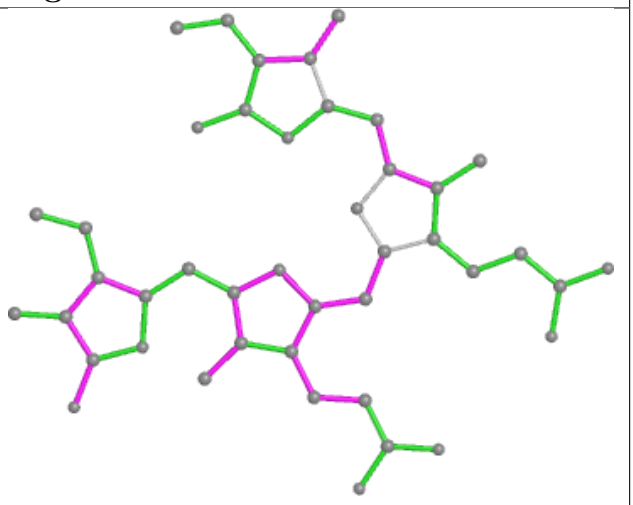

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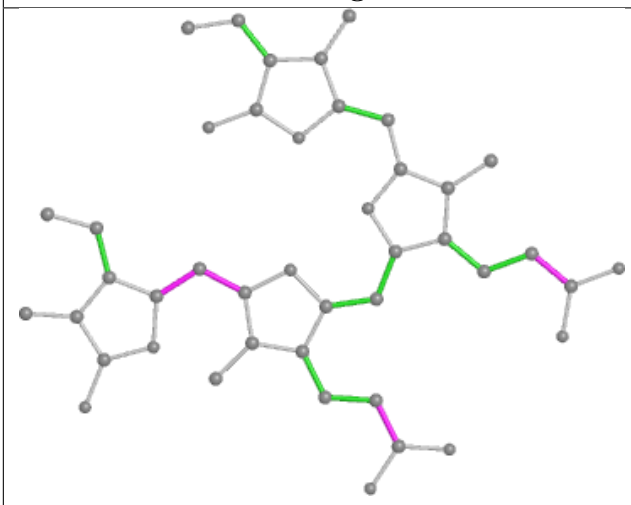

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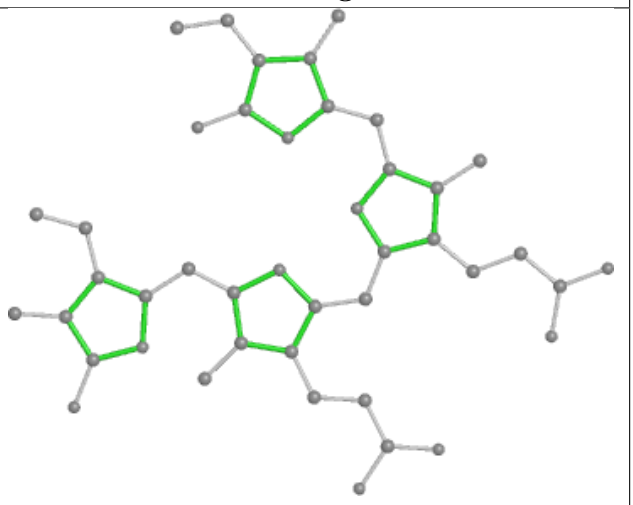
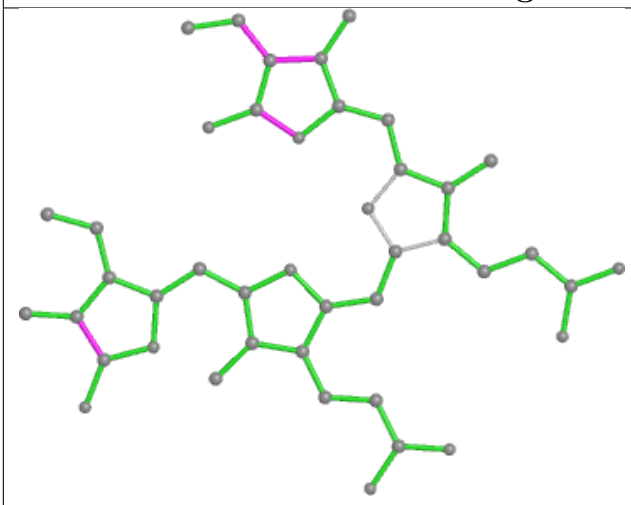


Rings

Ligand PEB hF 201



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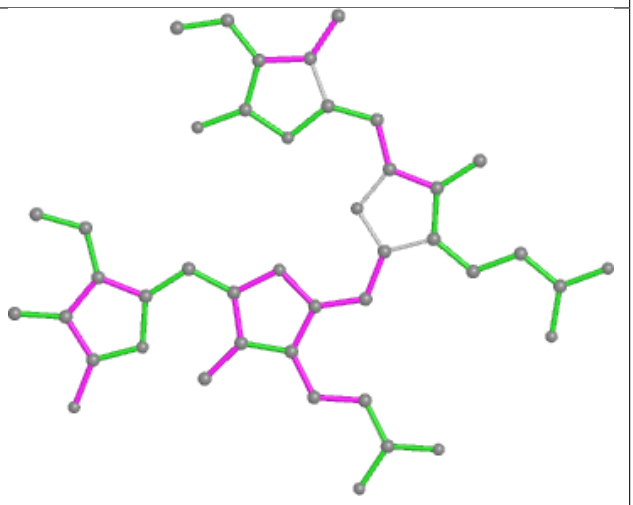

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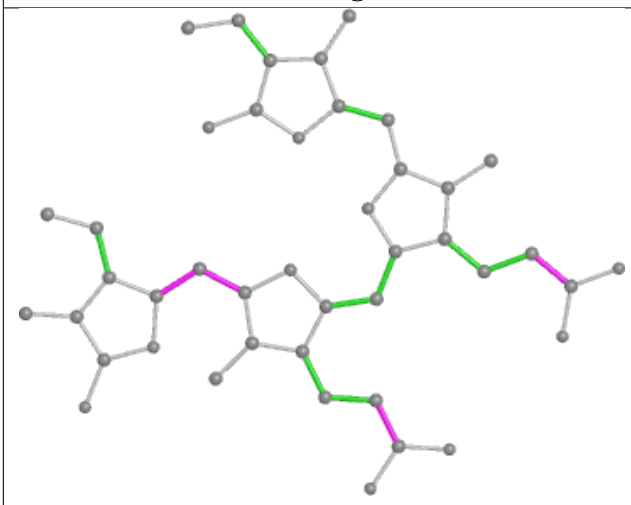

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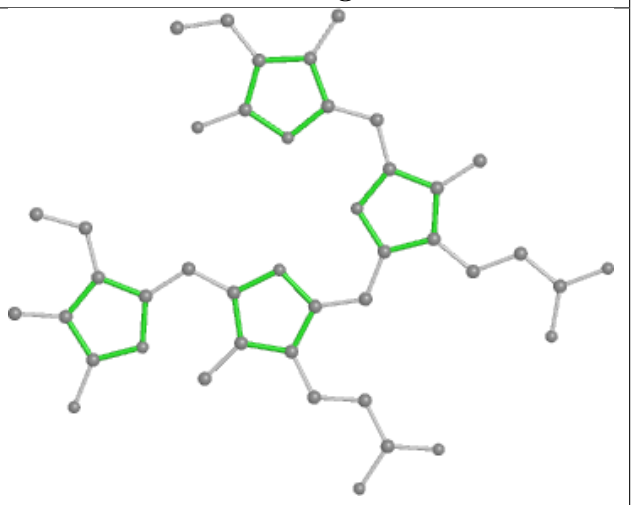
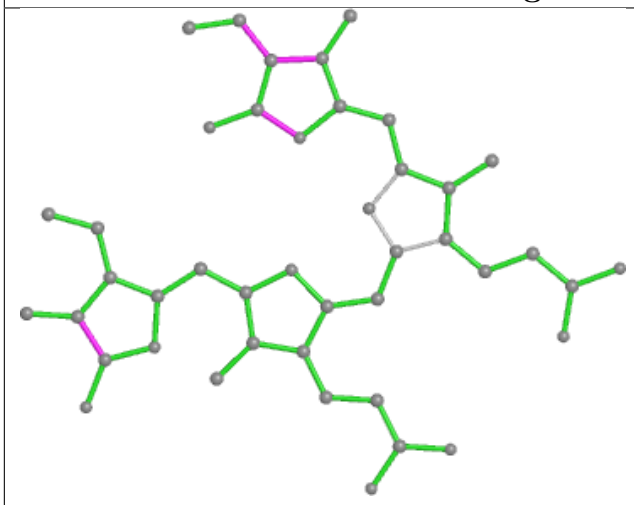


Rings

Ligand PEB bl 201



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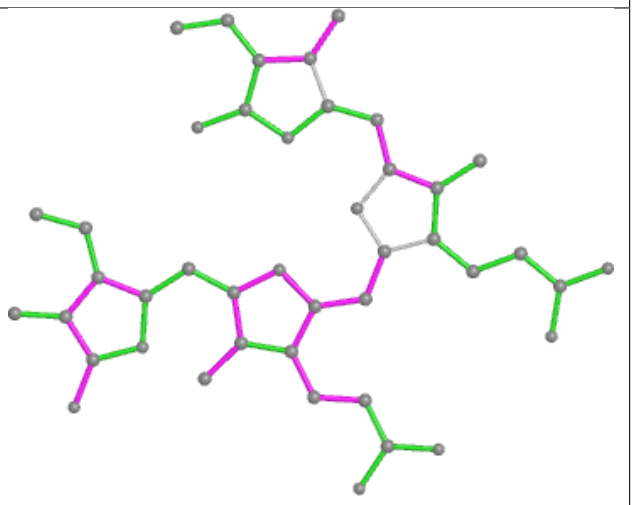

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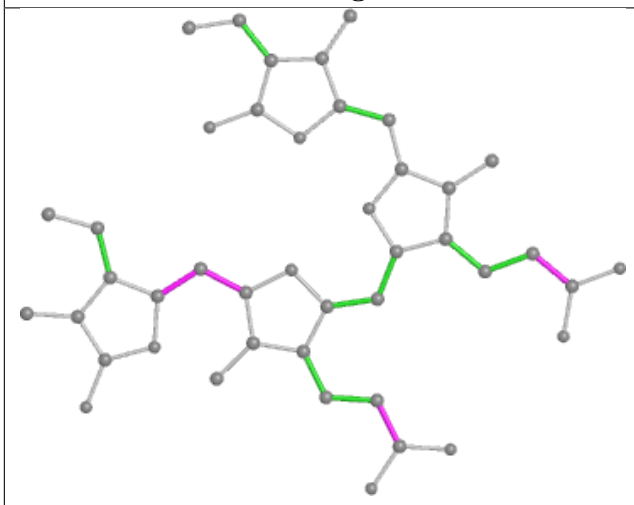

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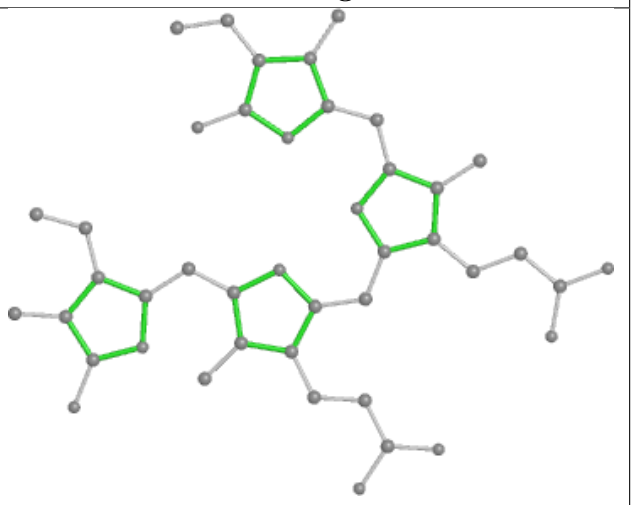
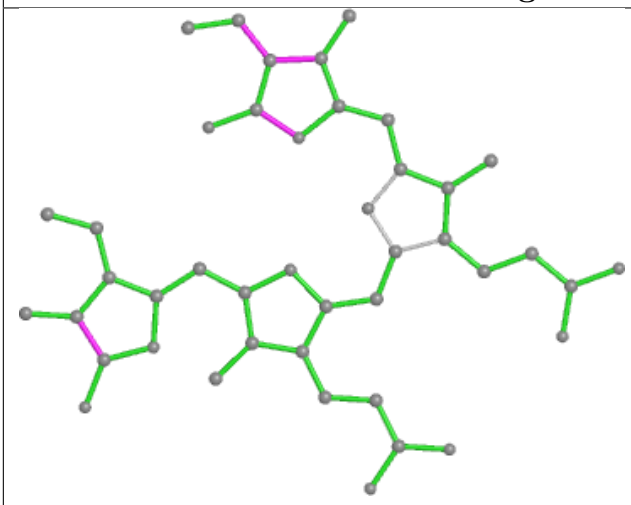


Rings

Ligand PEB dq 201



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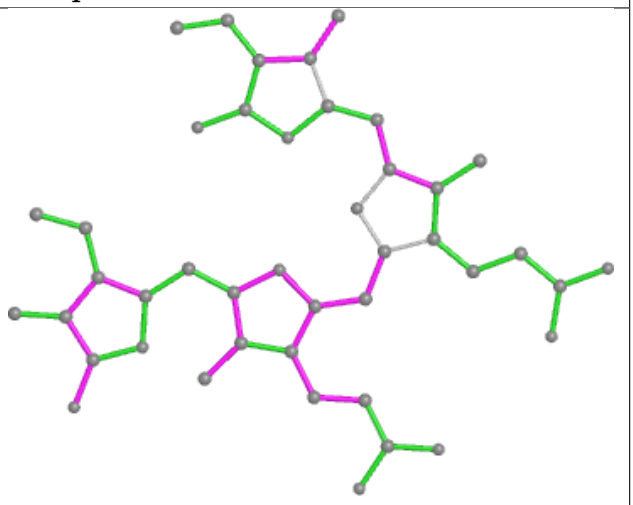

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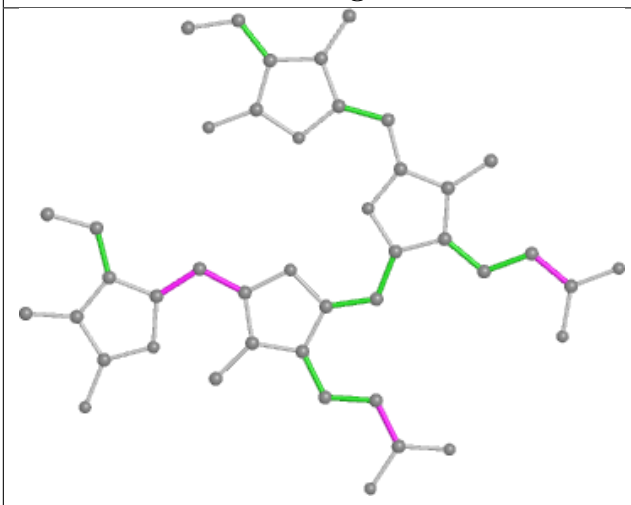

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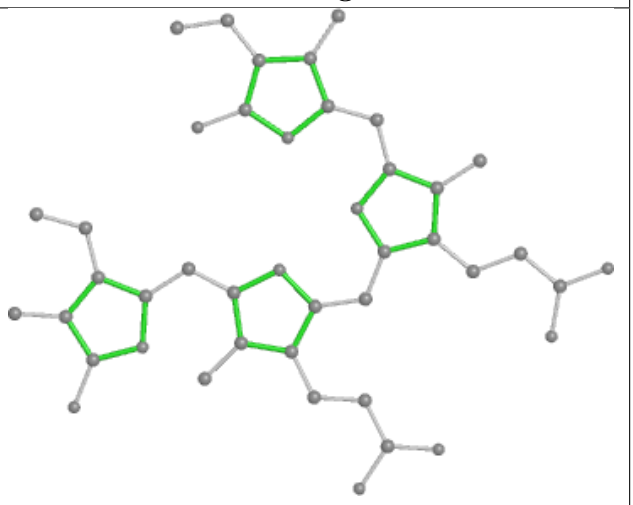
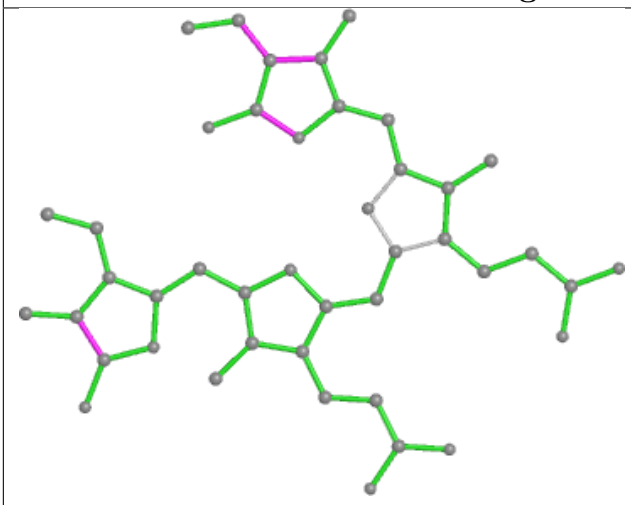


Rings

Ligand PEB k3 201



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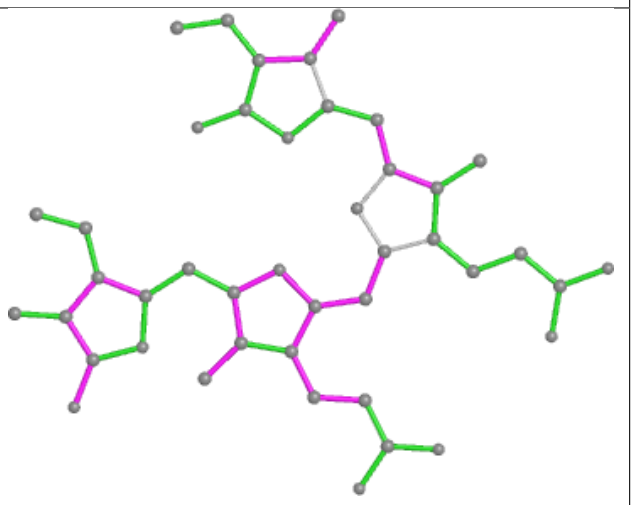

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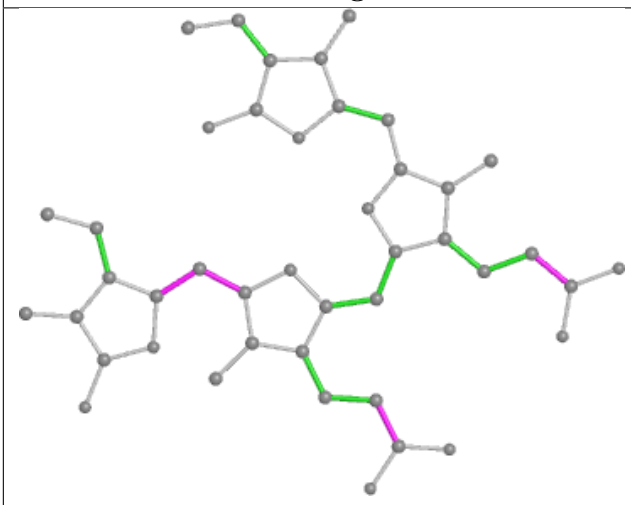

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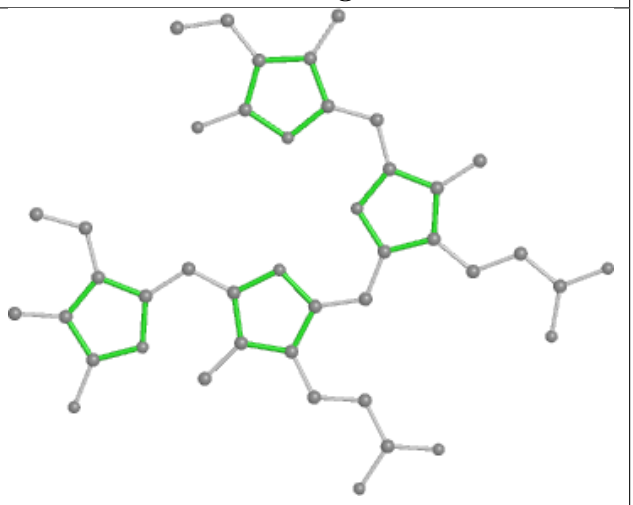
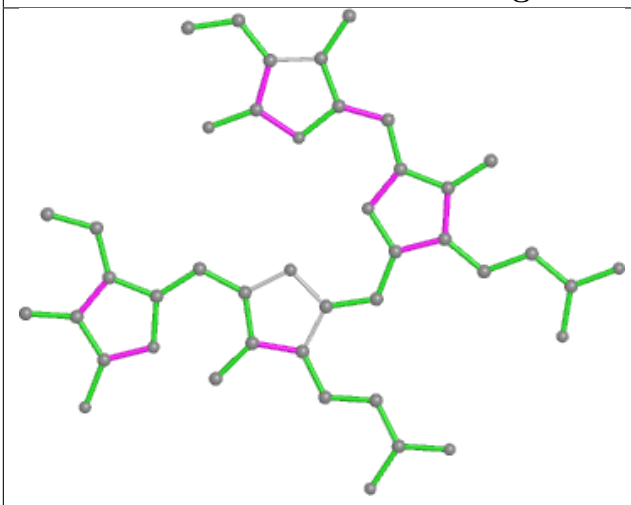


Rings

Ligand PUB dw 406



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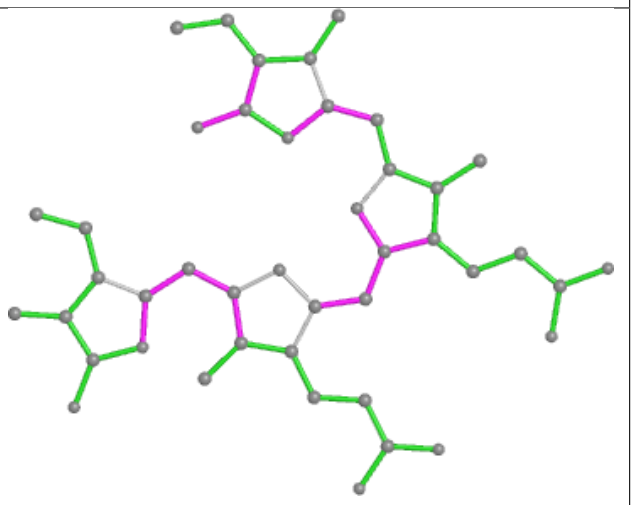

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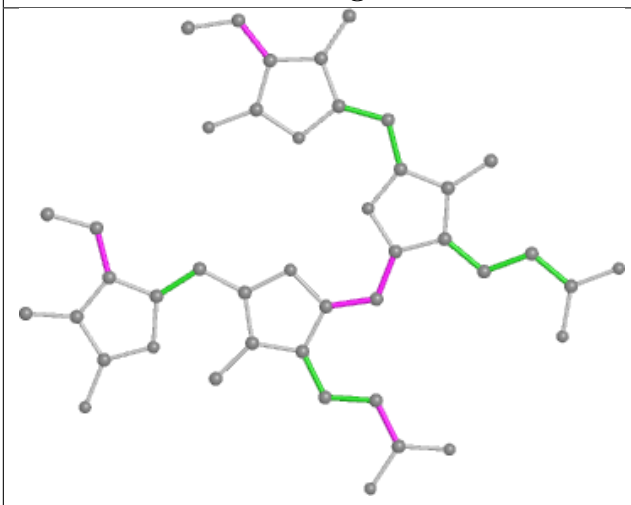

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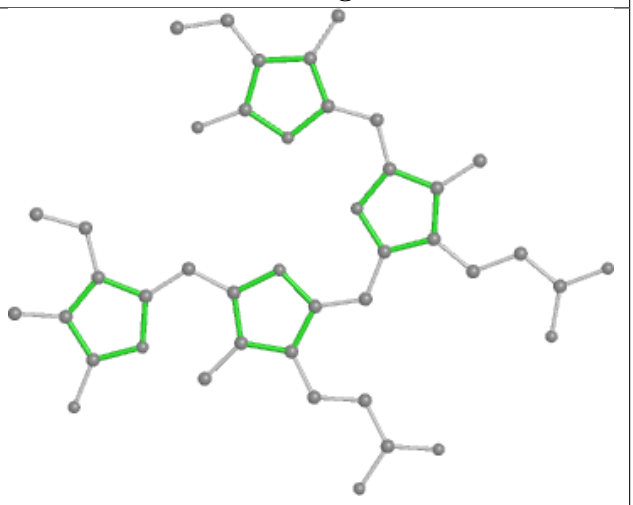
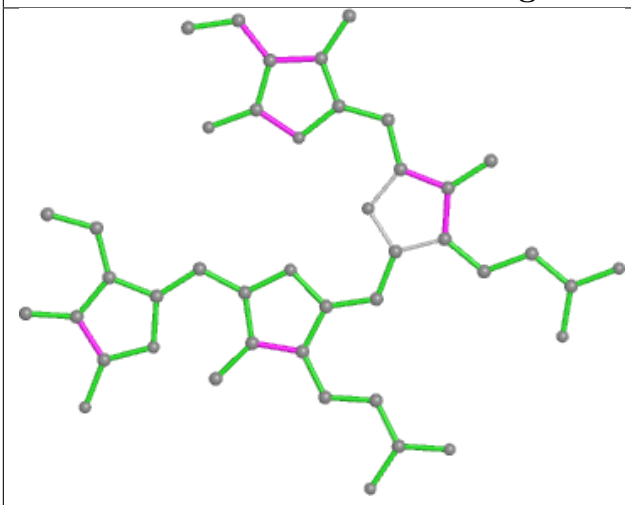


Rings

Ligand PEB p5 201



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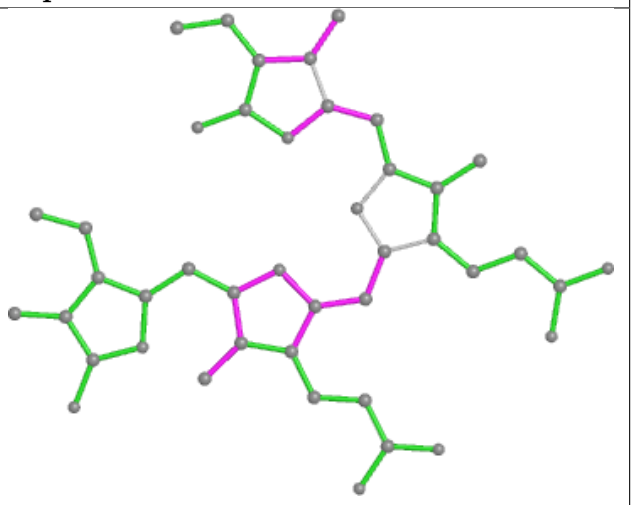

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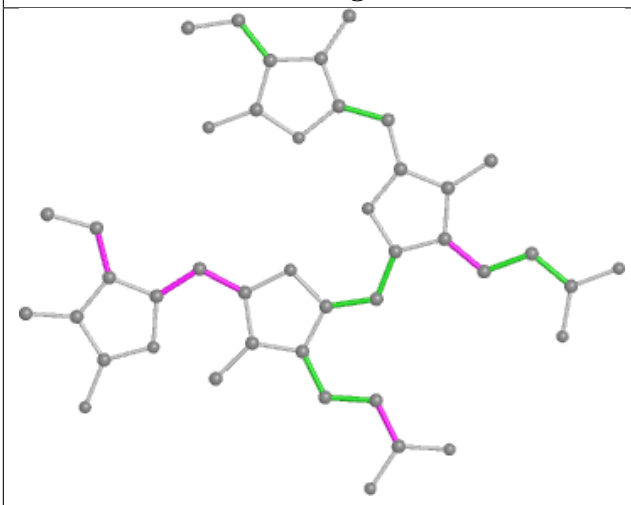

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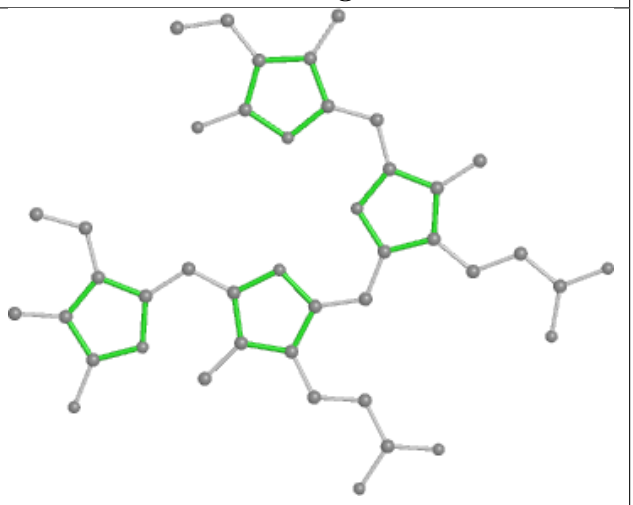
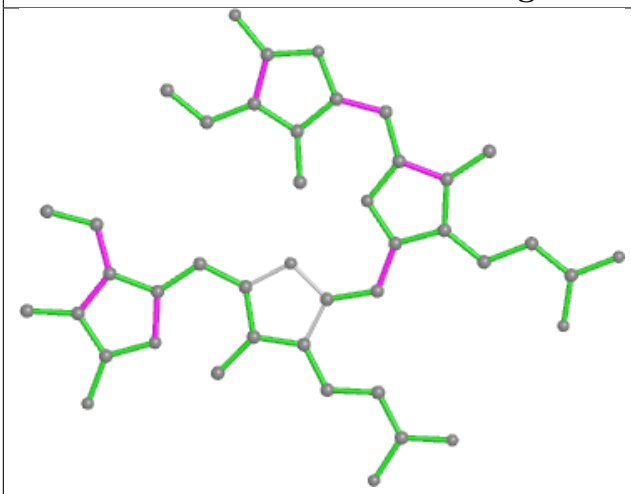


Rings

Ligand PVN c8 303



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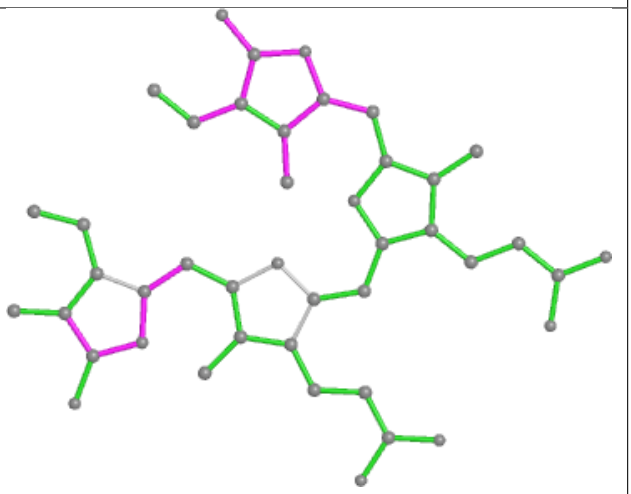

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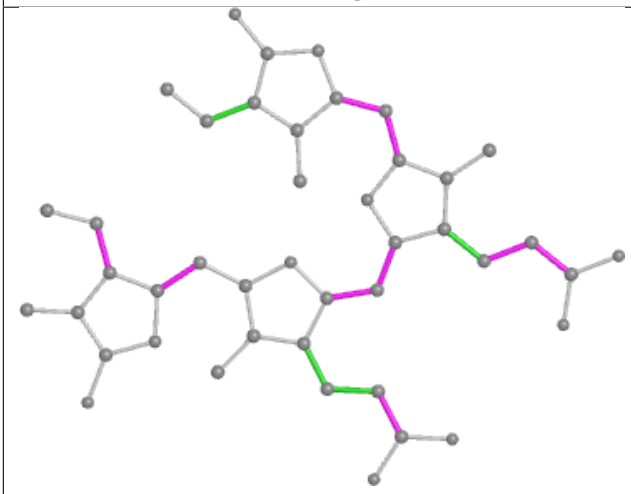

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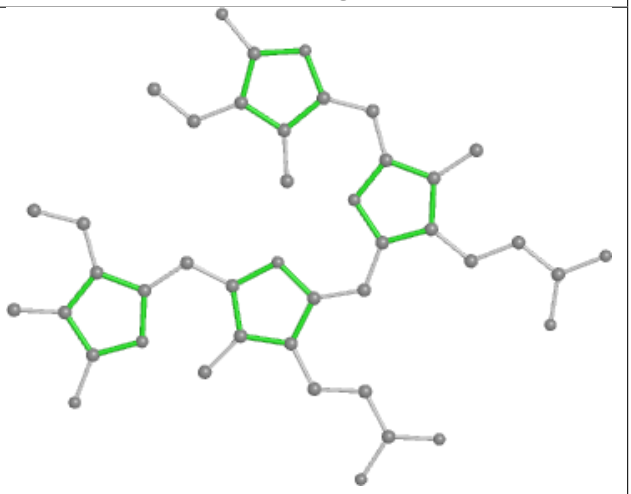
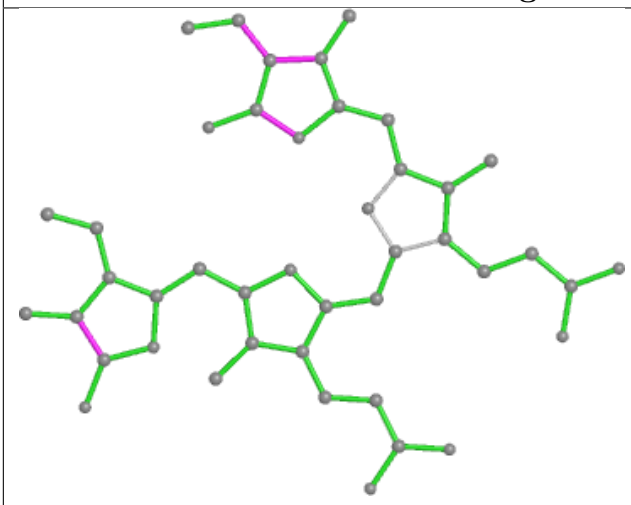


Rings

Ligand PEB gv 201



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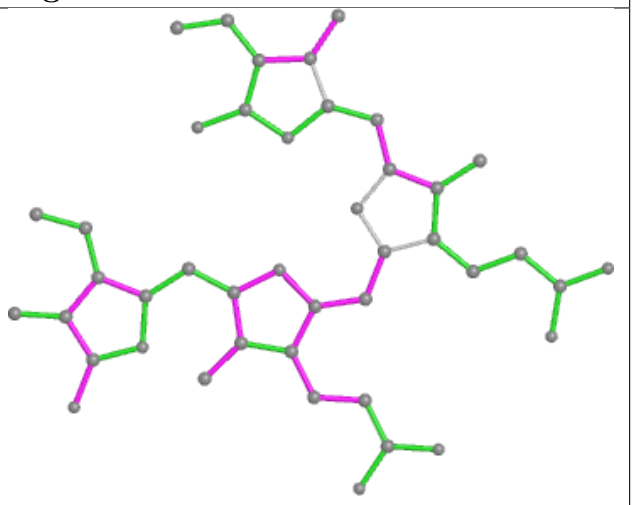

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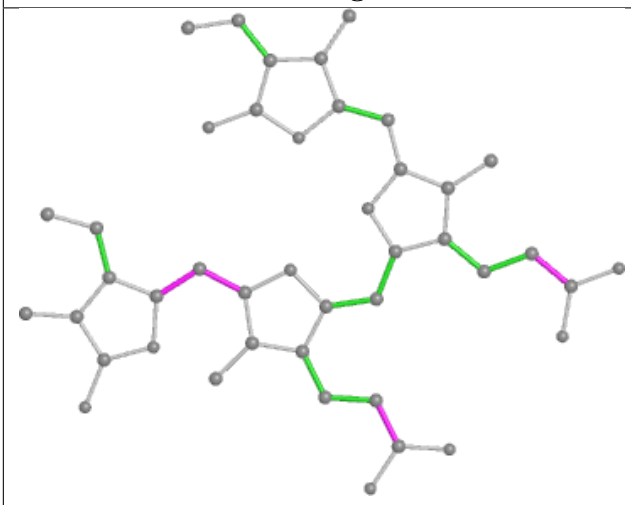

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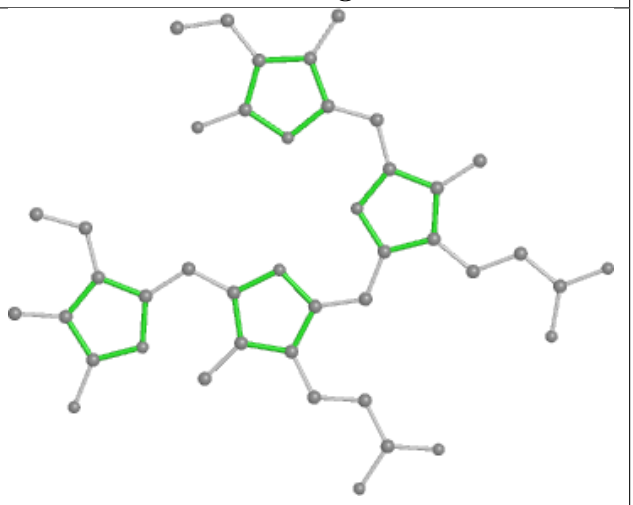
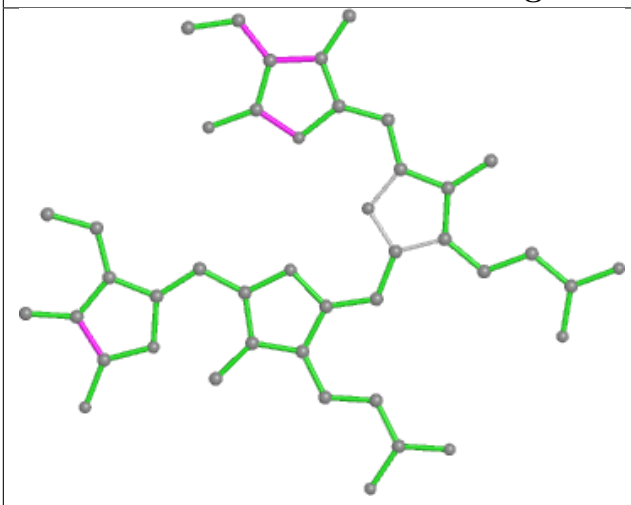


Rings

Ligand PEB el 201



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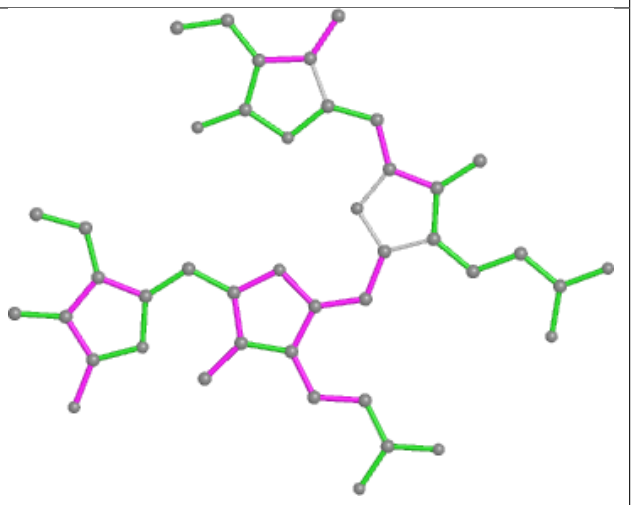

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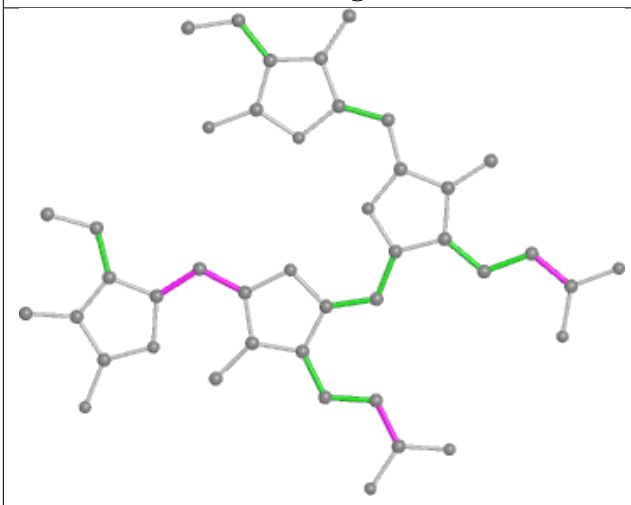

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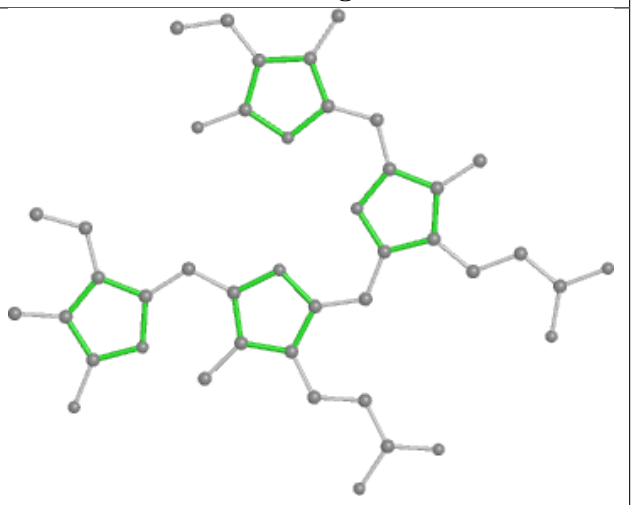
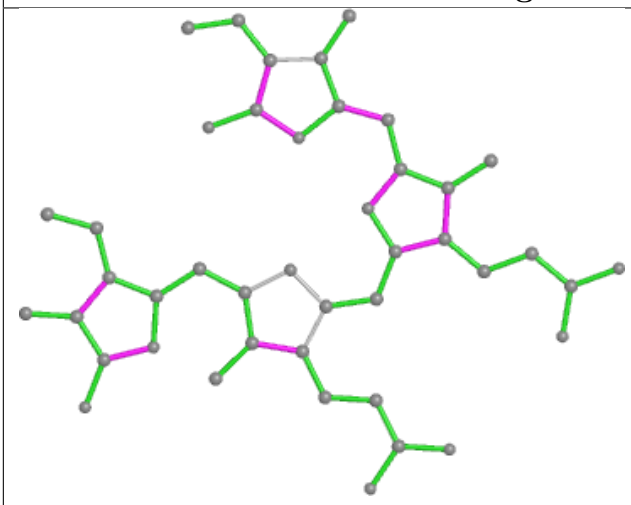


Rings

Ligand PUB Z5 305



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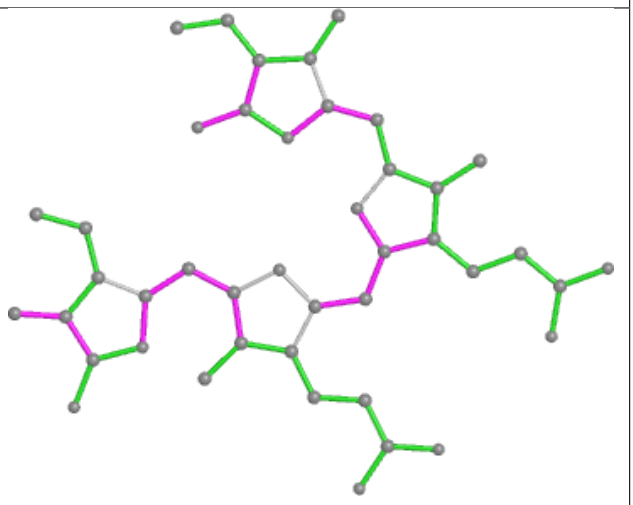

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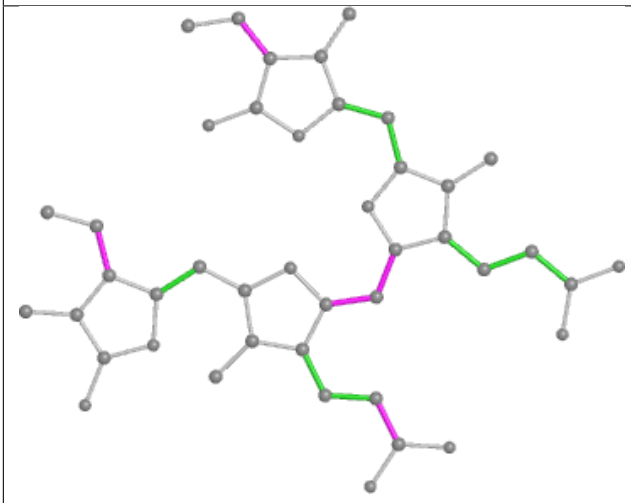

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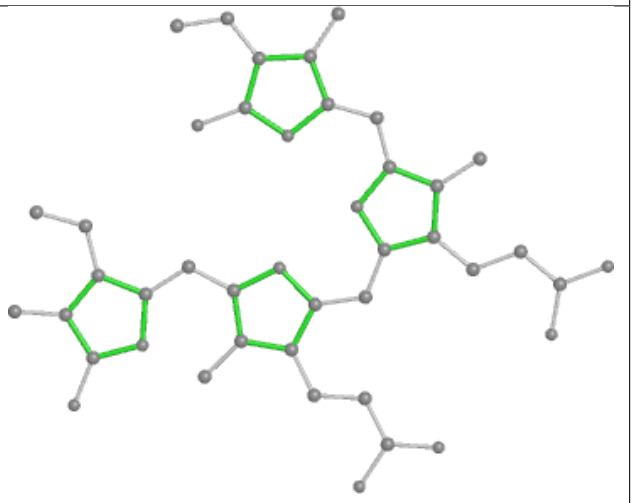

Rings

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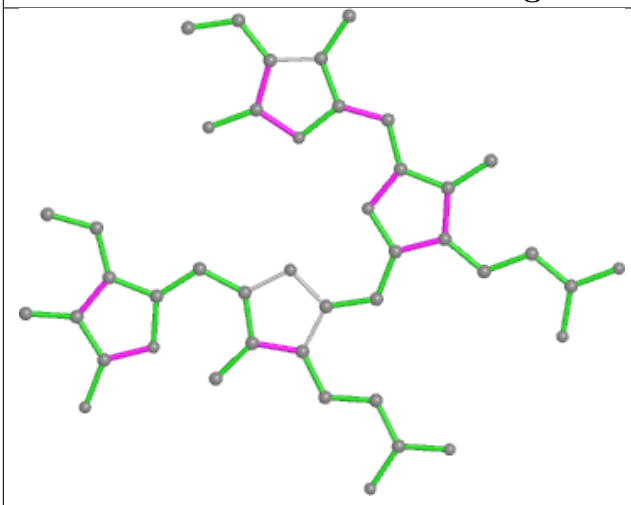

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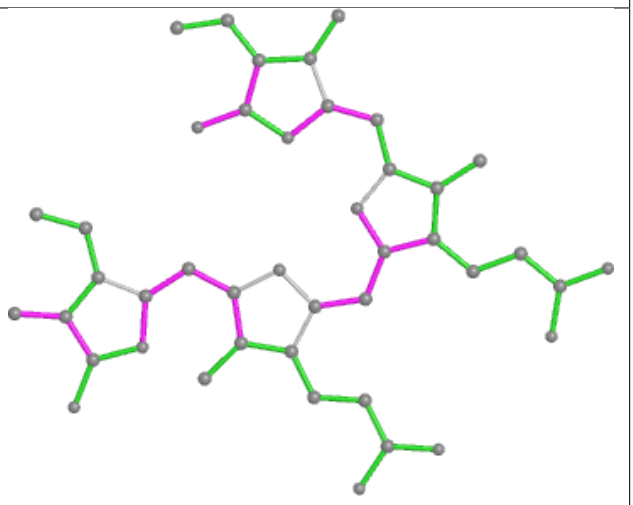

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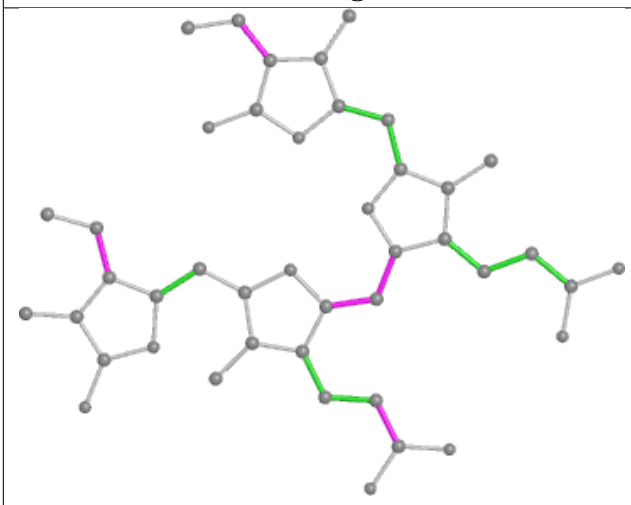

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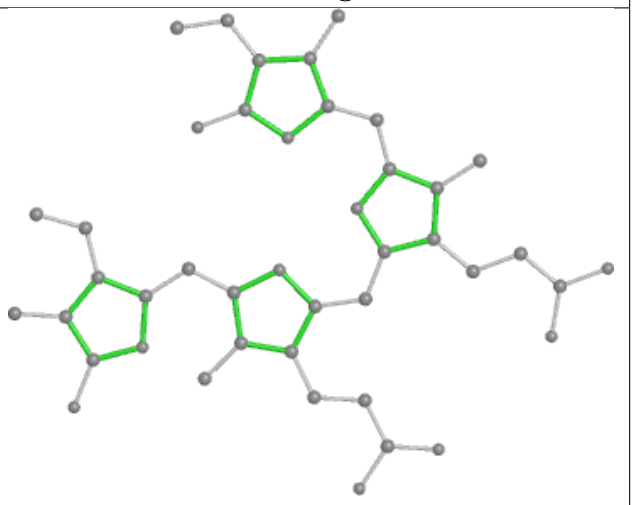
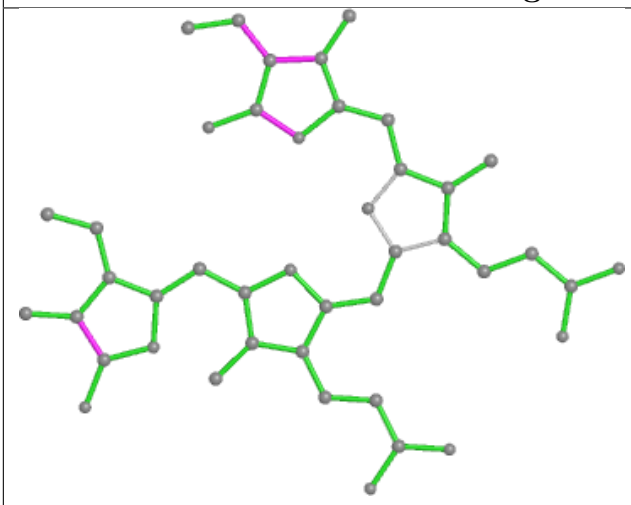


Rings

Ligand PEB j9 201



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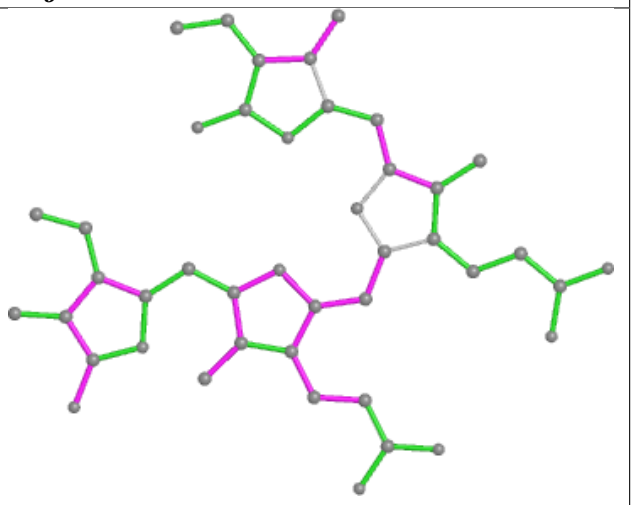
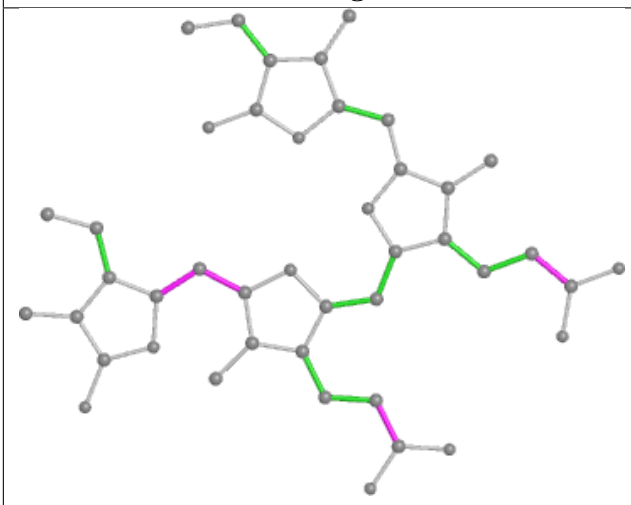
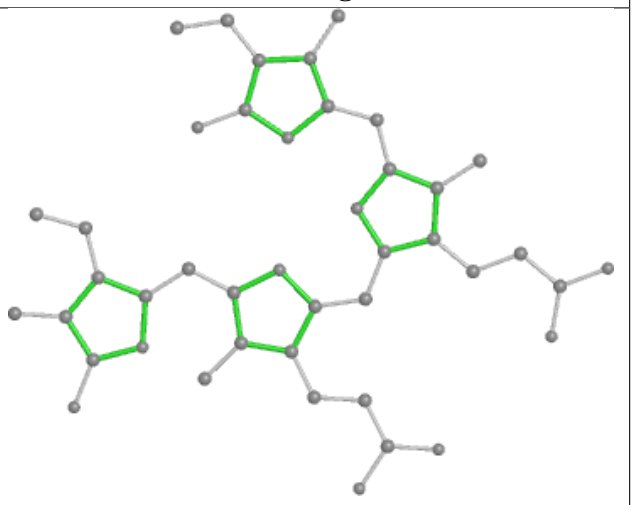


Bond angles

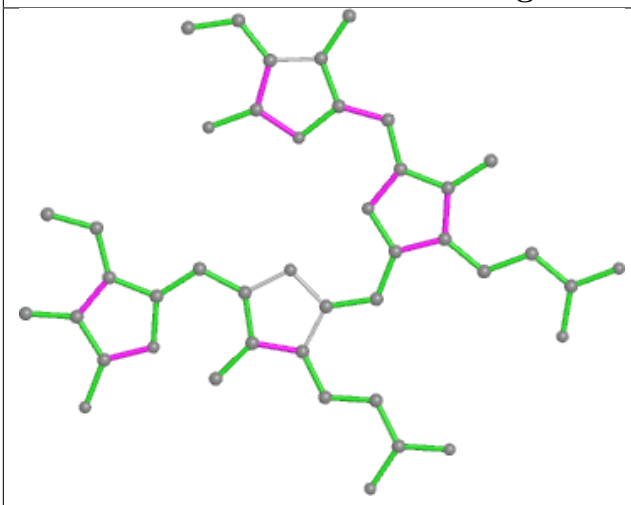


Torsions



Rings

Ligand PUB cF 202



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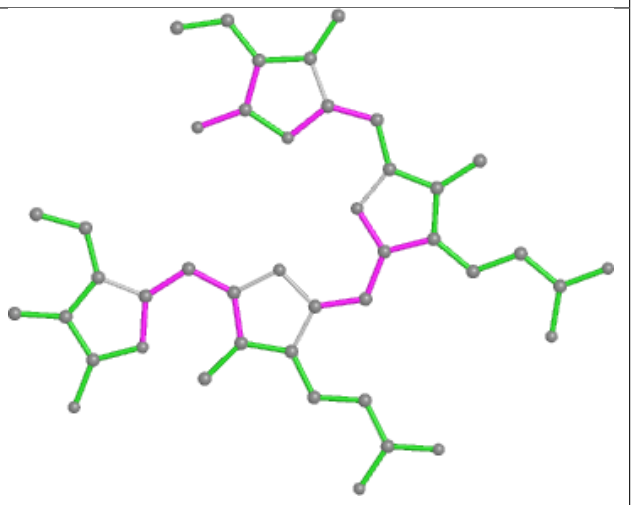
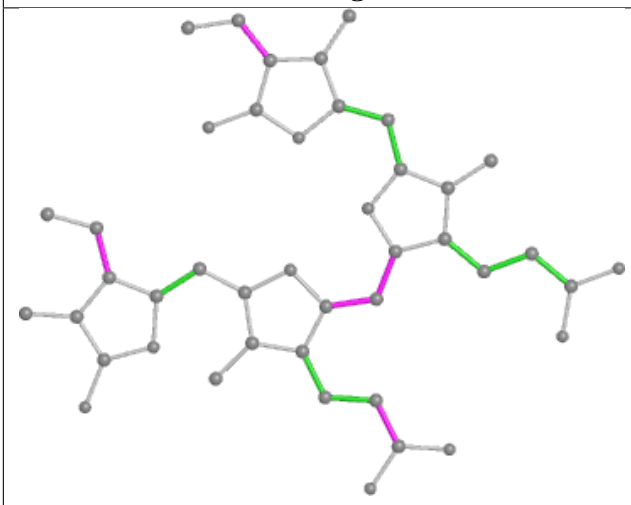


Bond angles



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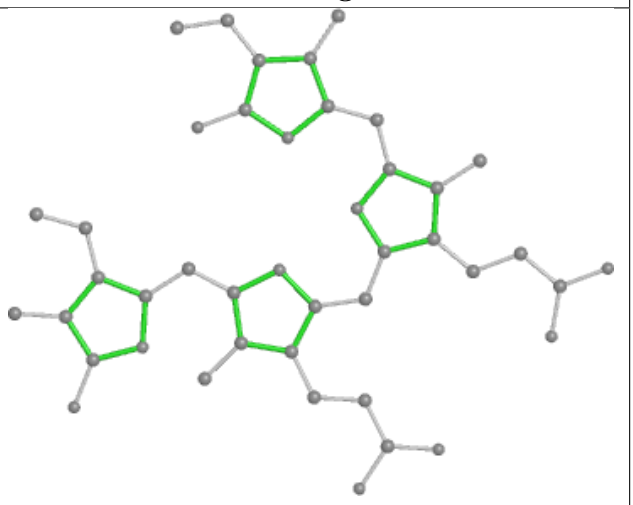
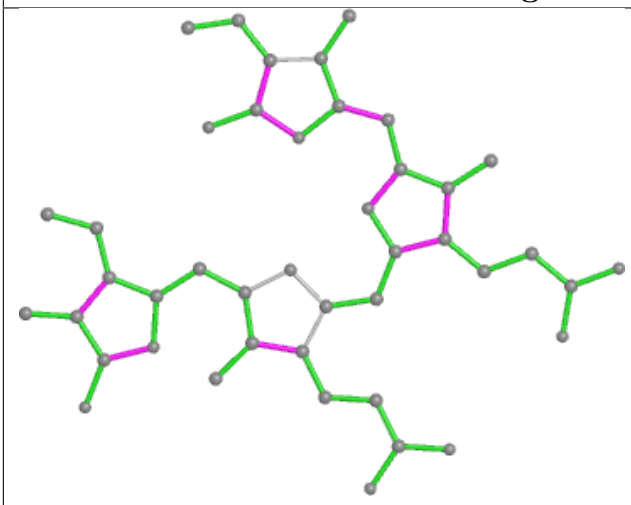


Rings

Ligand PUB ly 406



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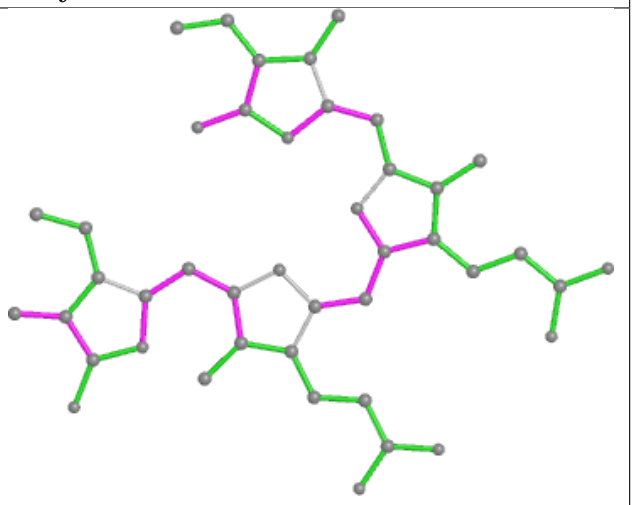

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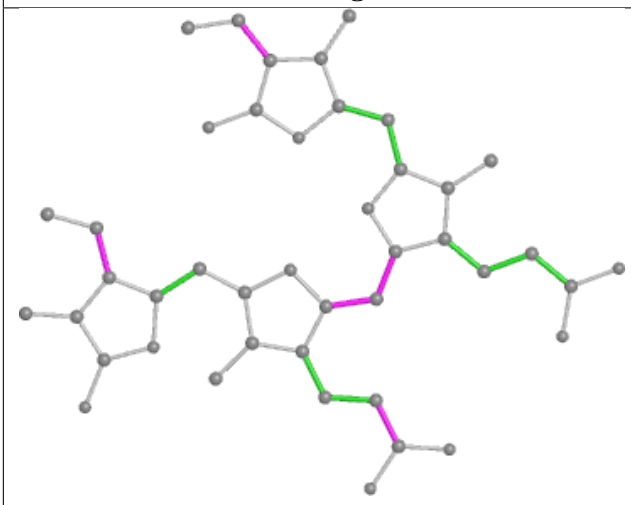

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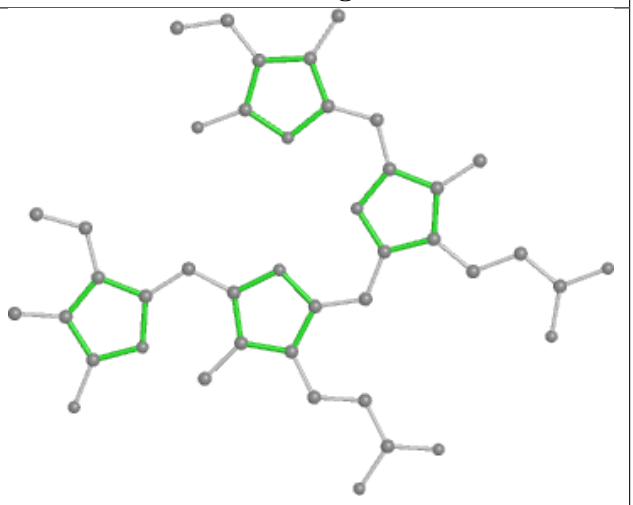
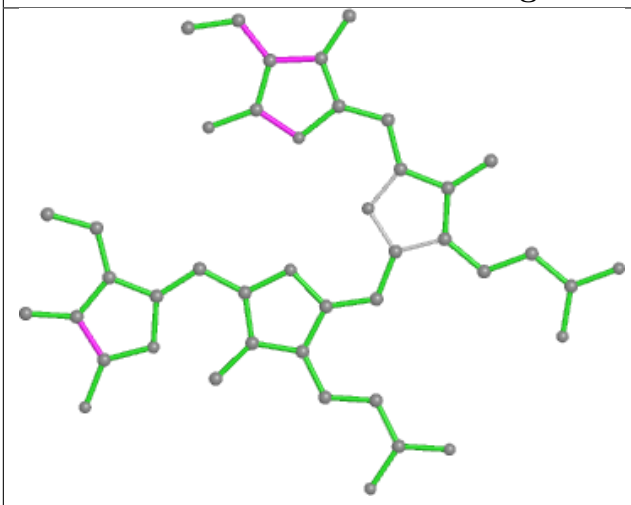


Rings

Ligand PEB dc 201



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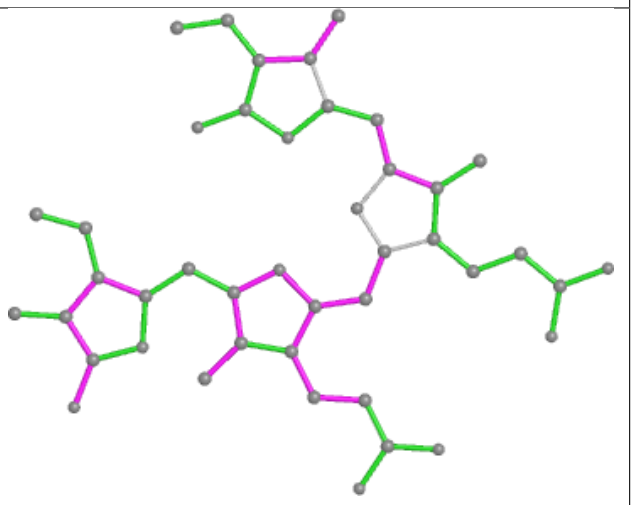

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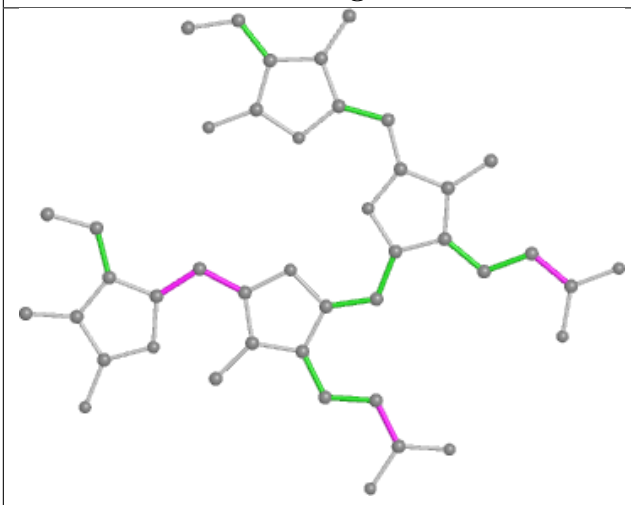

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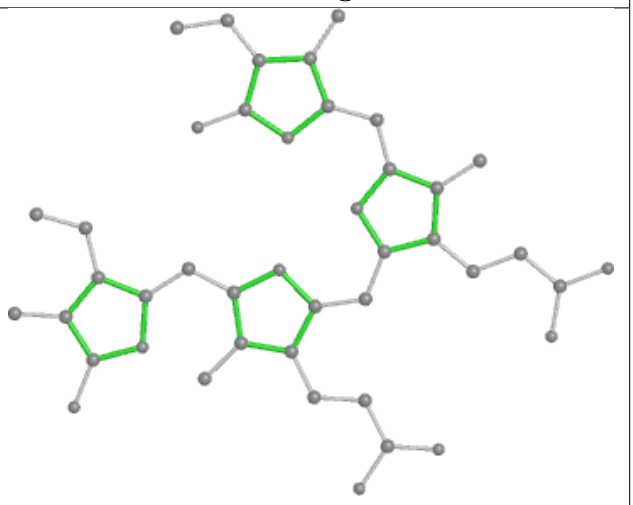
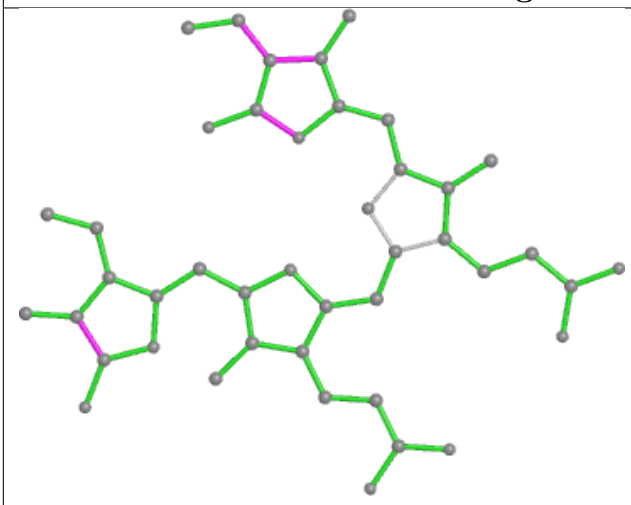


Rings

Ligand PEB eD 201



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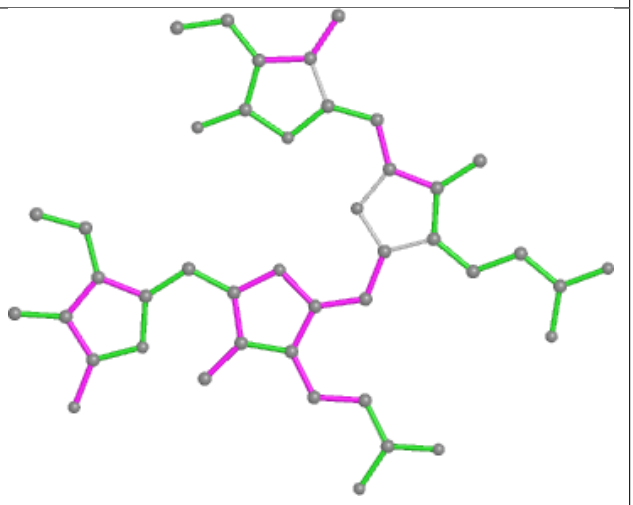

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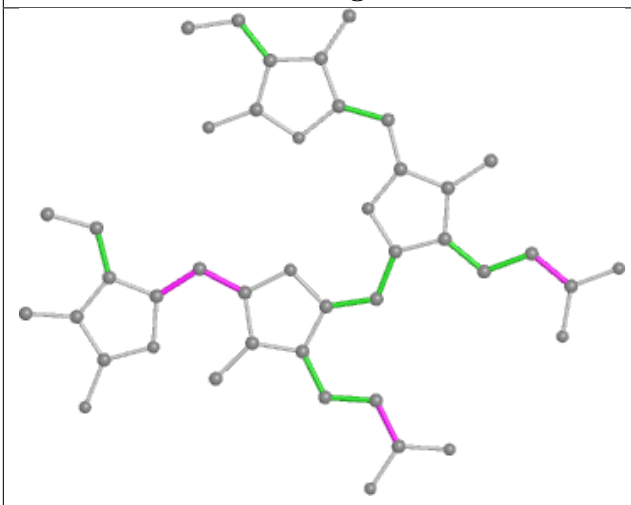

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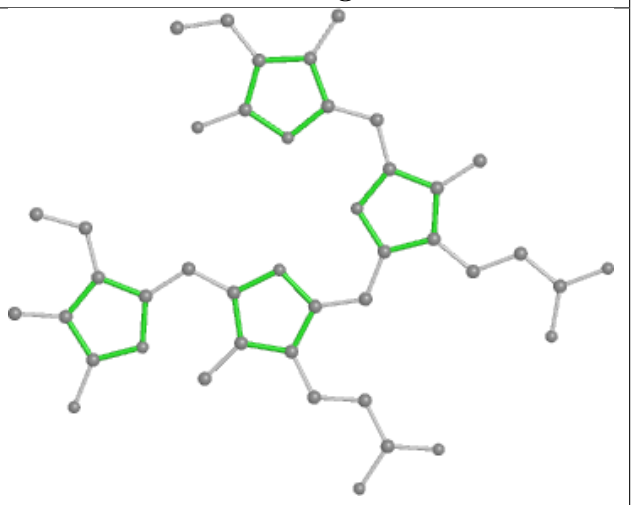

Rings

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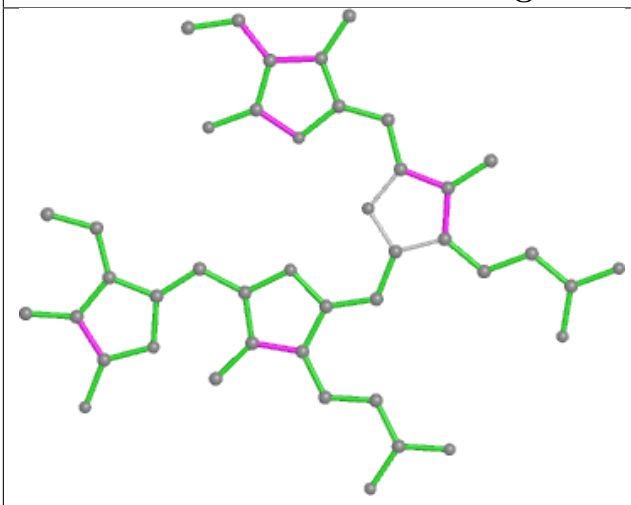

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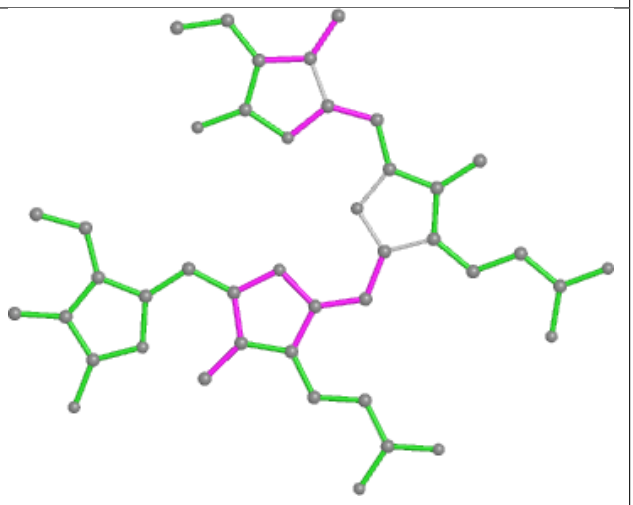

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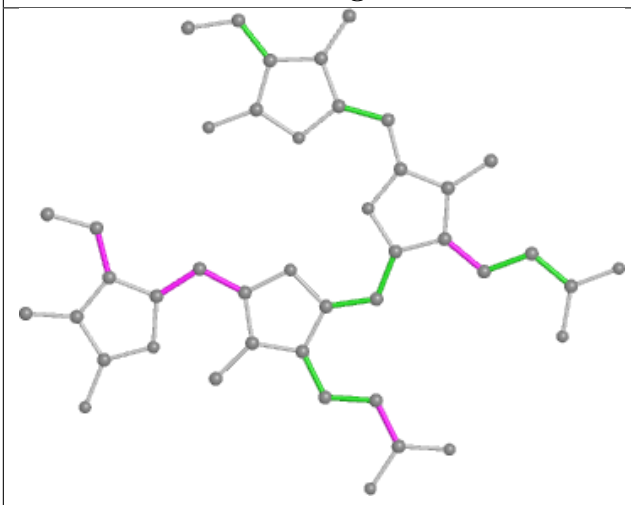

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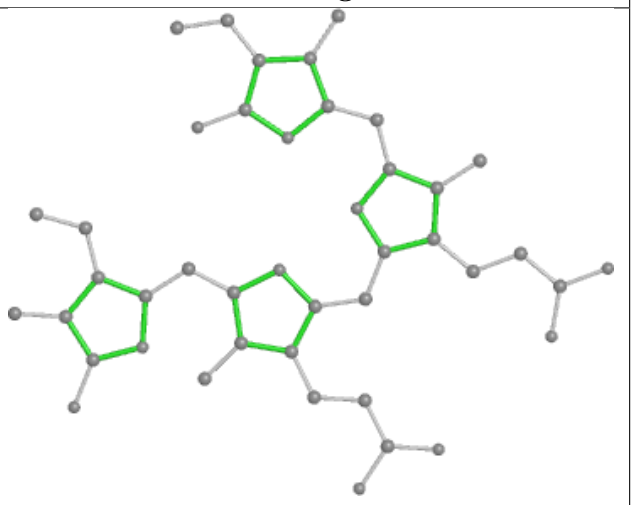
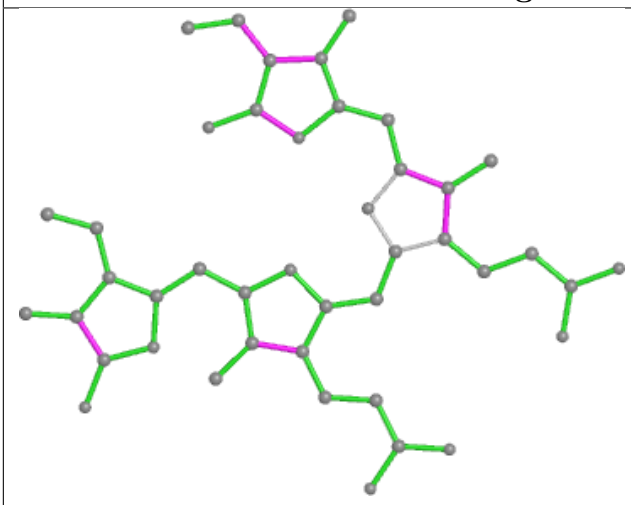


Rings

Ligand PEB hP 202



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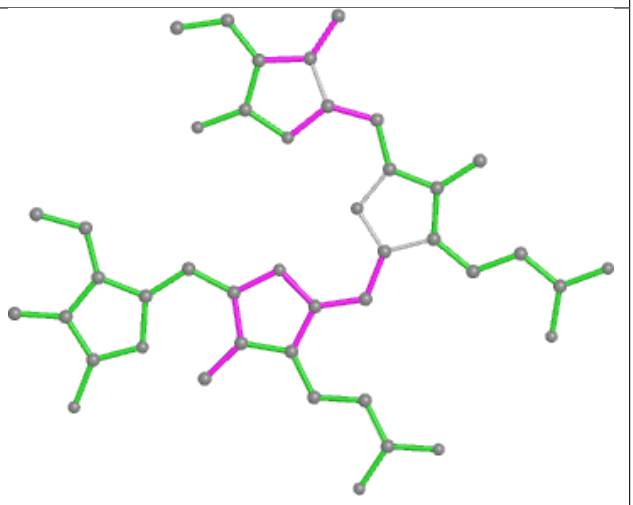

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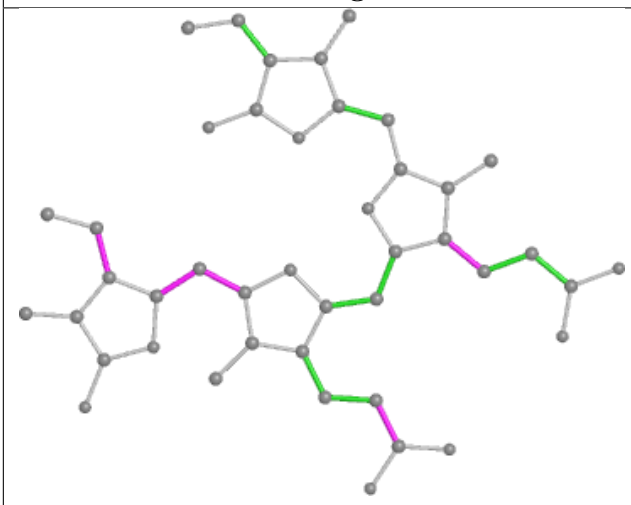

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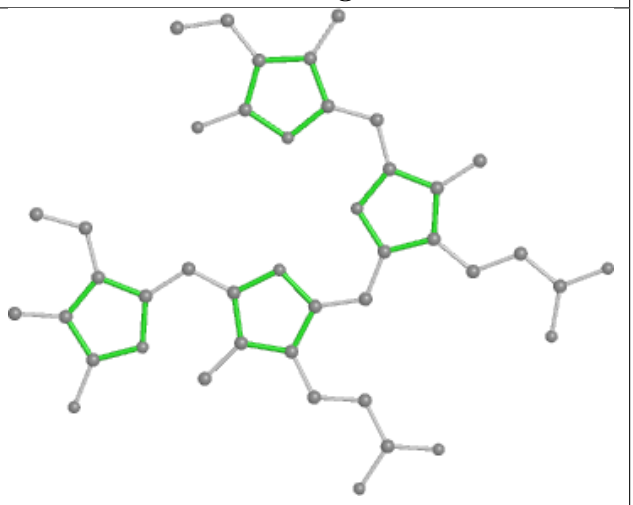

Rings

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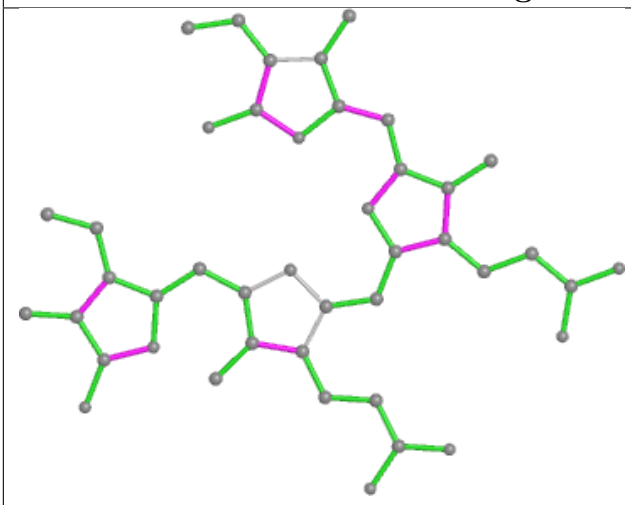

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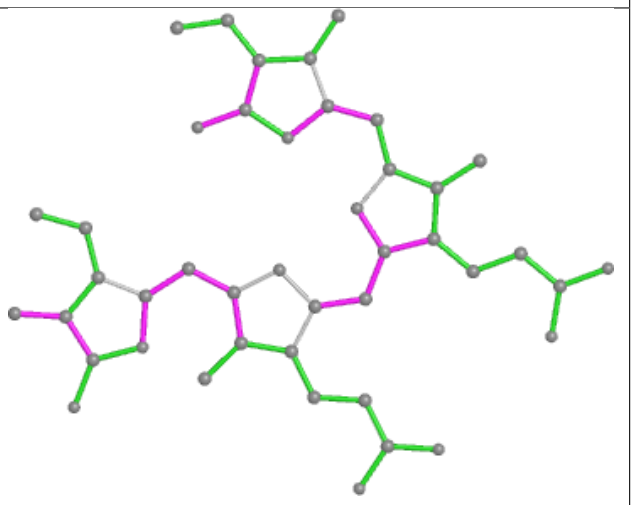

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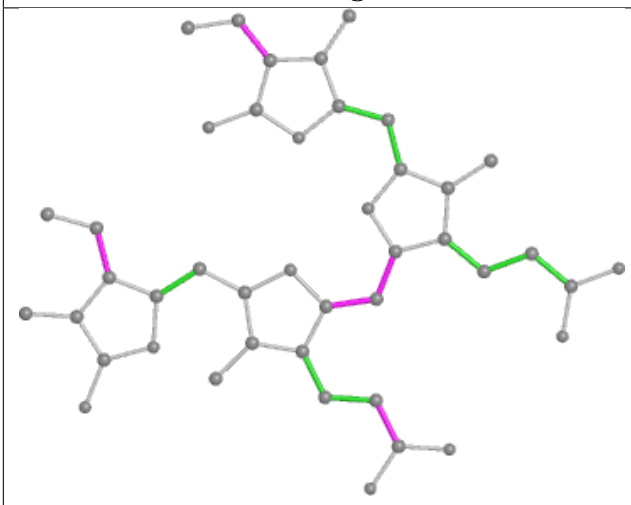

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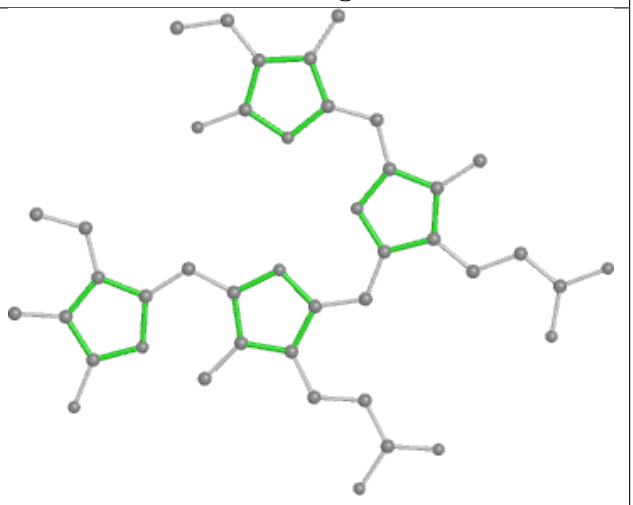
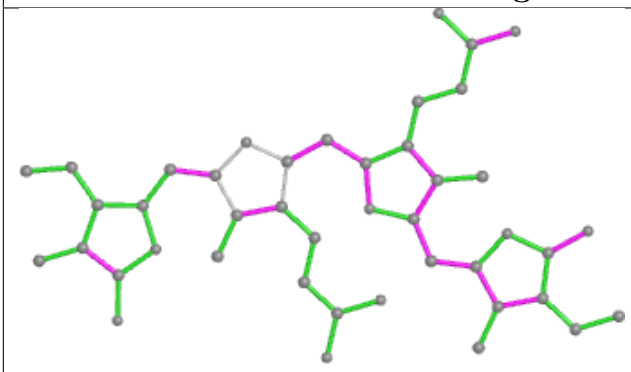


Rings

Ligand CYC w1 201



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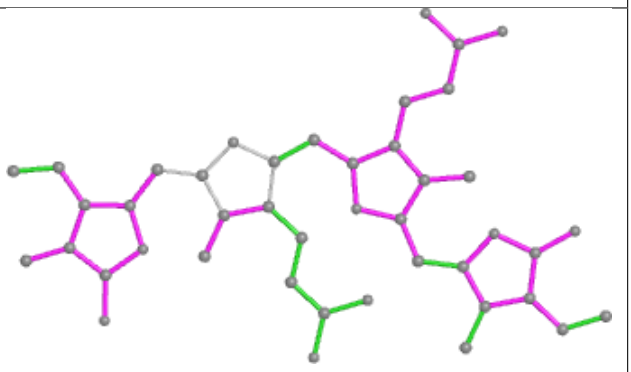

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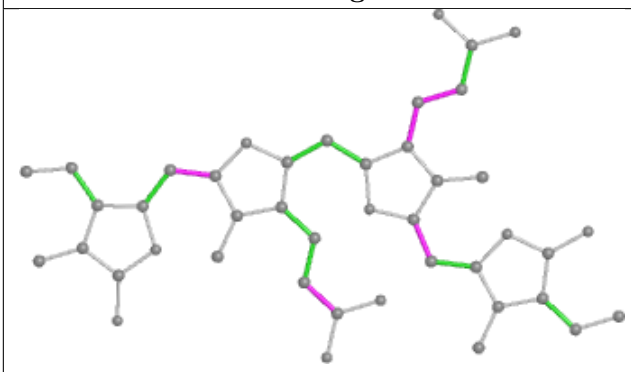

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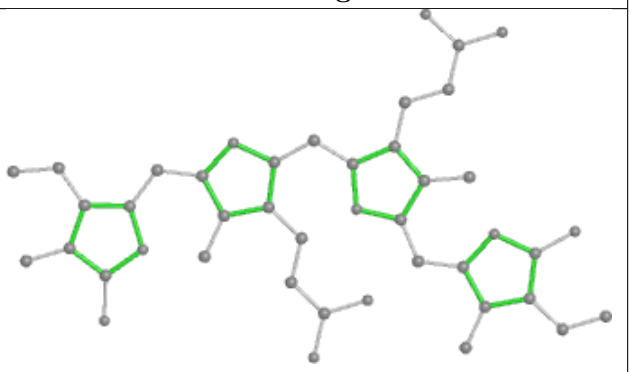

Rings

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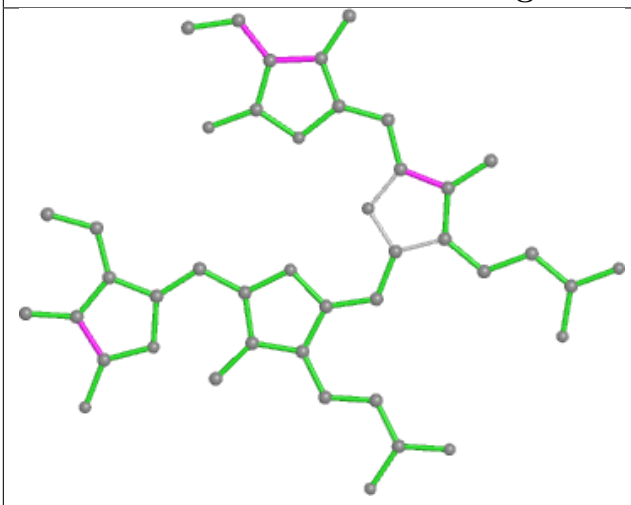

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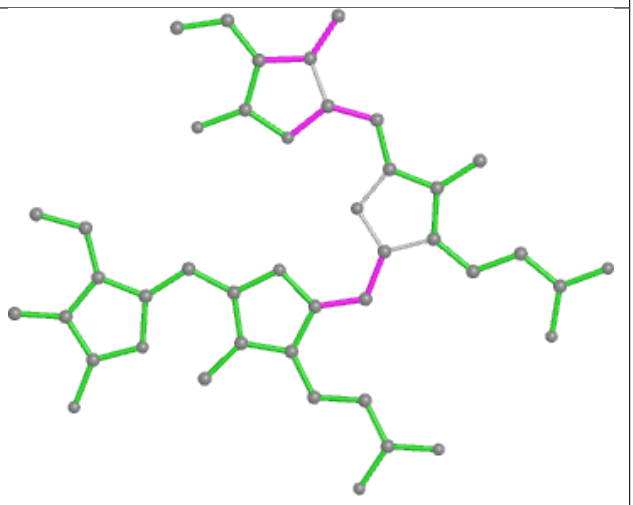

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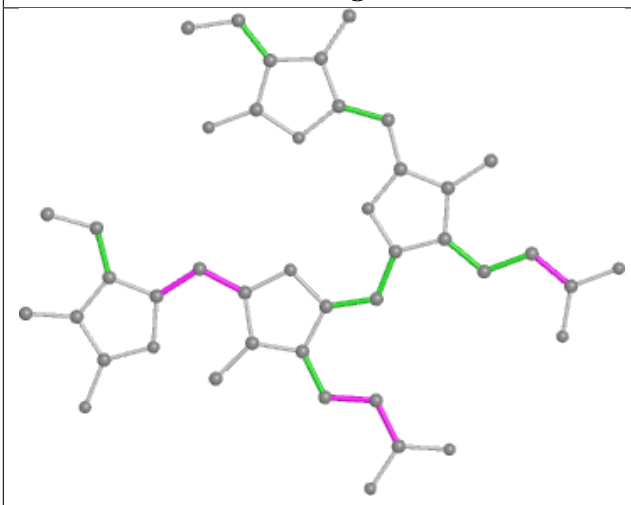

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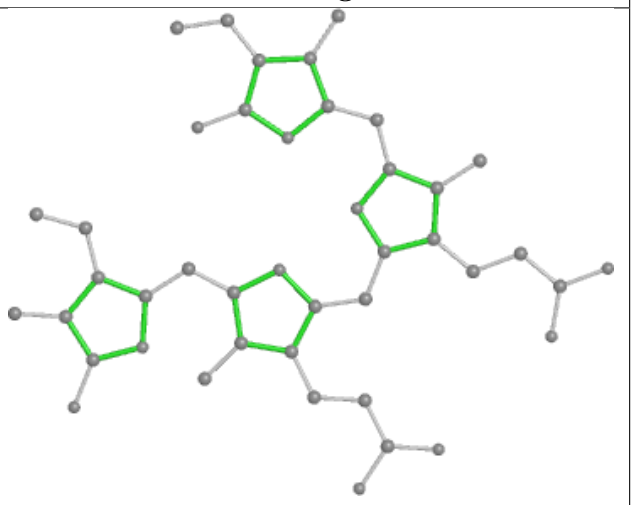

Rings

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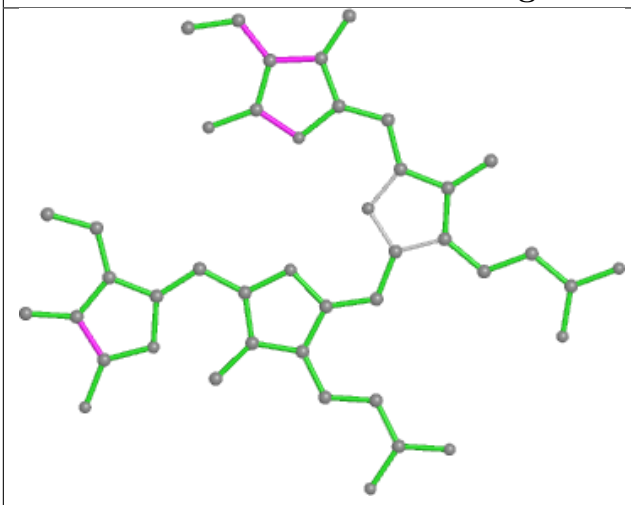

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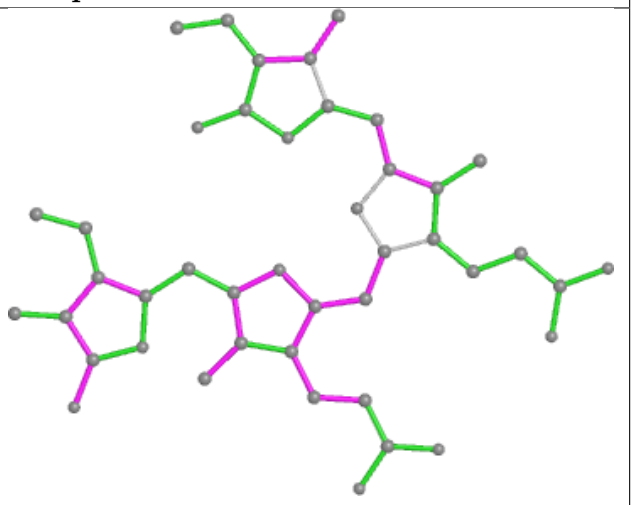

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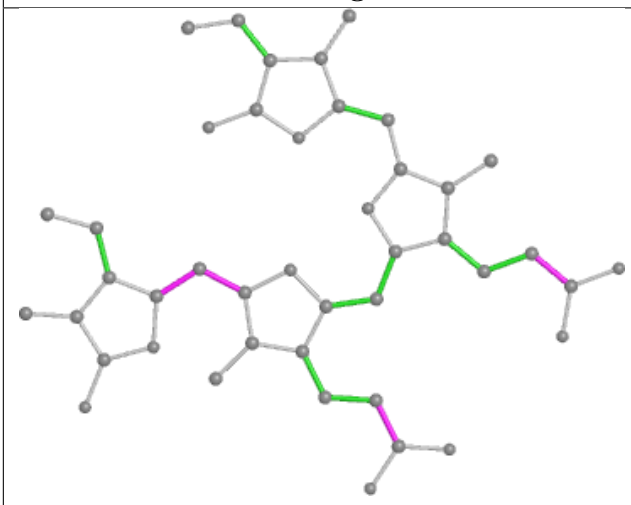

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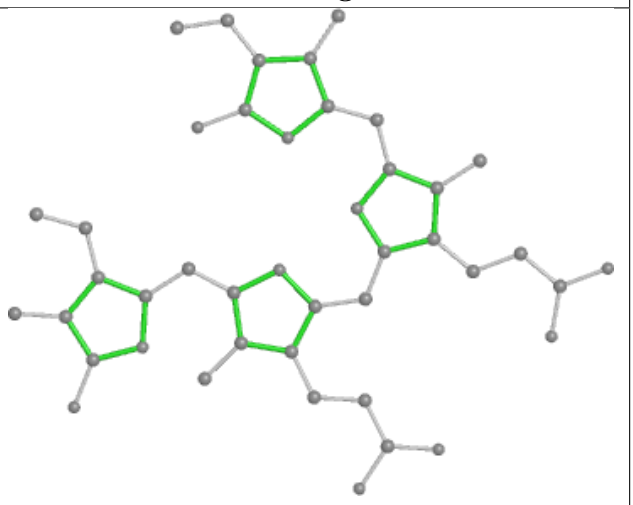
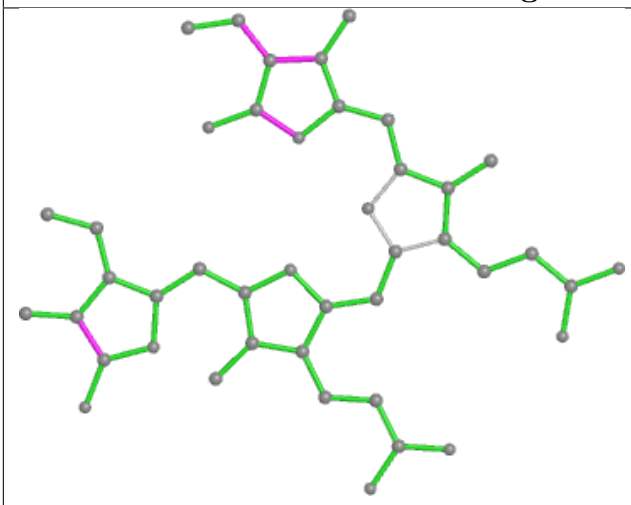


Rings

Ligand PEB eo 201



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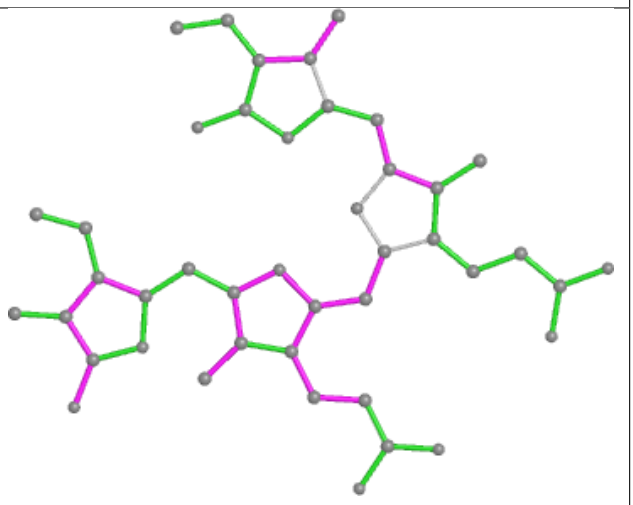

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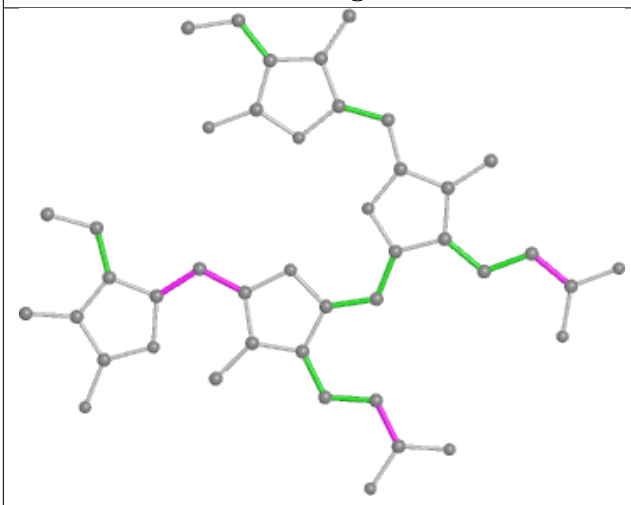

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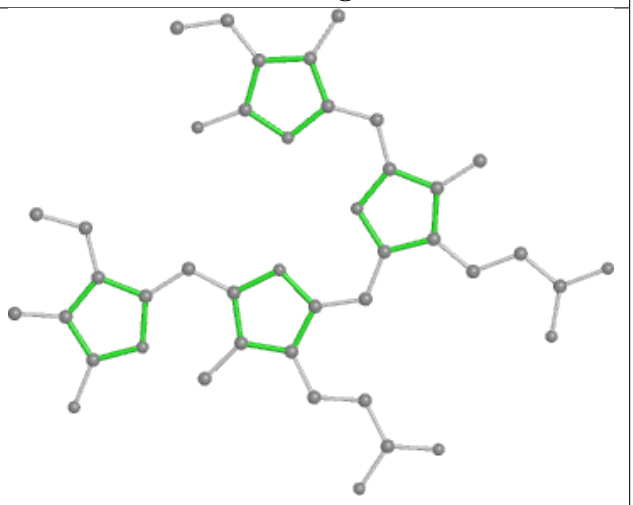
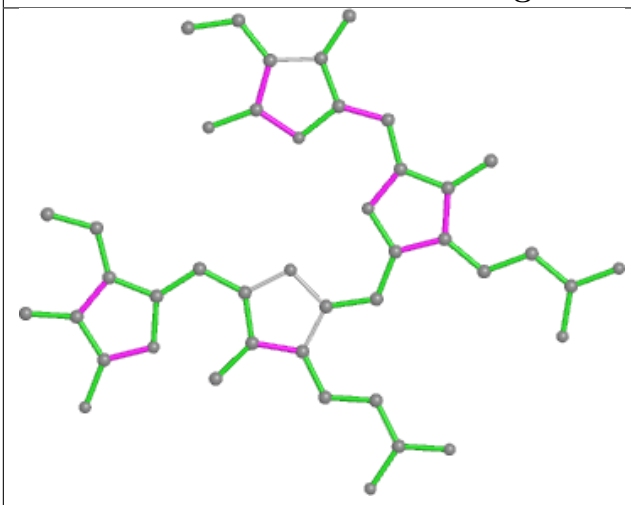


Rings

Ligand PUB B3 203



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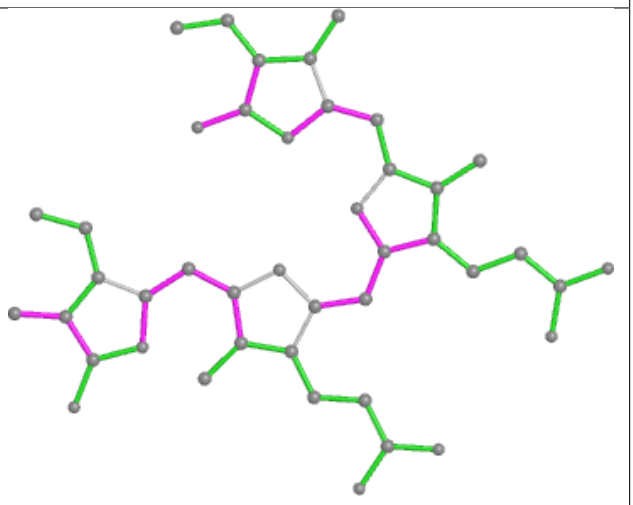

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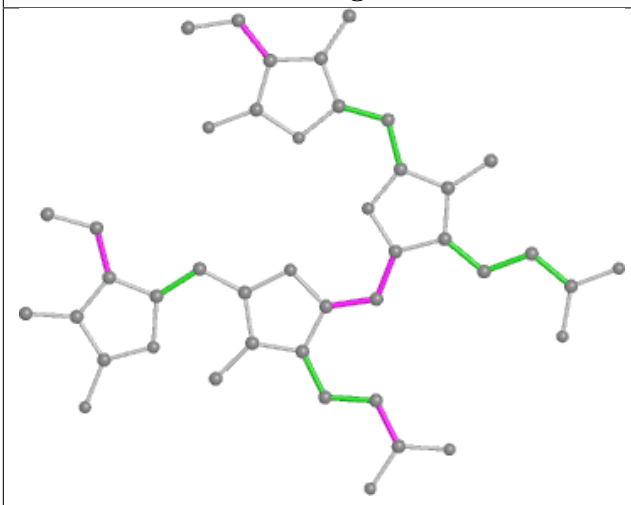

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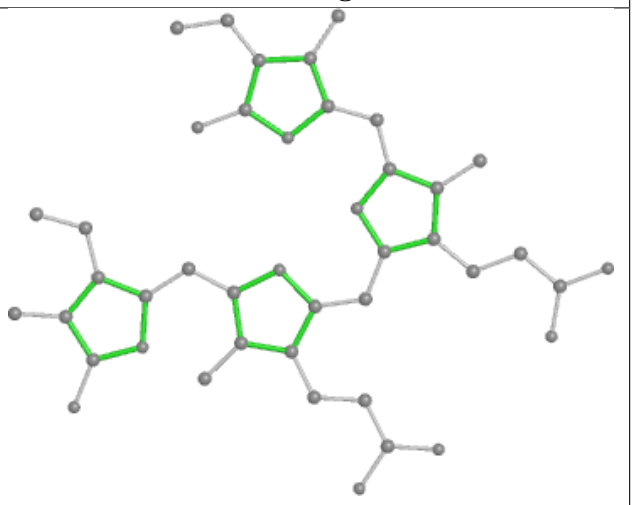

Rings

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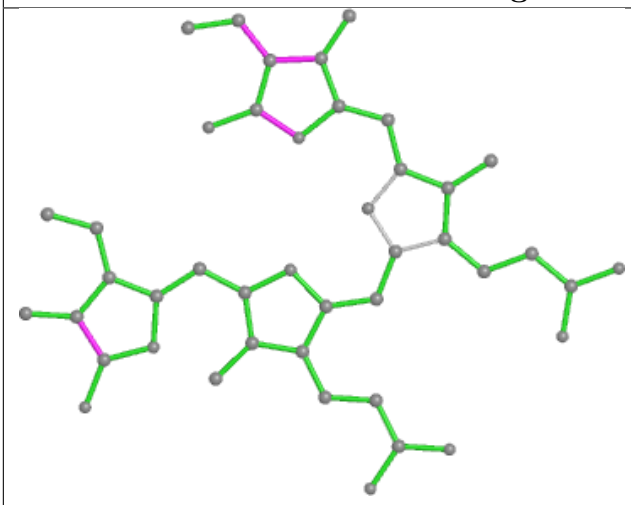

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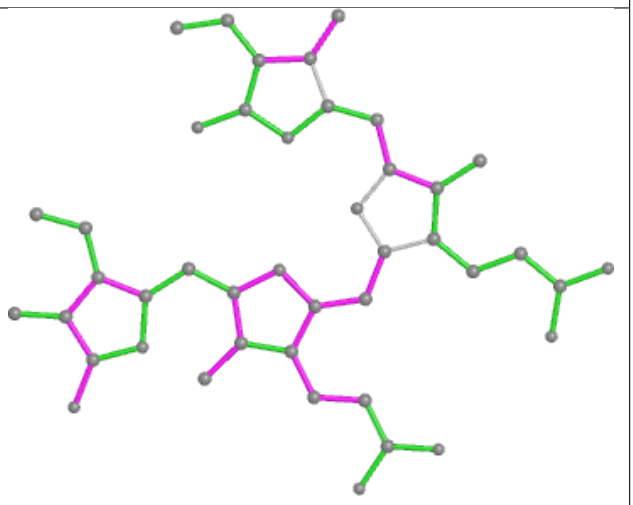

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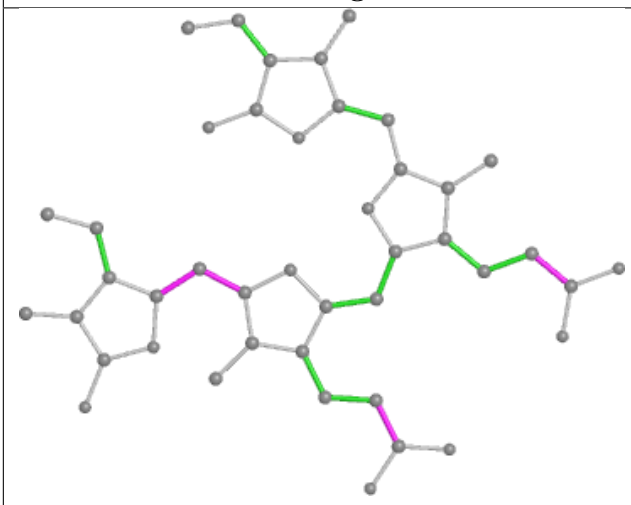

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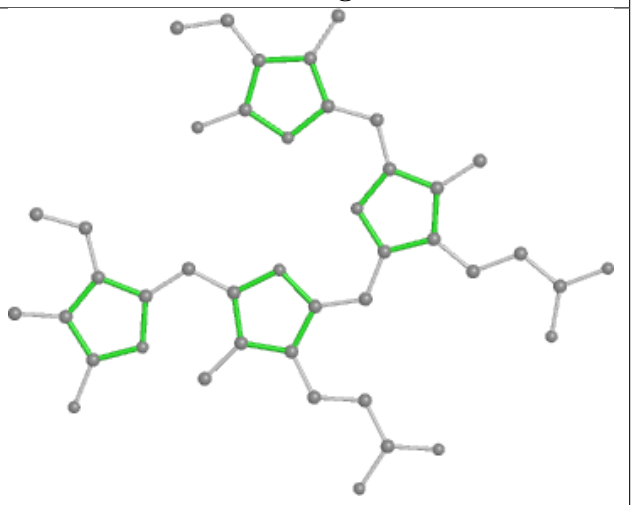
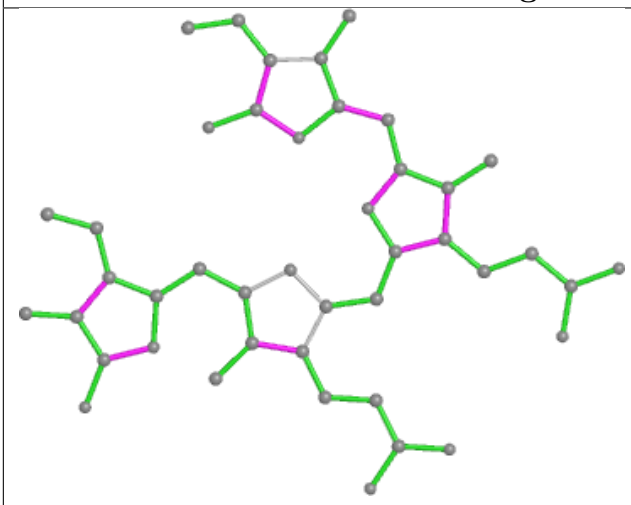


Rings

Ligand PUB t9 203



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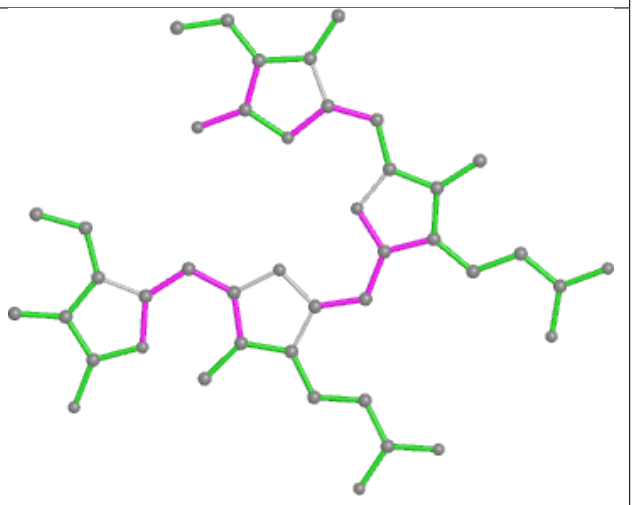

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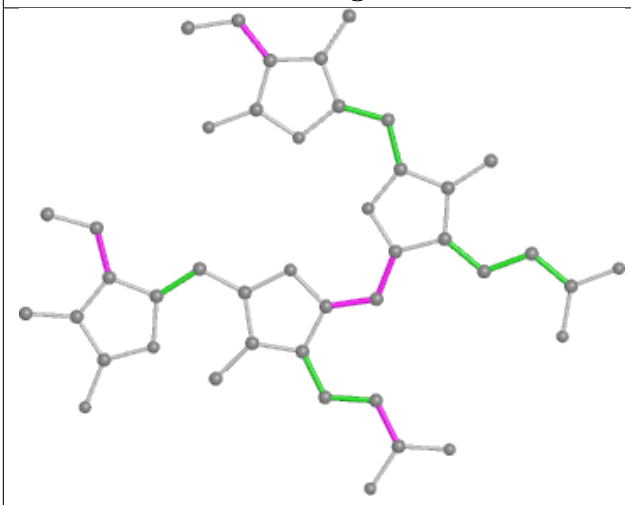
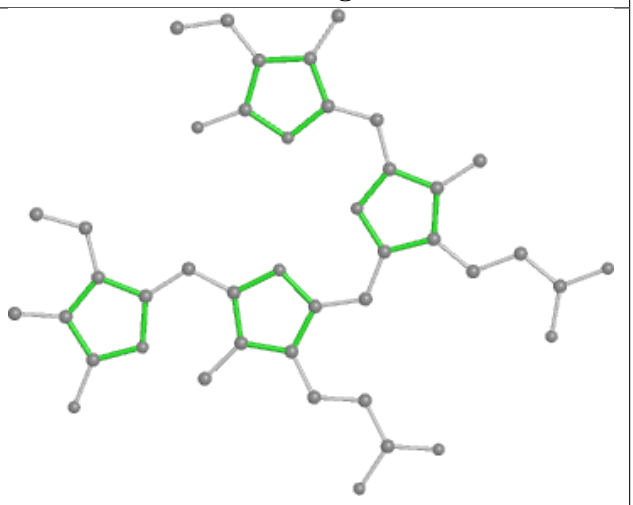
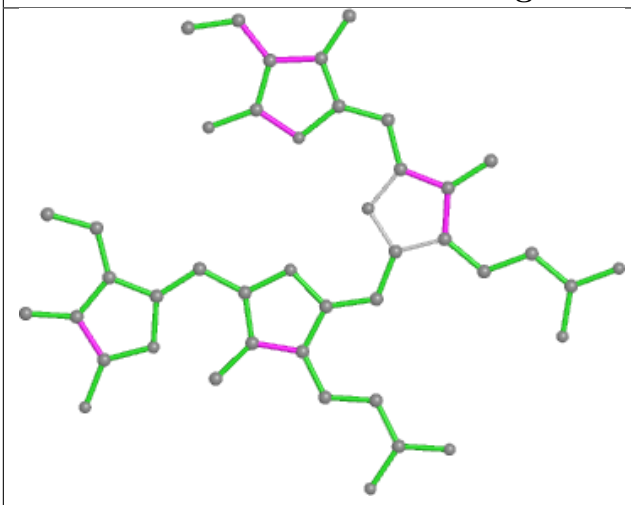


Torsions



Rings

Ligand PEB R5 202



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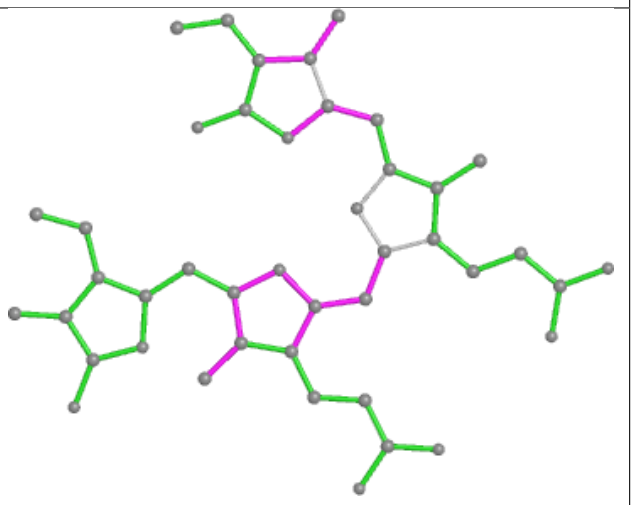

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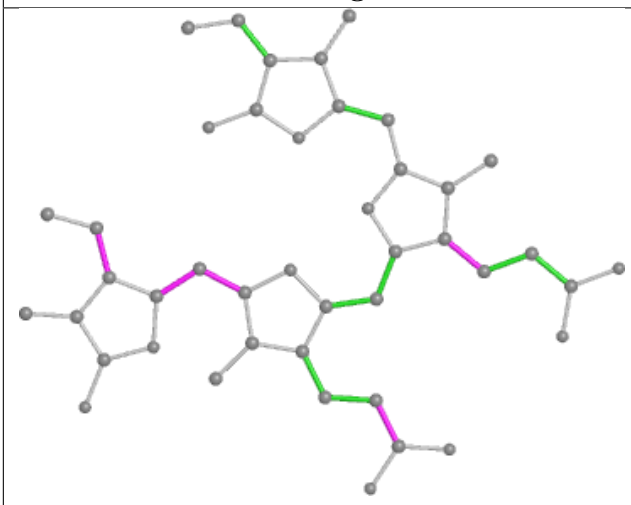

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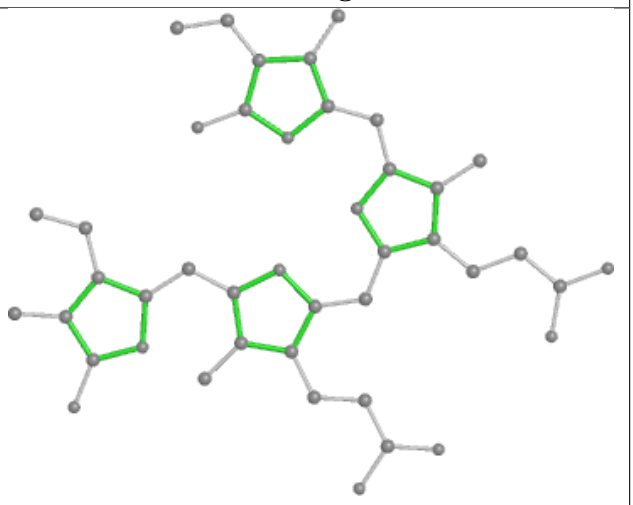
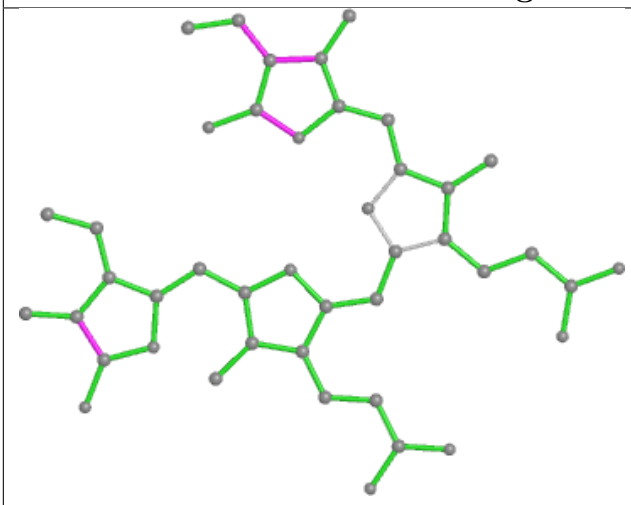


Rings

Ligand PEB eO 201



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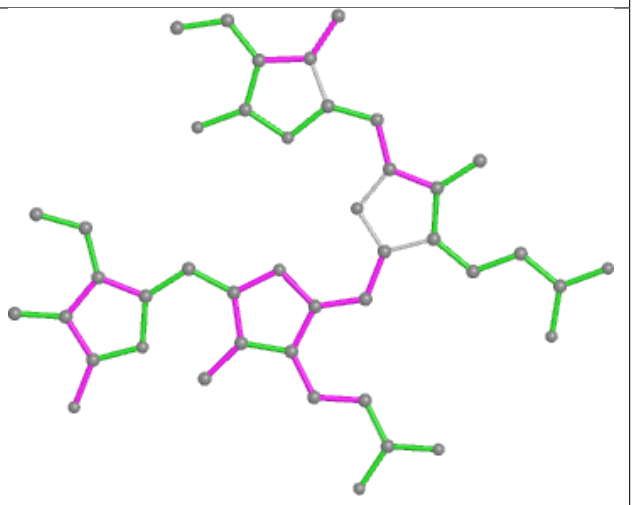

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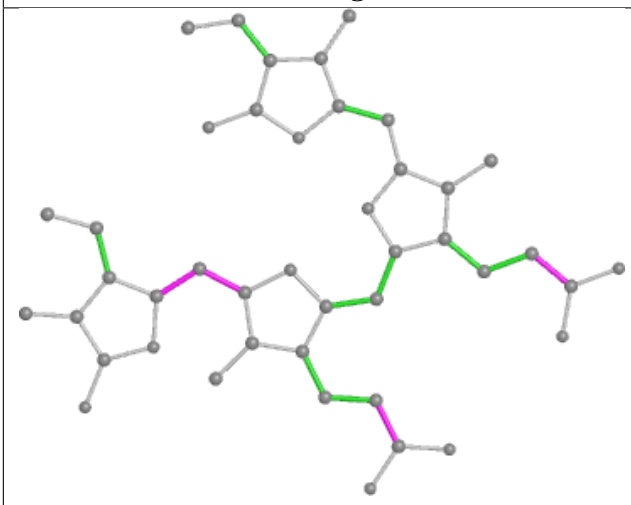

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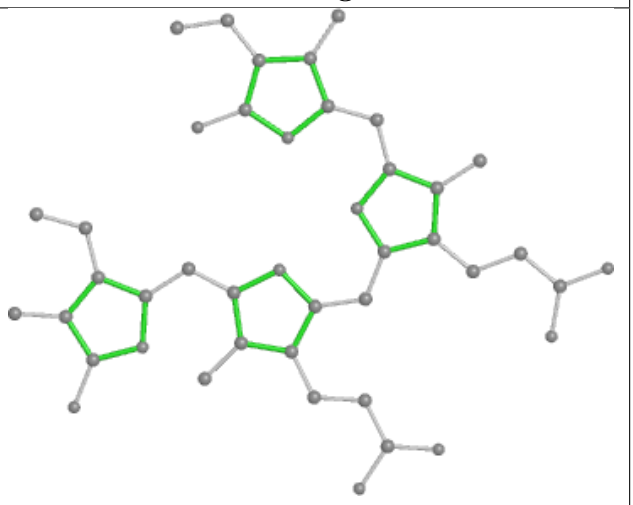
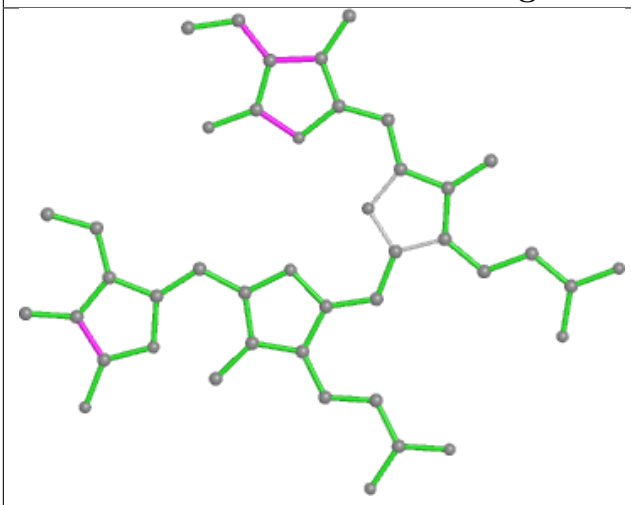


Rings

Ligand PEB b3 501



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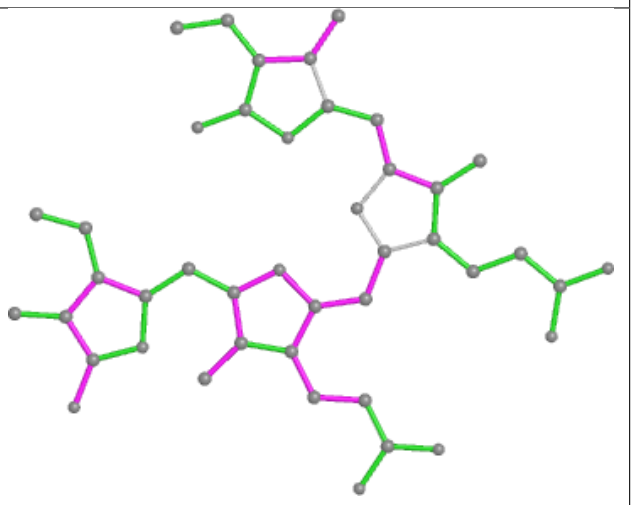

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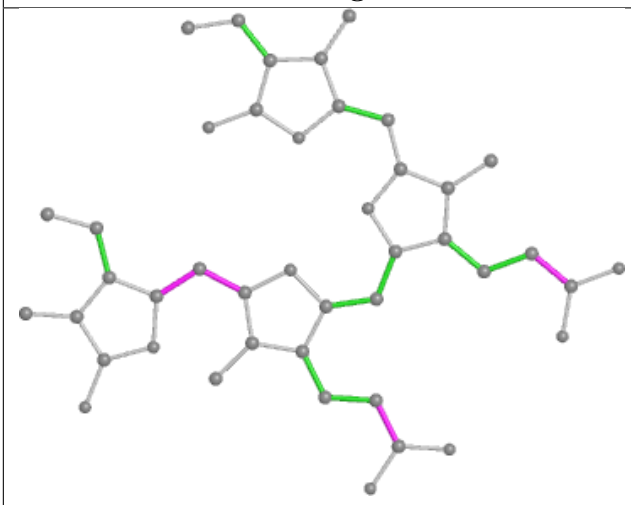

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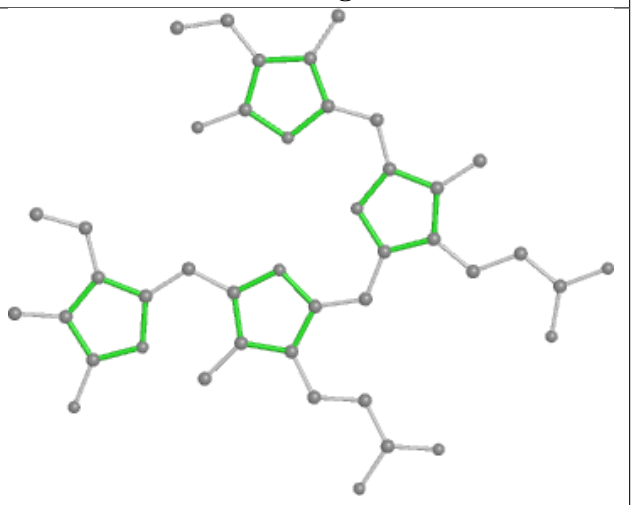
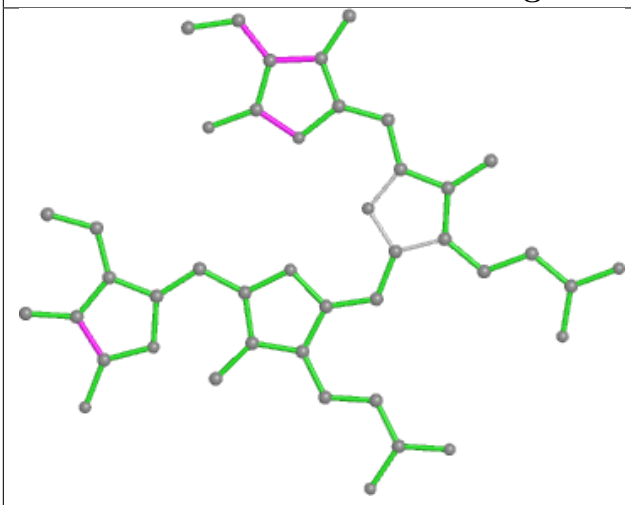


Rings

Ligand PEB l9 201



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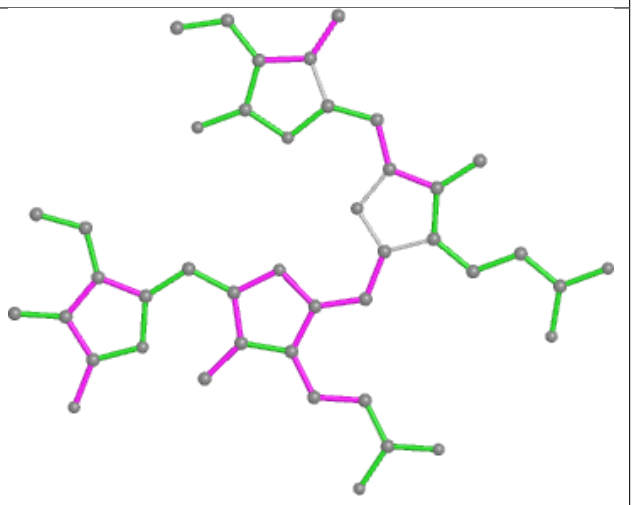

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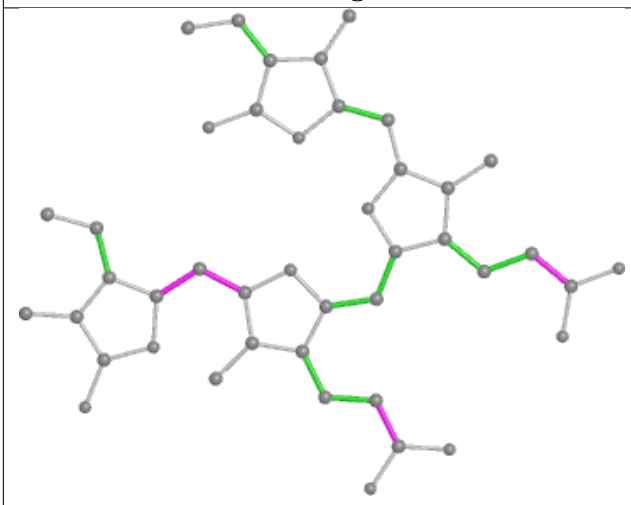

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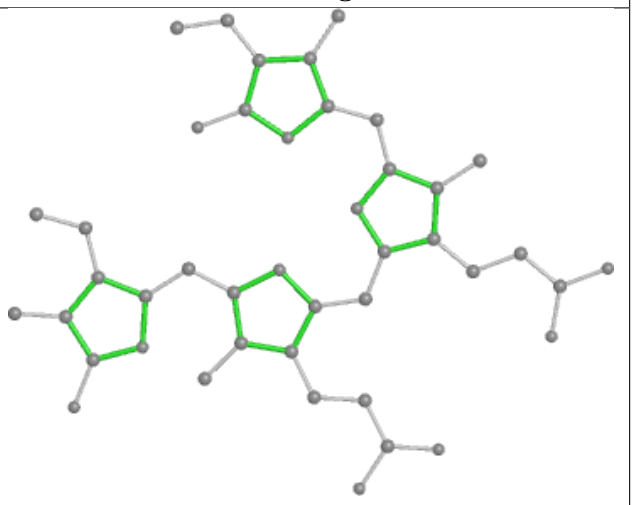
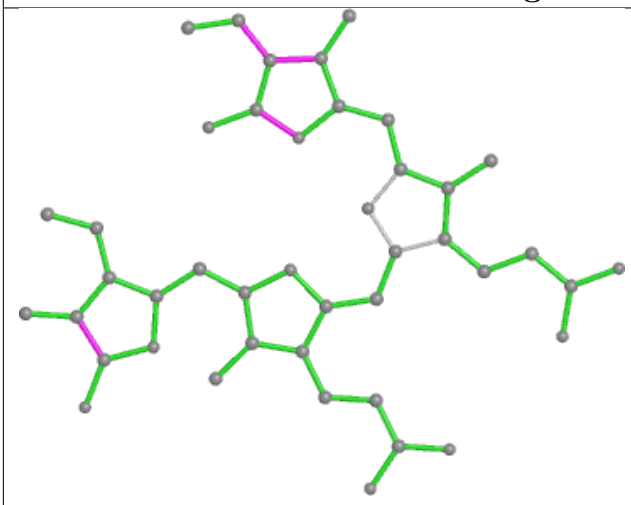


Rings

Ligand PEB l7 201



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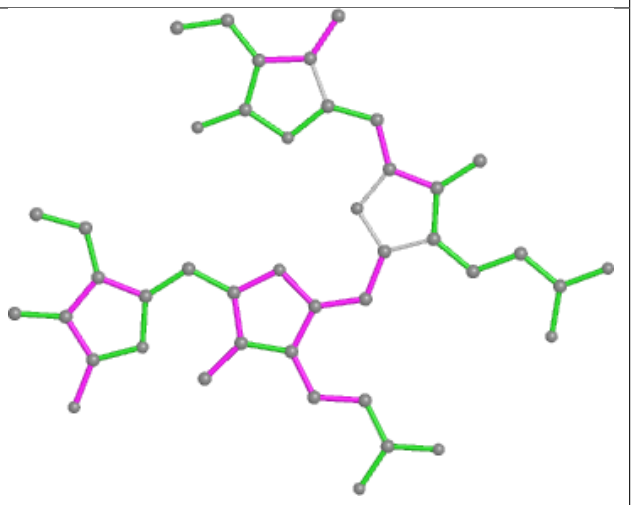

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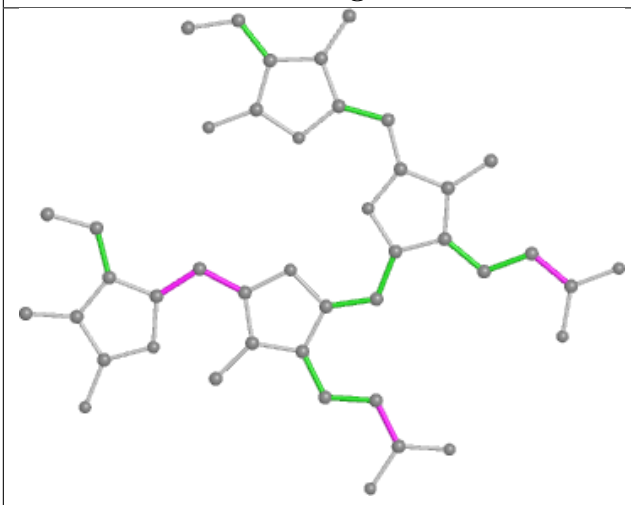

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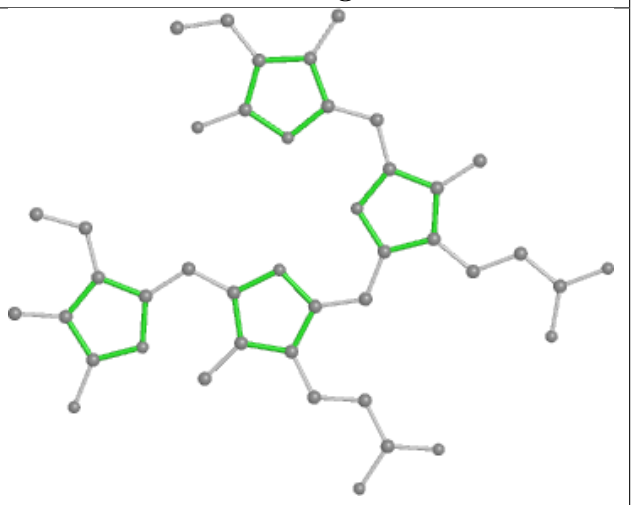
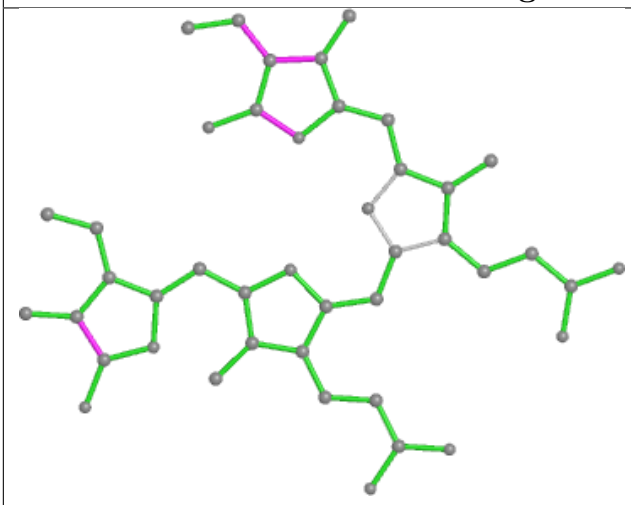


Rings

Ligand PEB b6 201



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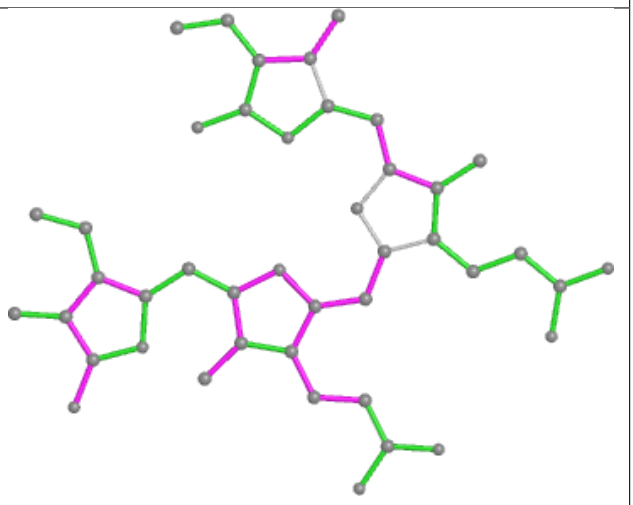

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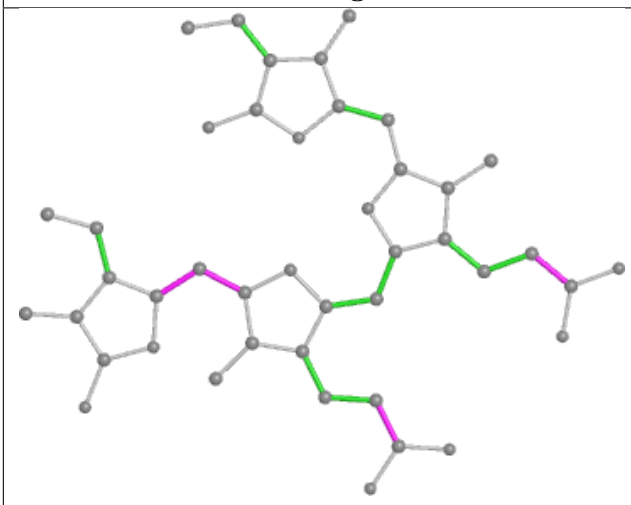

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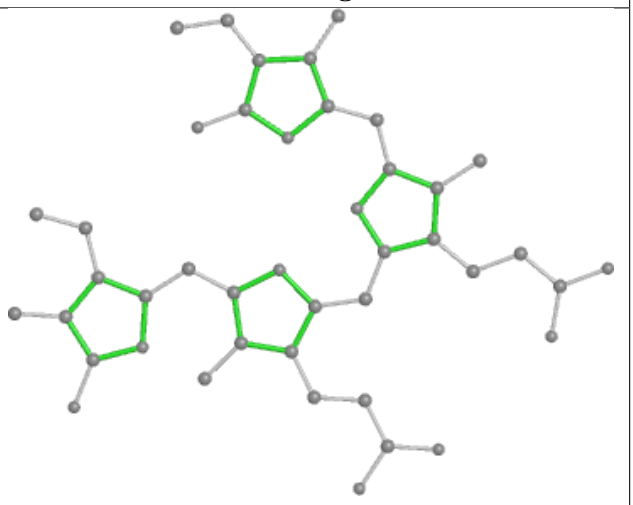
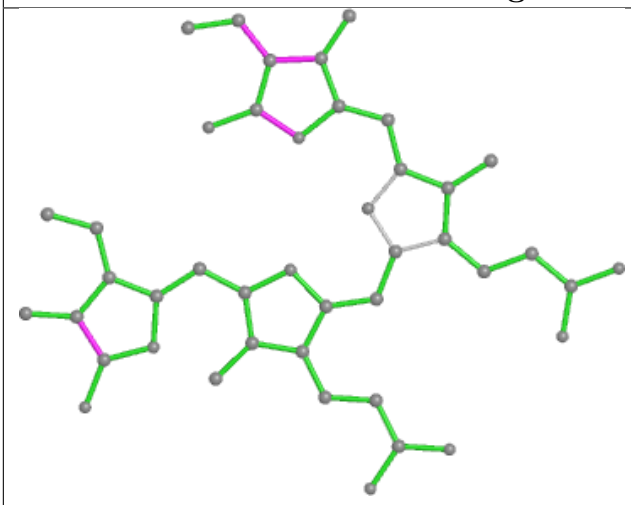


Rings

Ligand PEB cC 1001



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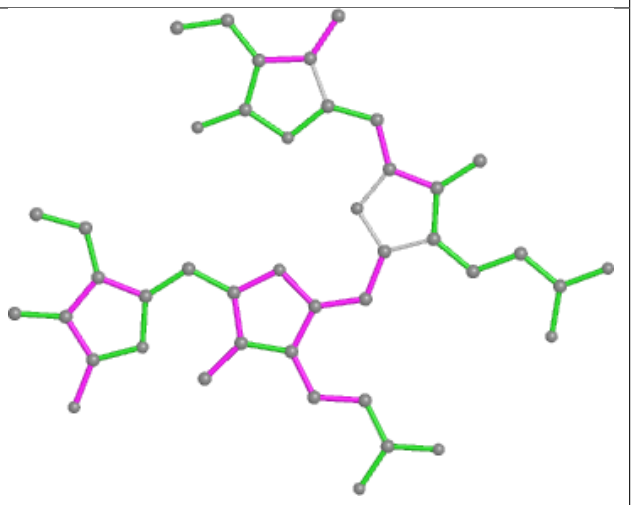

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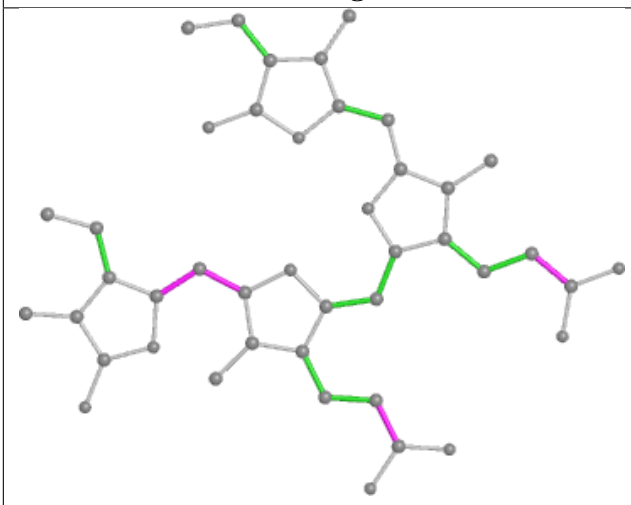

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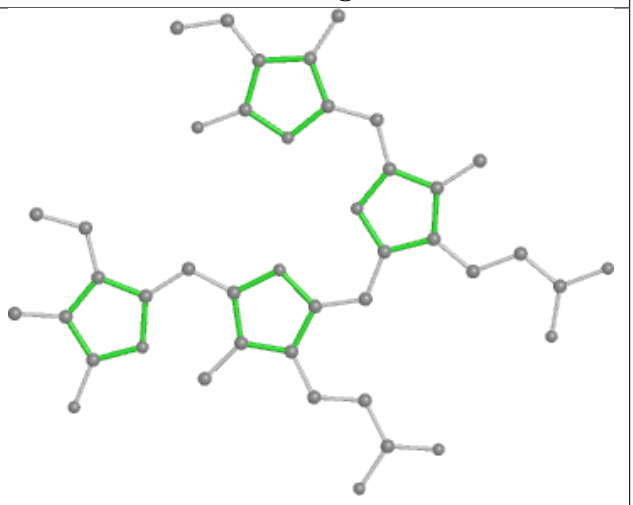

Rings

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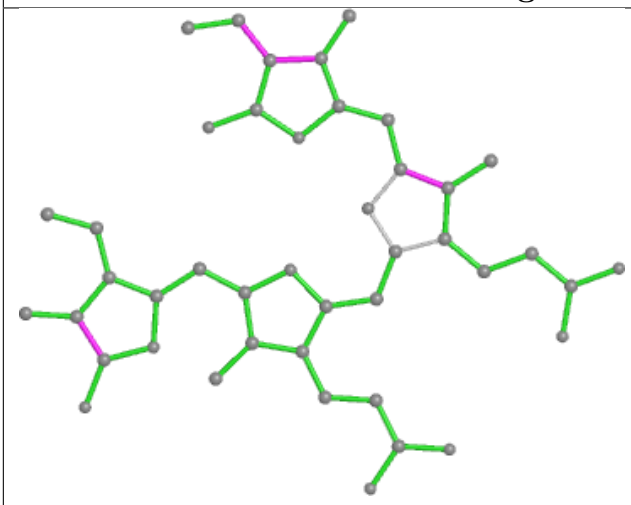

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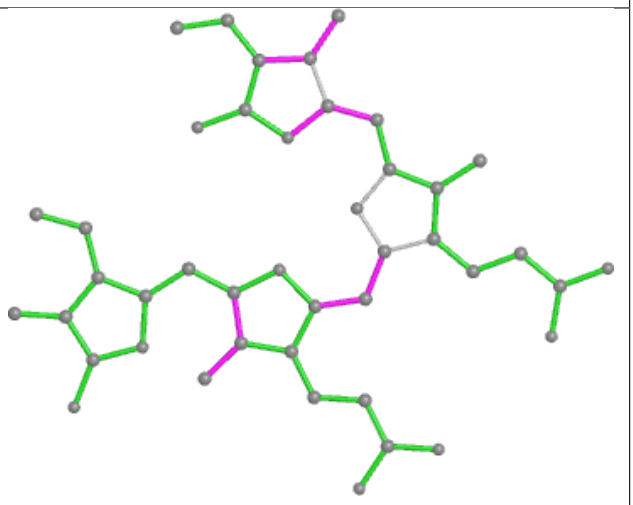

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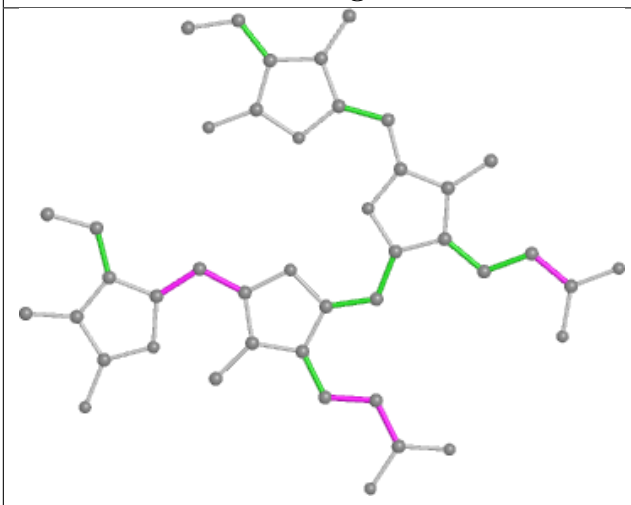

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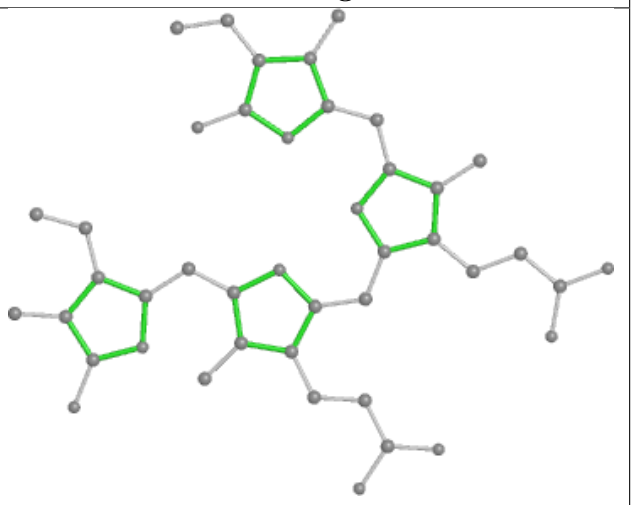

Rings

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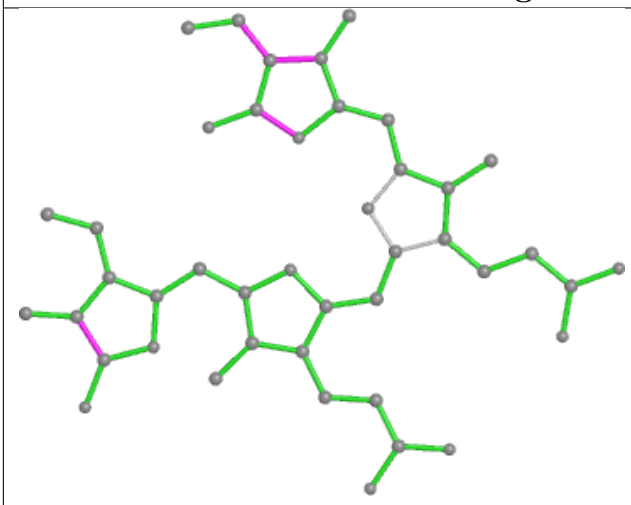

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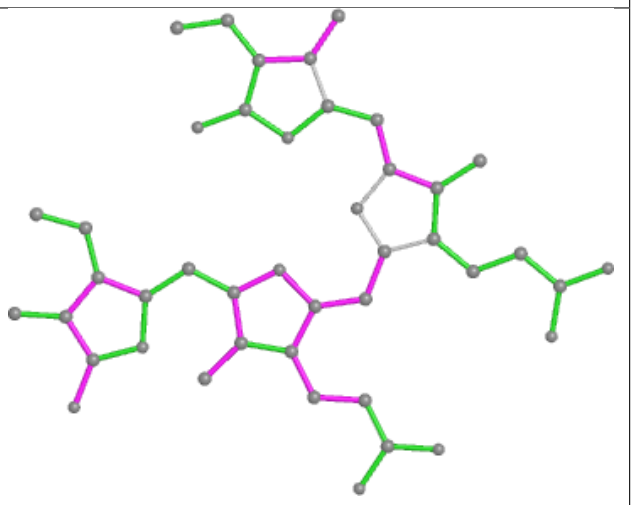

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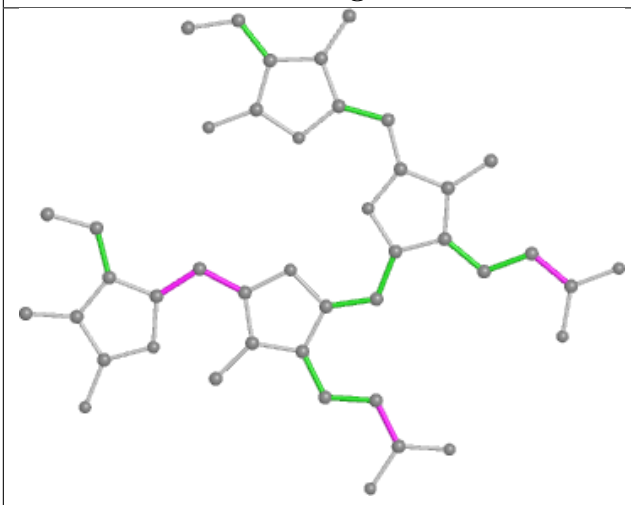

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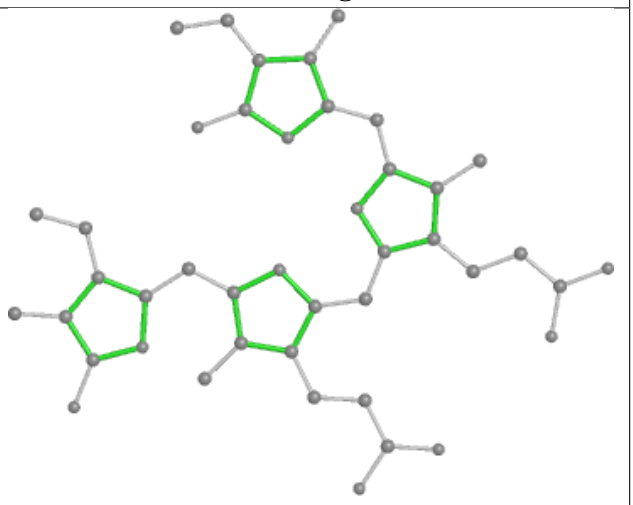

Rings

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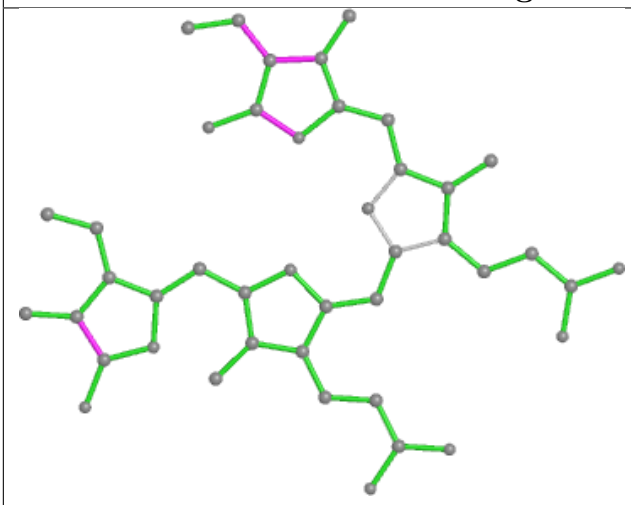

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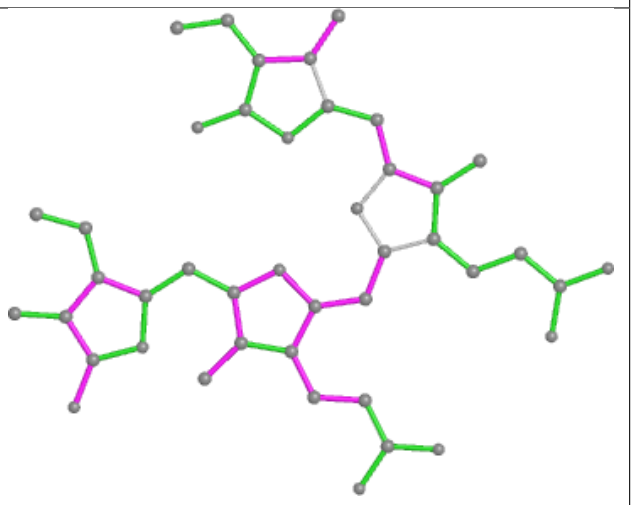

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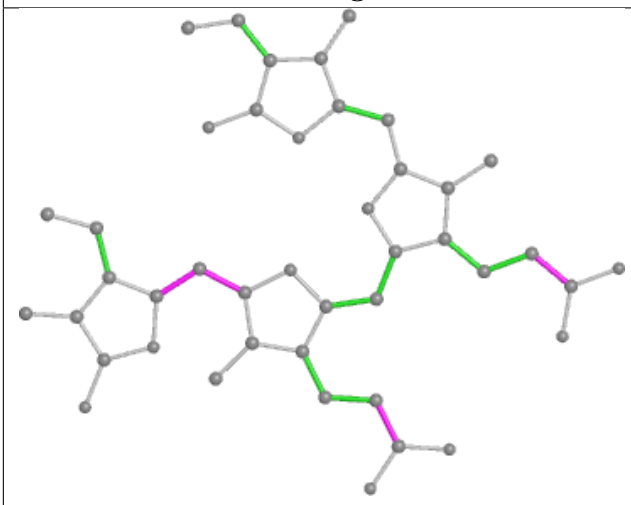

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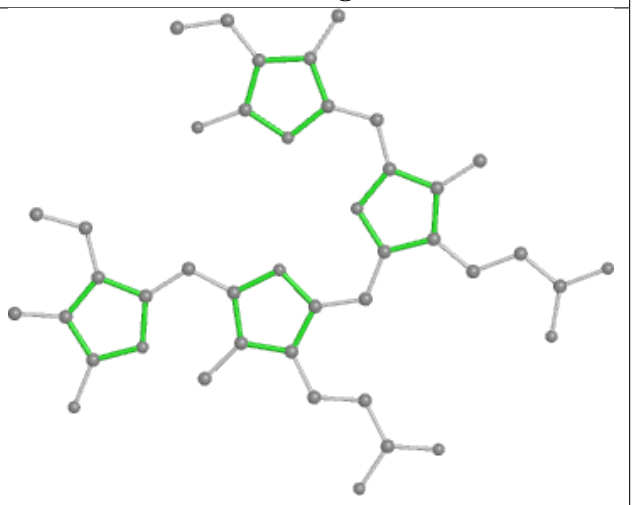
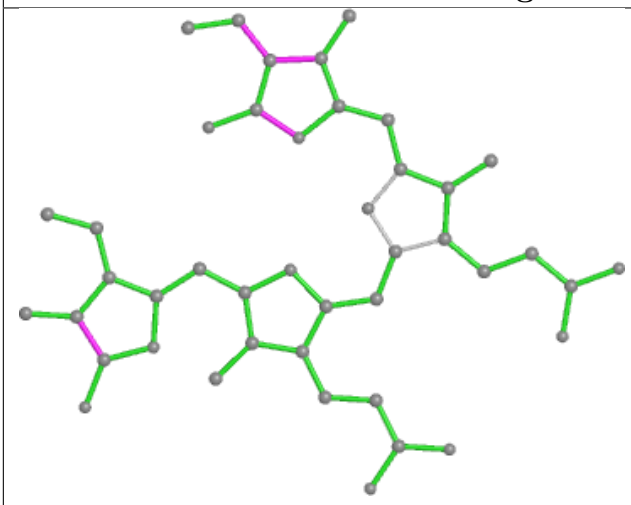


Rings

Ligand PEB T4 201



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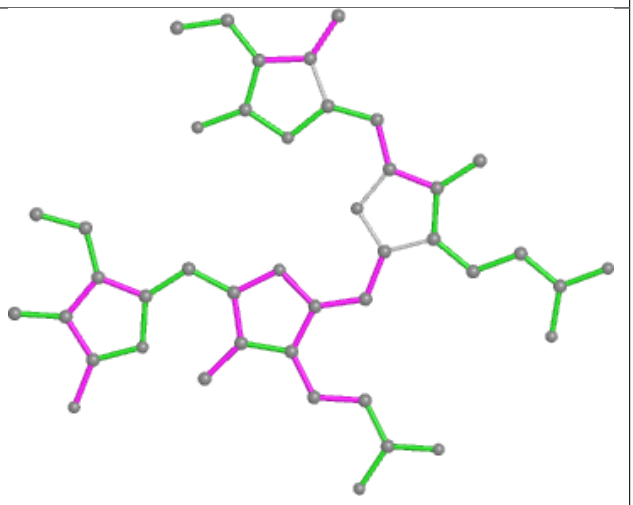

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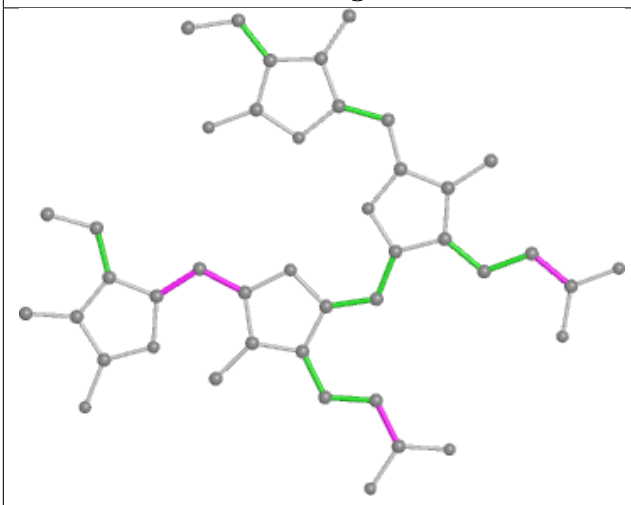

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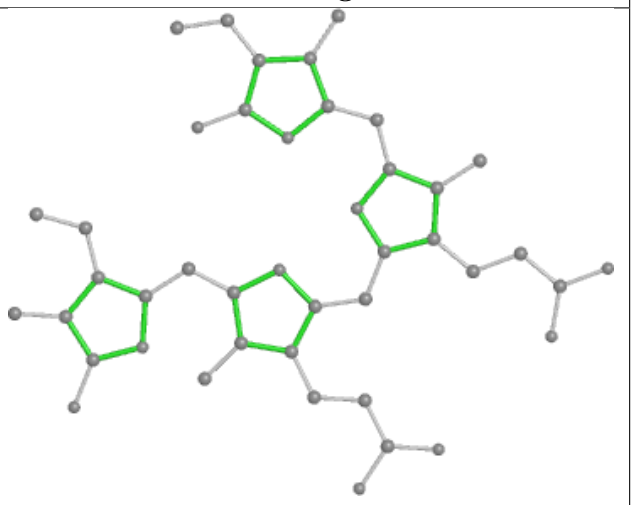

Rings

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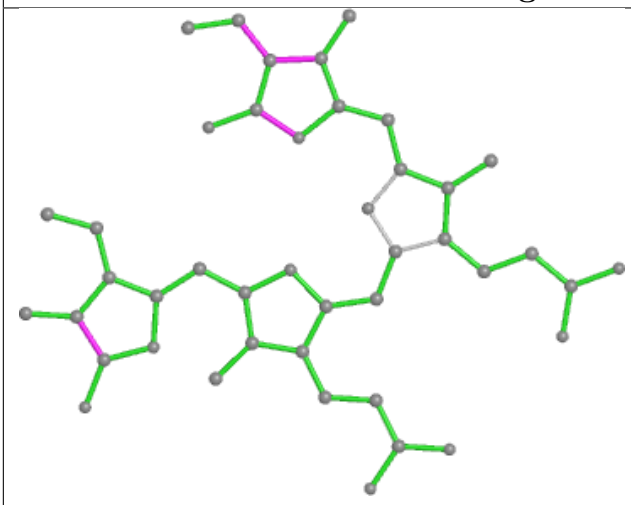

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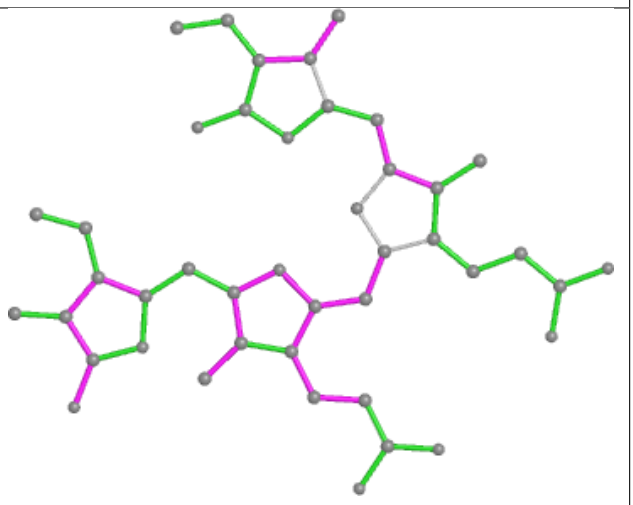

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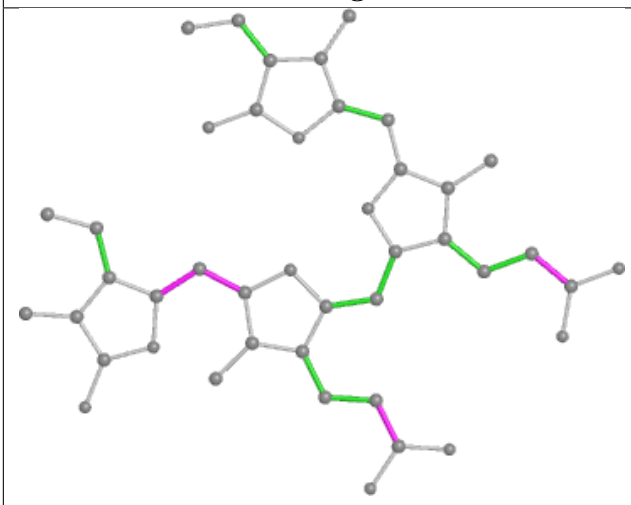

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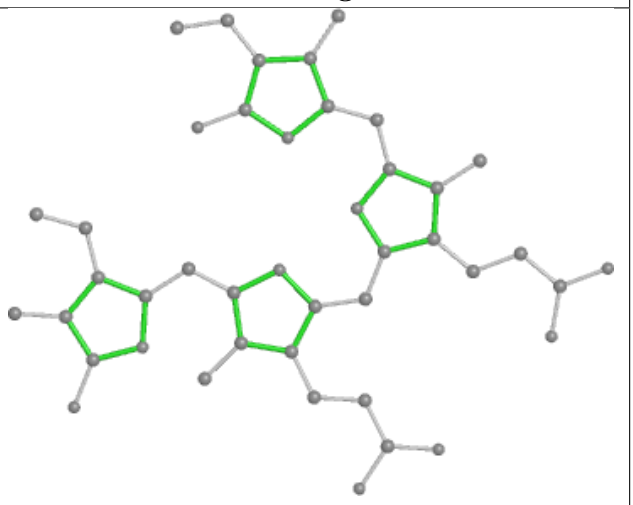
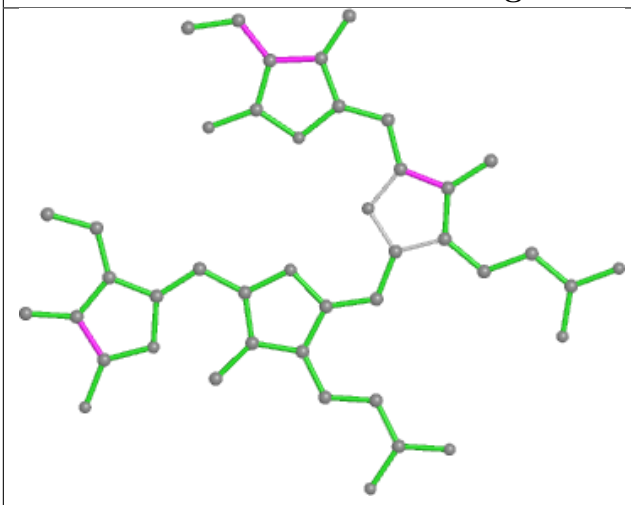


Rings

Ligand PEB bK 1002



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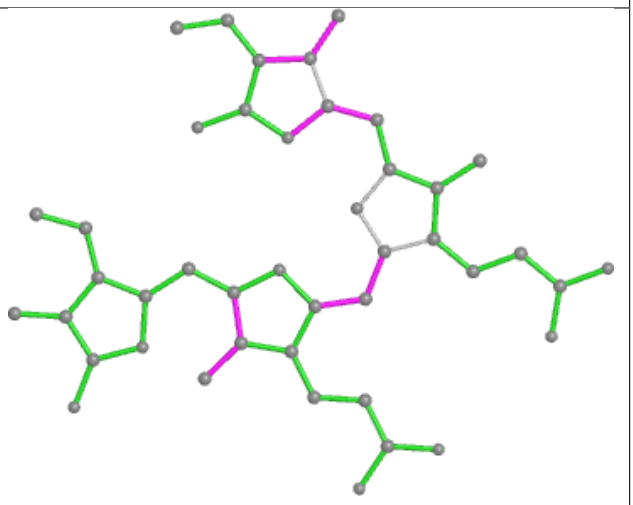
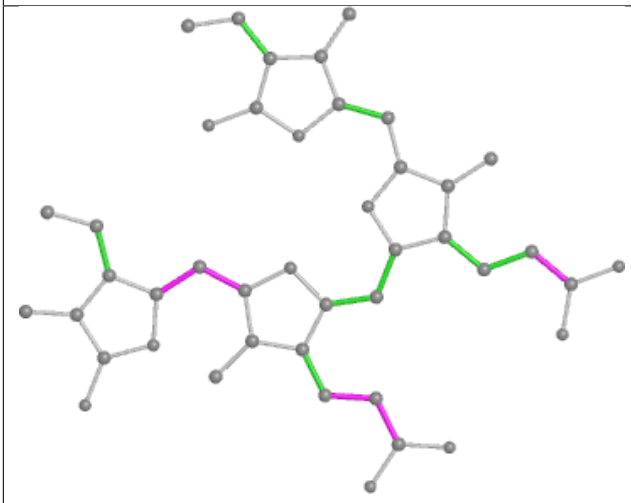
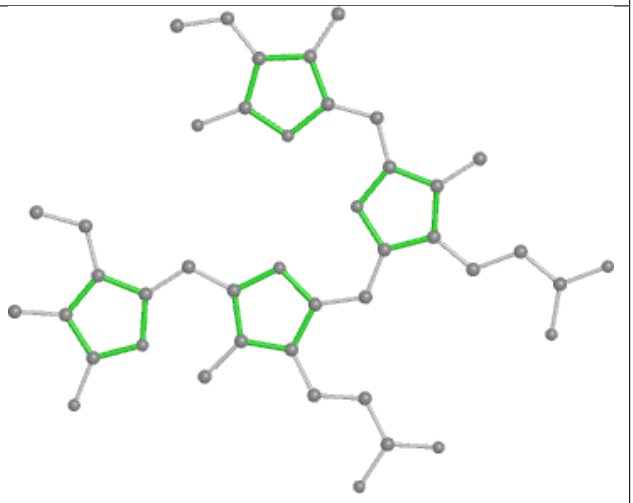


Bond angles

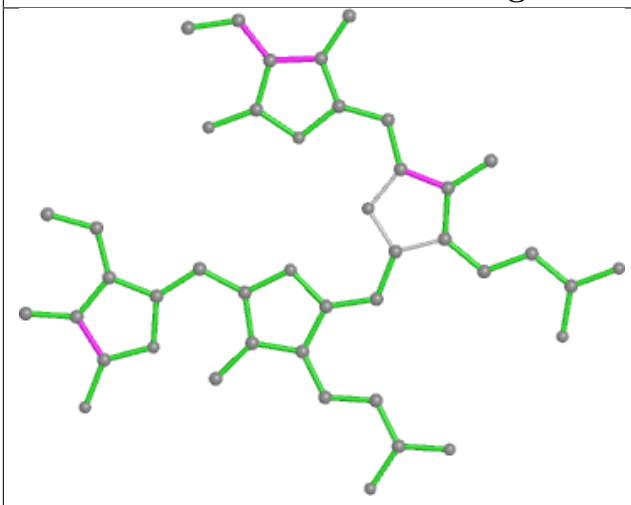


Torsions



Rings

Ligand PEB E2 1002



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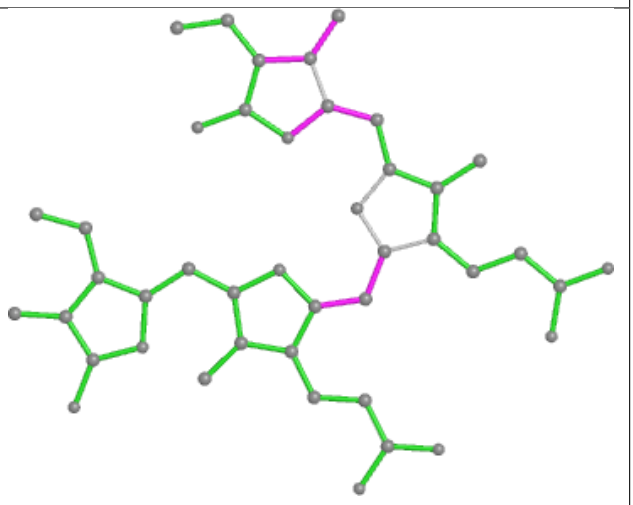

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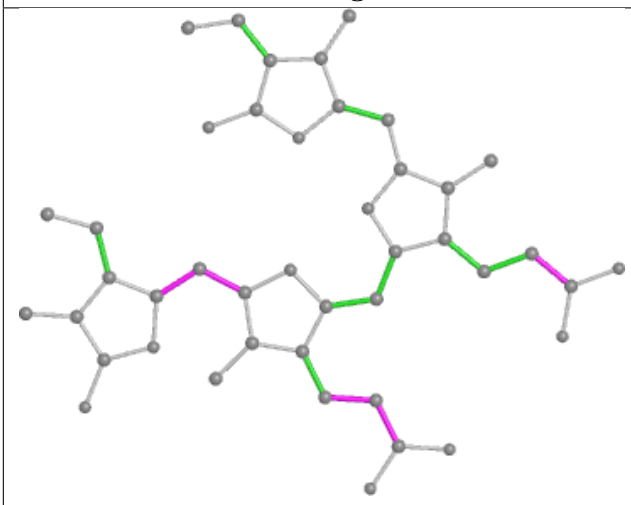

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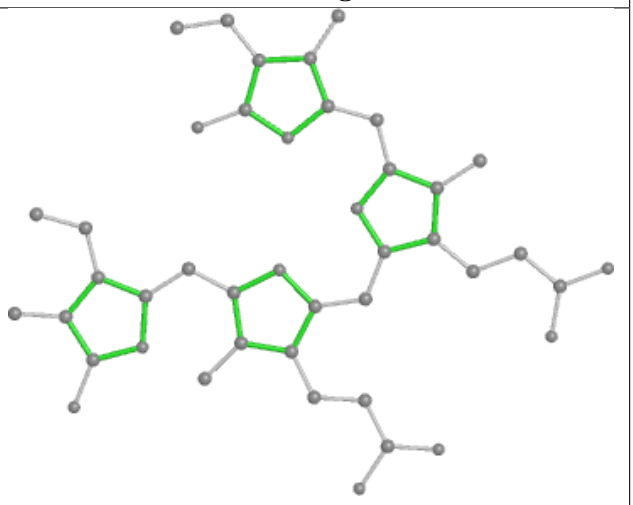
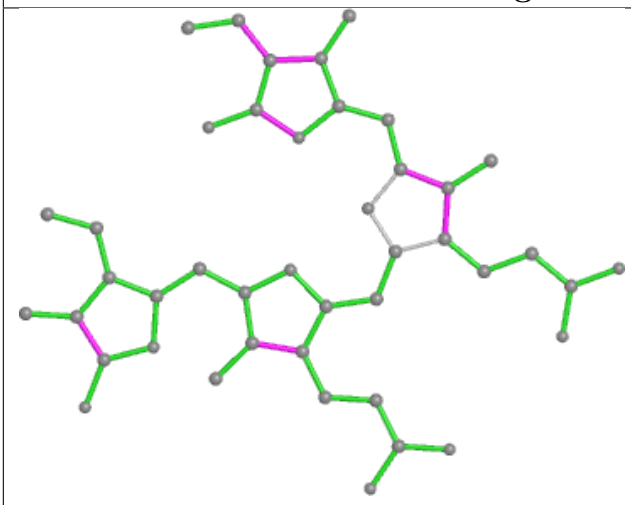


Rings

Ligand PEB hX 202



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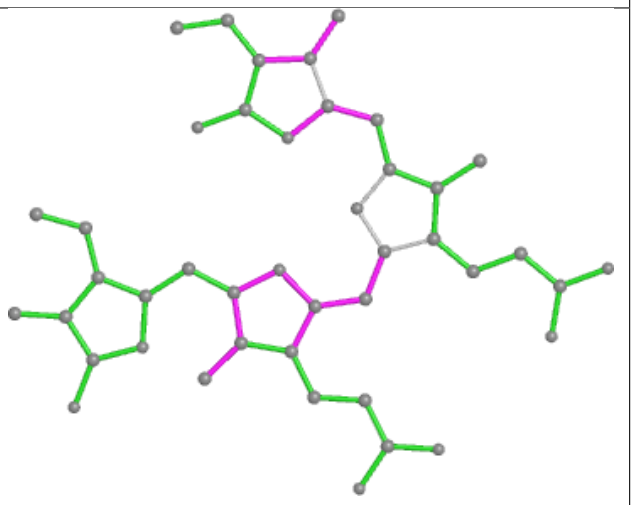

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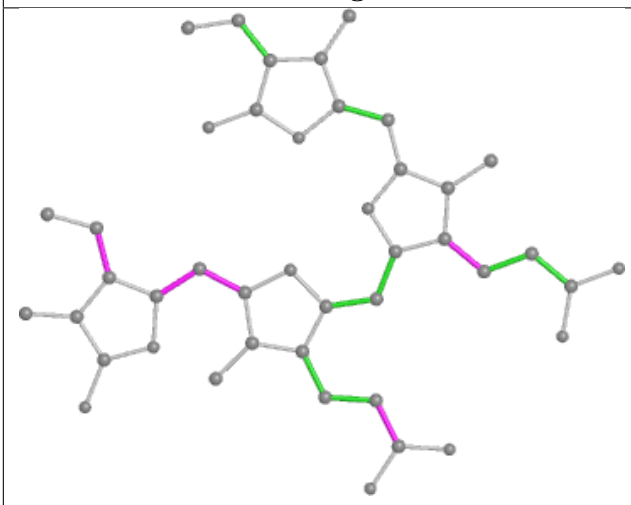

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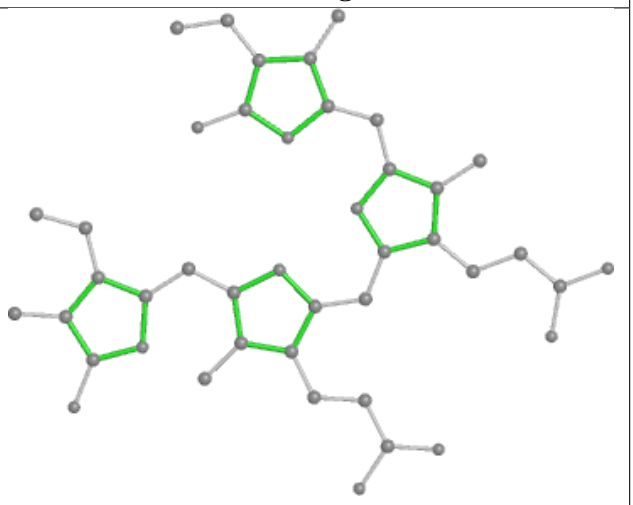
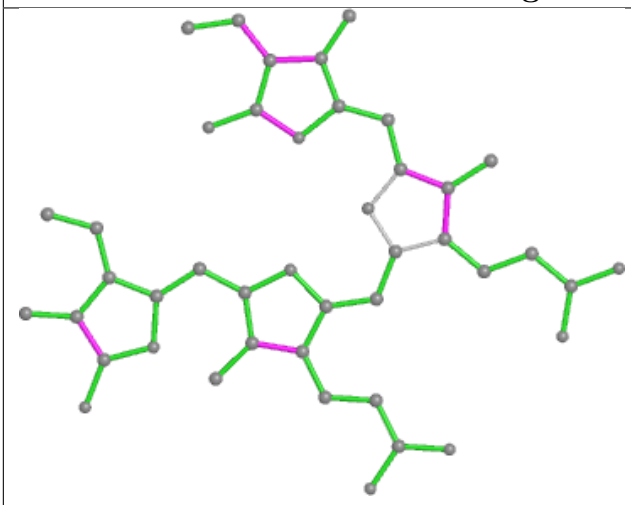


Rings

Ligand PEB at 202



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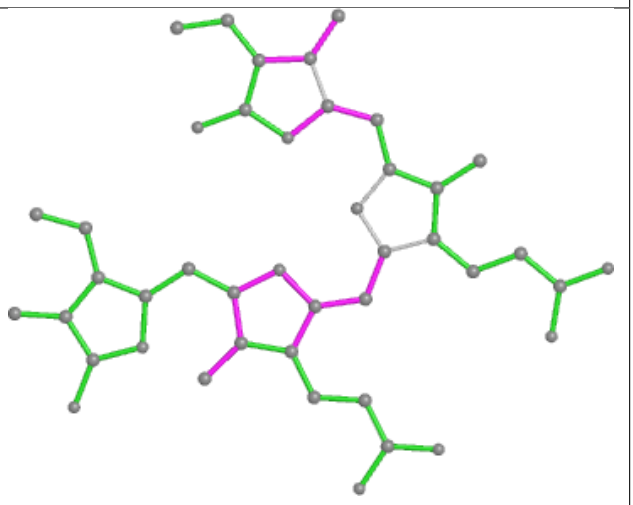

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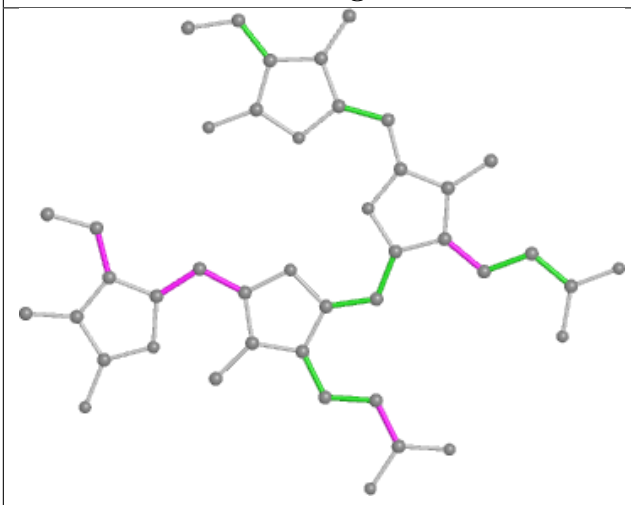

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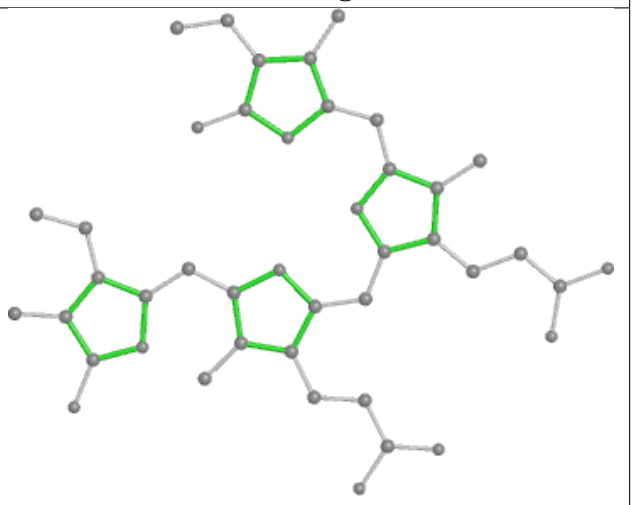
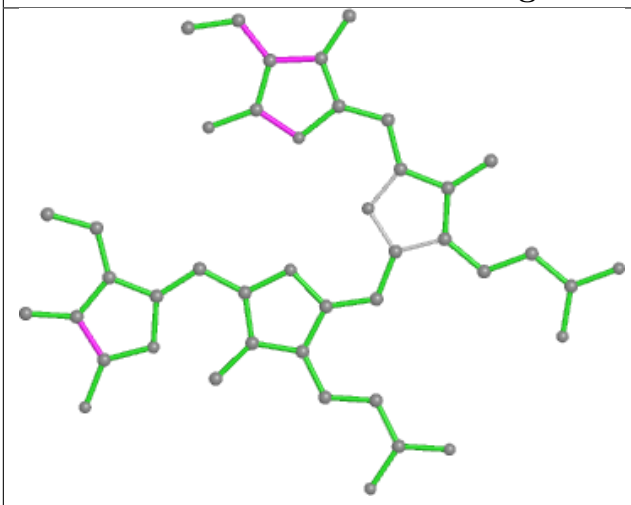


Rings

Ligand PEB n9 201



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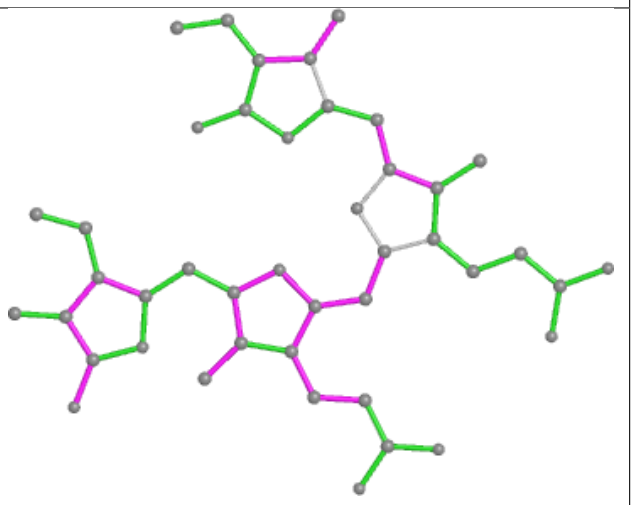

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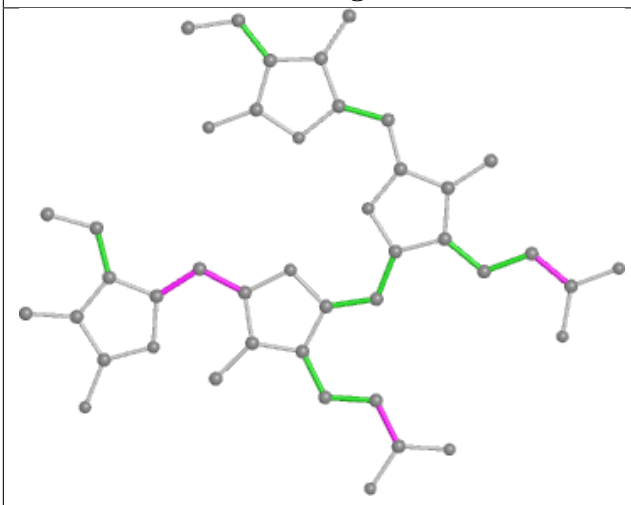

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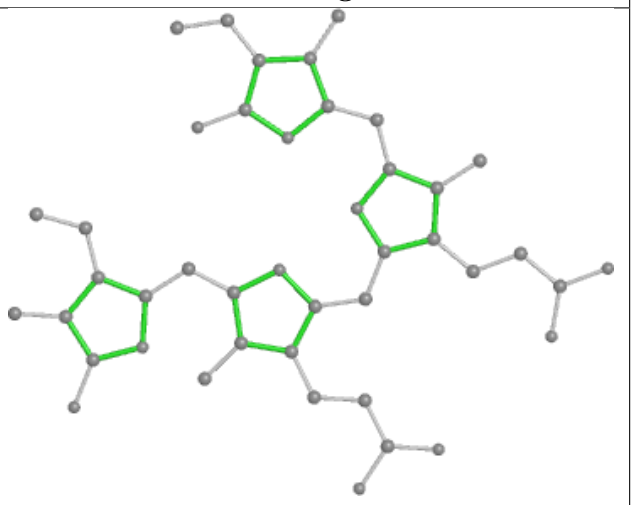
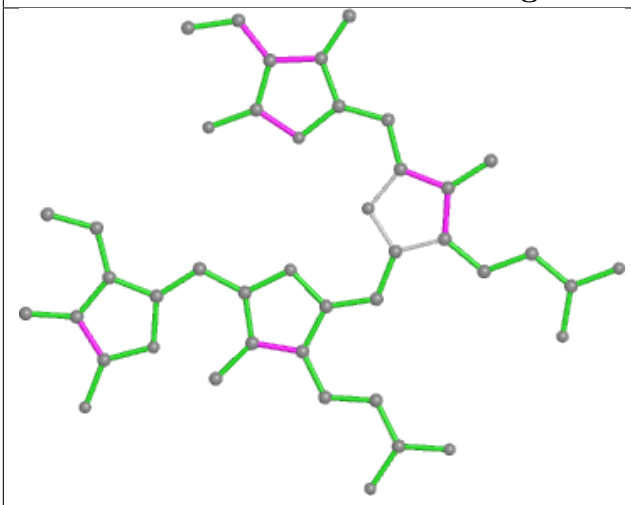


Rings

Ligand PEB z7 202



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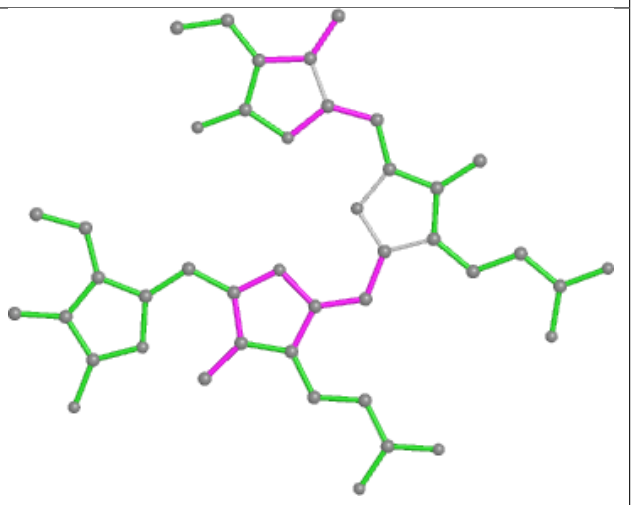

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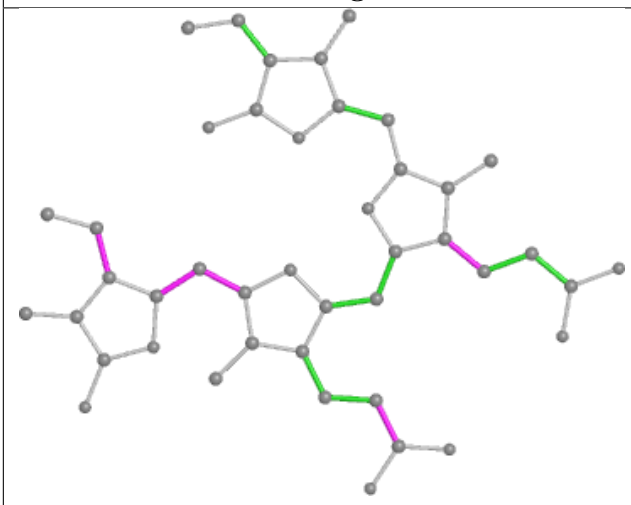

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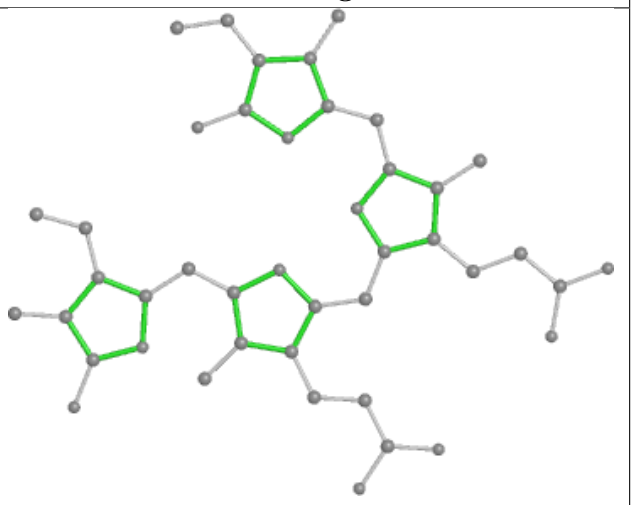
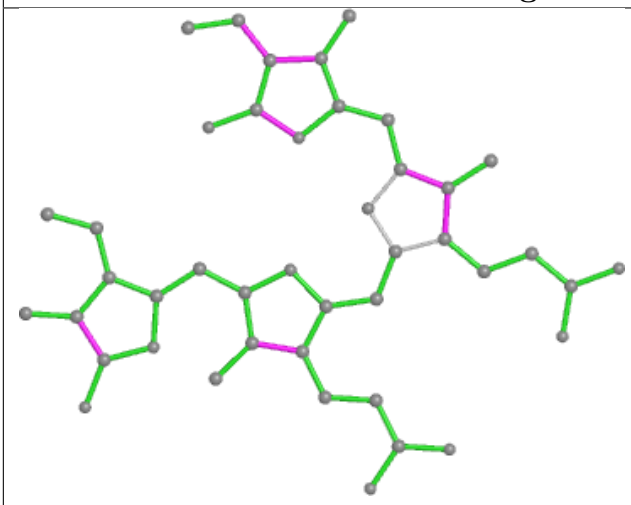


Rings

Ligand PEB cp 202



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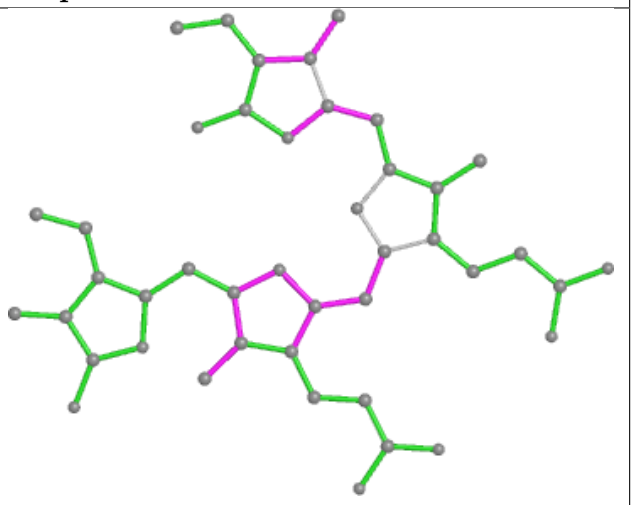

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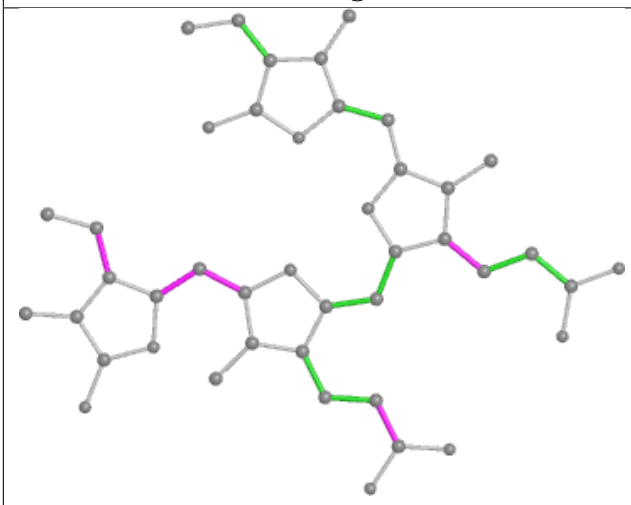

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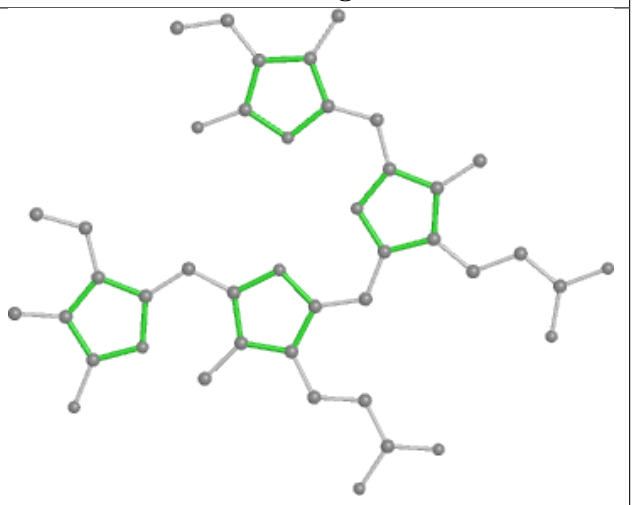
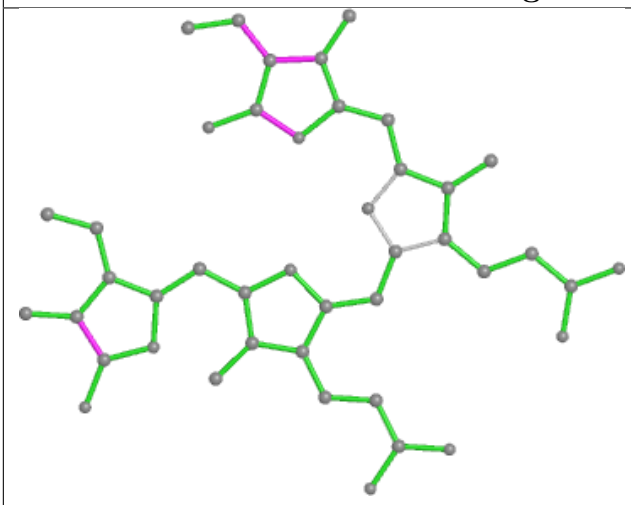


Rings

Ligand PEB fx 201



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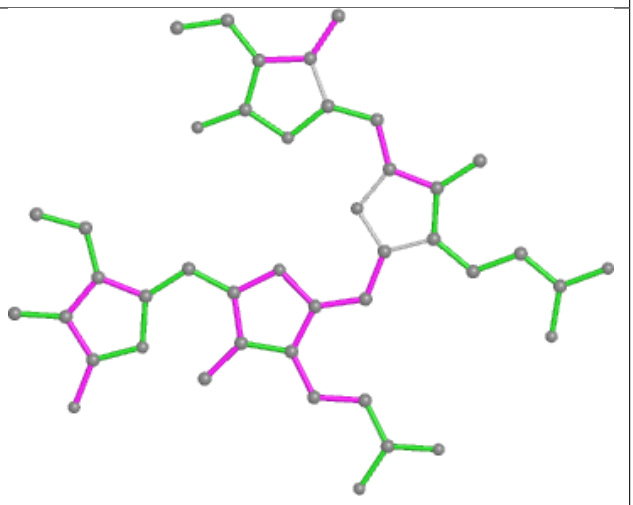

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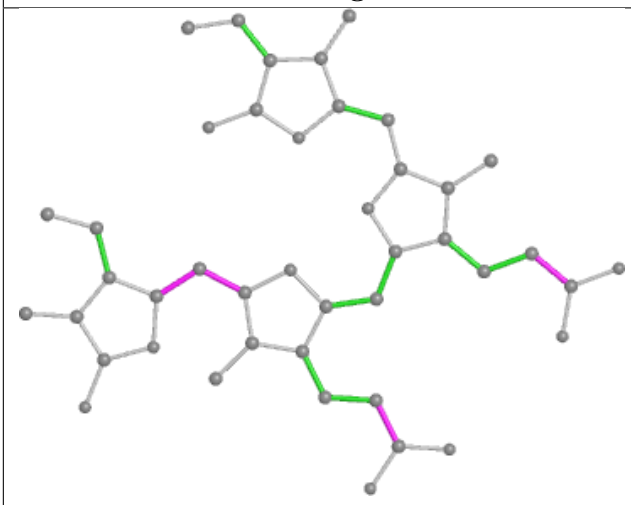

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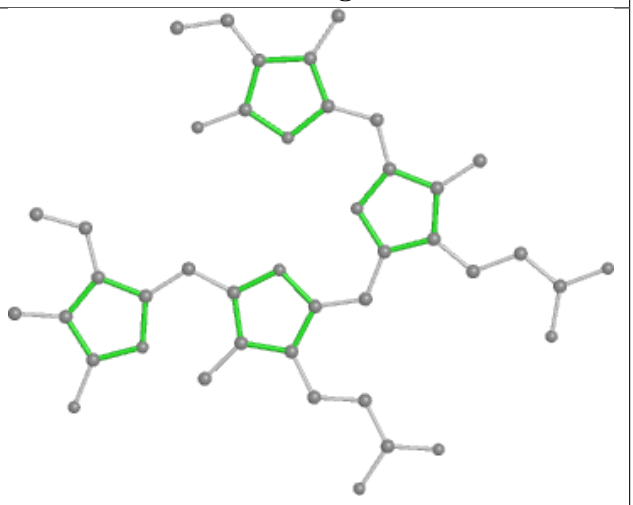
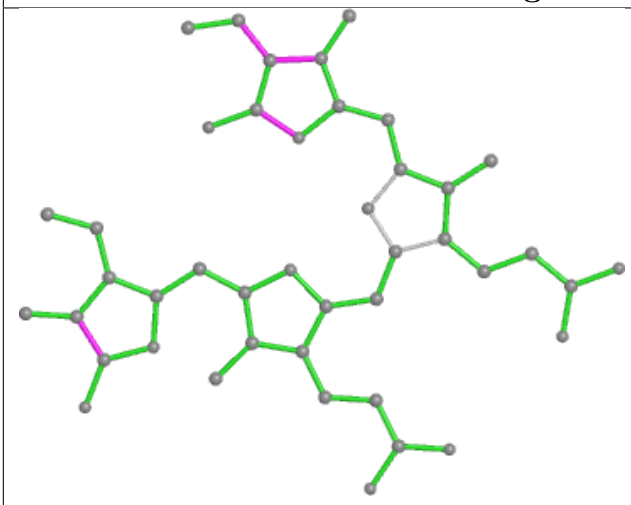


Rings

Ligand PEB l9 202



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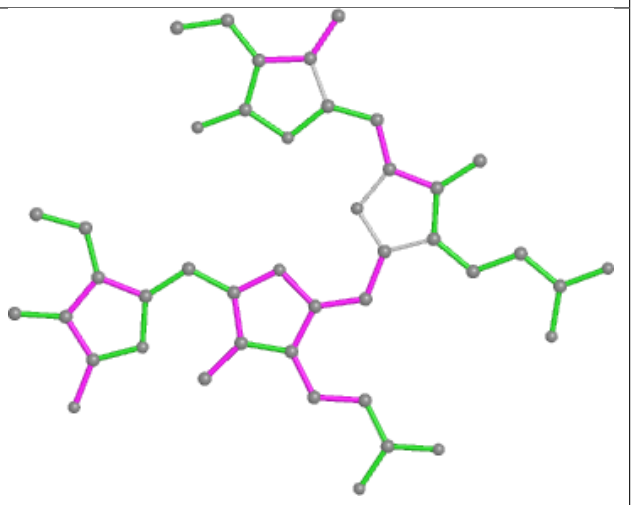

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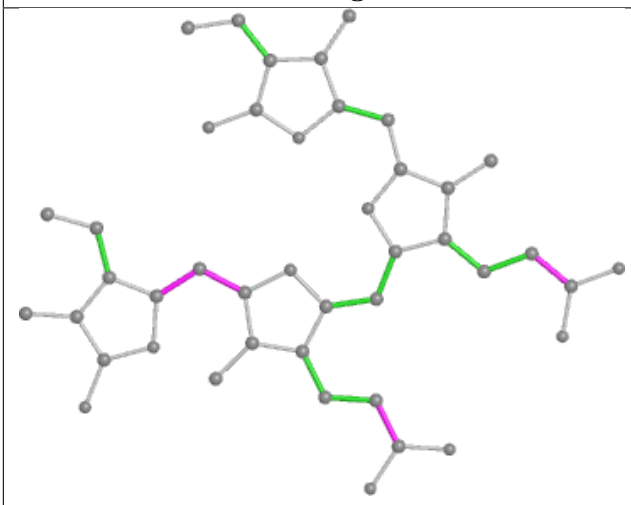

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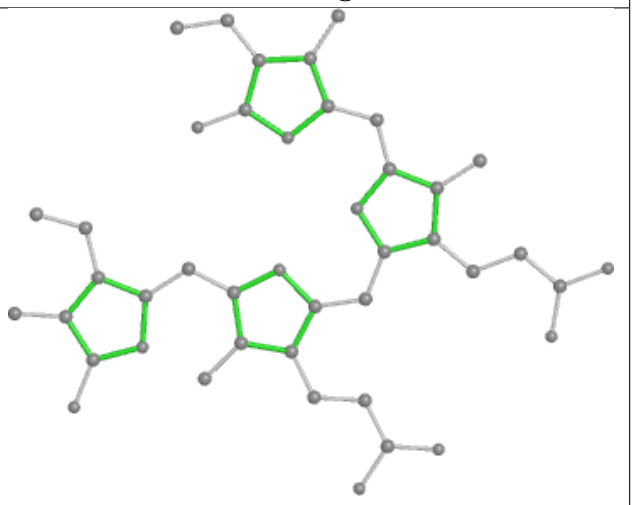
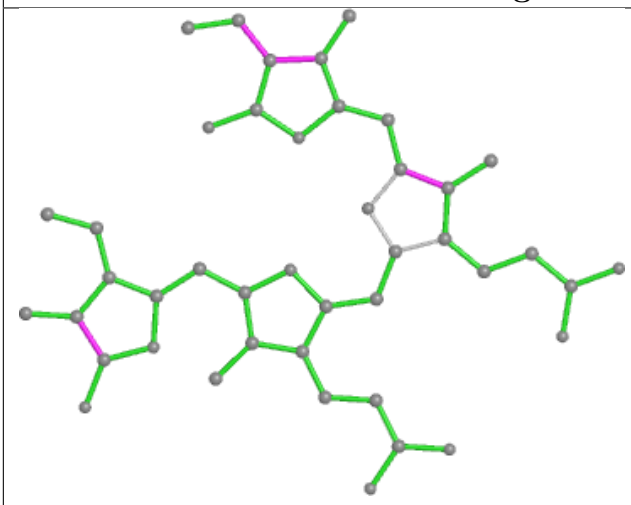


Rings

Ligand PEB fn 1002



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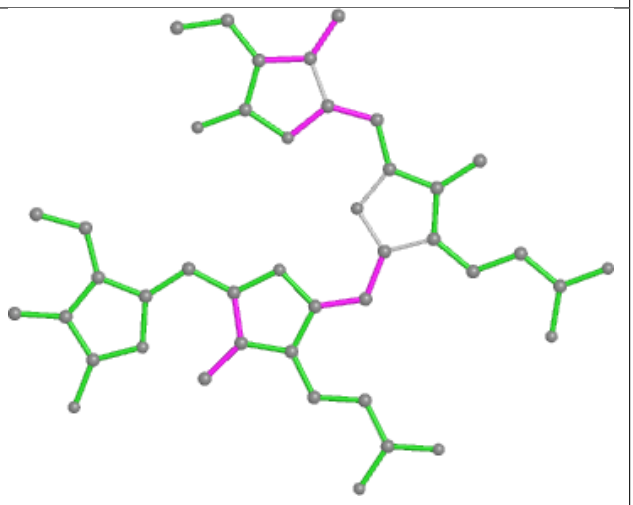

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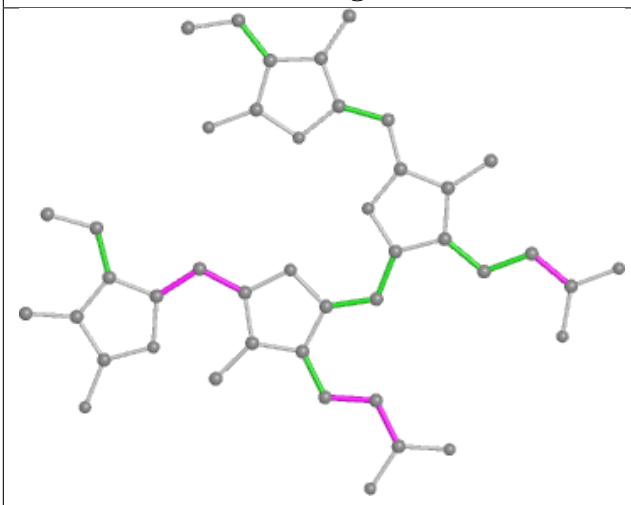

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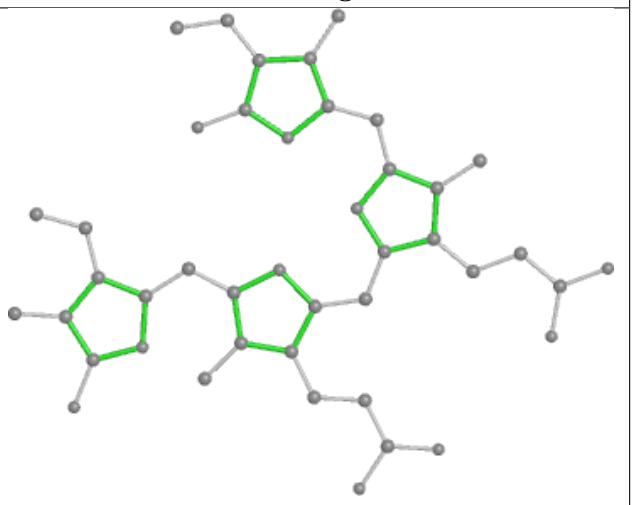
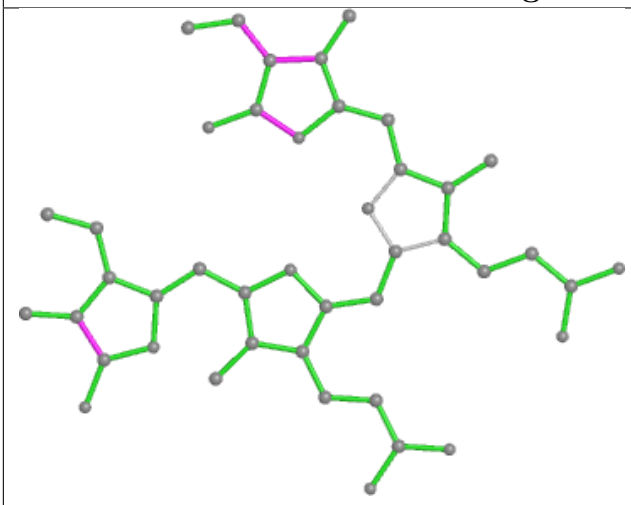


Rings

Ligand PEB er 201



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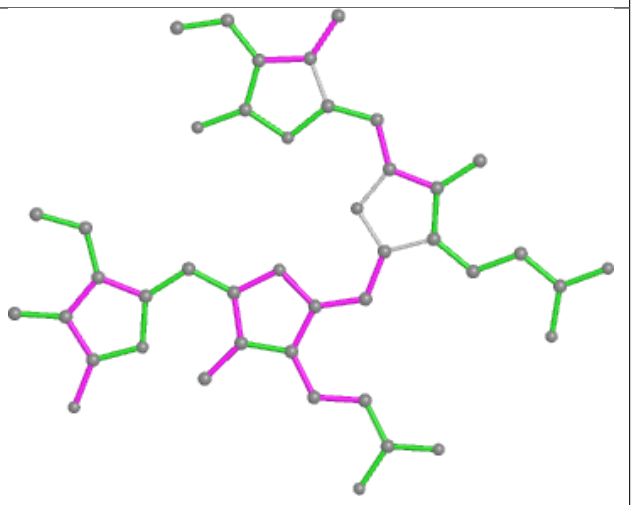

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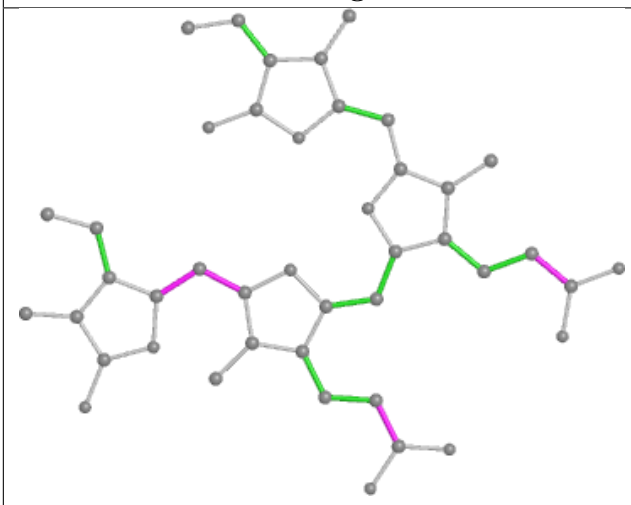

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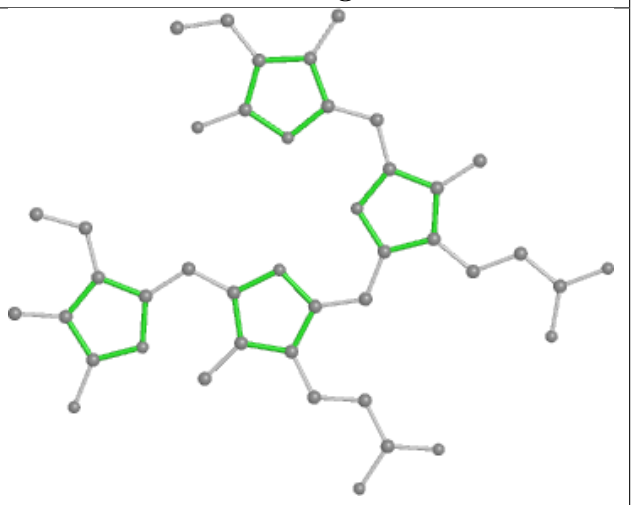
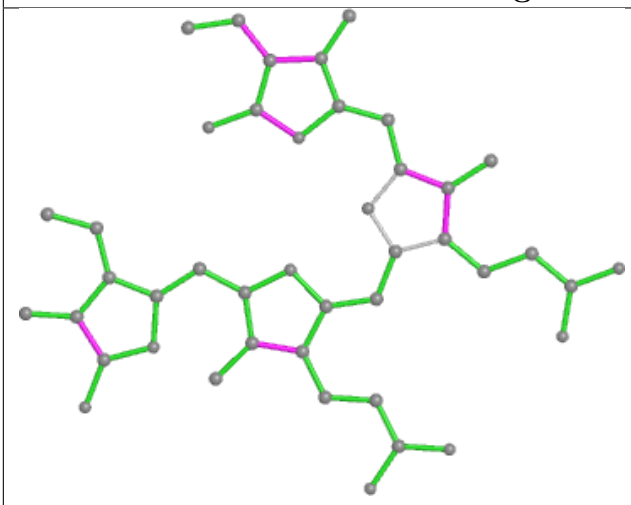


Rings

Ligand PEB hH 202



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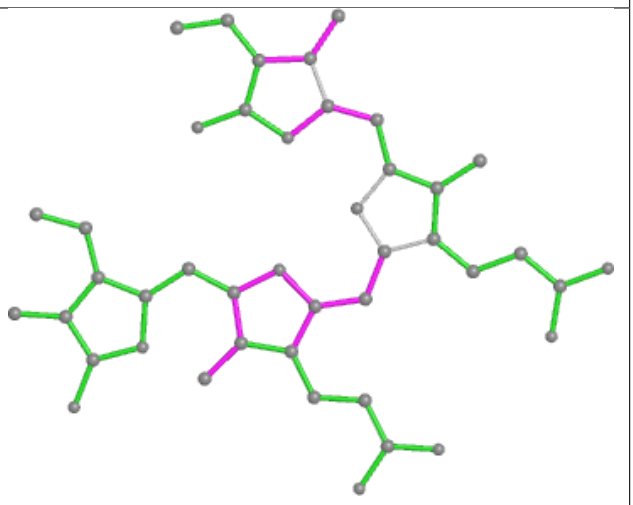

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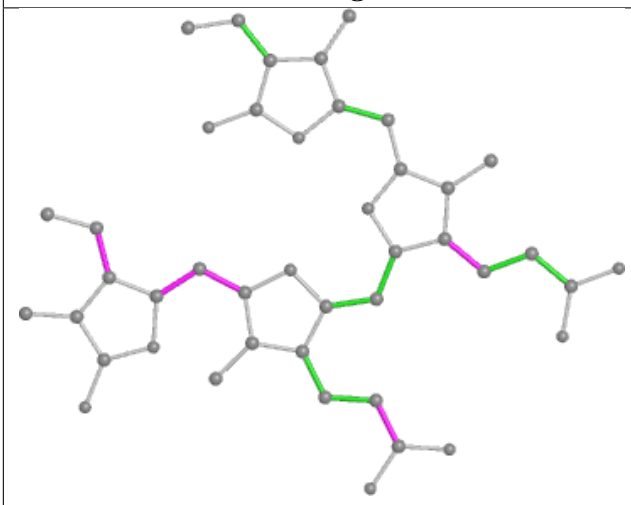

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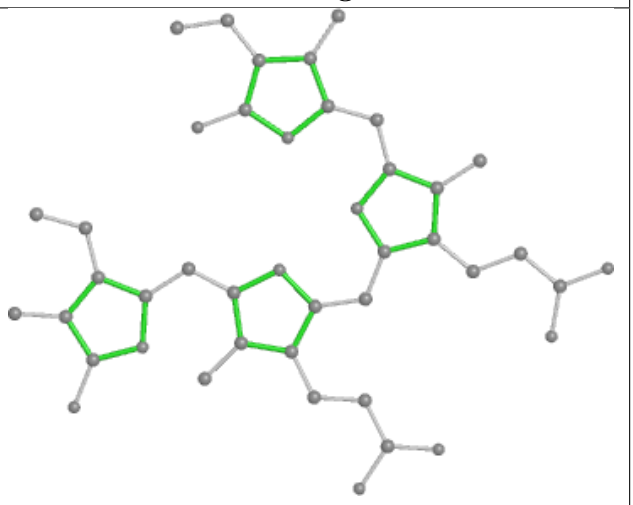
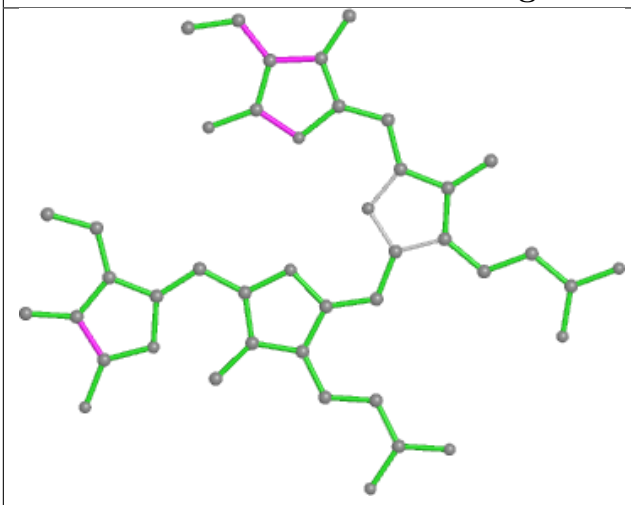


Rings

Ligand PEB p2 201



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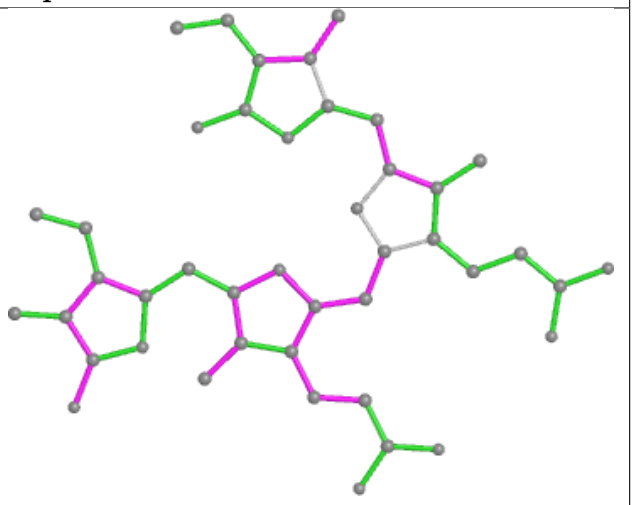

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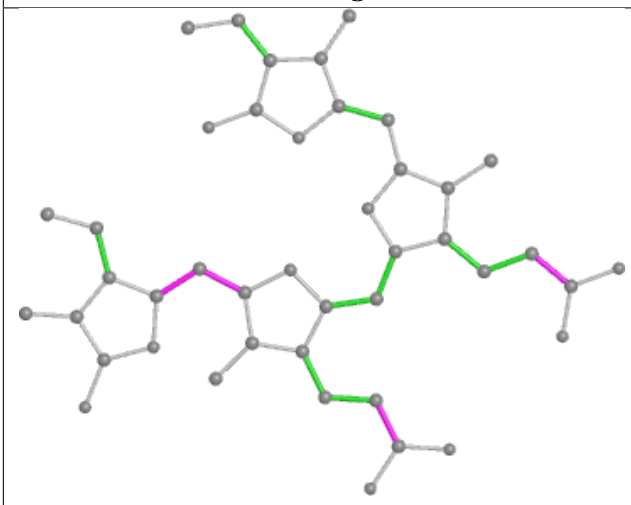

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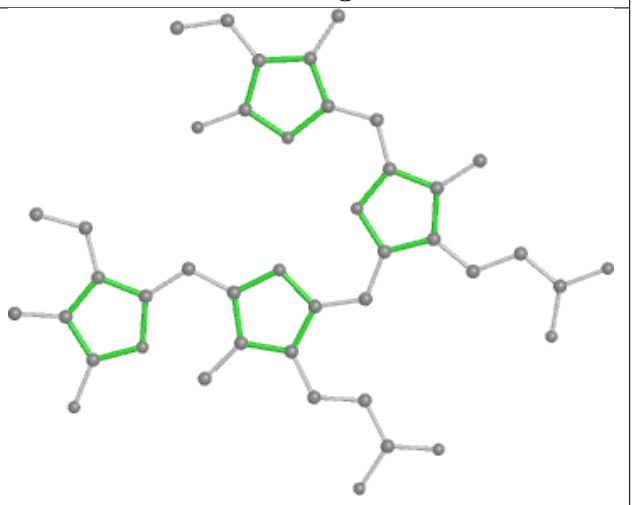
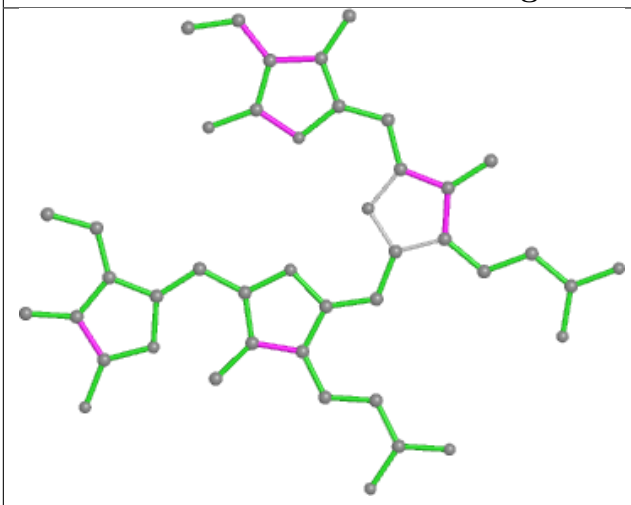


Rings

Ligand PEB eg 202



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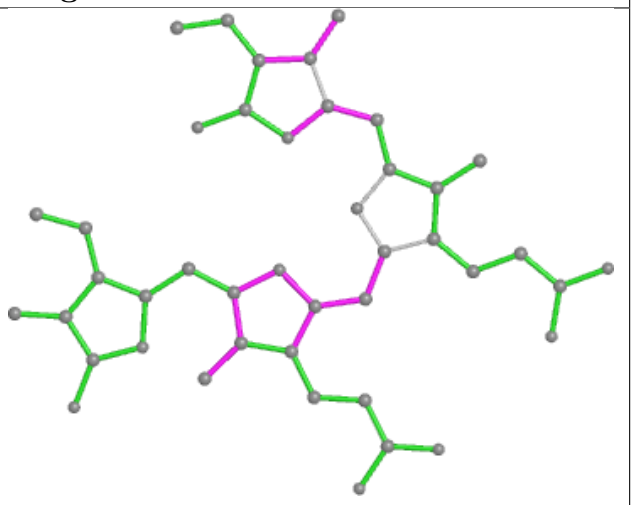

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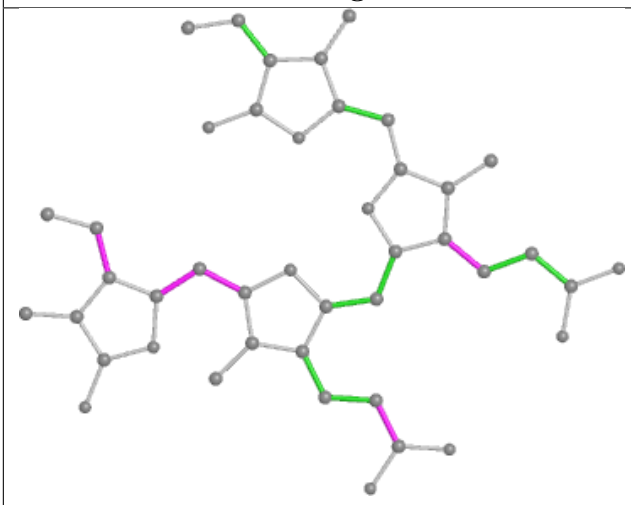
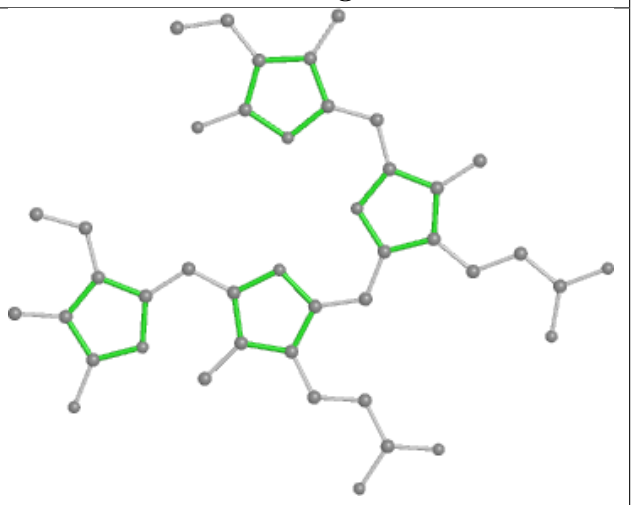
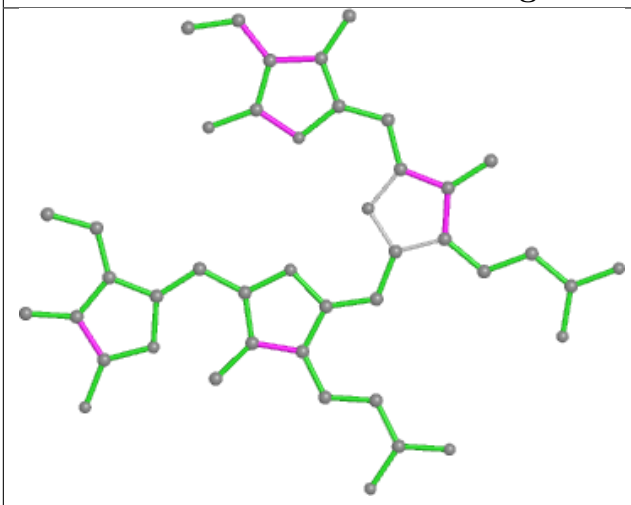


Torsions



Rings

Ligand PEB y8 202



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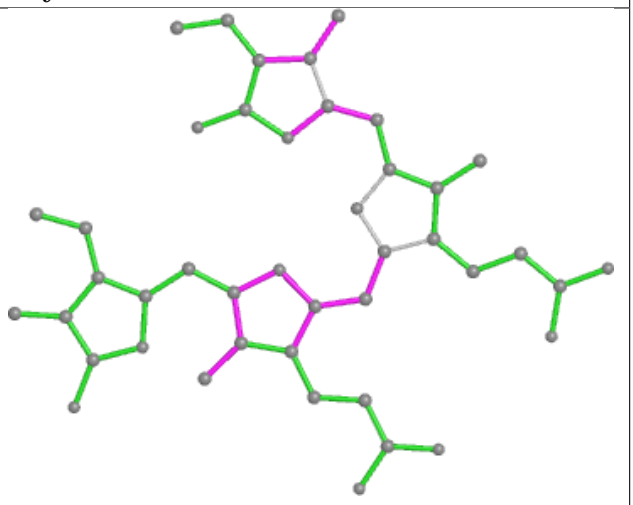

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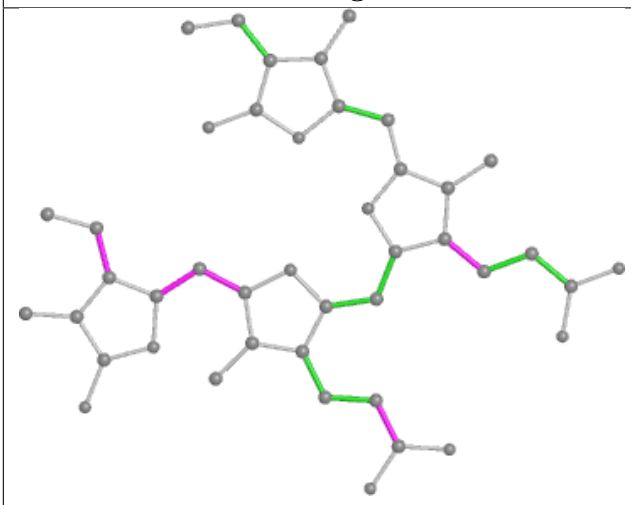

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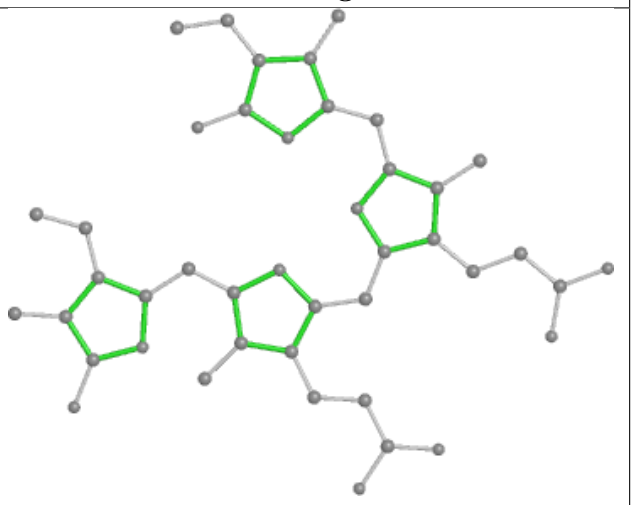
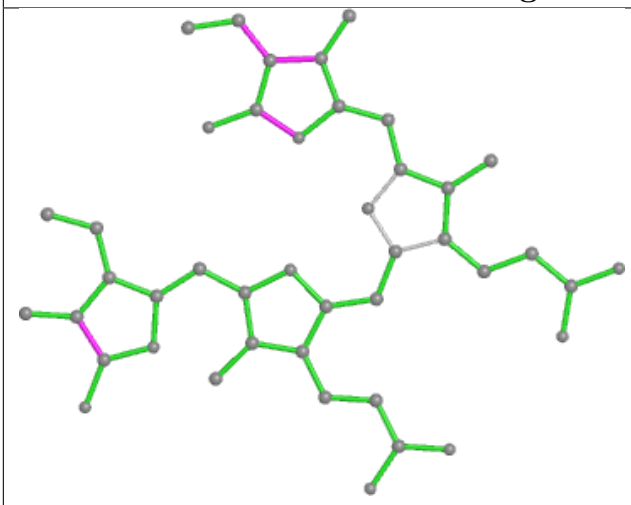


Rings

Ligand PEB o4 202



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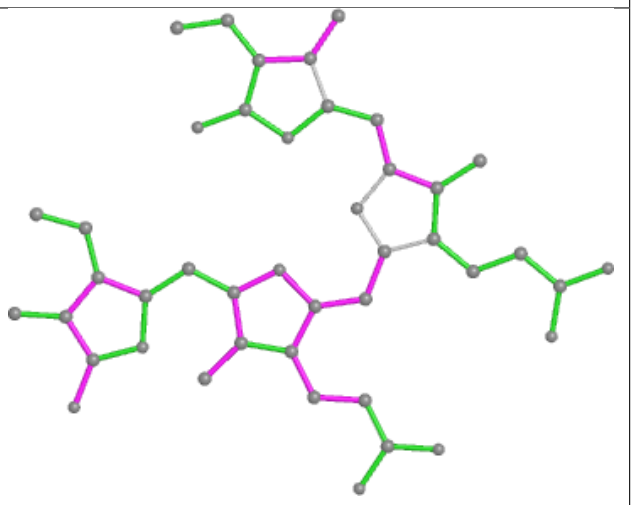

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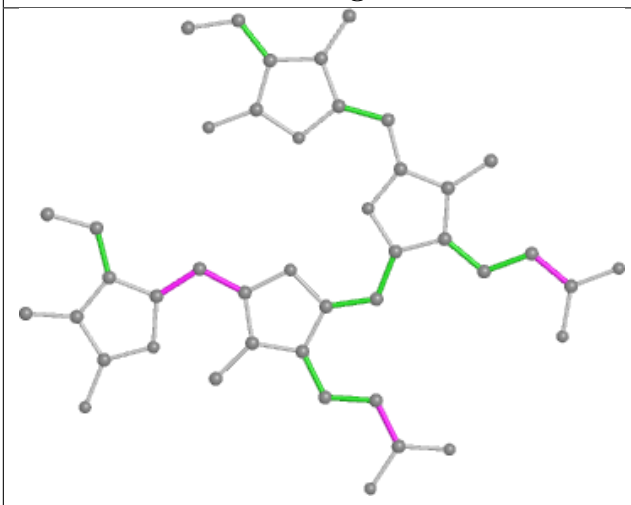

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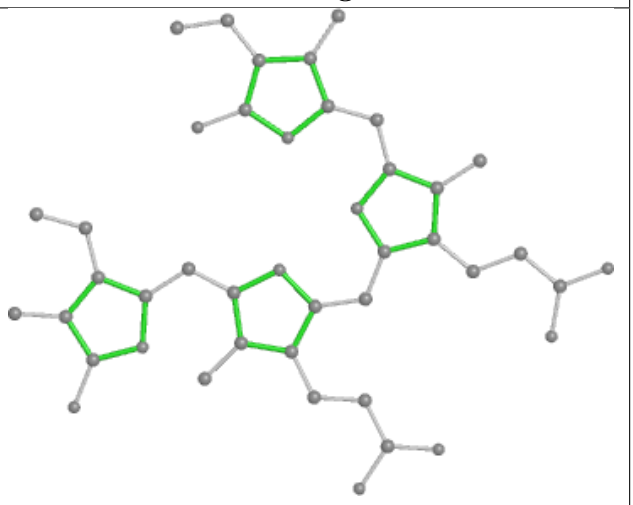
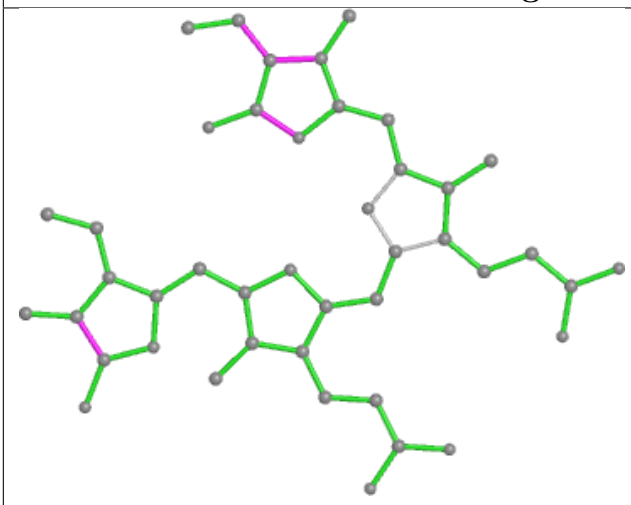


Rings

Ligand PEB I6 202



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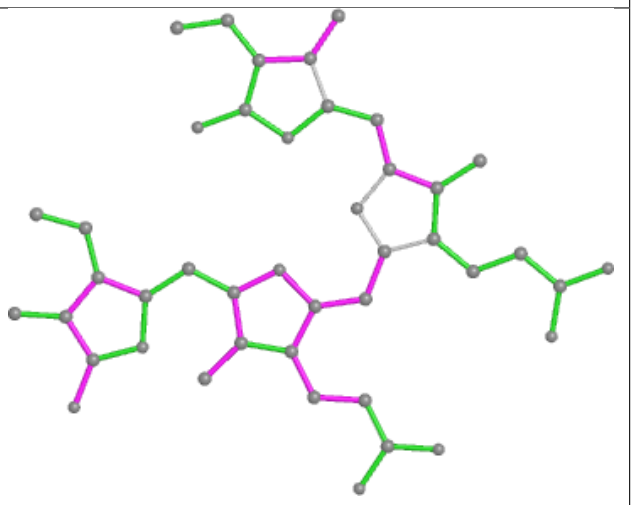

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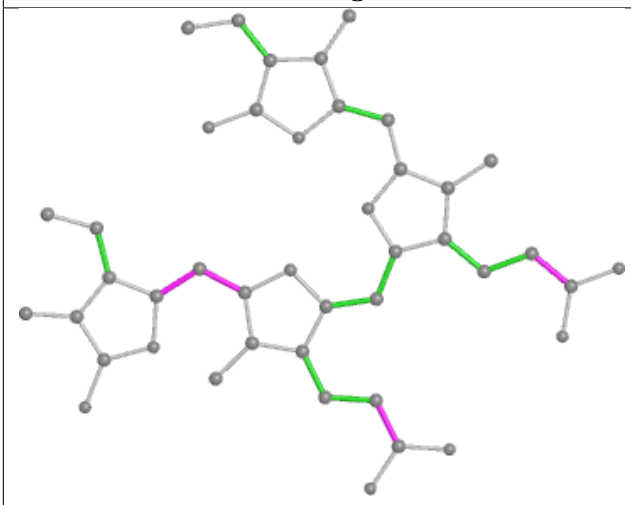

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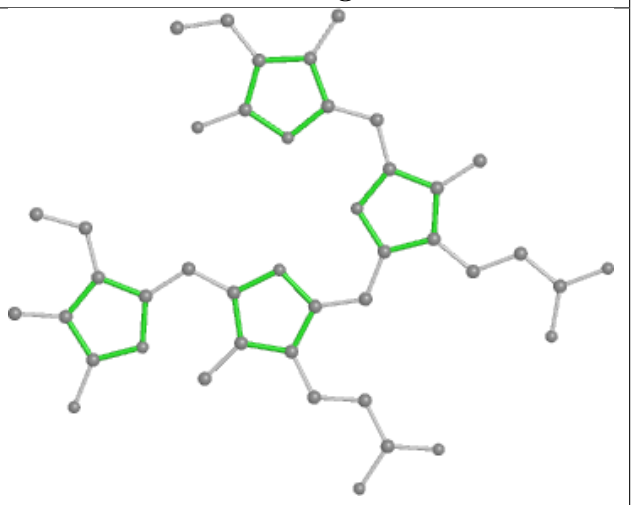
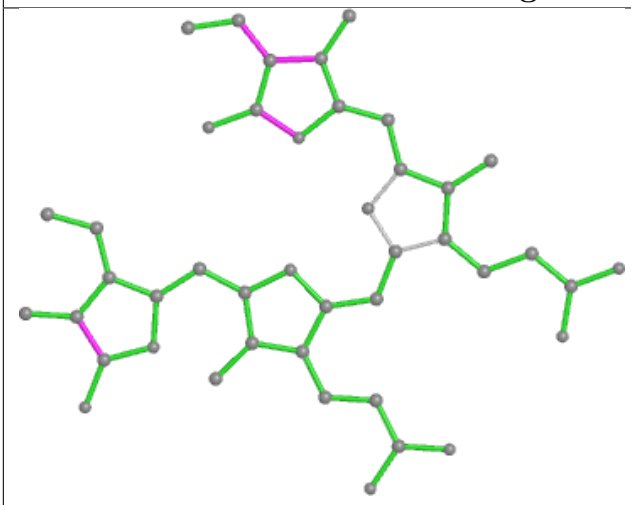


Rings

Ligand PEB o4 201



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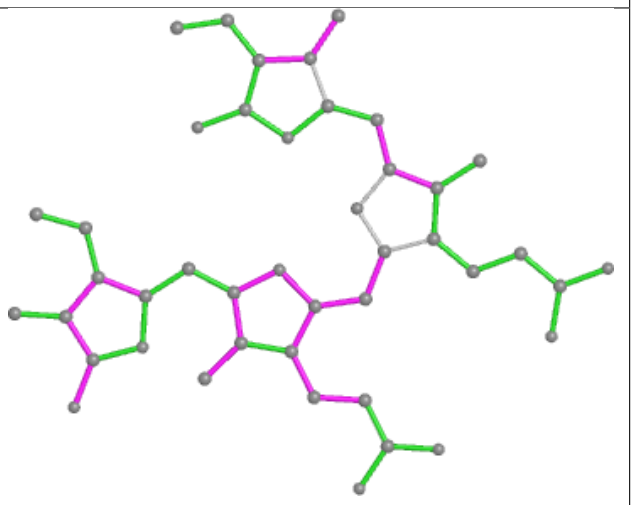

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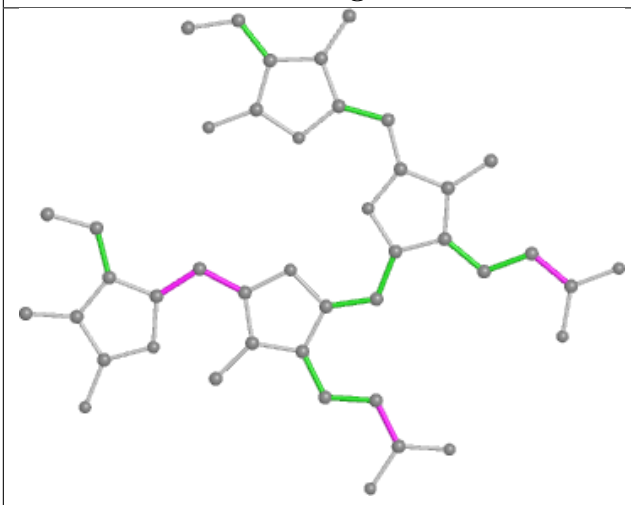

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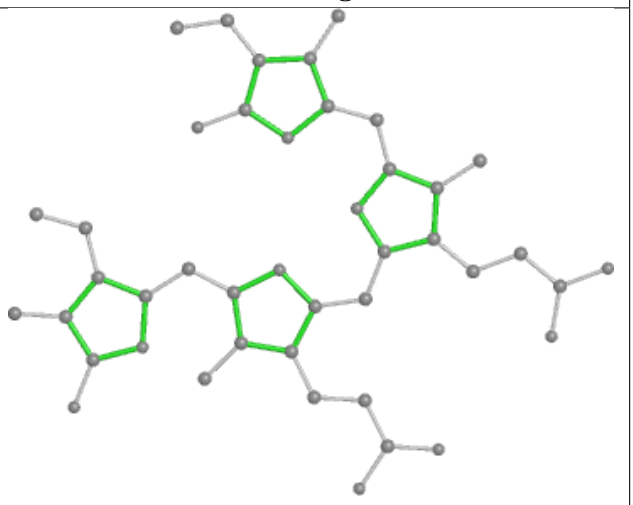
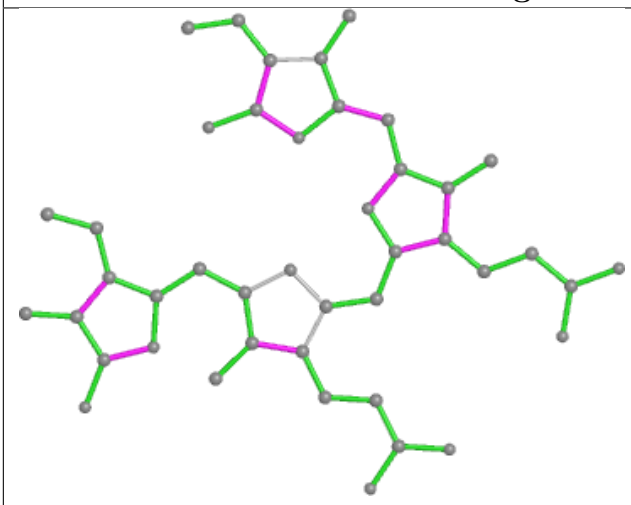


Rings

Ligand PUB R7 203



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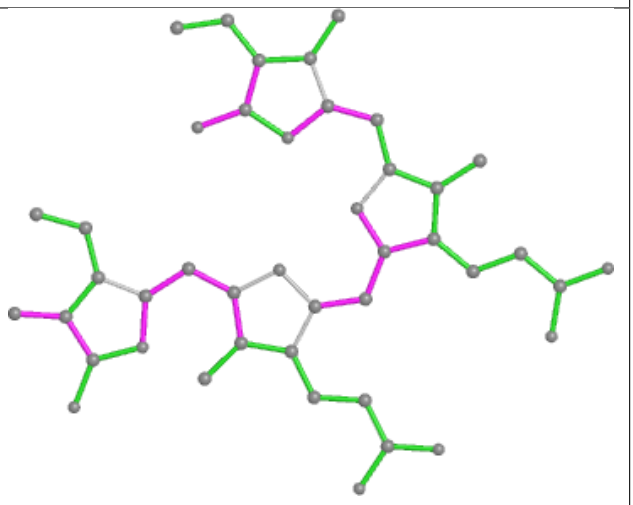

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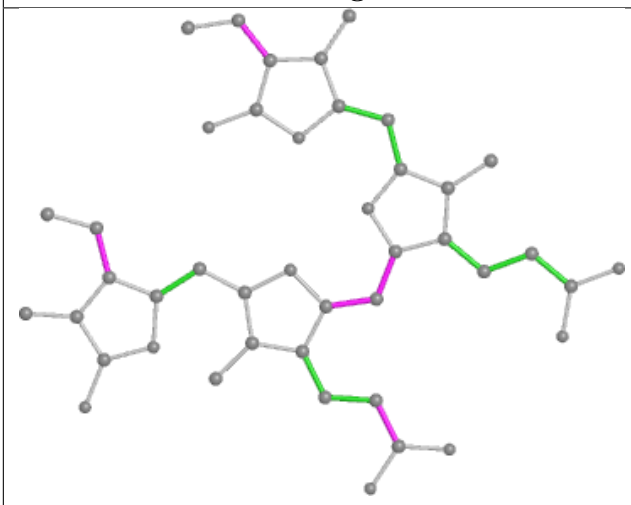

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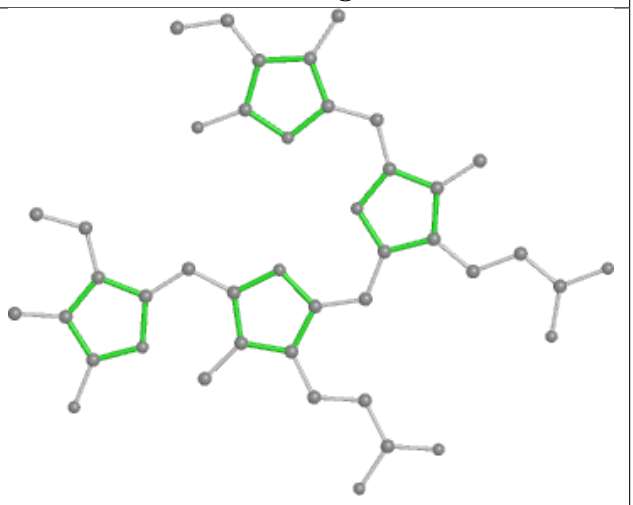
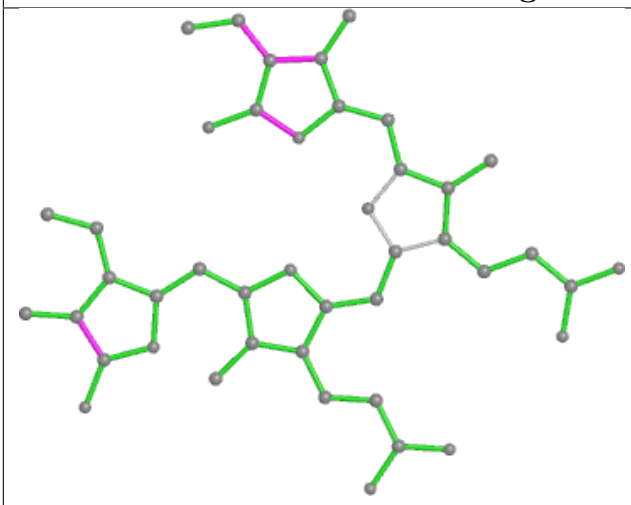


Rings

Ligand PEB v6 201



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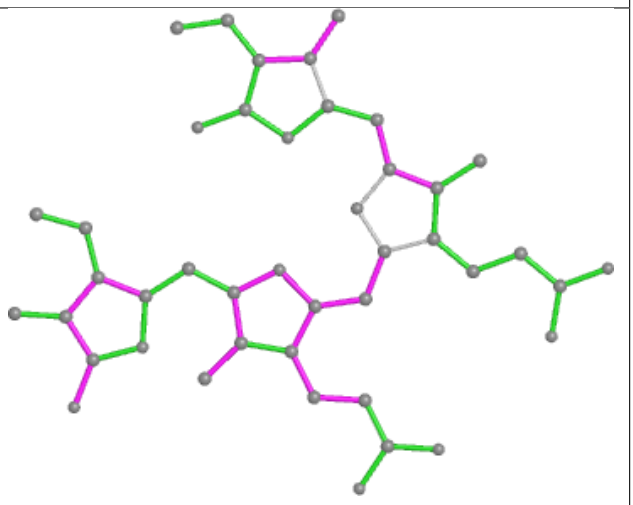

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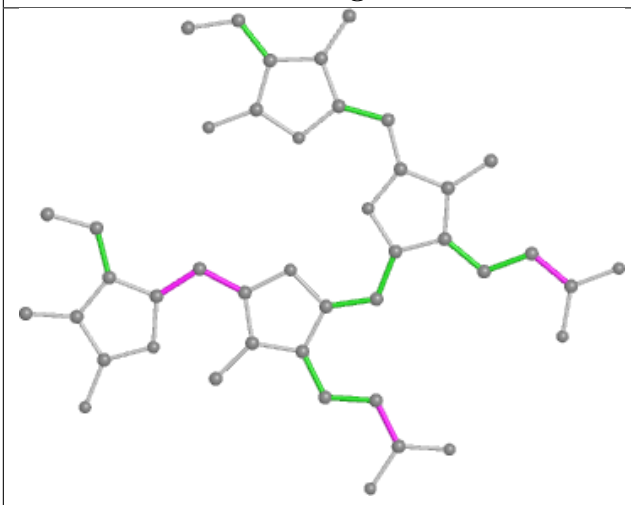

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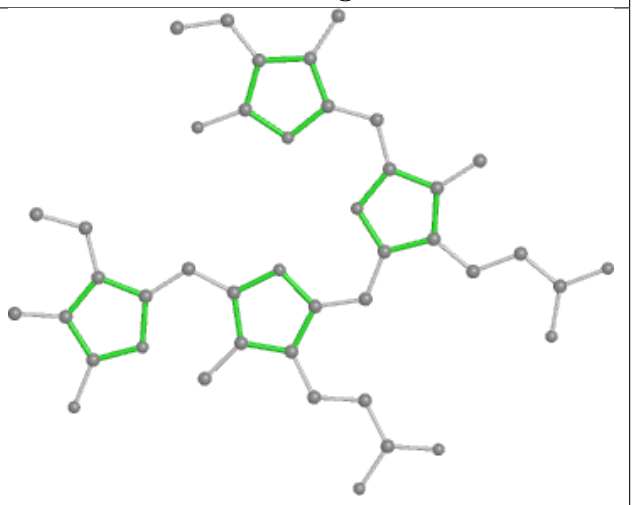

Rings

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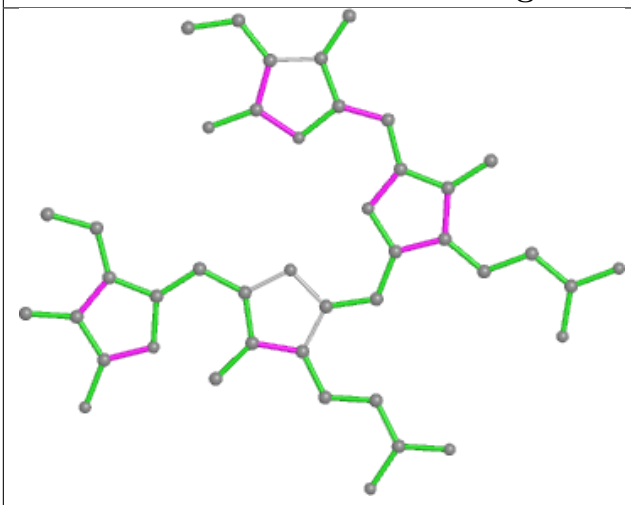

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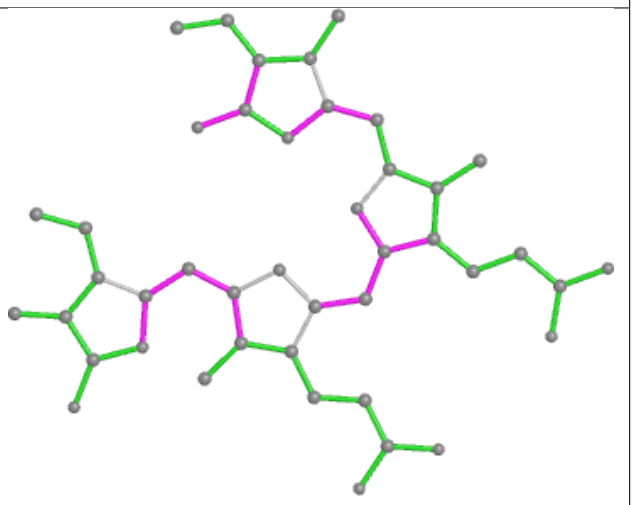

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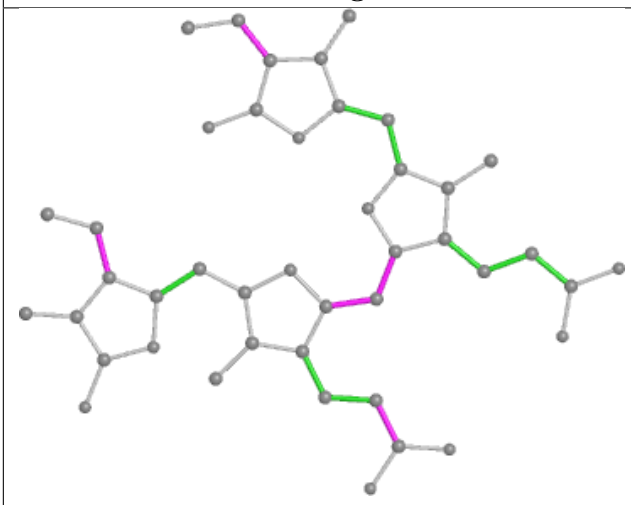

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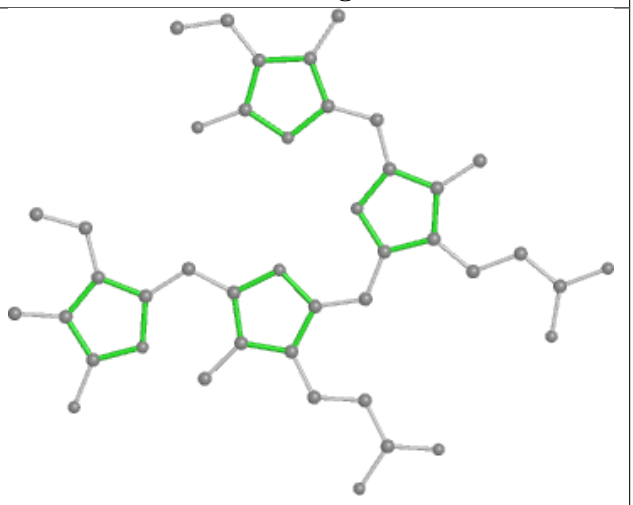
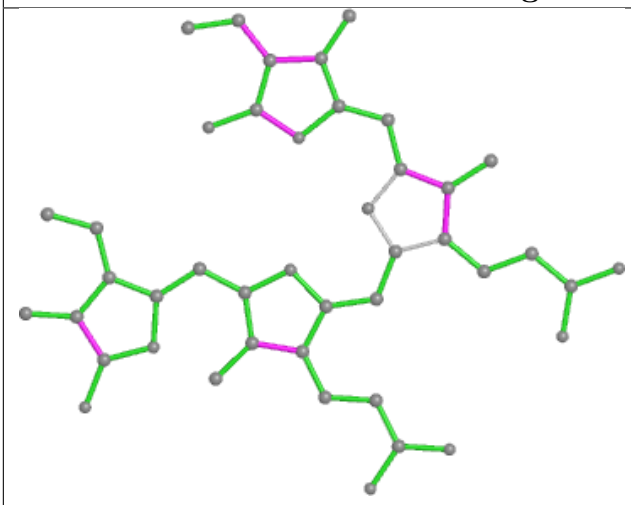


Rings

Ligand PEB r7 202



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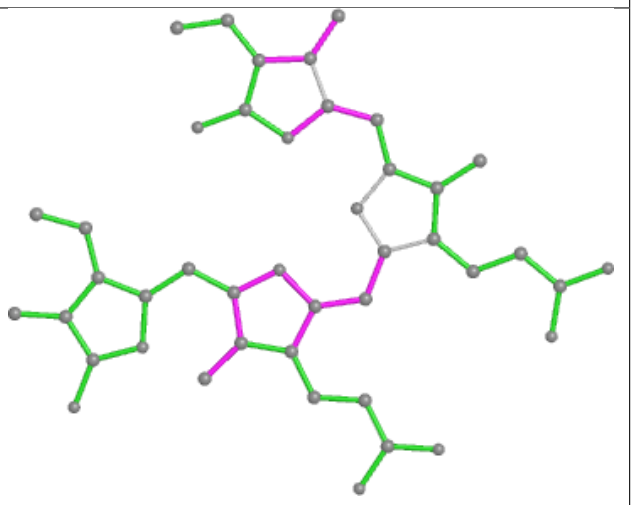

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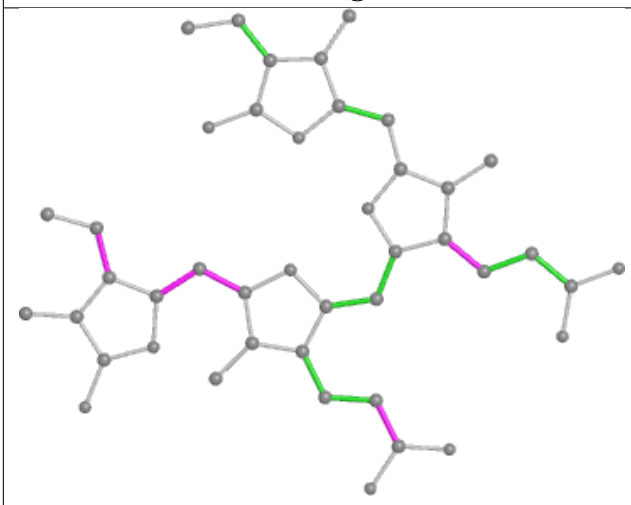

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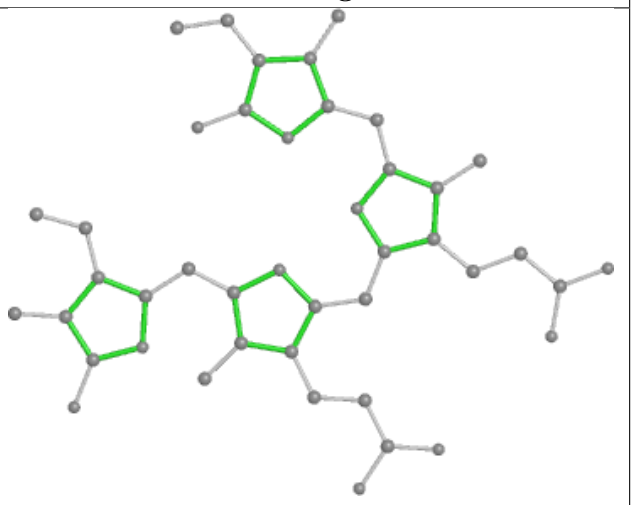
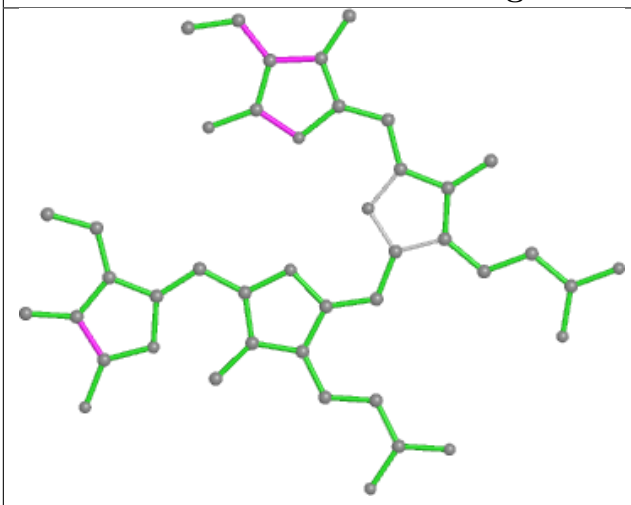


Rings

Ligand PEB A6 1002



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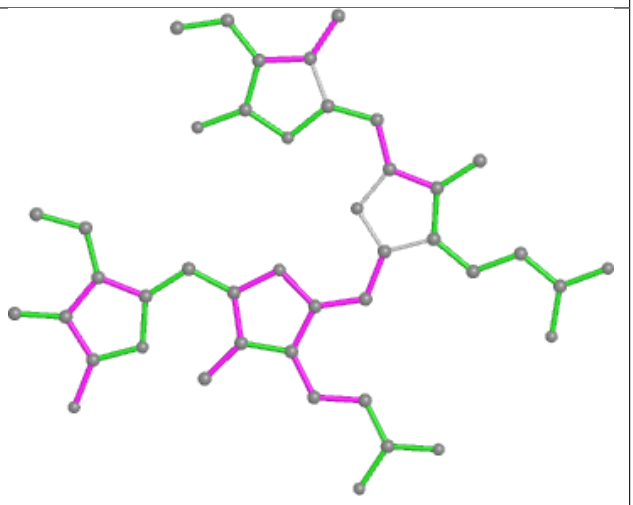

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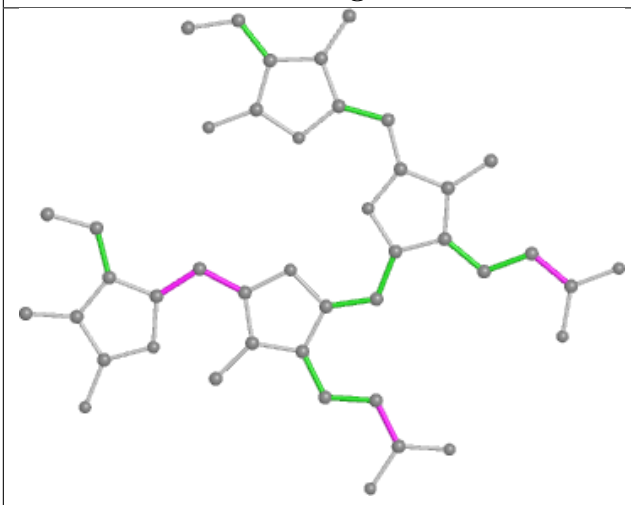

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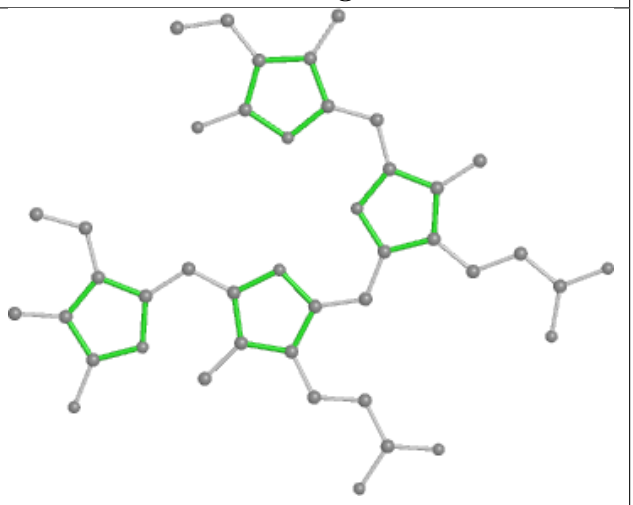
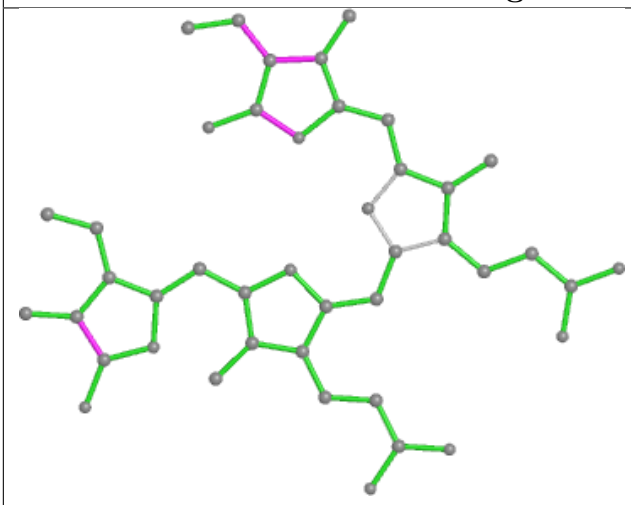


Rings

Ligand PEB O3 1001



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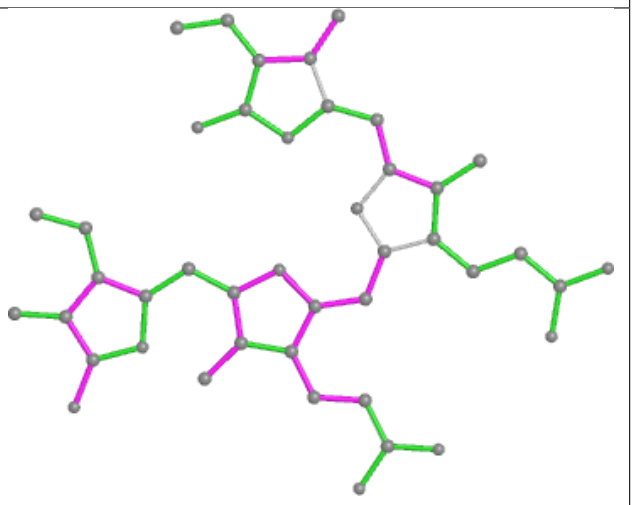

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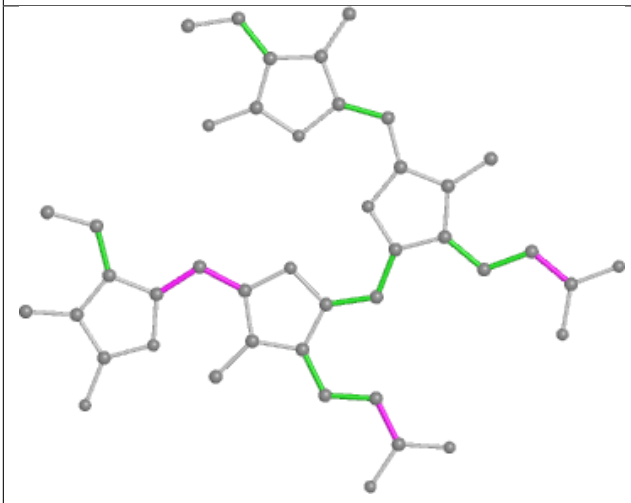

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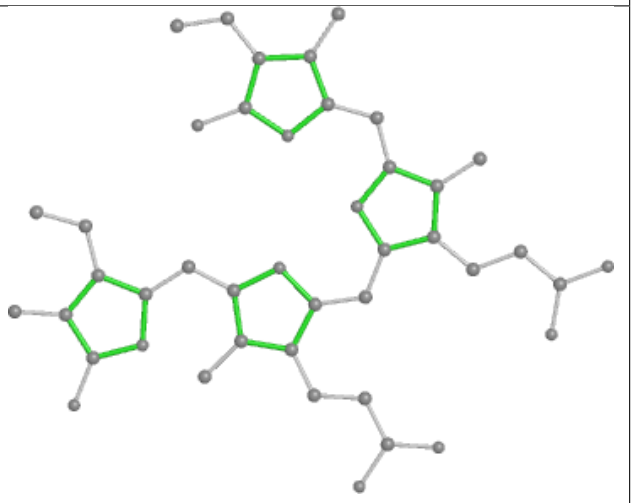
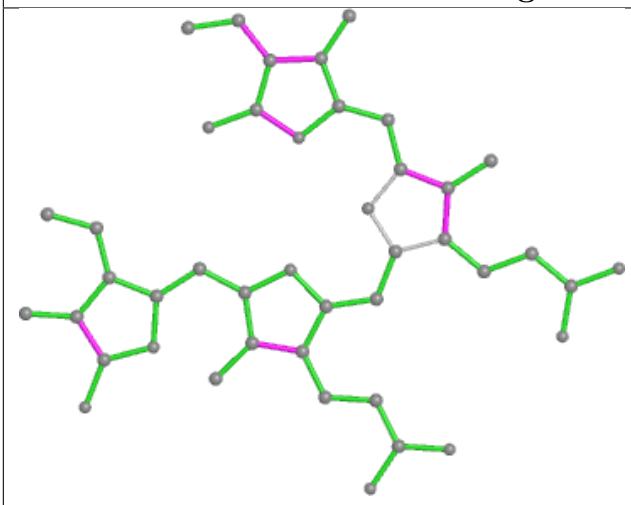


Rings

Ligand PEB Z7 202



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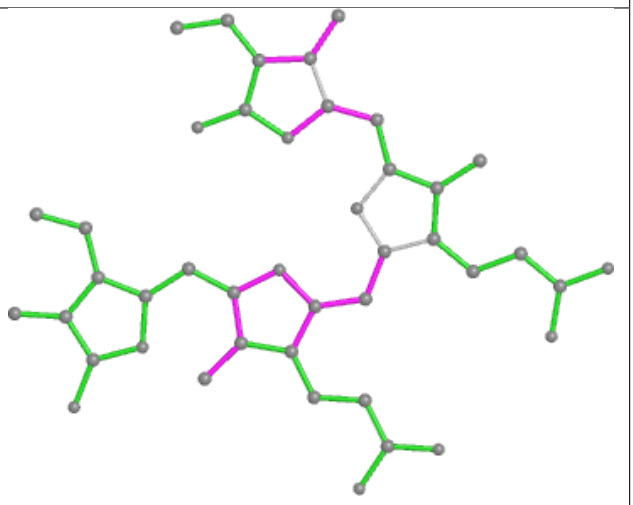

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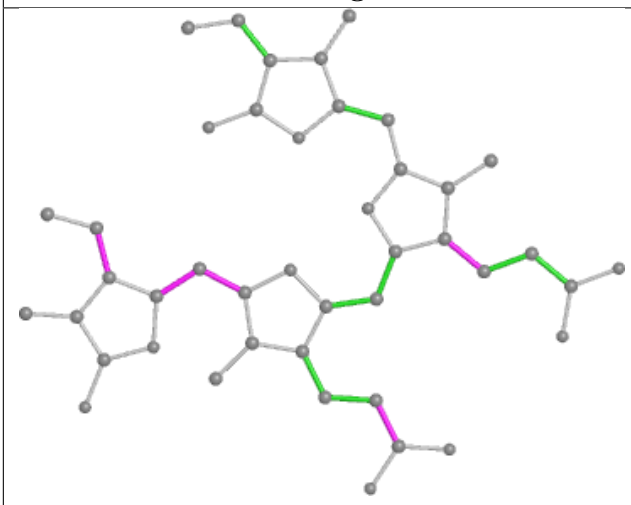

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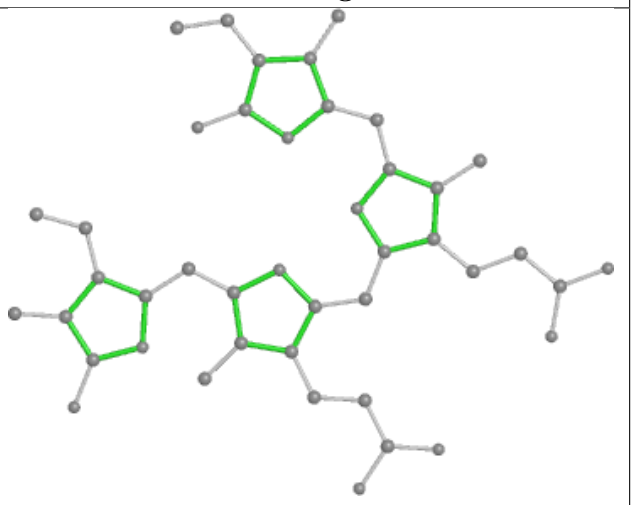
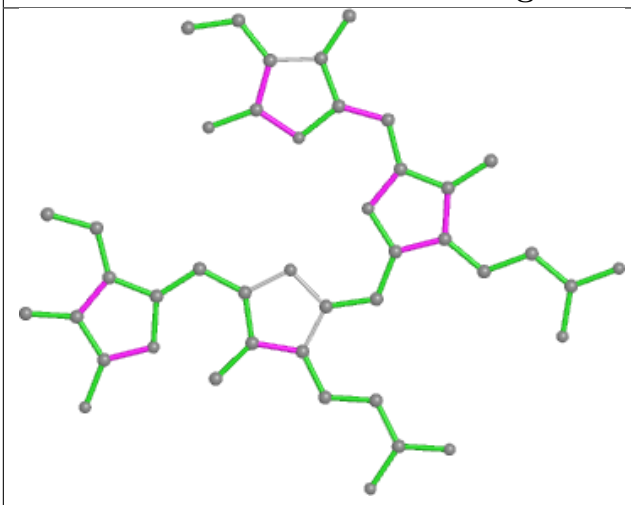


Rings

Ligand PUB p4 203



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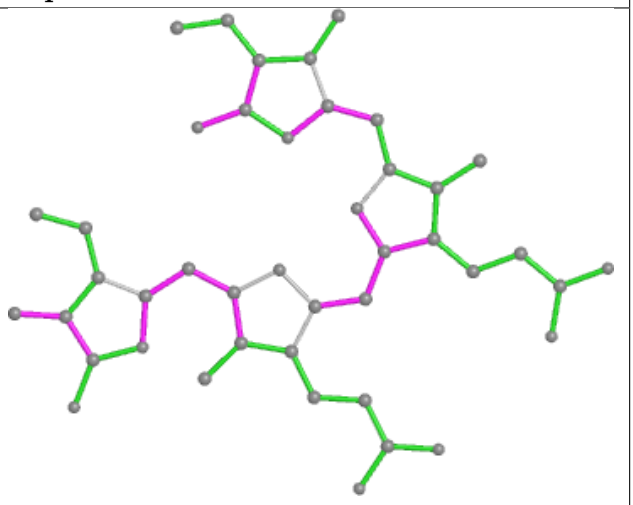

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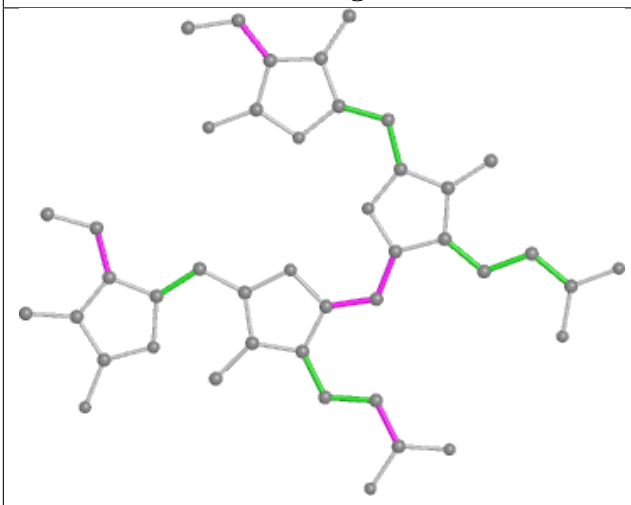

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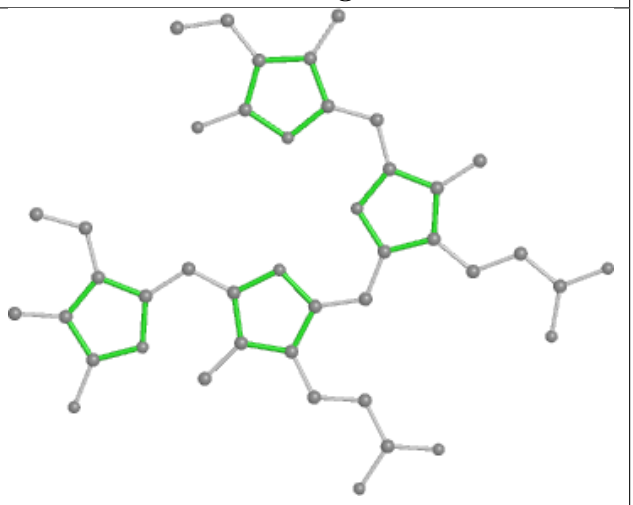
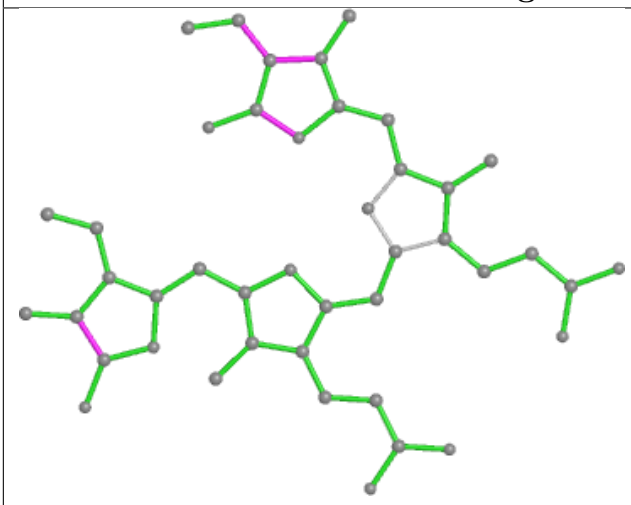


Rings

Ligand PEB Z4 201



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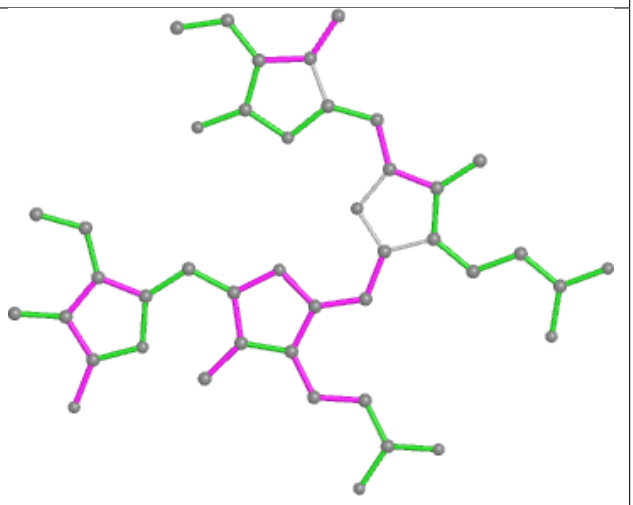
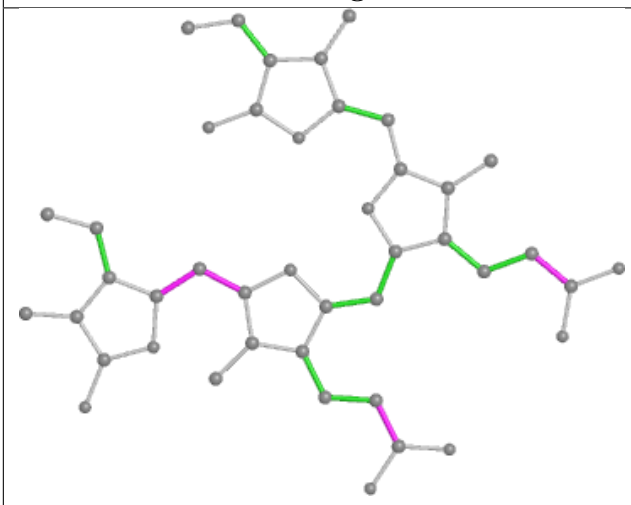


Bond angles



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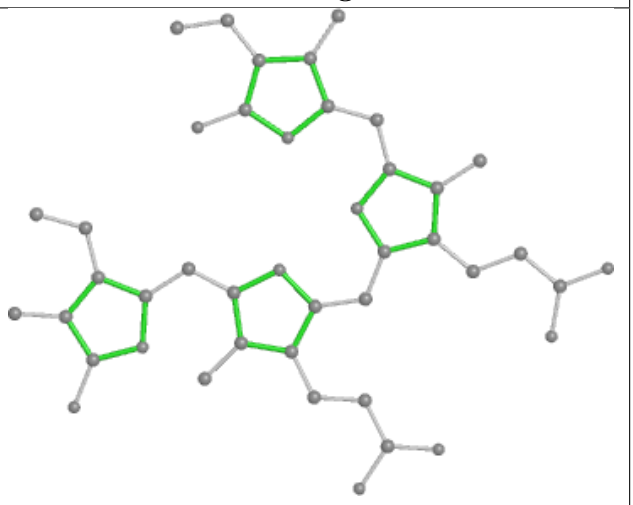
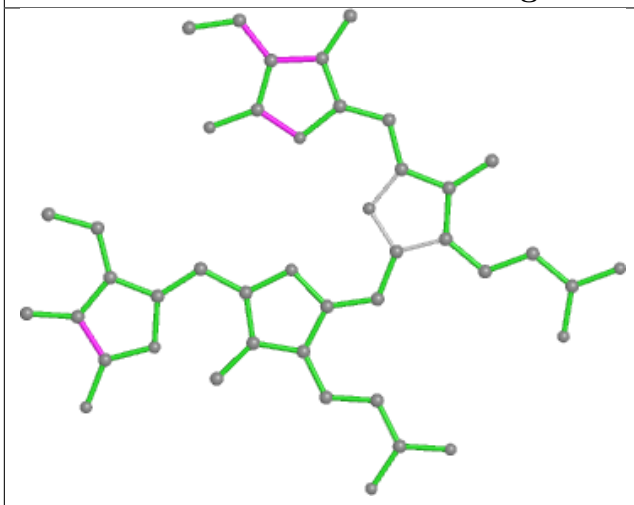
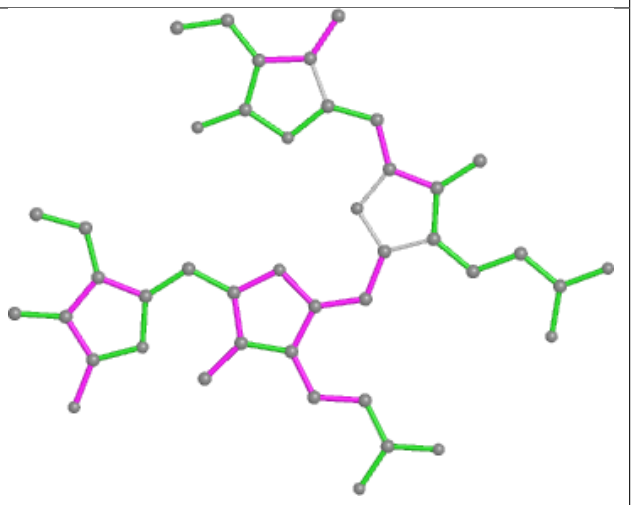


Rings

Ligand PEB J5 201



Bond lengths



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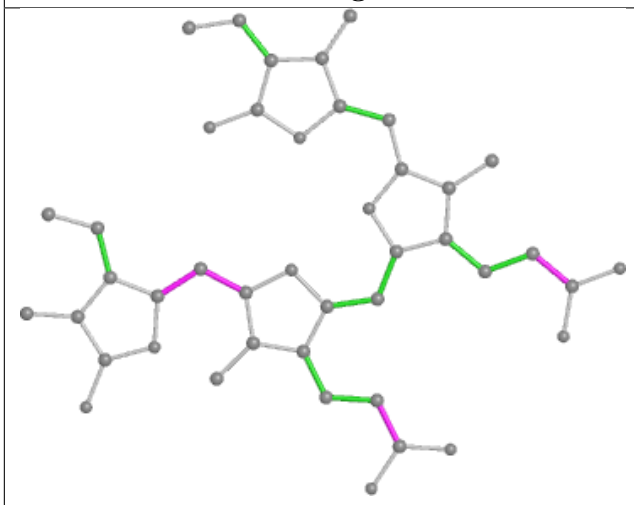
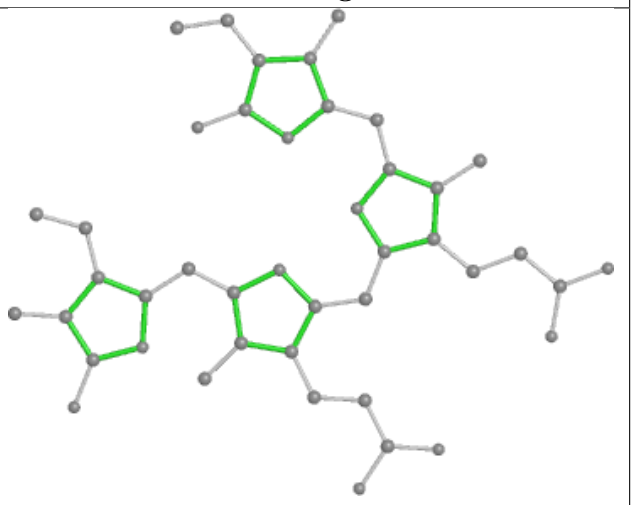
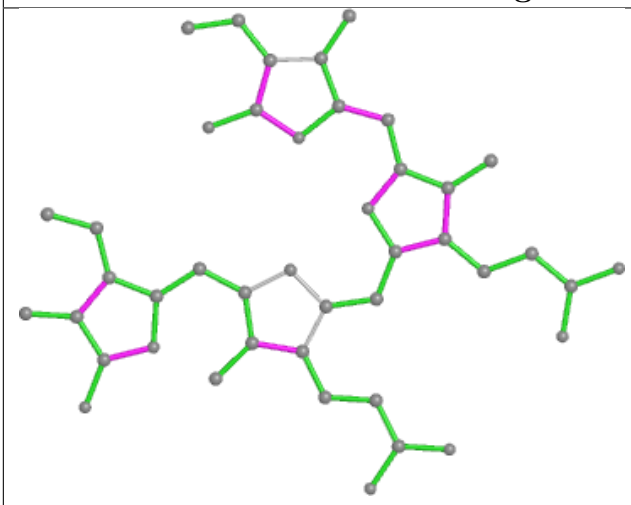


Torsions



Rings

Ligand PUB dF 203



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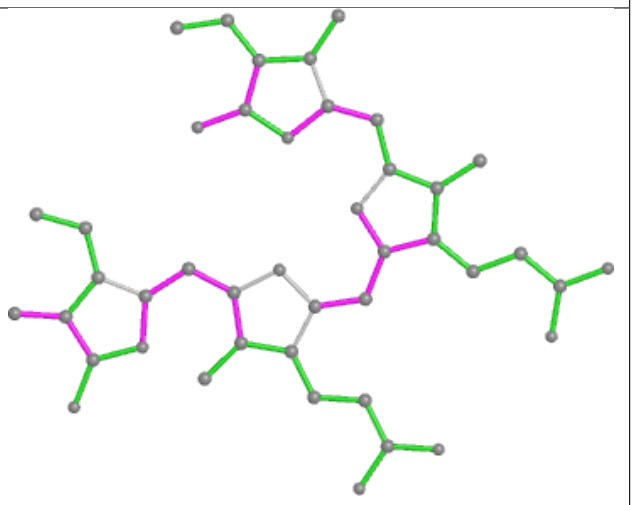

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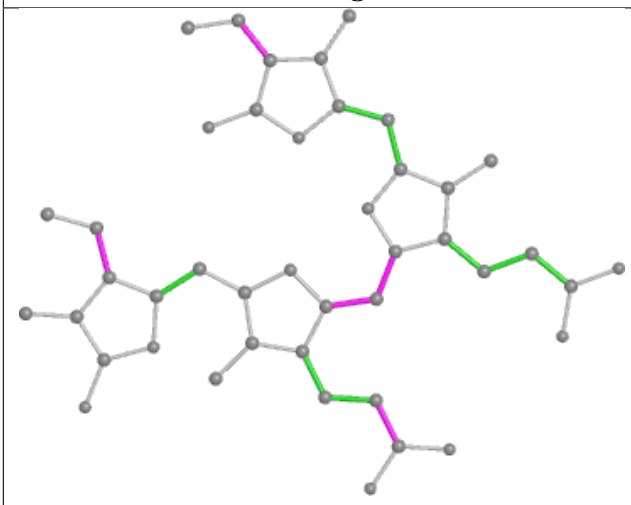

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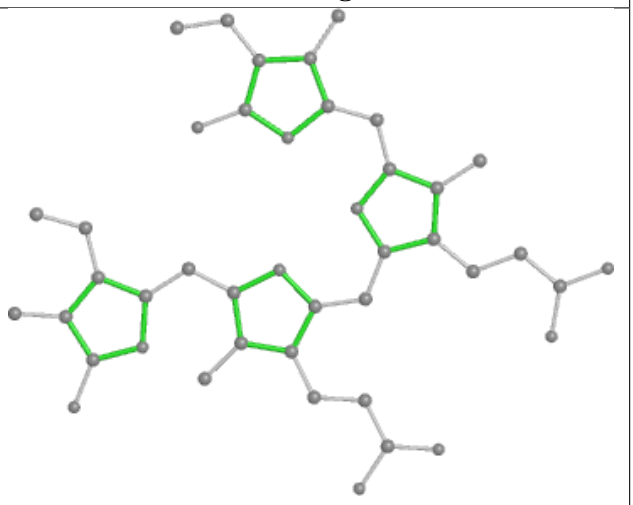
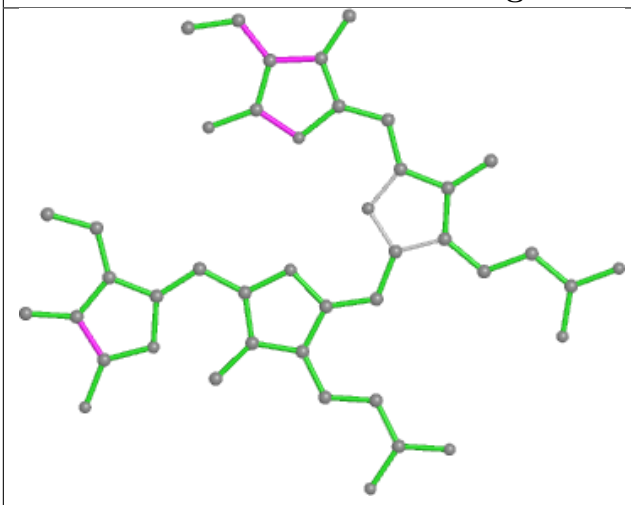


Rings

Ligand PEB O4 1002



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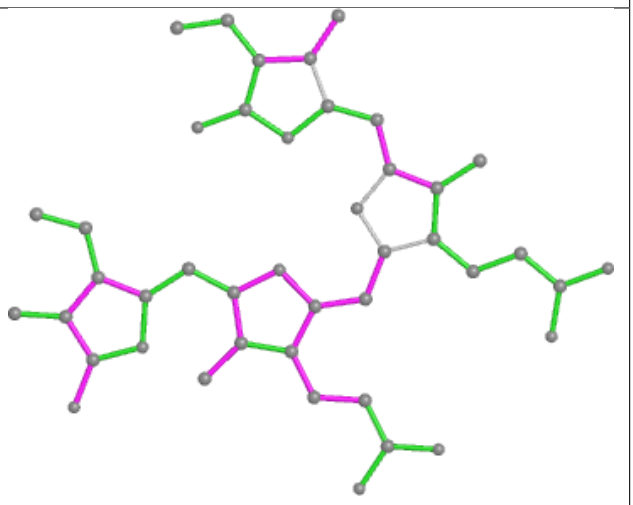

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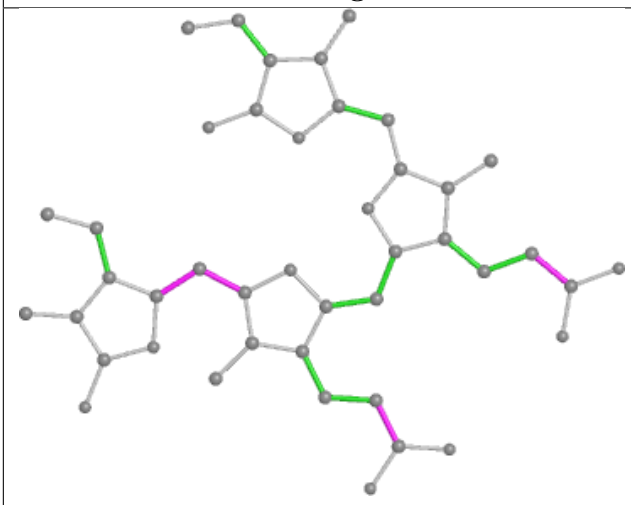

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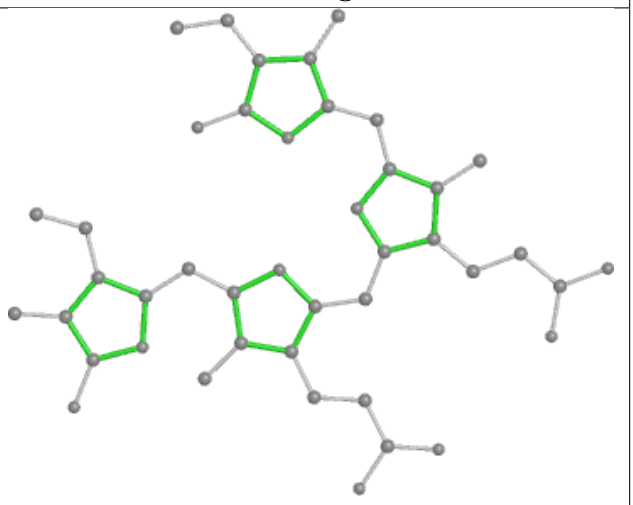

Rings

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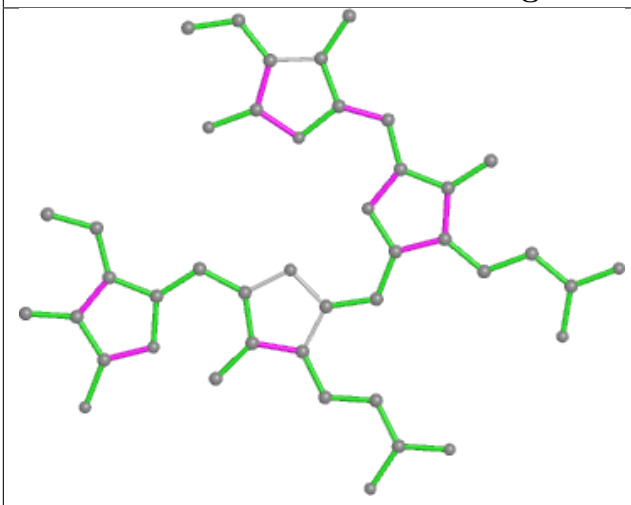

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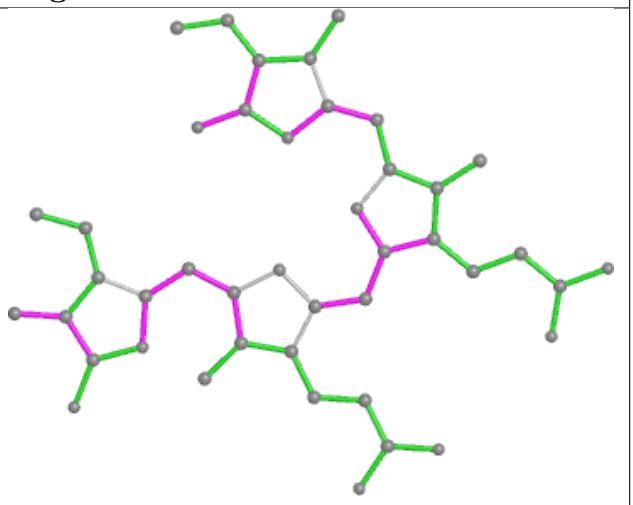

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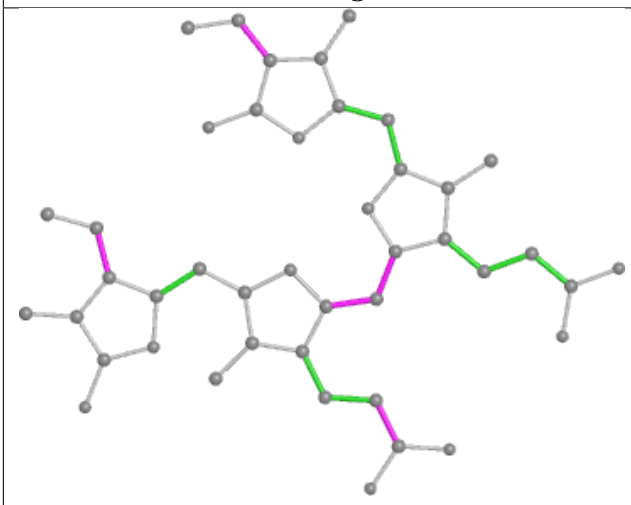

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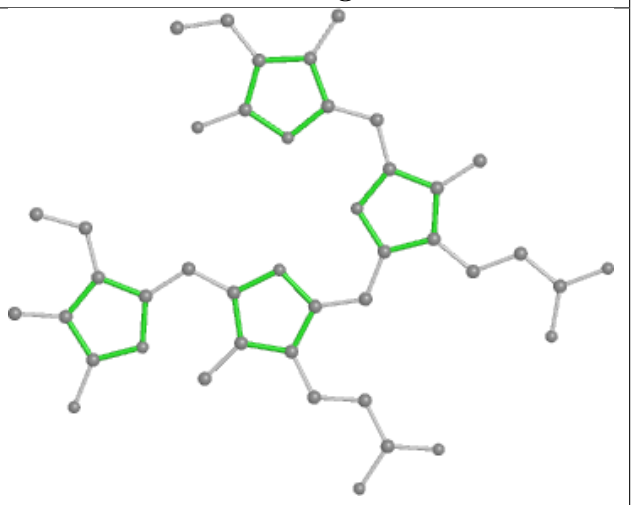

Rings

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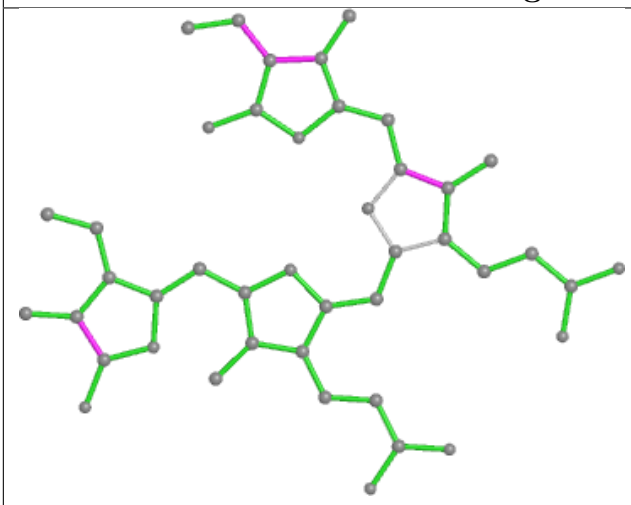

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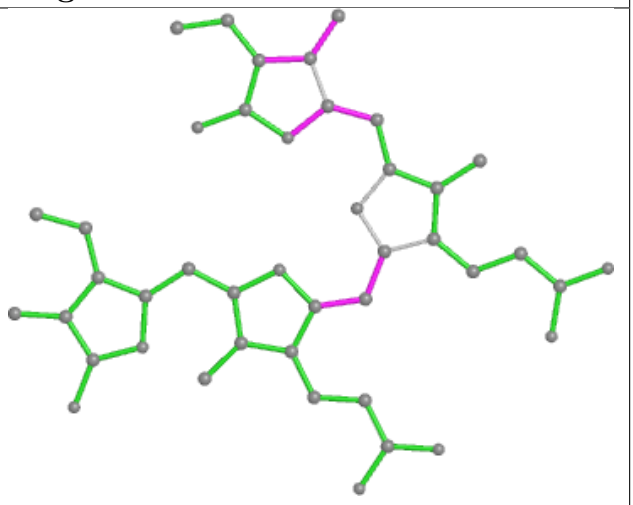

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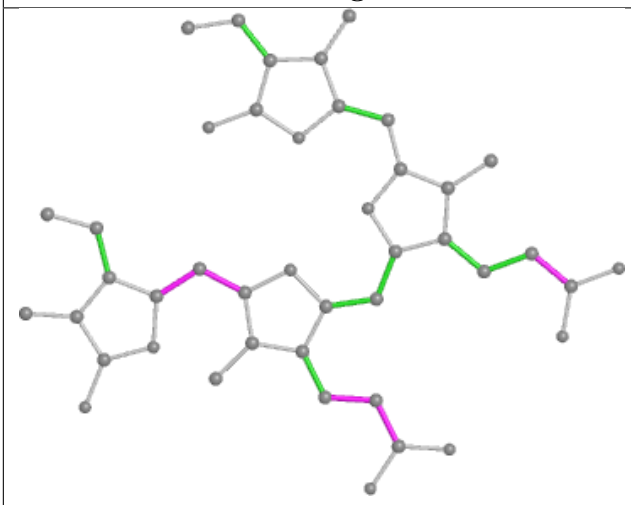

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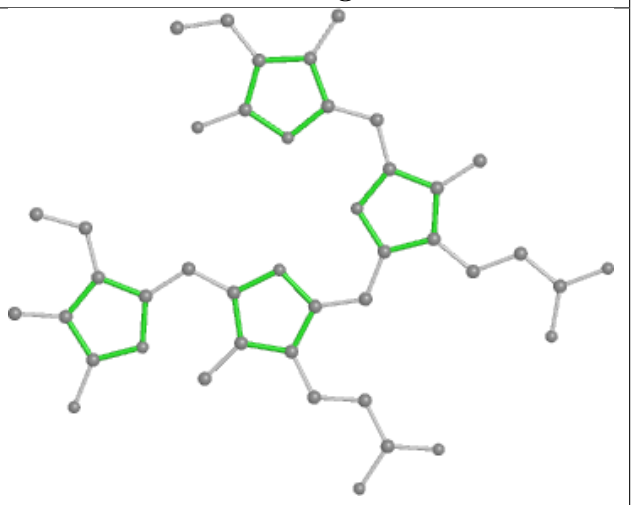

Rings

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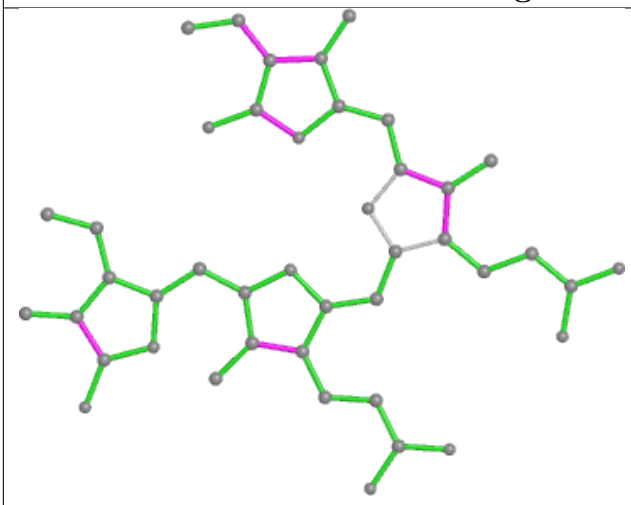

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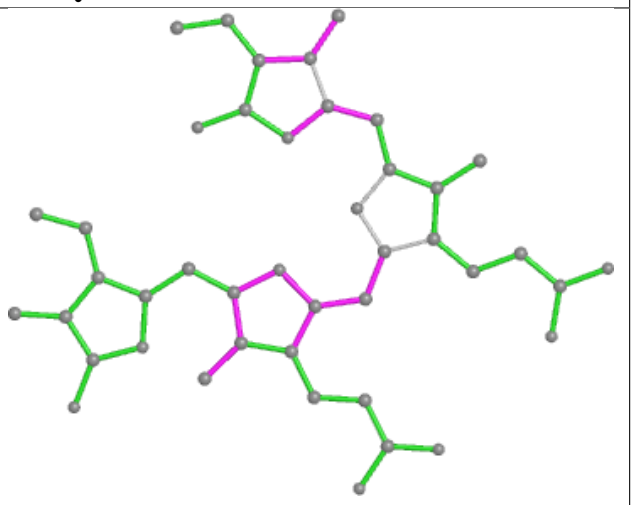

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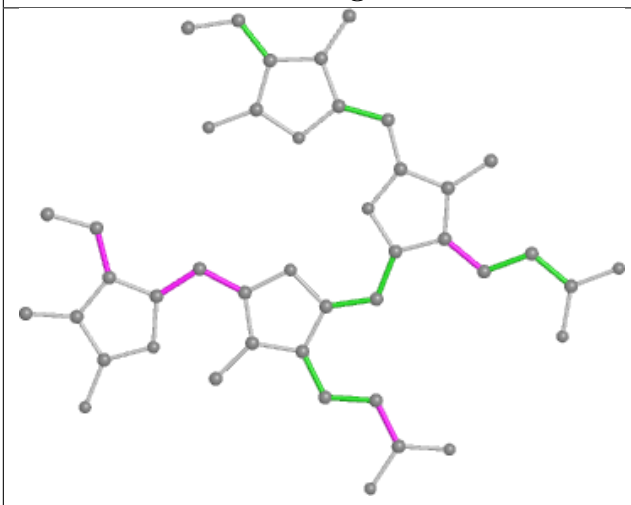

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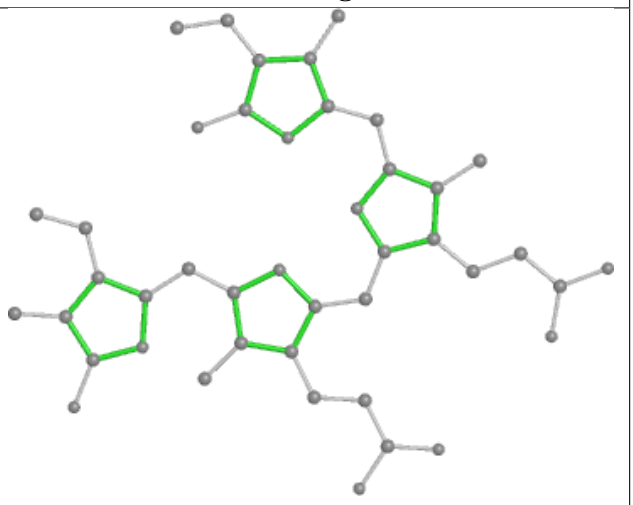

Rings

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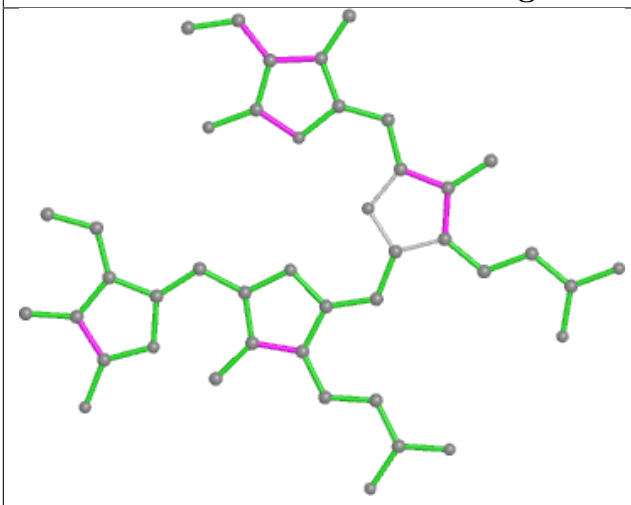

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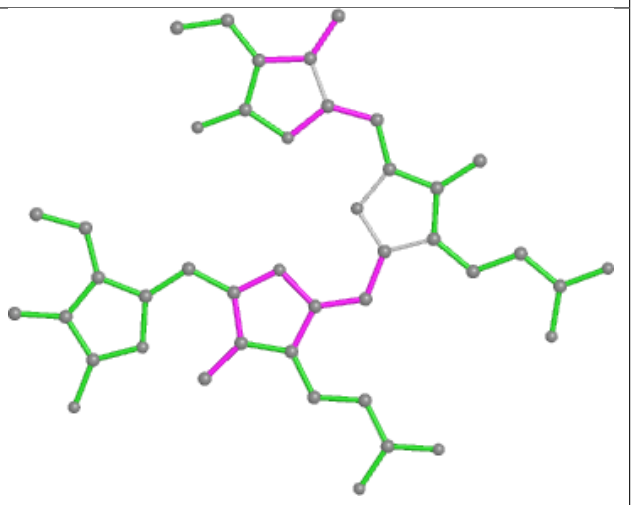

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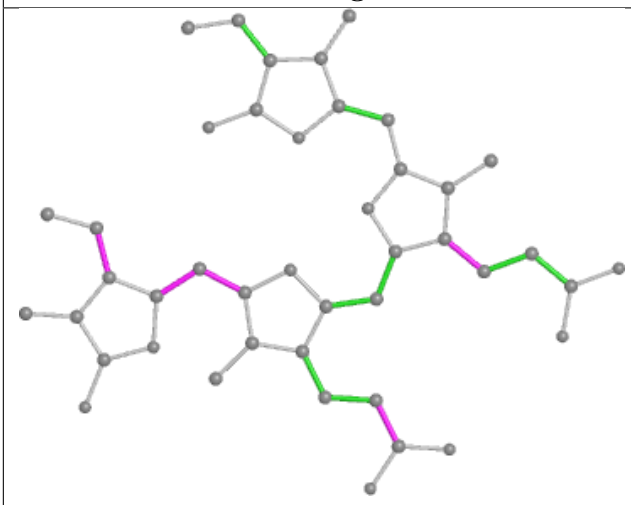

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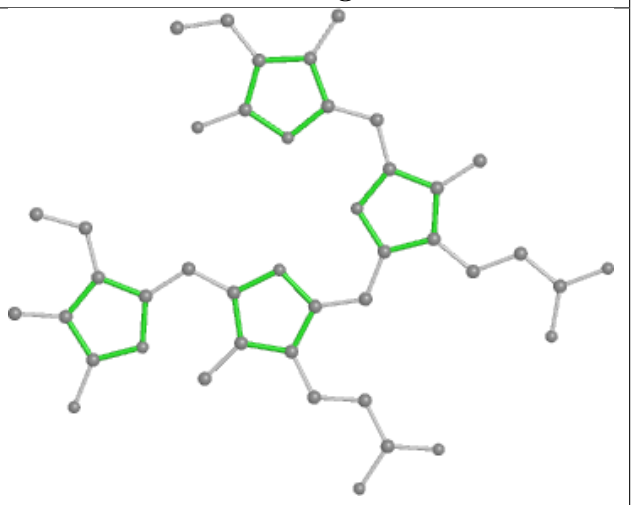
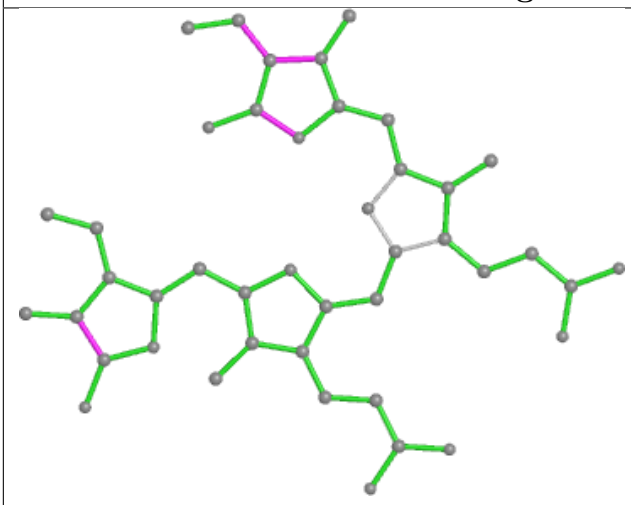


Rings

Ligand PEB cA 201



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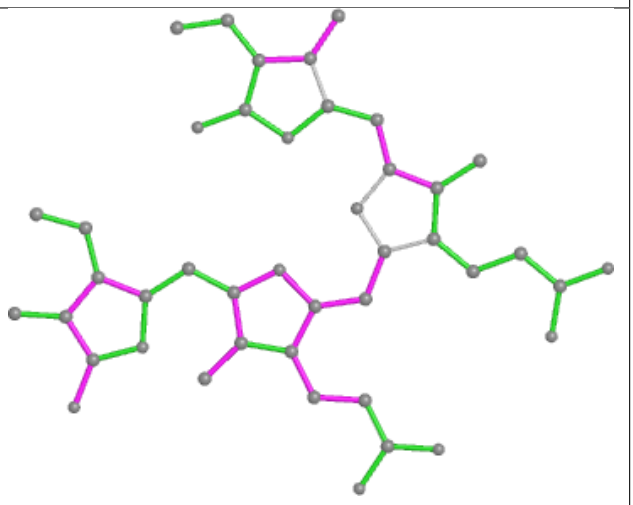

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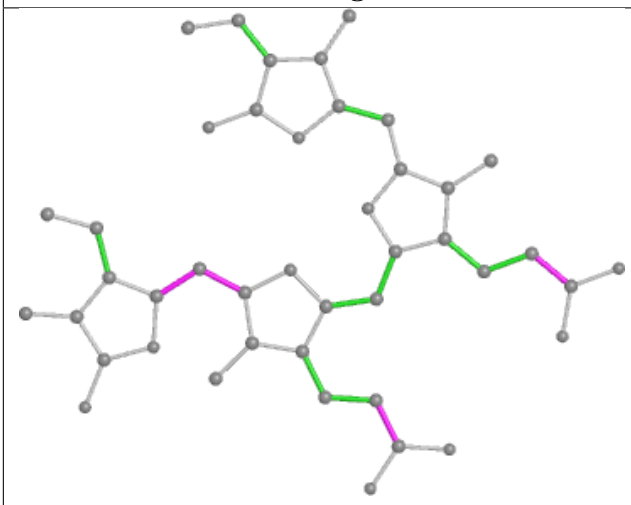

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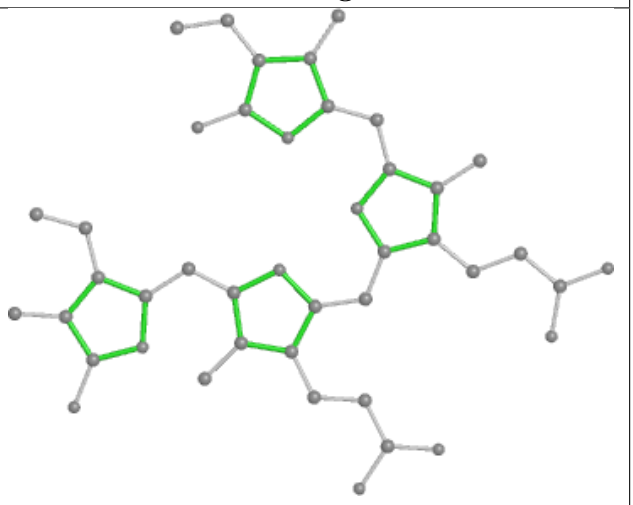

Rings

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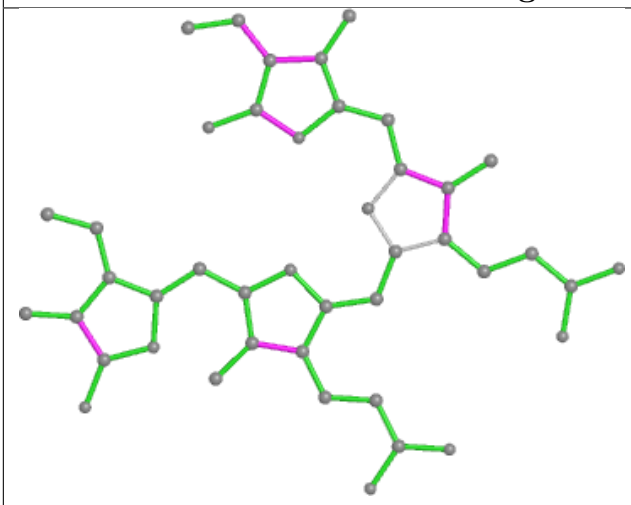

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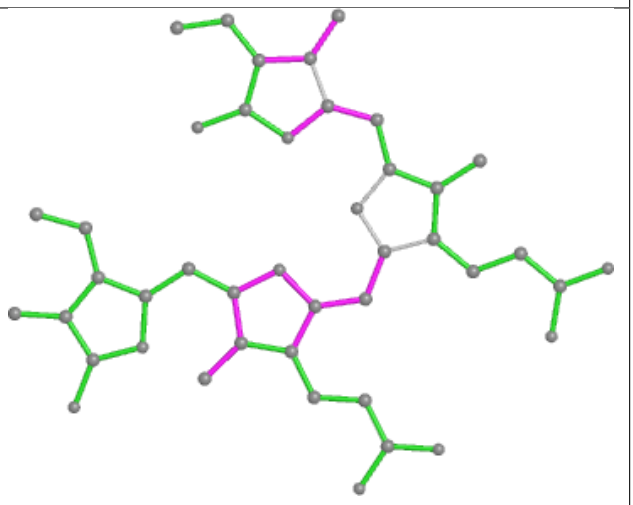

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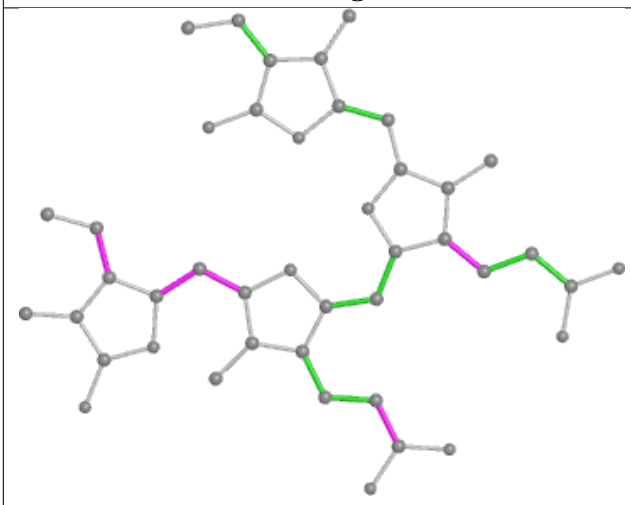

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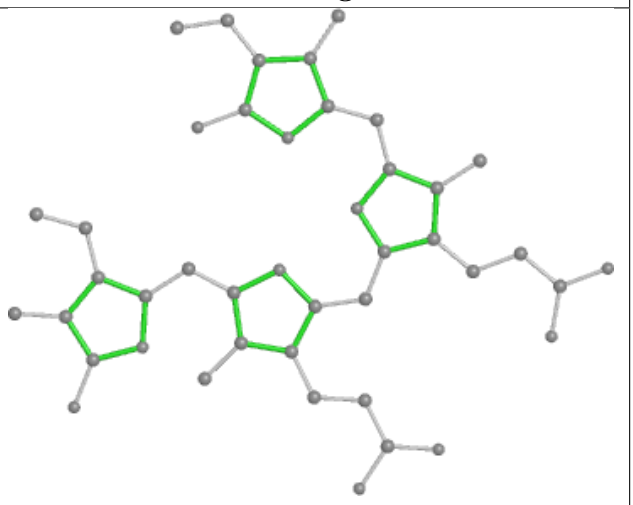

Rings

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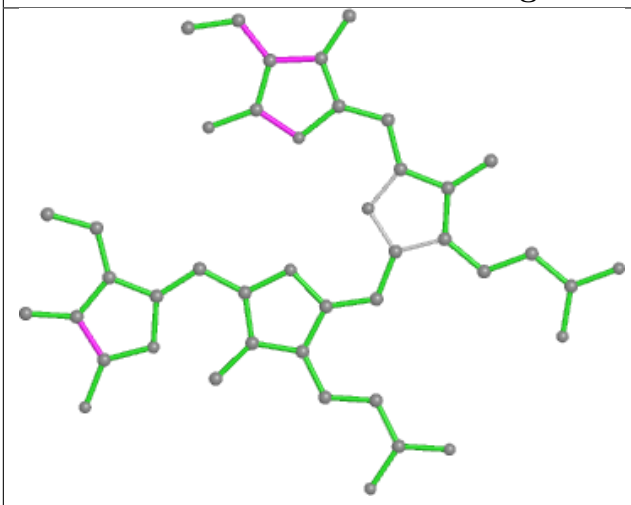

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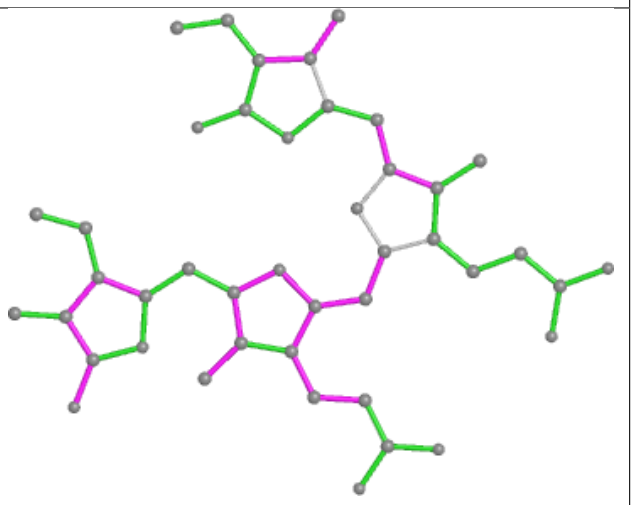

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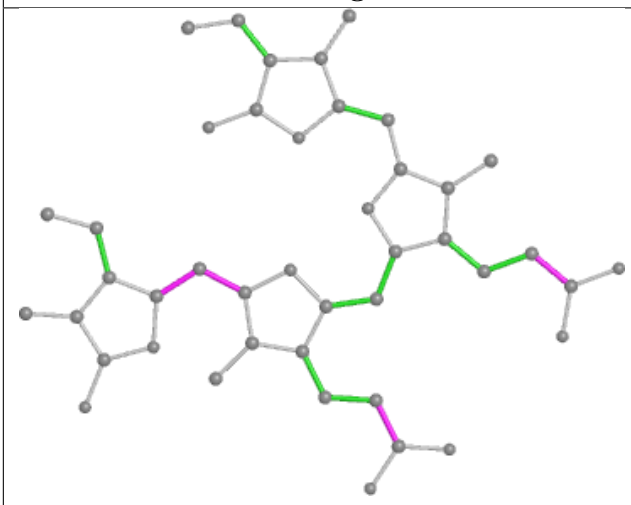

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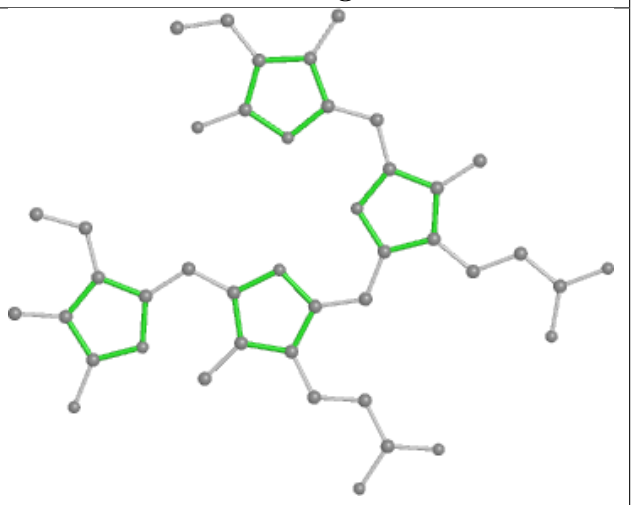
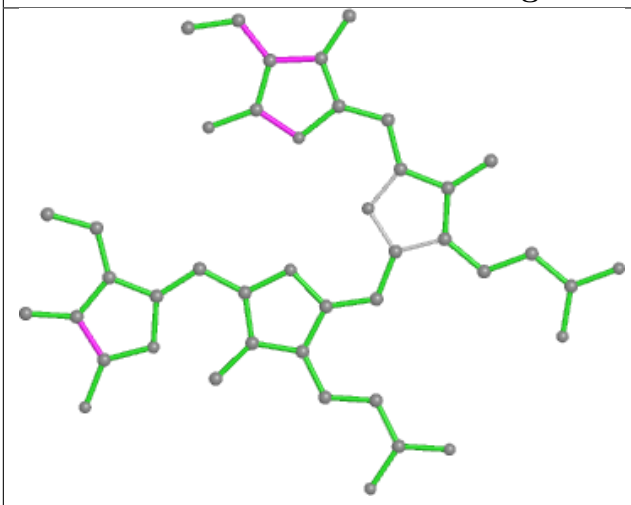


Rings

Ligand PEB r6 201



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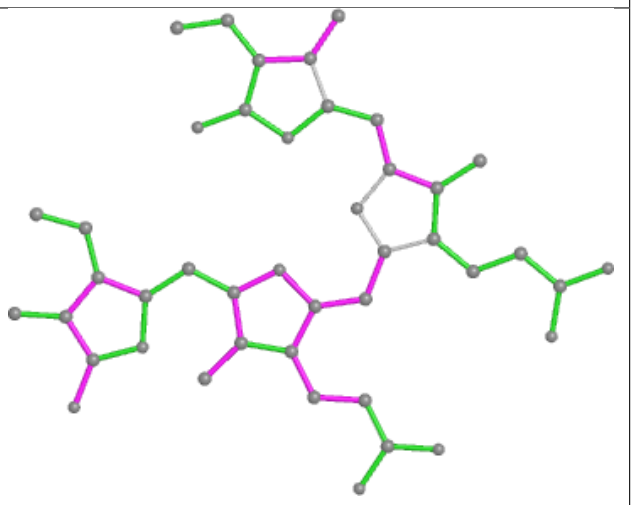

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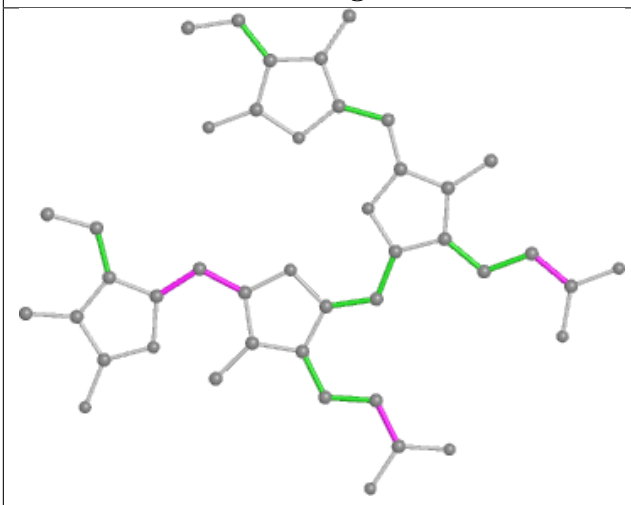

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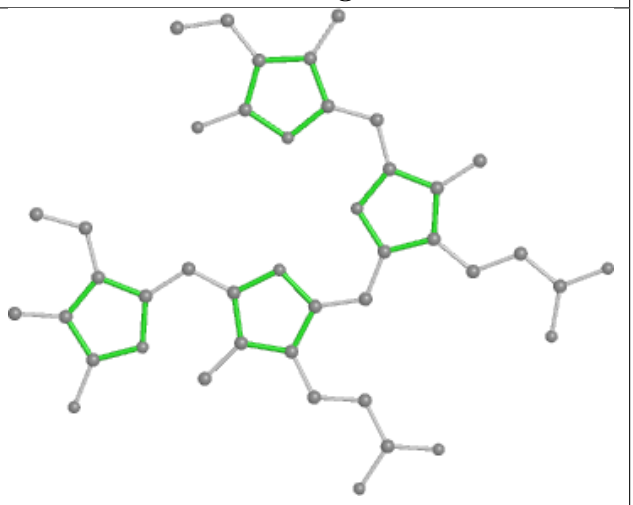
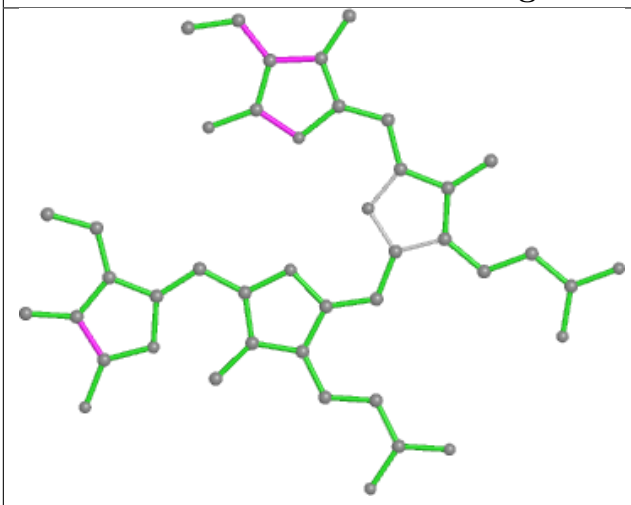


Rings

Ligand PEB h7 201



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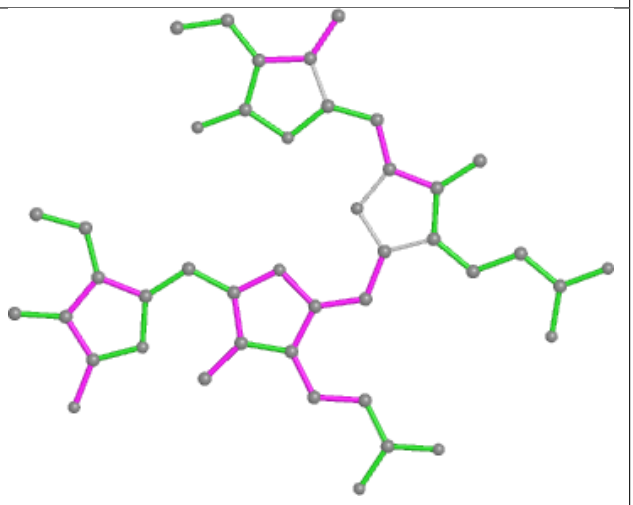

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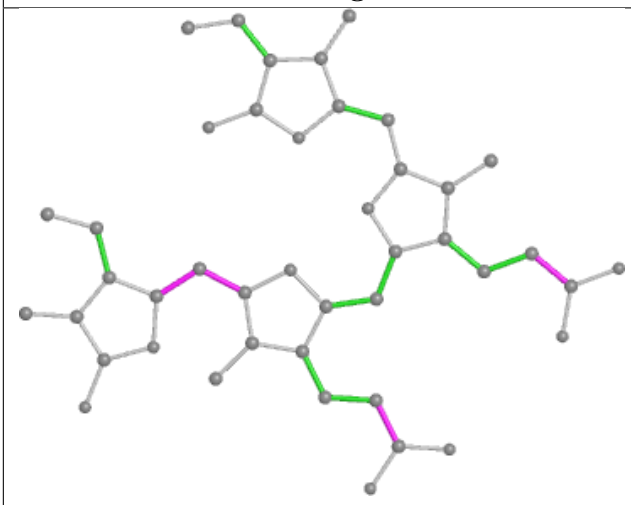

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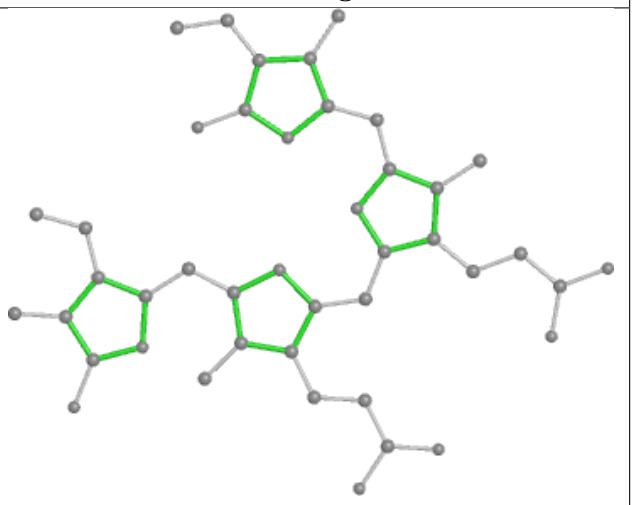
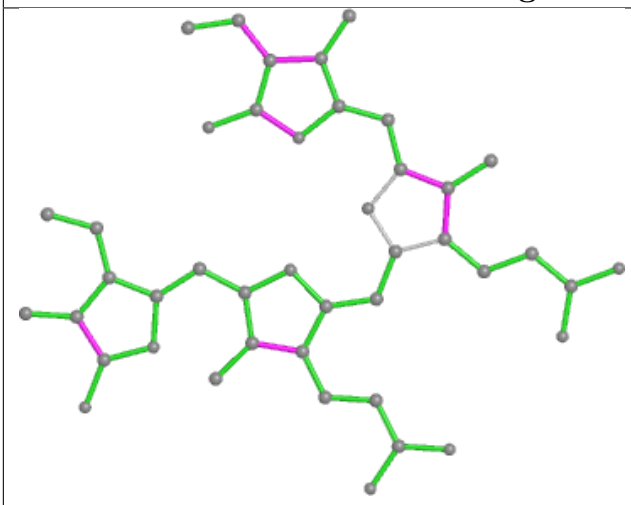


Rings

Ligand PEB n7 202



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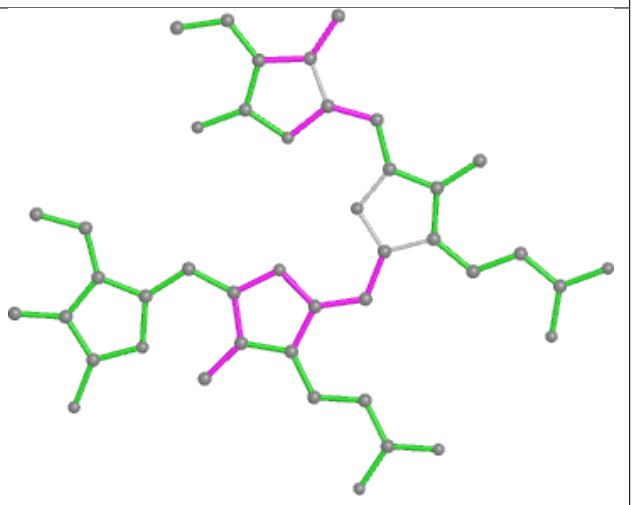

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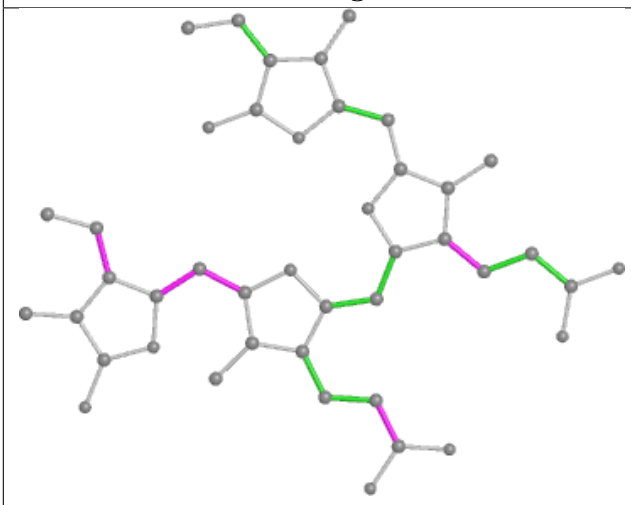

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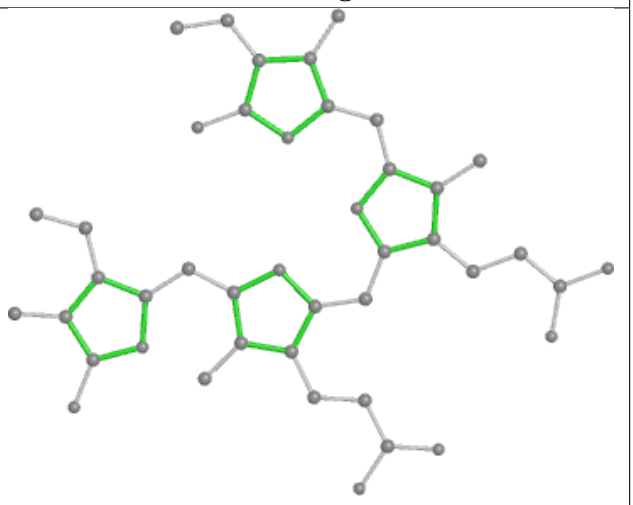
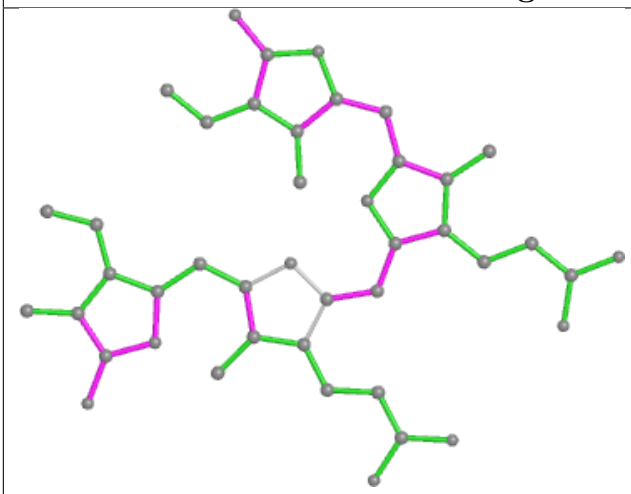


Rings

Ligand PVN gz 304



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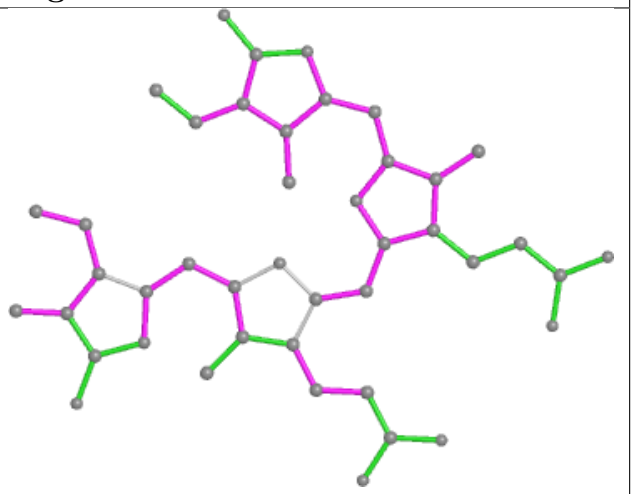
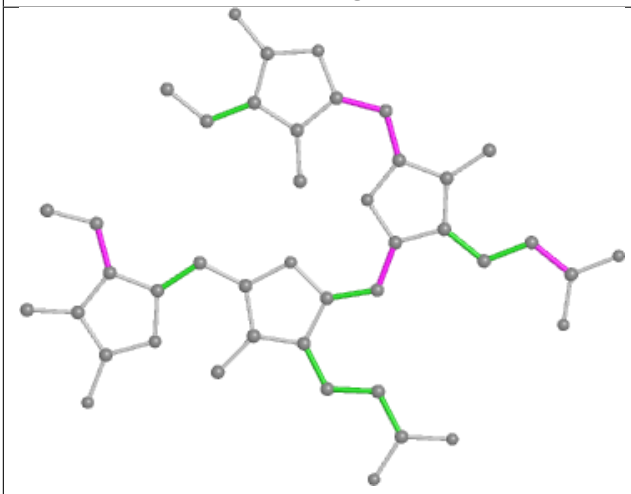
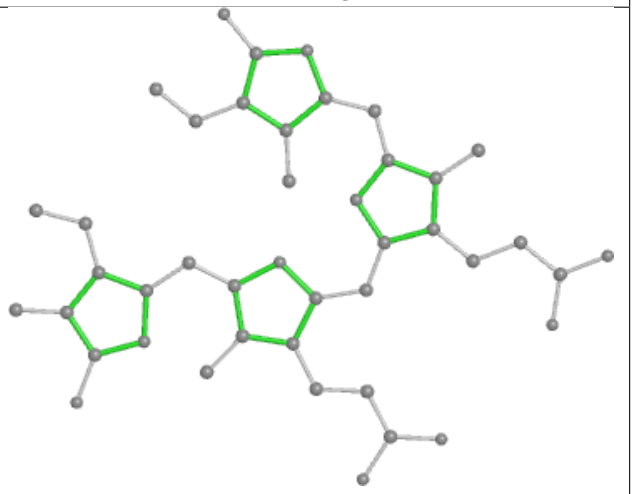


Bond angles

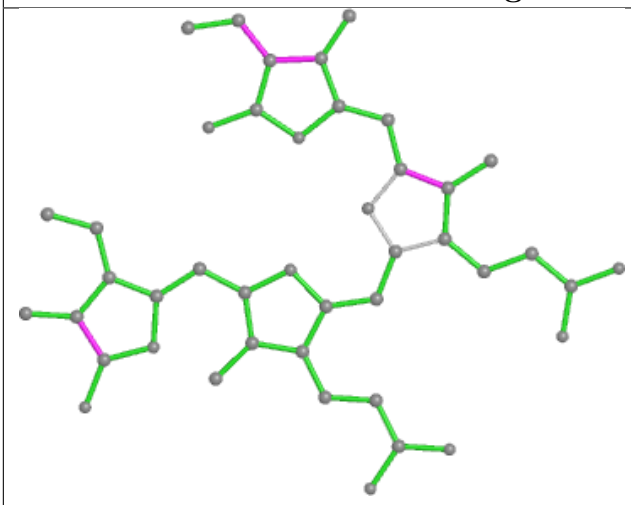


Torsions



Rings

Ligand PEB gm 1002



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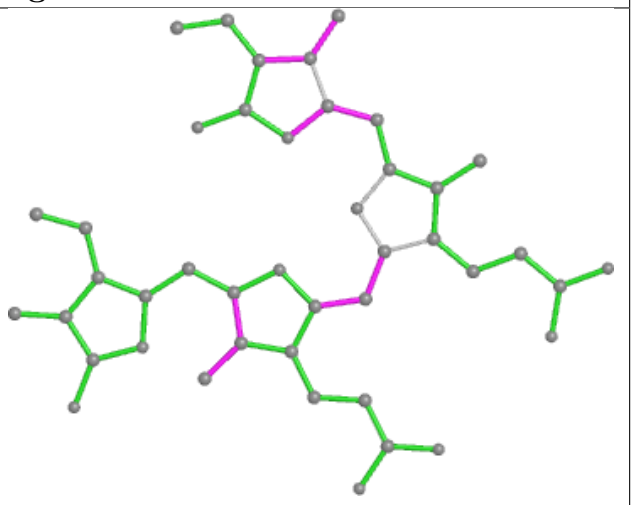

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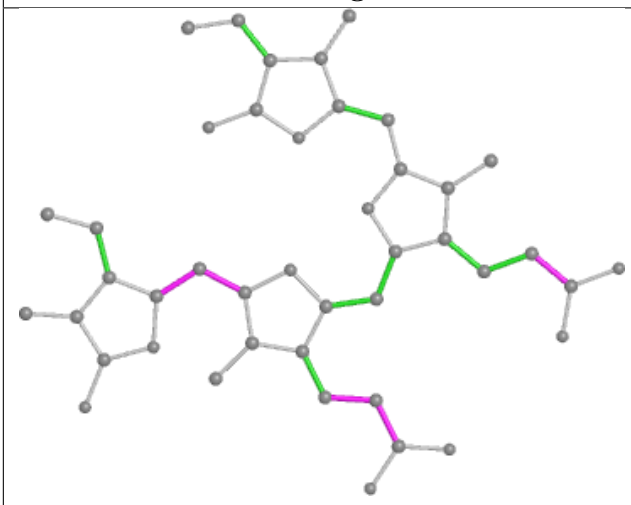

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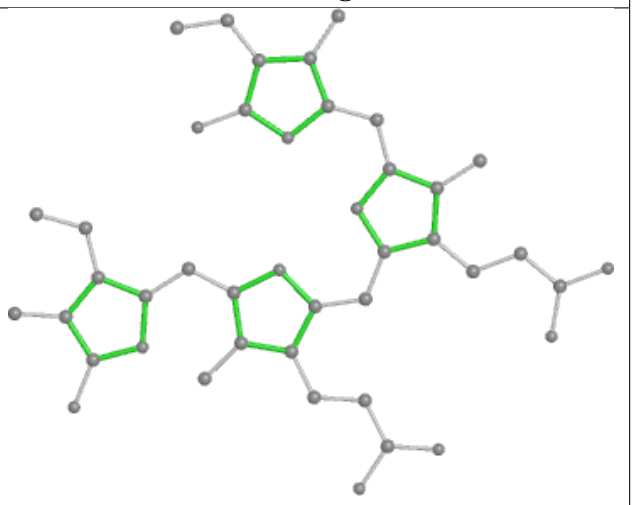
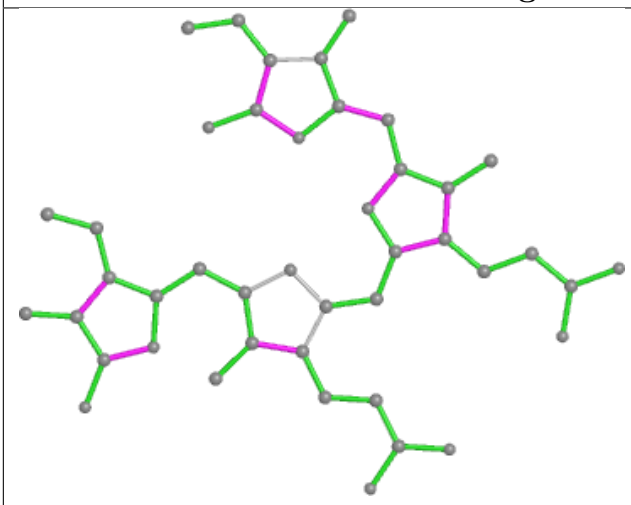


Rings

Ligand PUB c9 304



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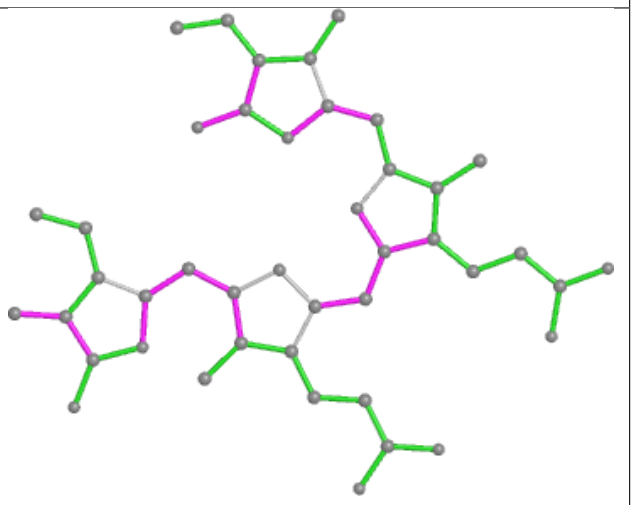

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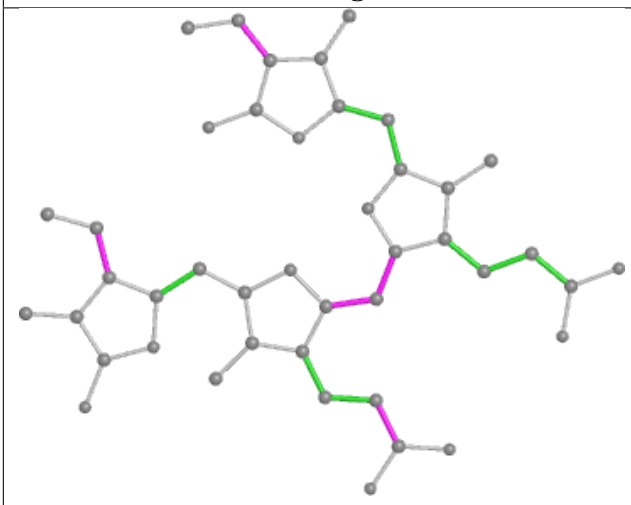

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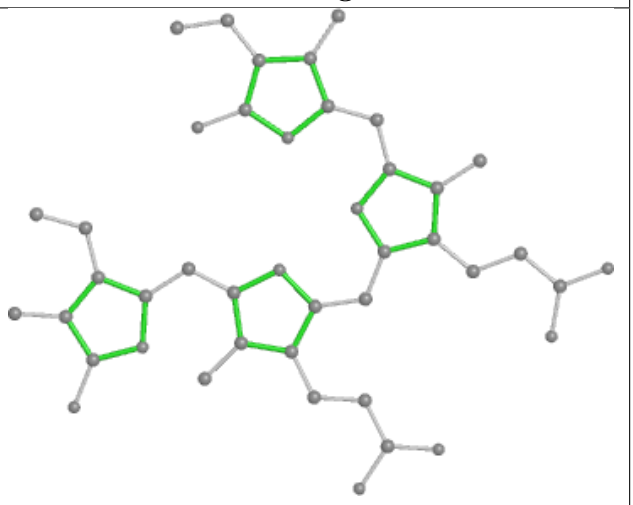
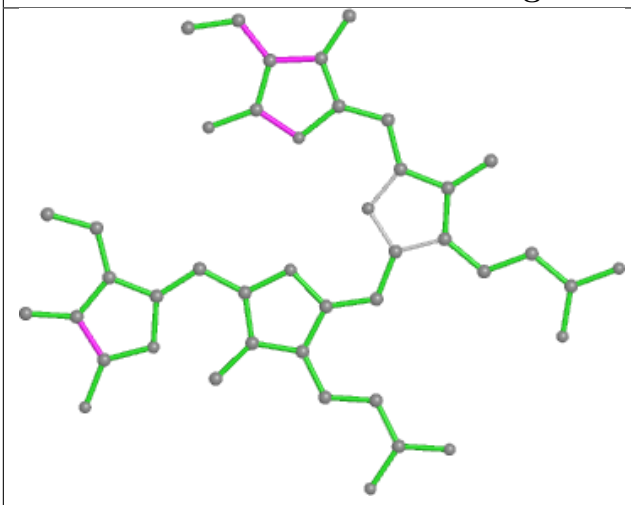


Rings

Ligand PEB ly 401



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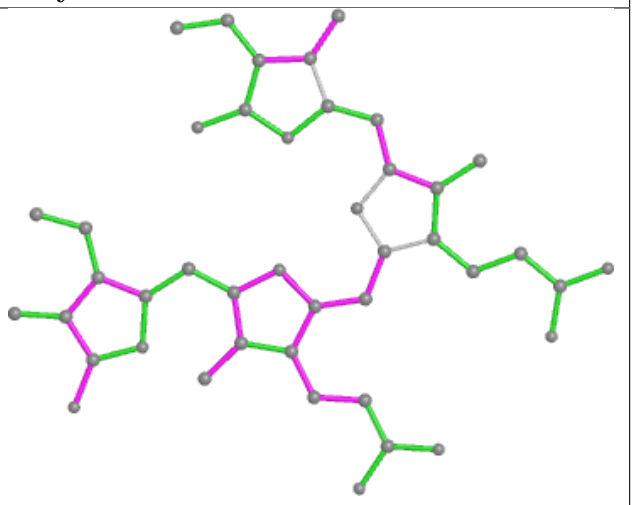
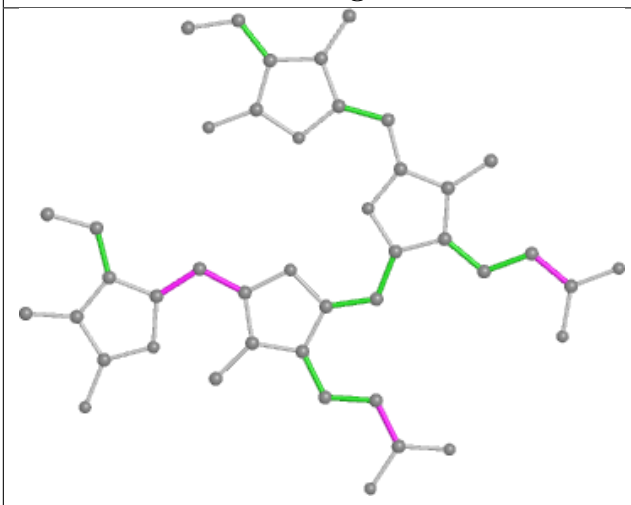


Bond angles



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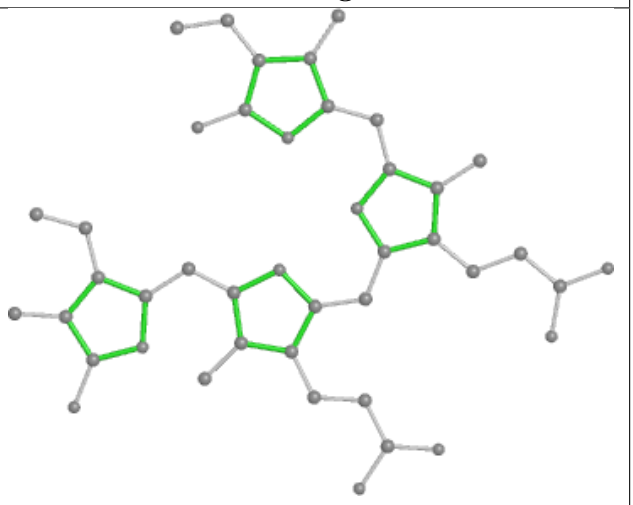
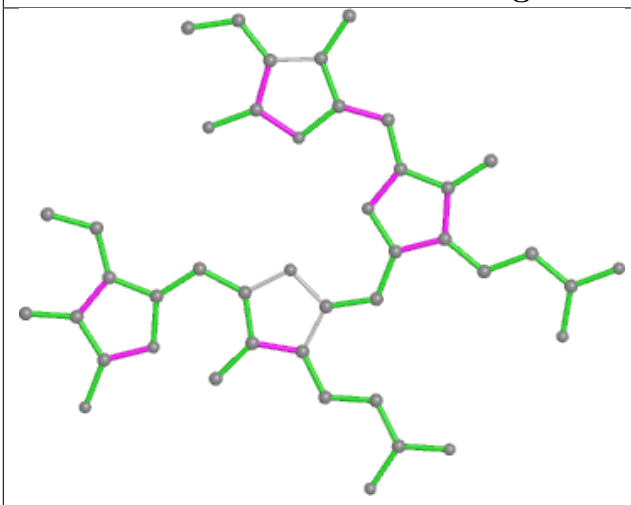


Rings

Ligand PUB H5 202



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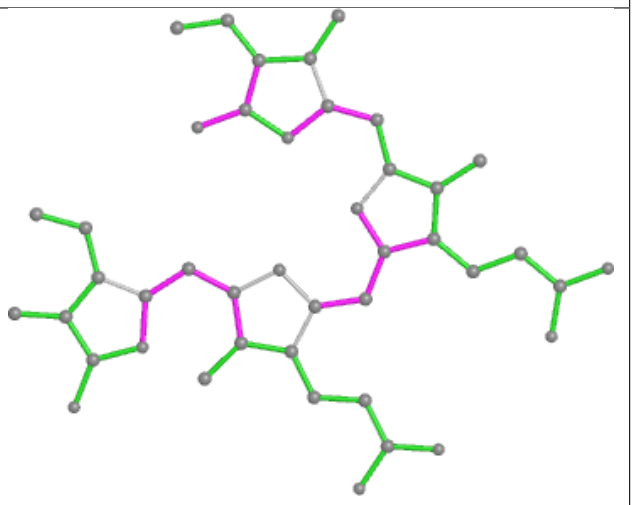

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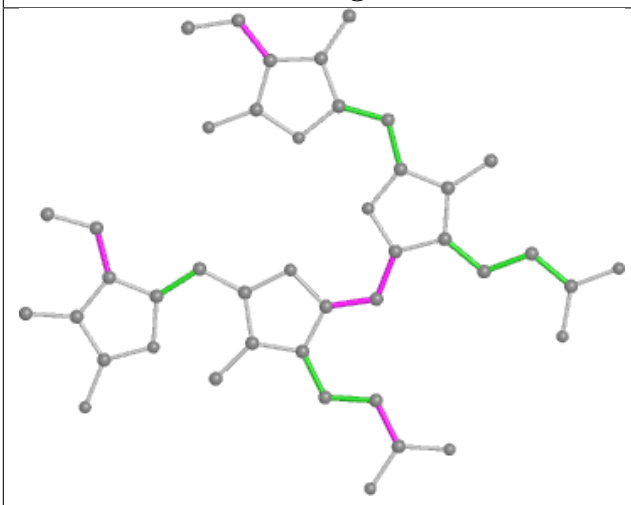

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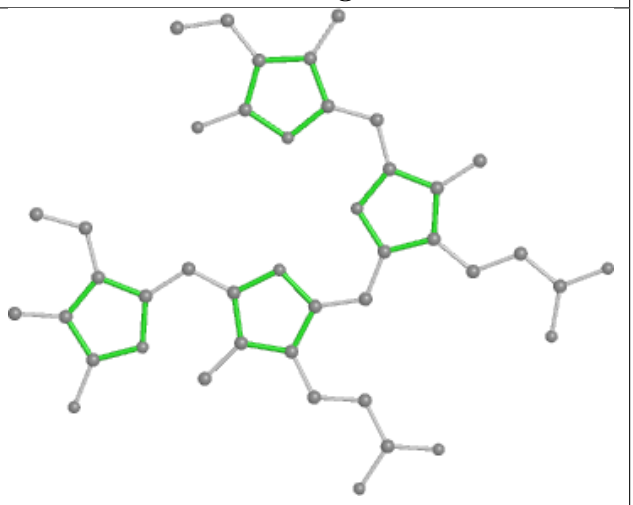
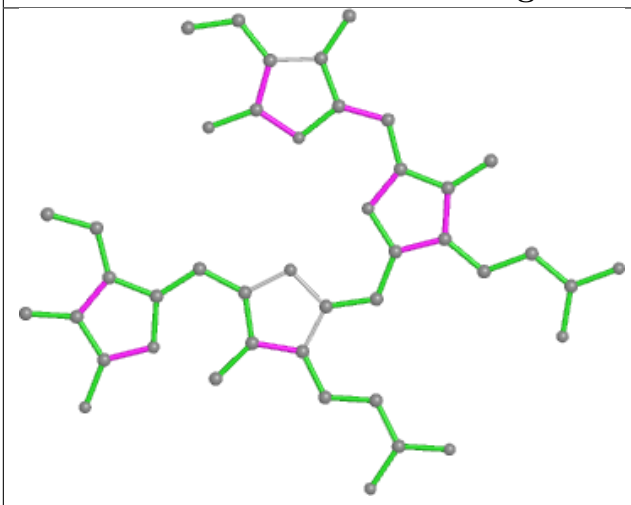


Rings

Ligand PUB v9 203



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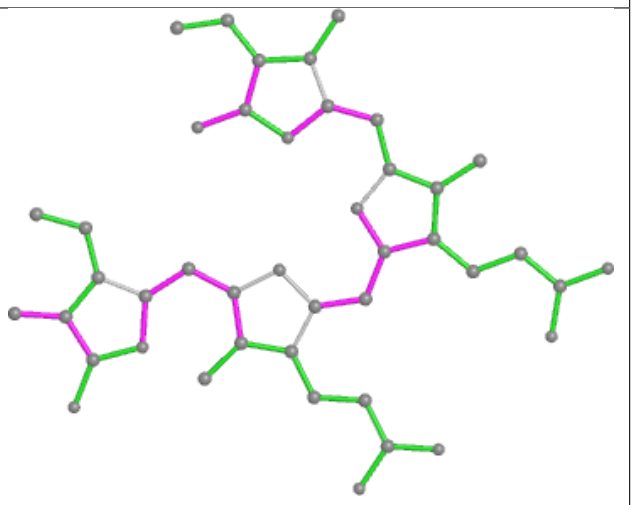

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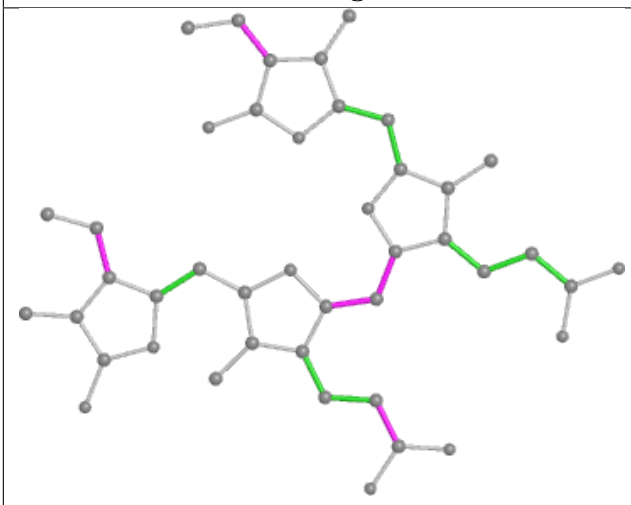

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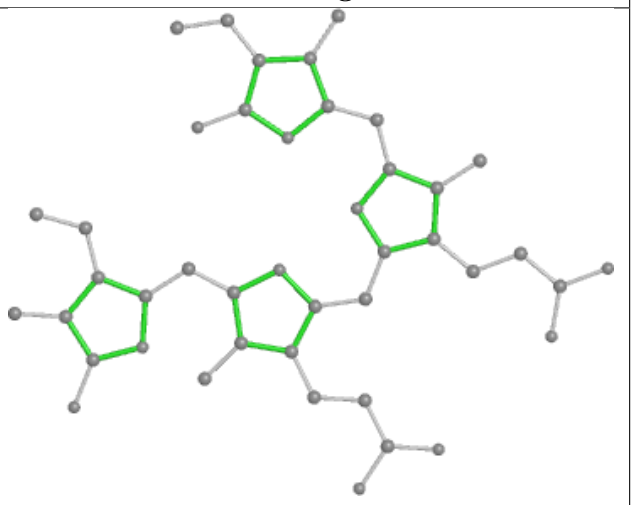
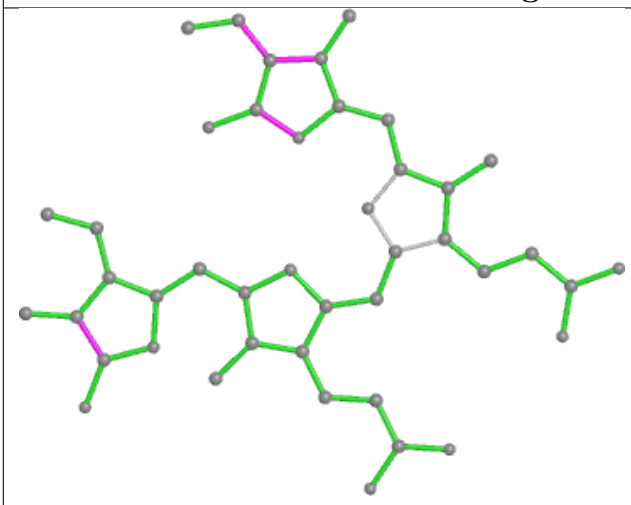


Rings

Ligand PEB t2 202



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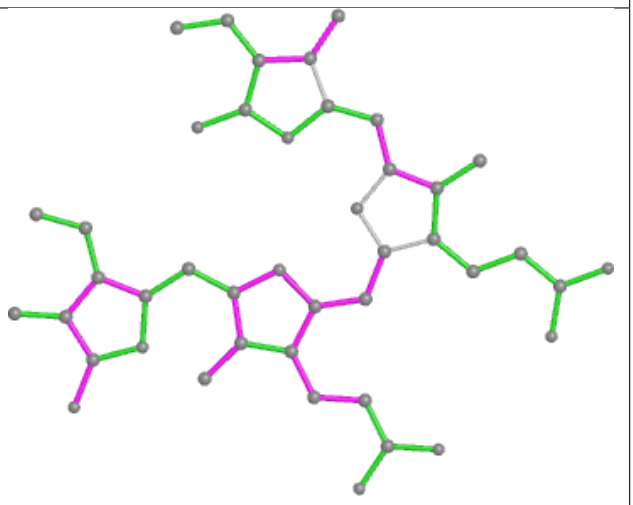

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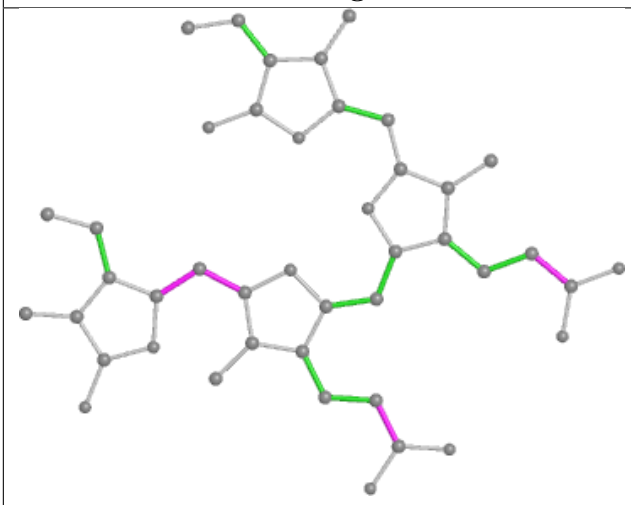

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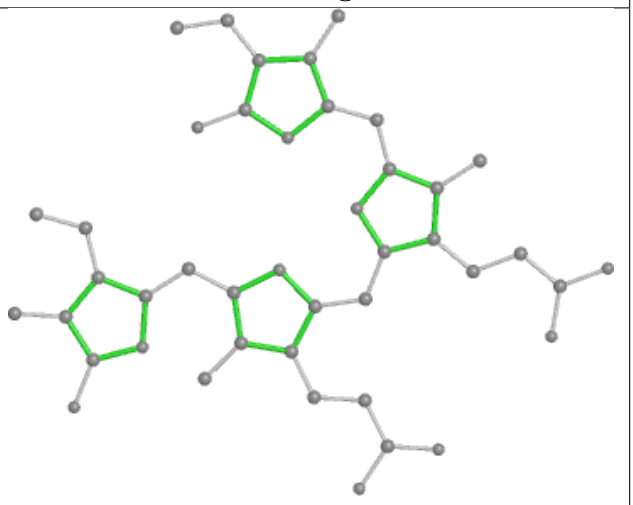
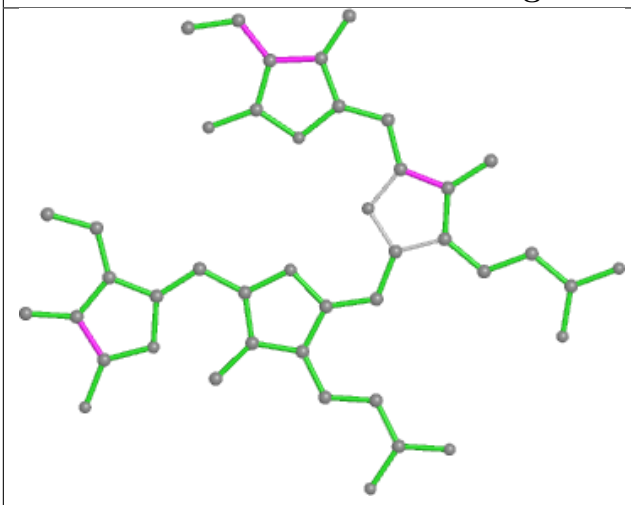


Rings

Ligand PEB gf 202



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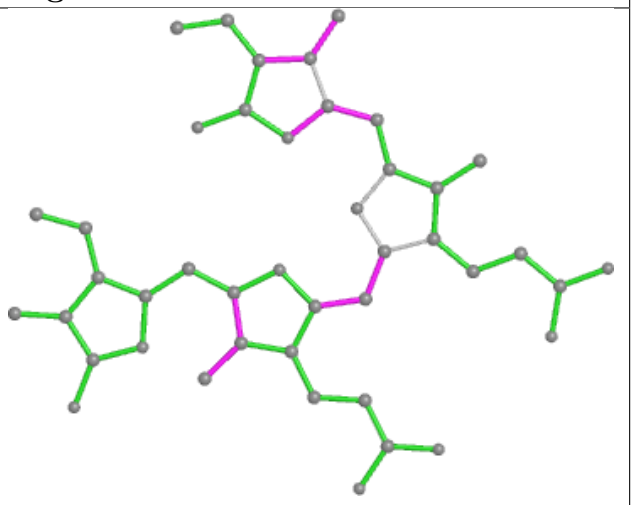

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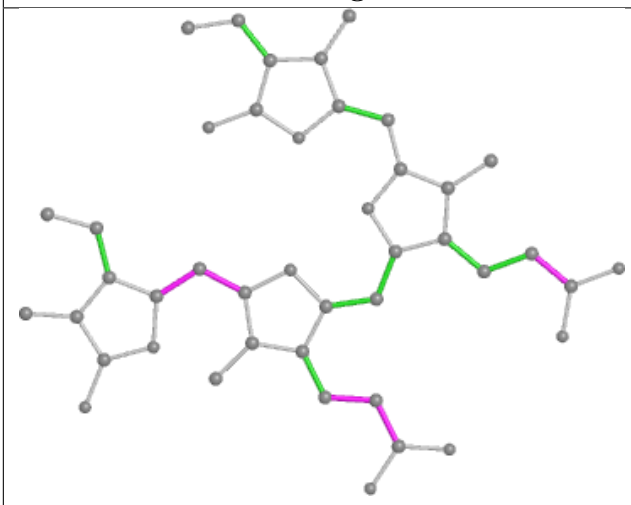

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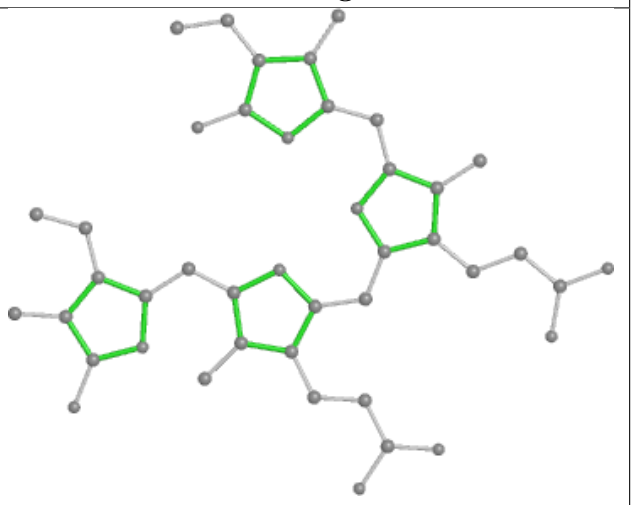
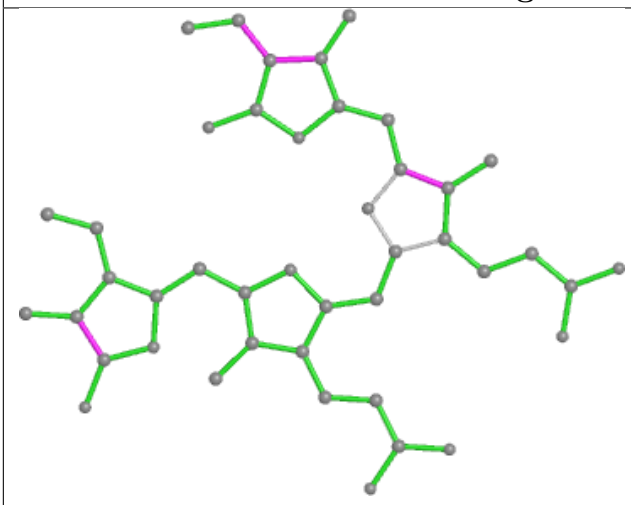


Rings

Ligand PEB bZ 302



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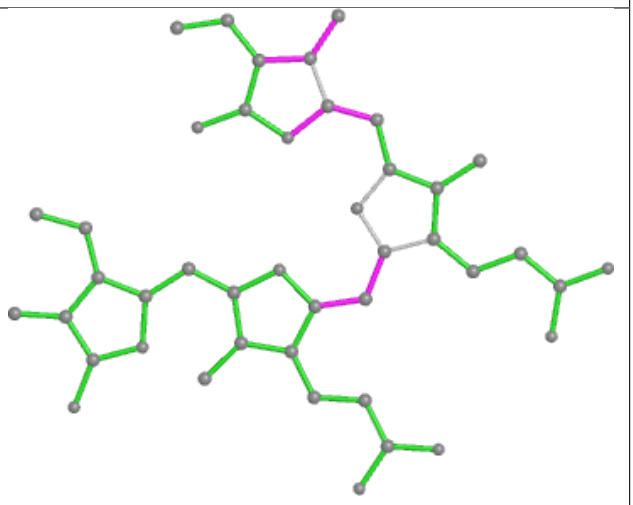
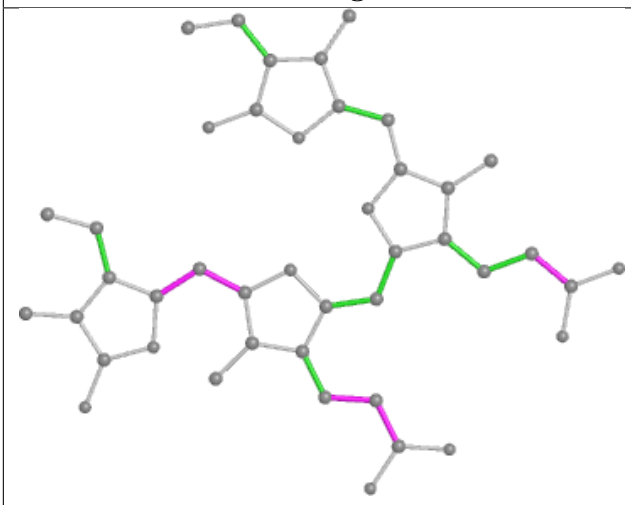


Bond angles



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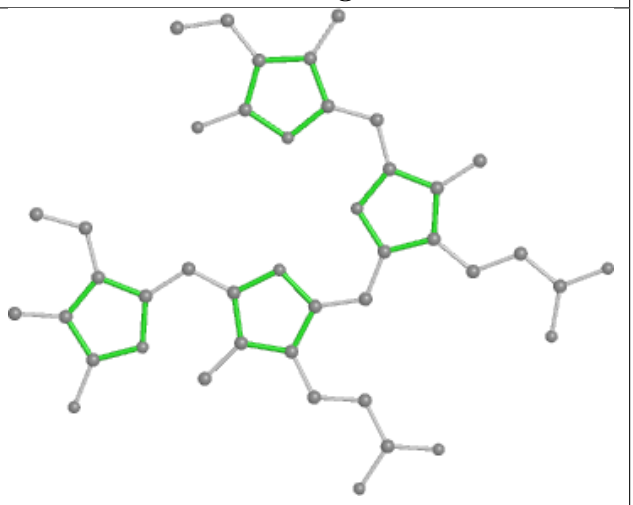

Rings

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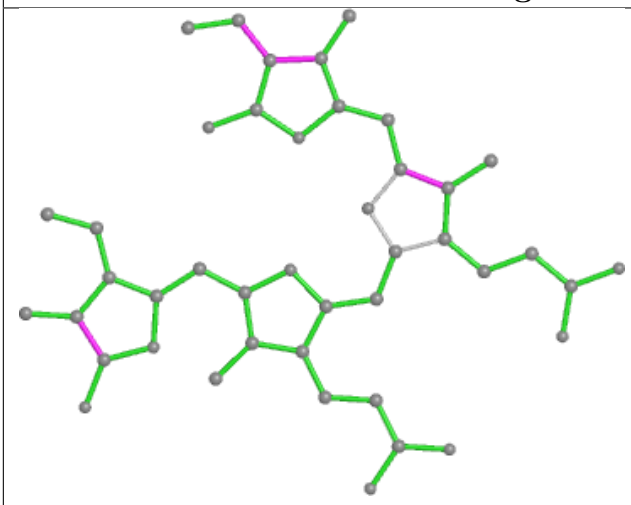

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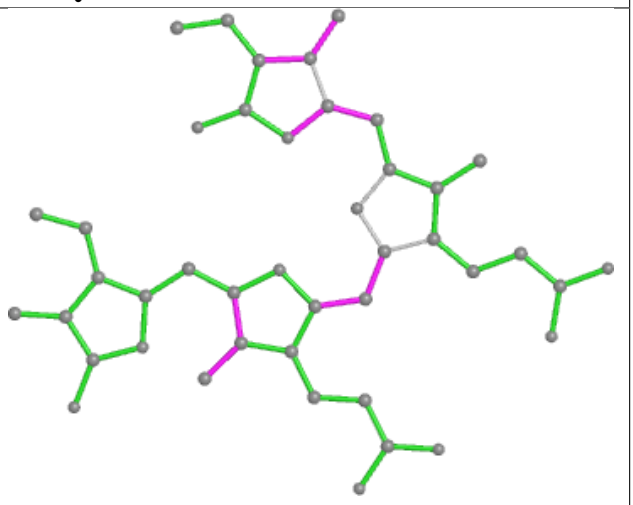

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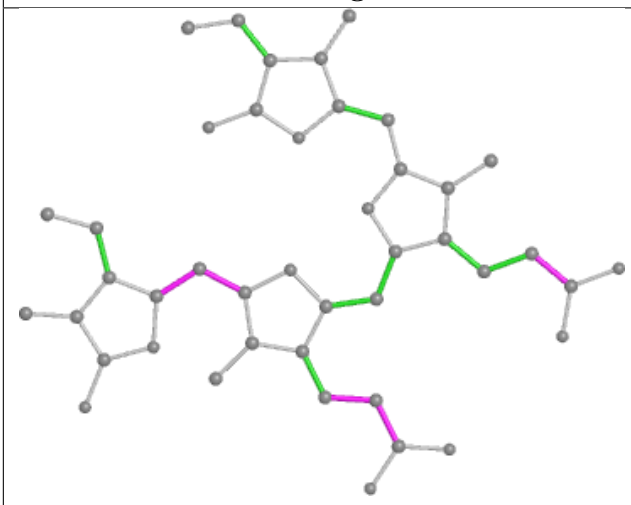

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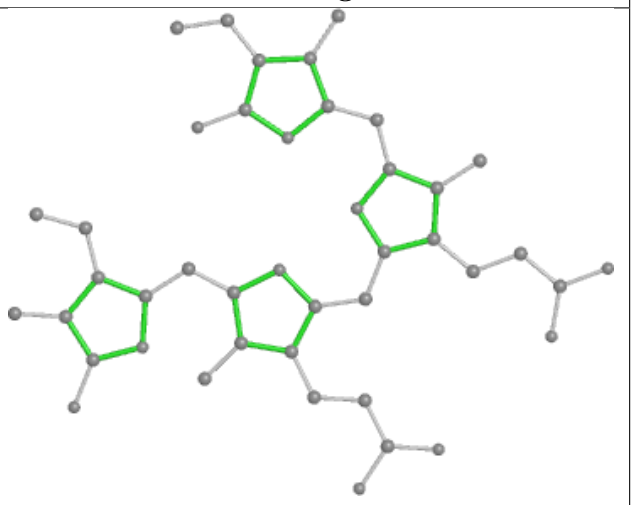
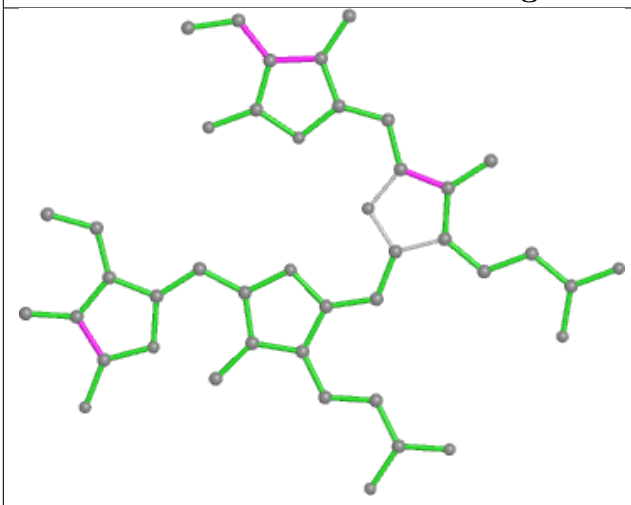


Rings

Ligand PEB c5 201



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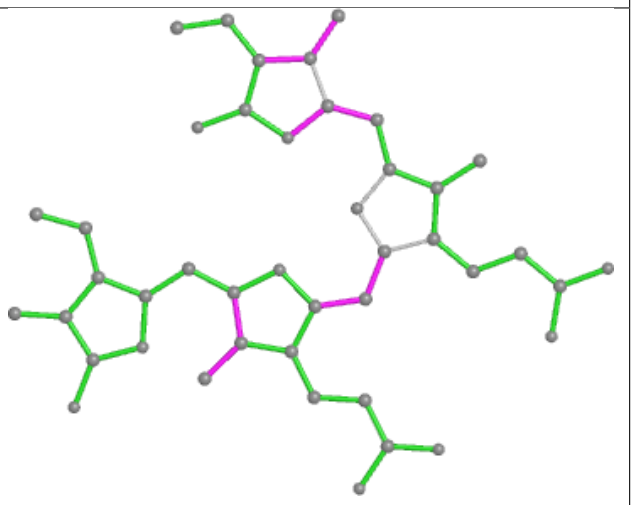

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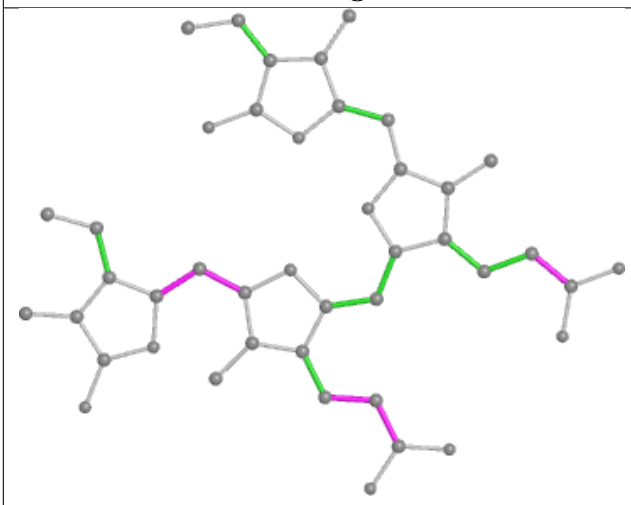

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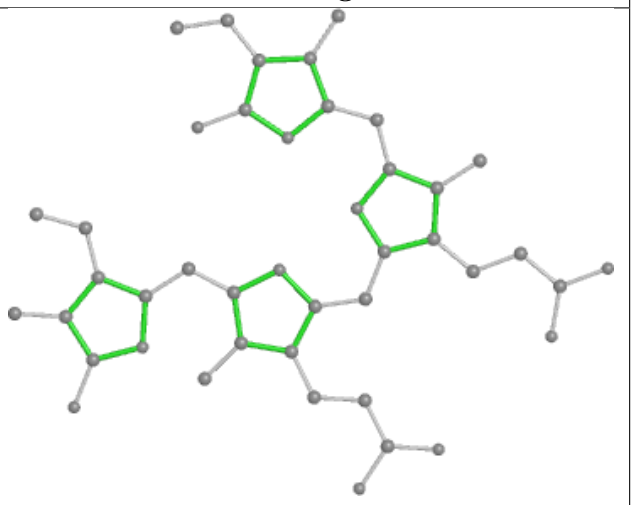
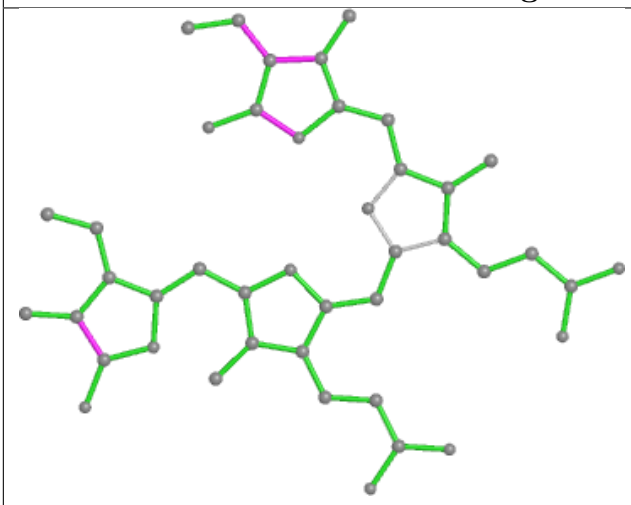


Rings

Ligand PEB c9 301



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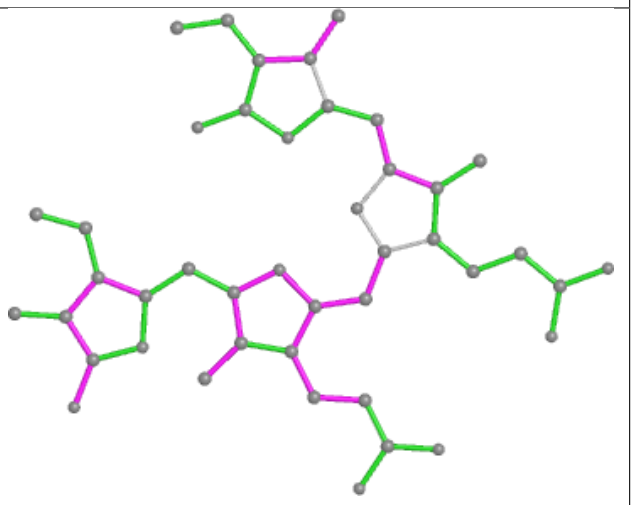
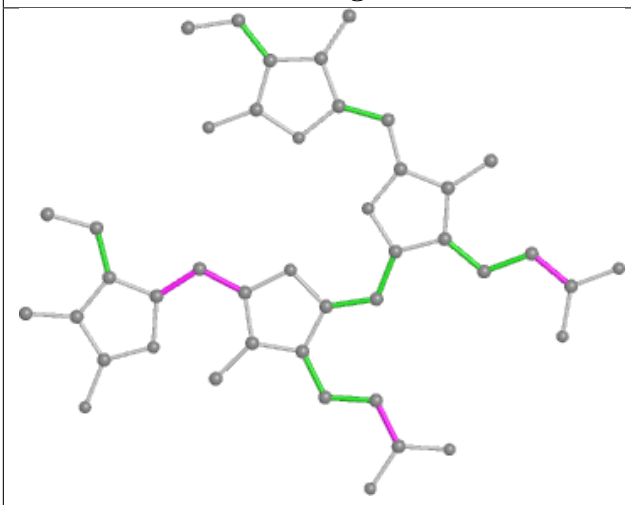


Bond angles



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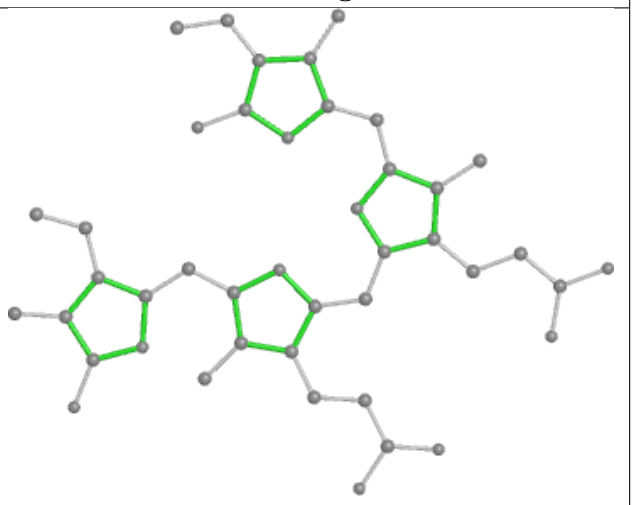
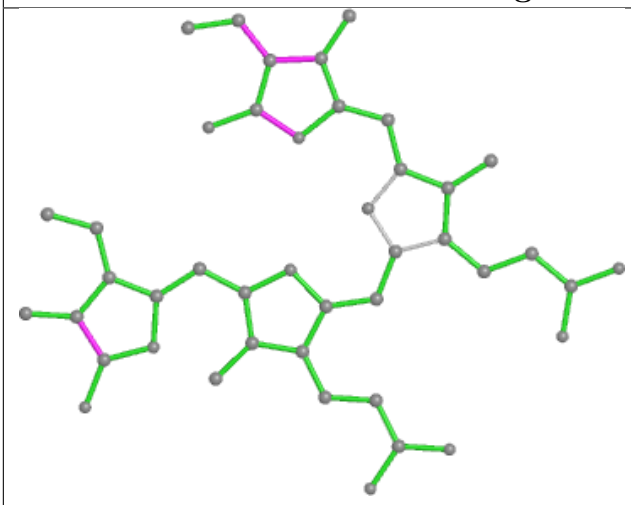


Rings

Ligand PEB bA 201



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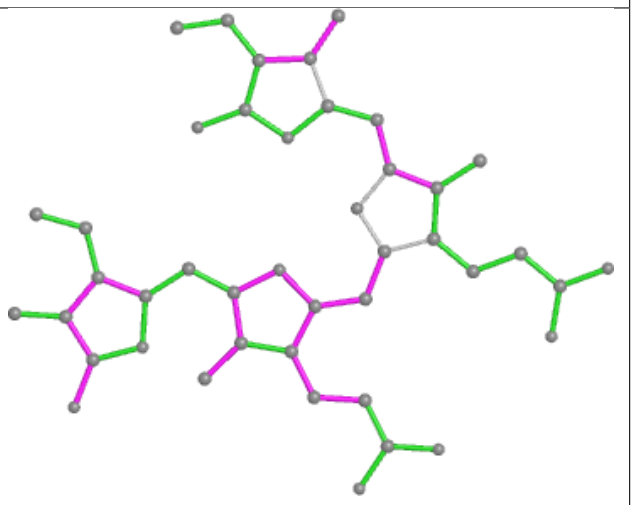
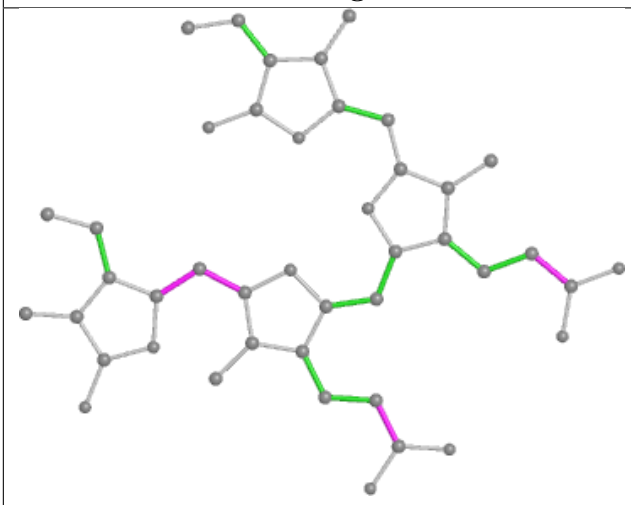


Bond angles



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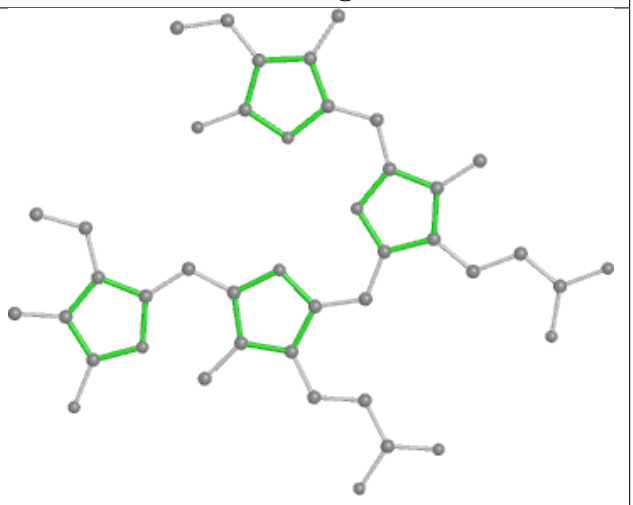
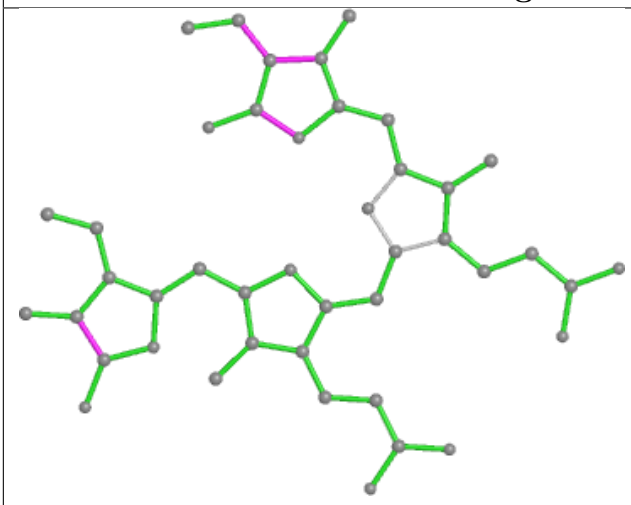


Rings

Ligand PEB bB 201



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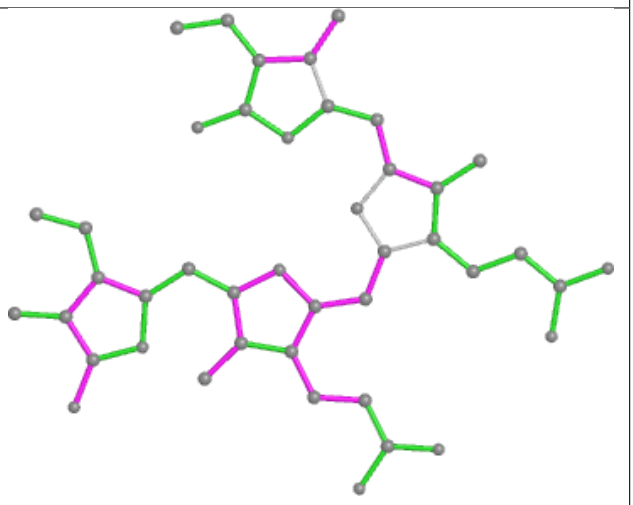
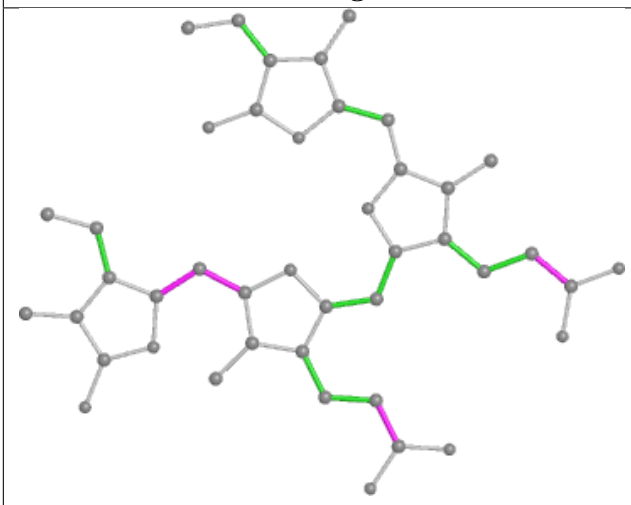
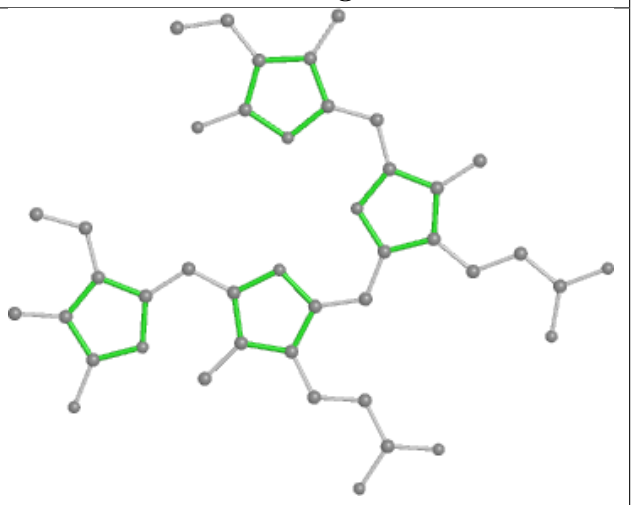


Bond angles

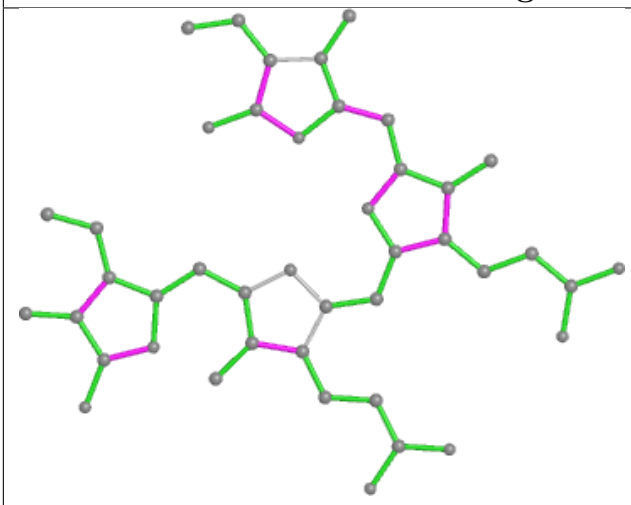


Torsions



Rings

Ligand PUB gn 203



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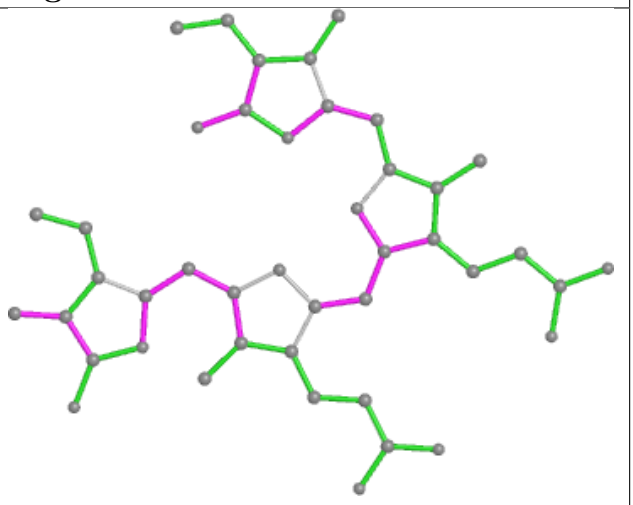

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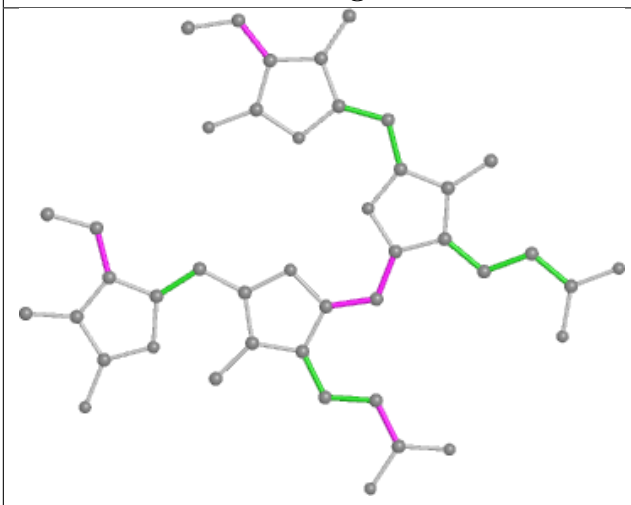

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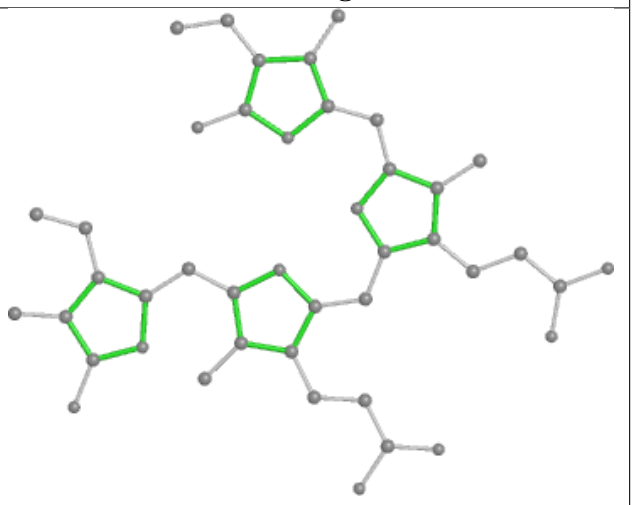
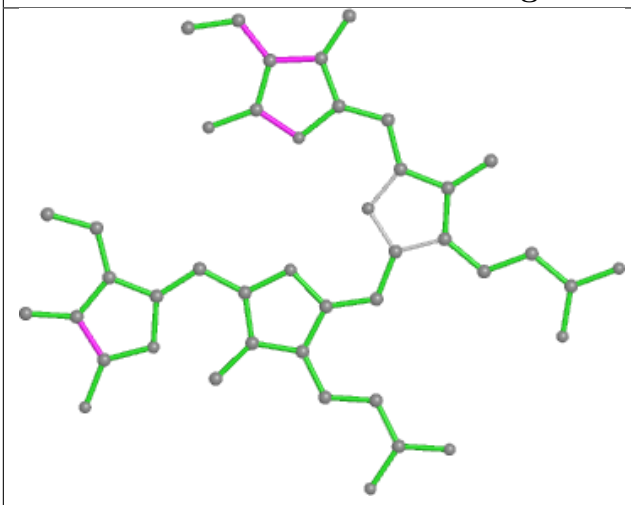


Rings

Ligand PEB bt 202



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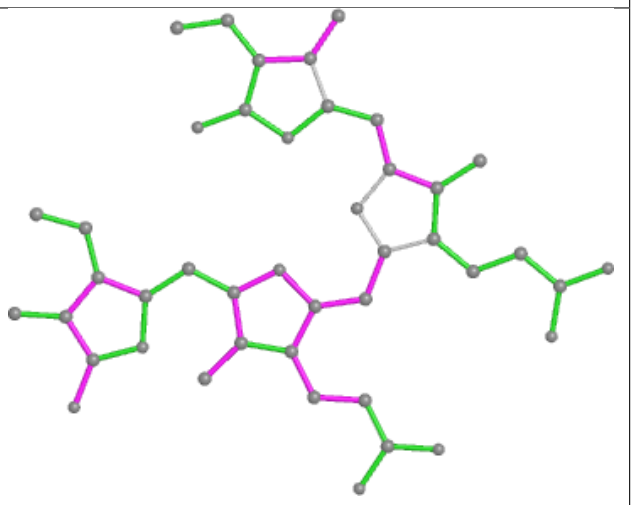

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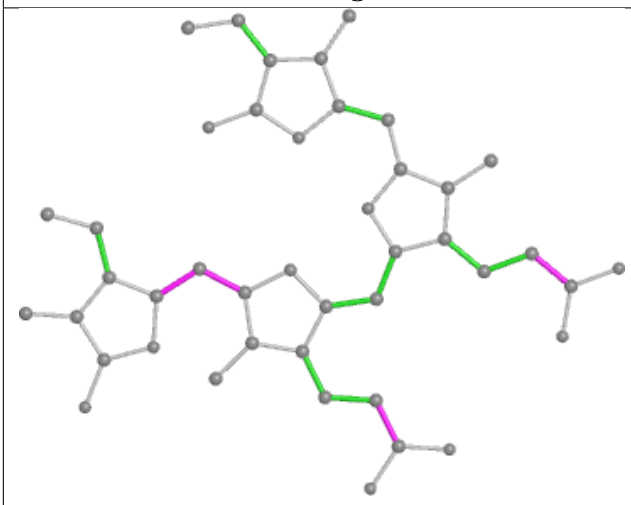

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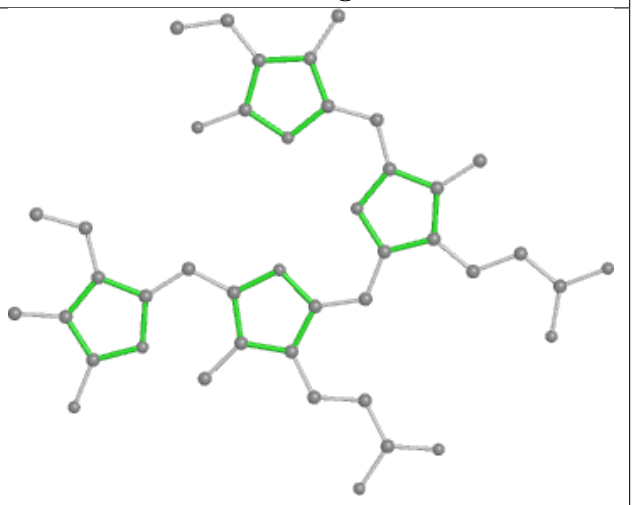
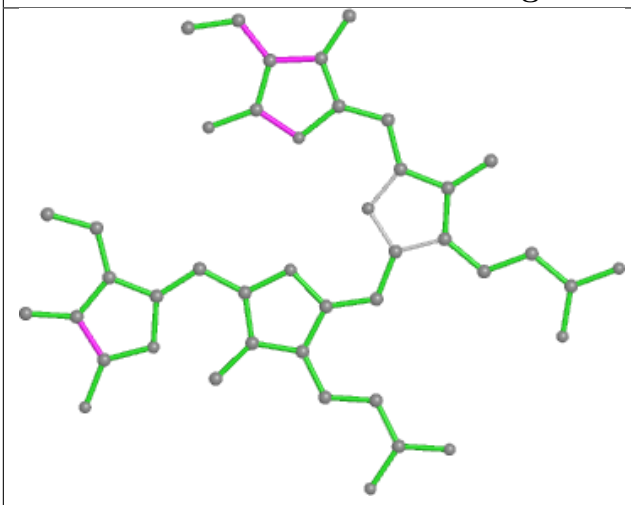


Rings

Ligand PEB s7 201



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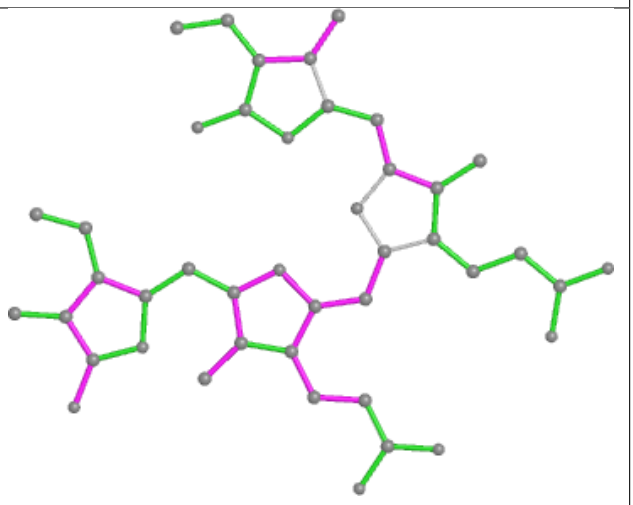

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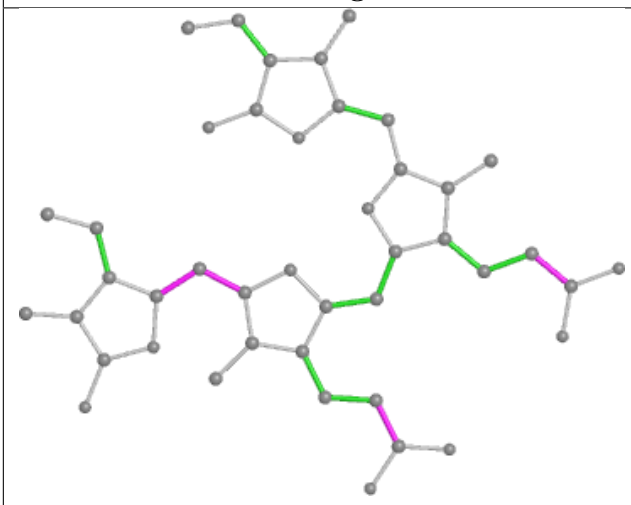

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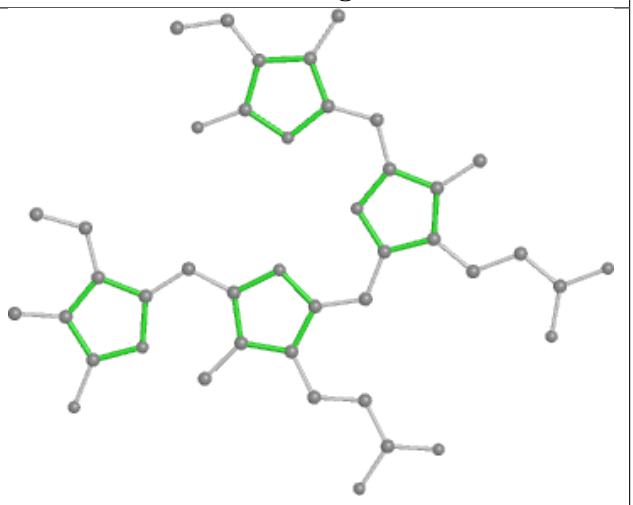
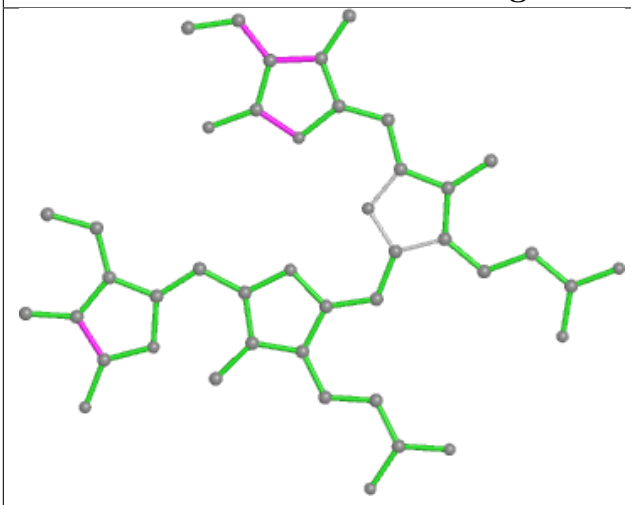


Rings

Ligand PEB jN 1001



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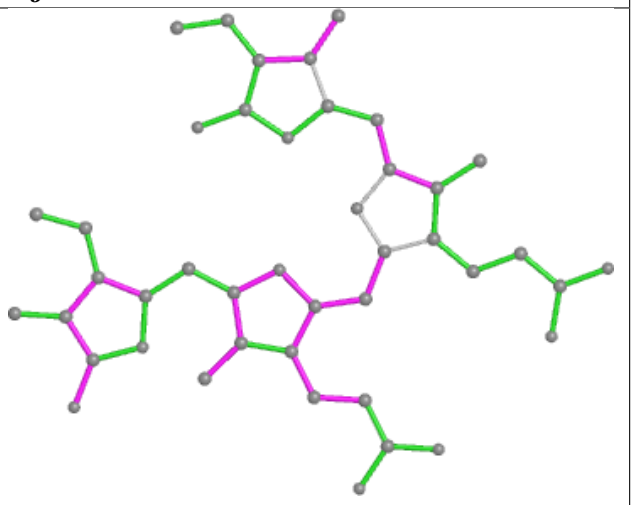

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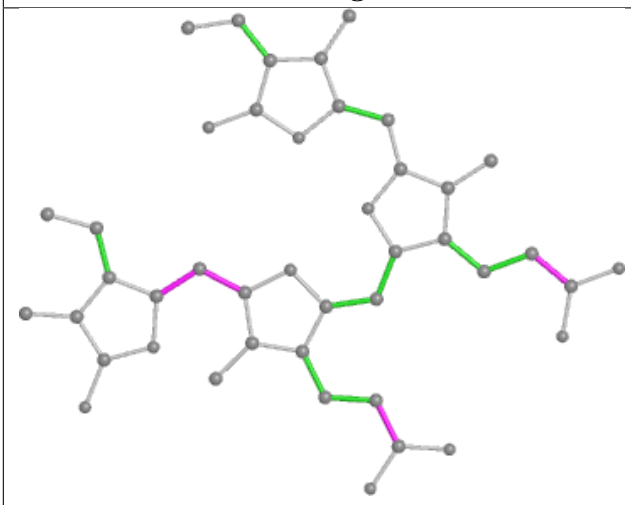

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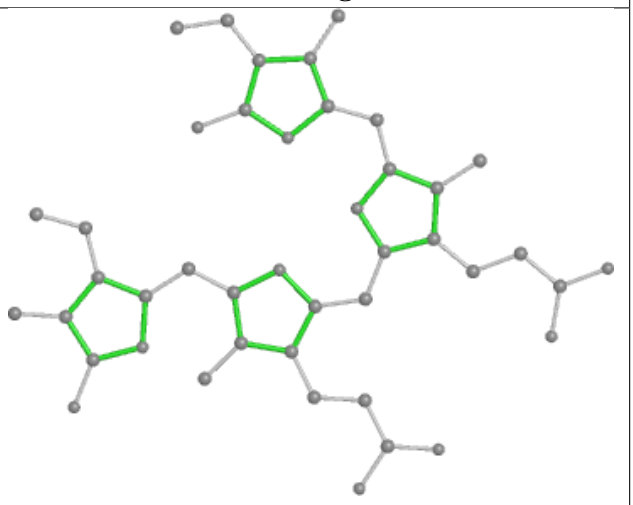
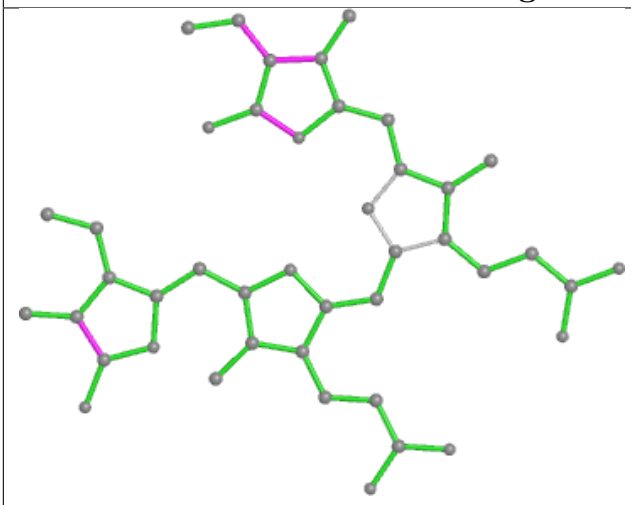


Rings

Ligand PEB bg 201



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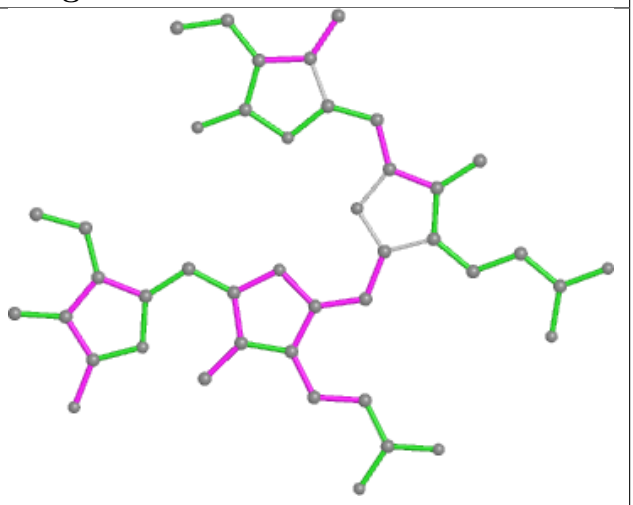

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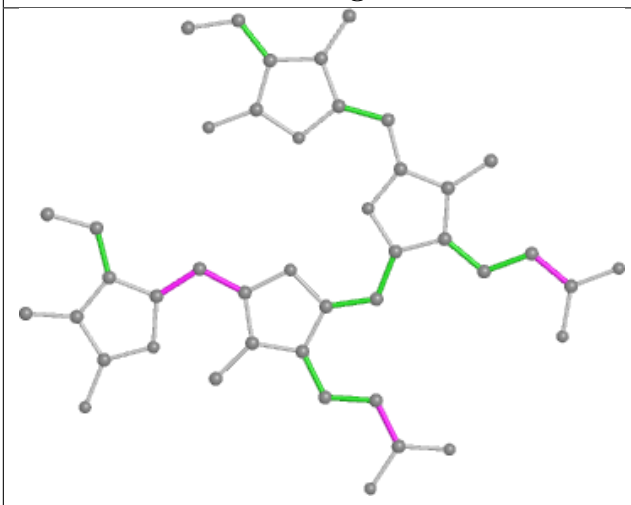

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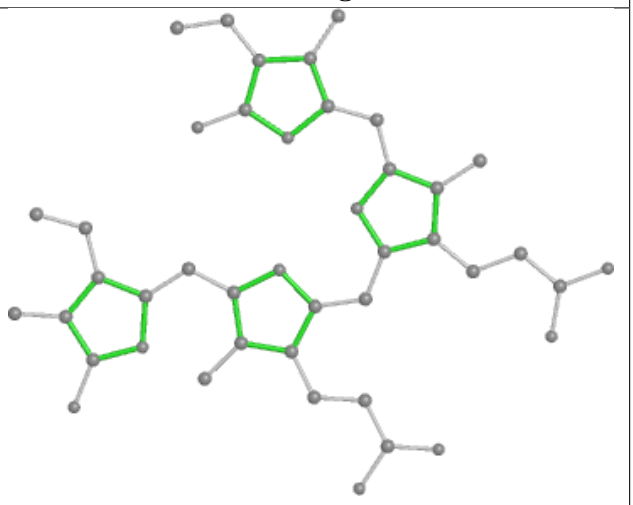
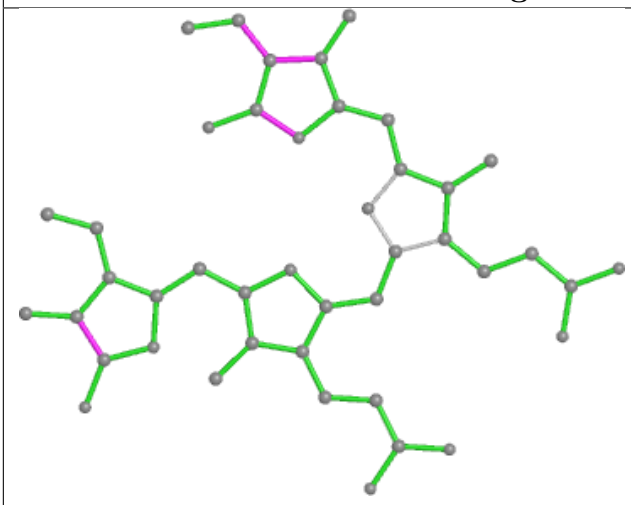


Rings

Ligand PEB W4 201



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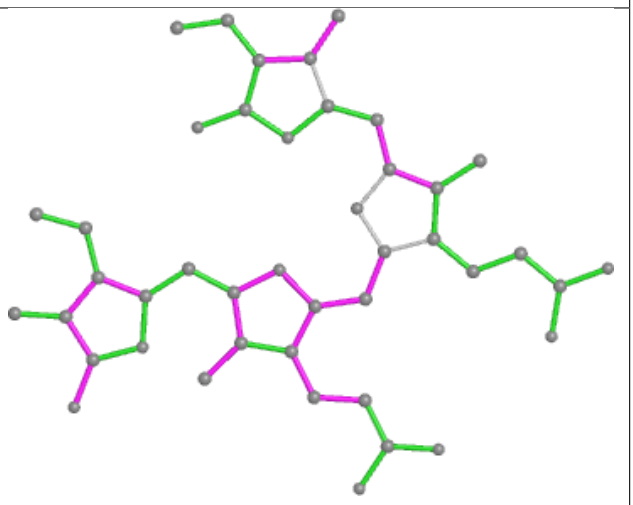

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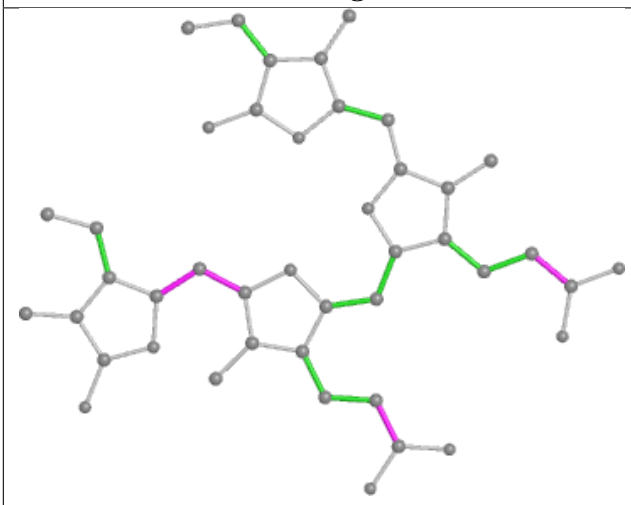

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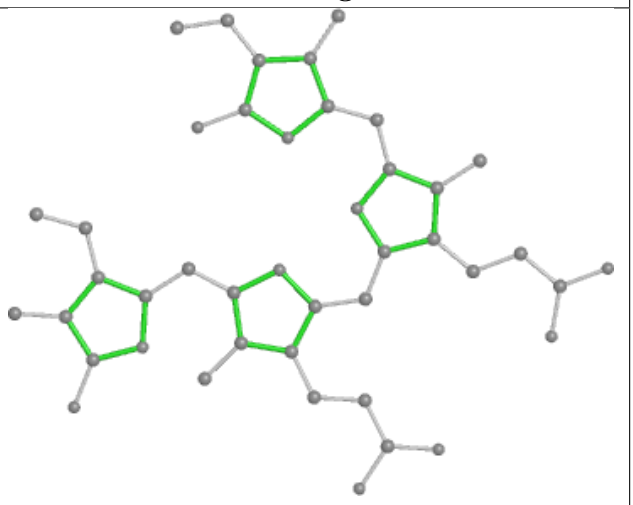
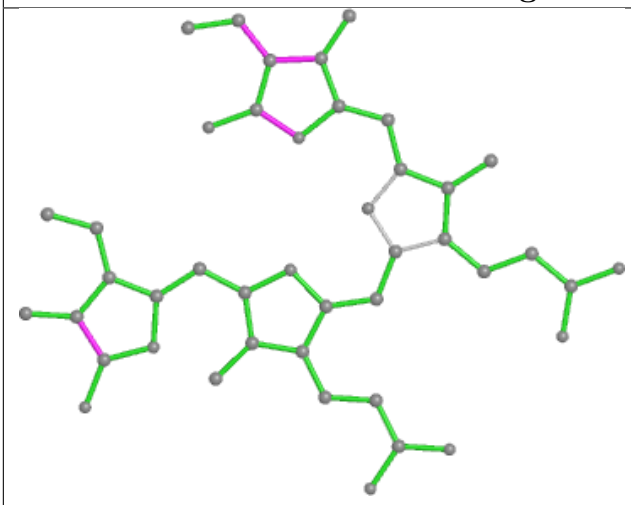


Rings

Ligand PEB q2 202



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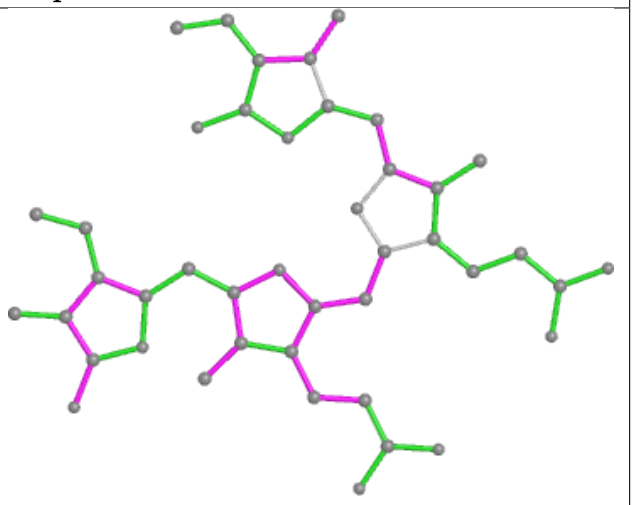

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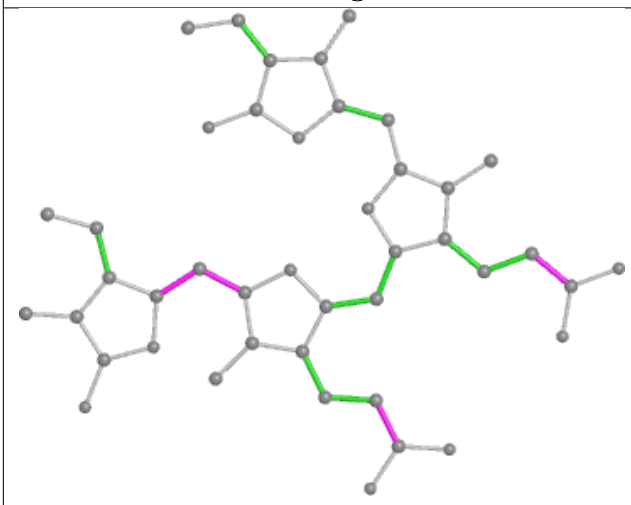

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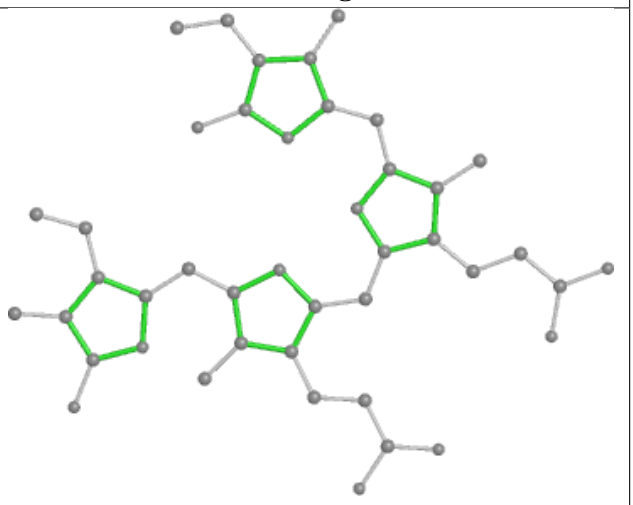

Rings

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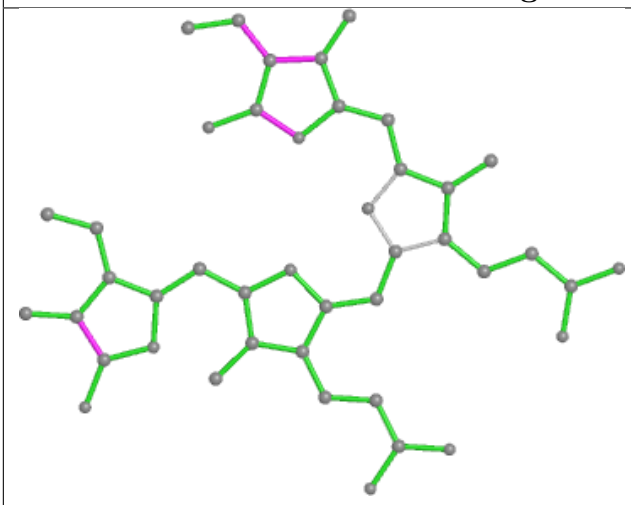

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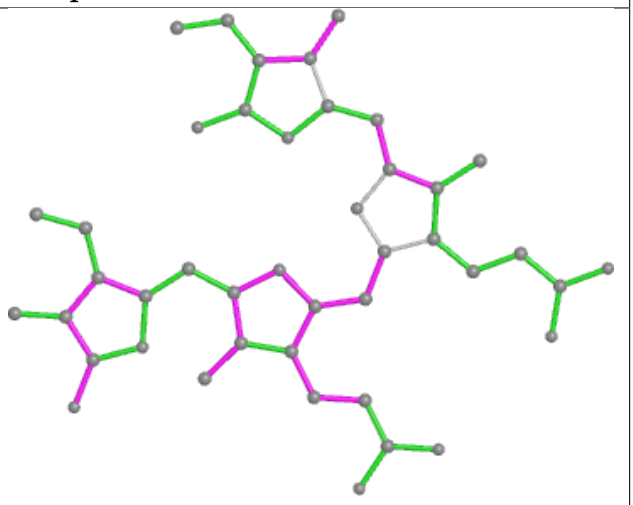

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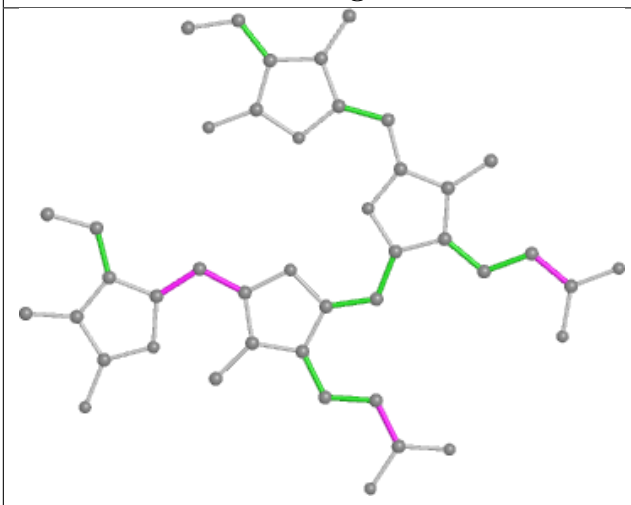

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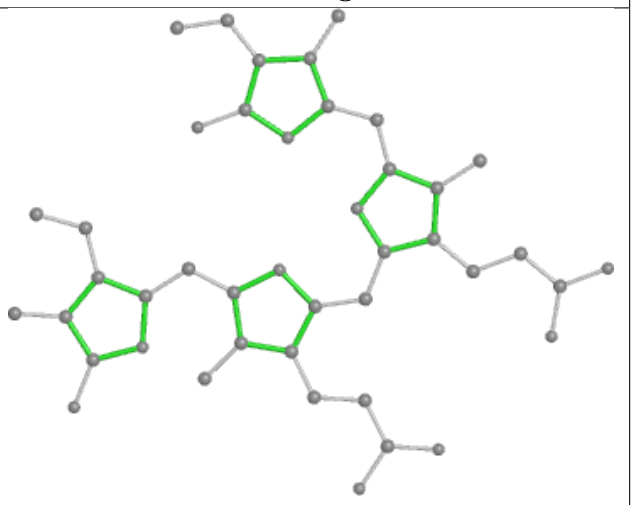

Rings

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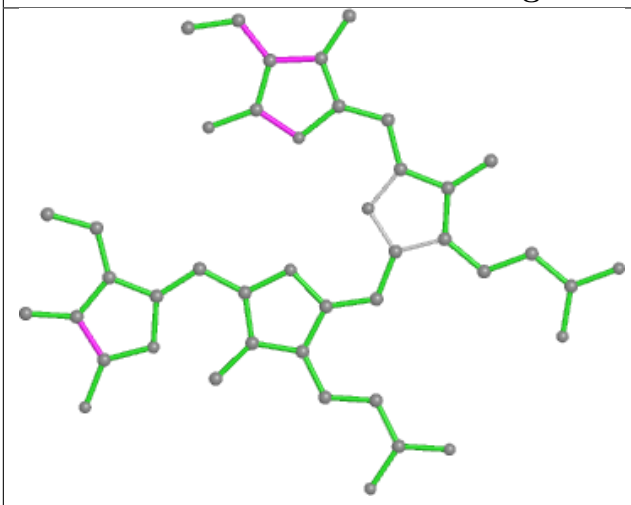

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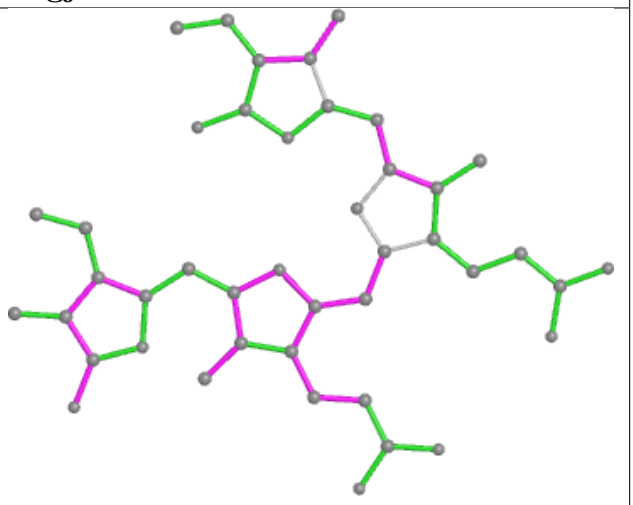

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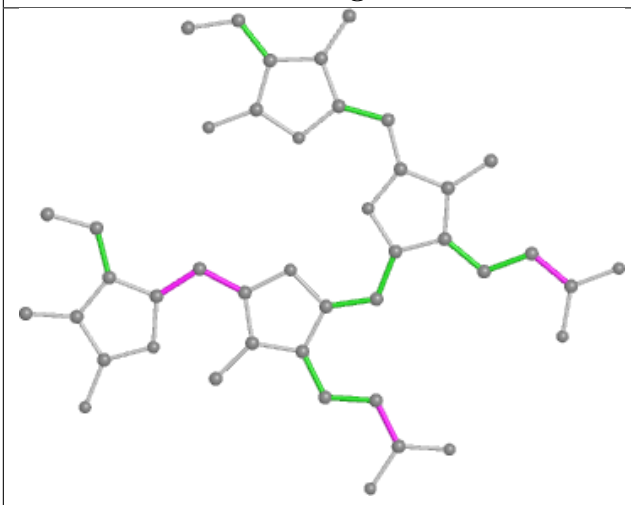

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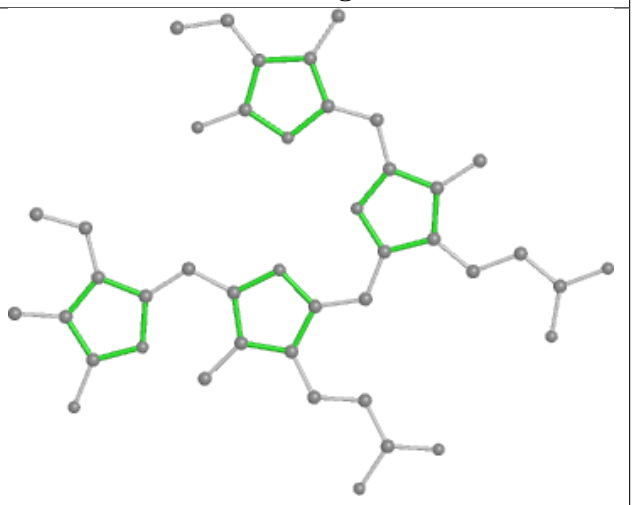
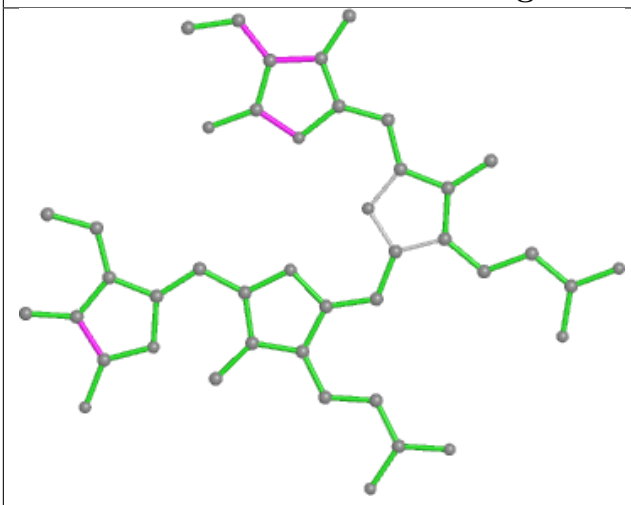


Rings

Ligand PEB aP 202



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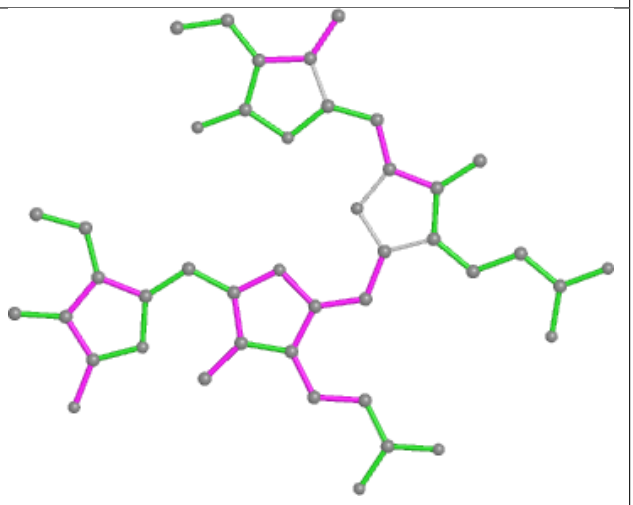

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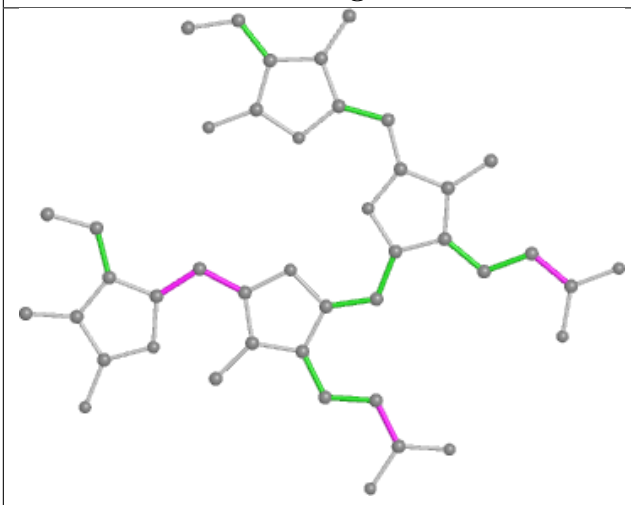

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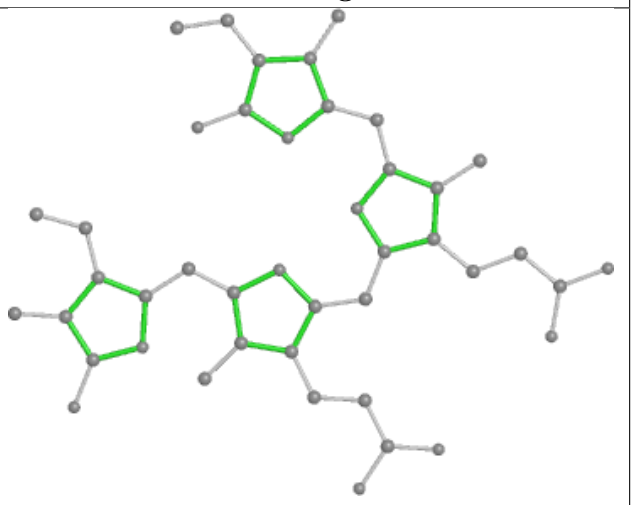
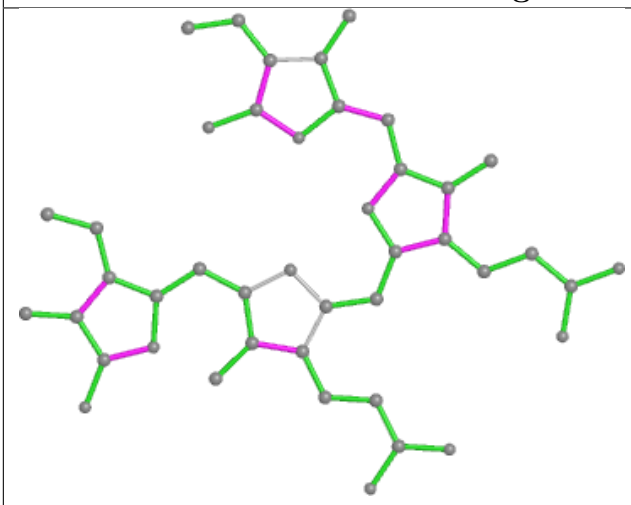


Rings

Ligand PUB H4 203



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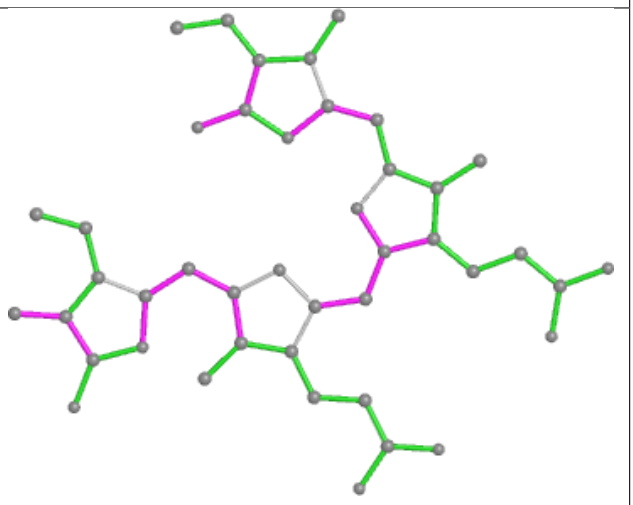

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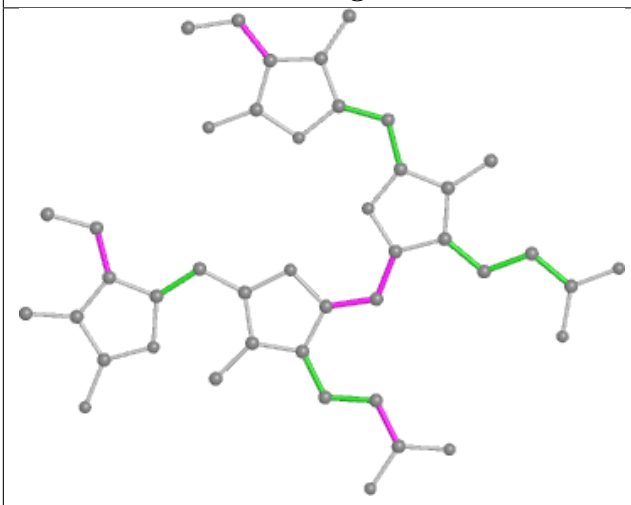

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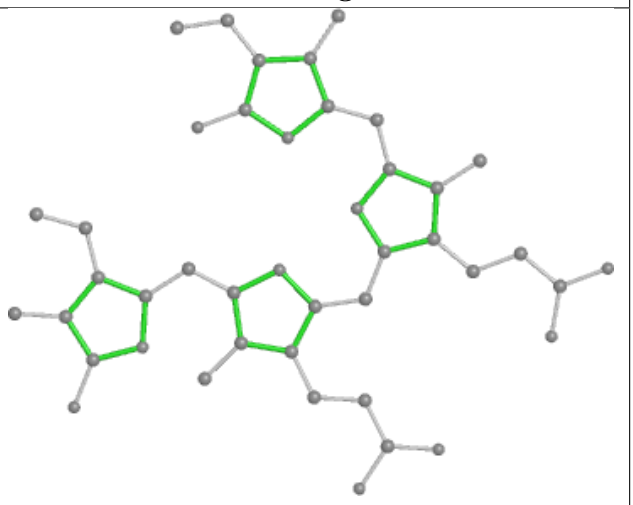
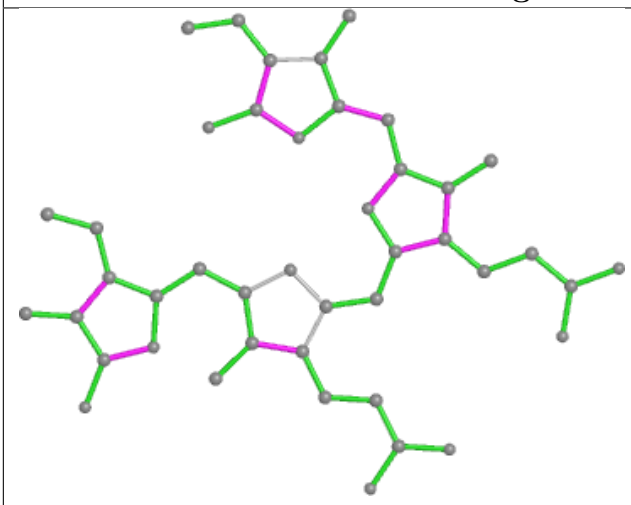


Rings

Ligand PUB N4 203



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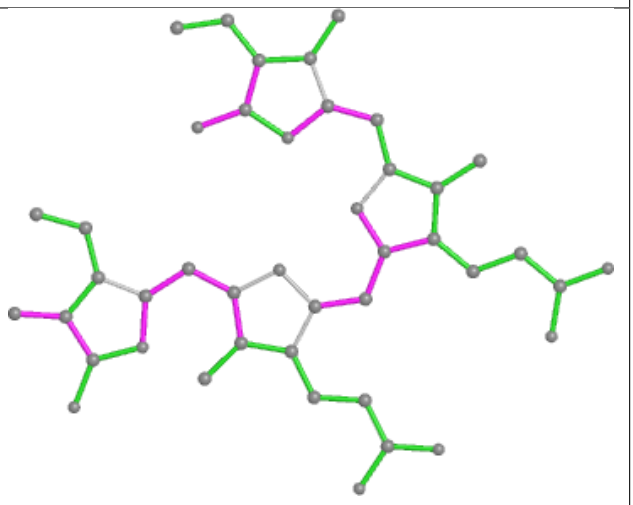

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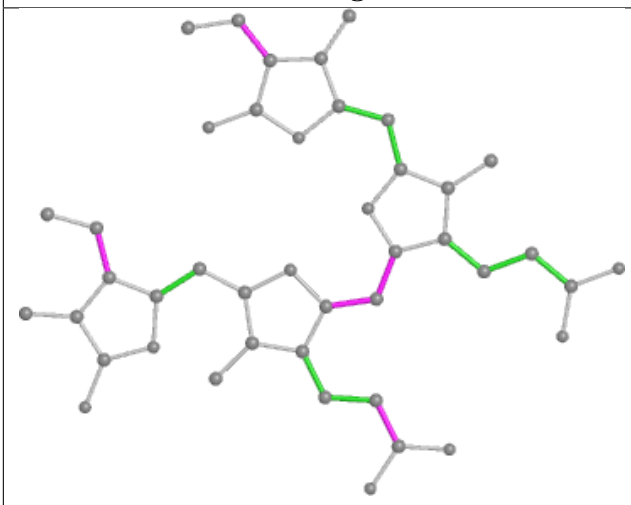

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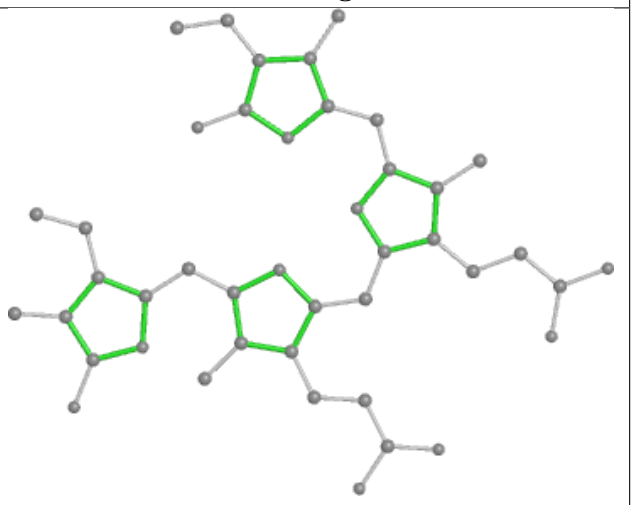
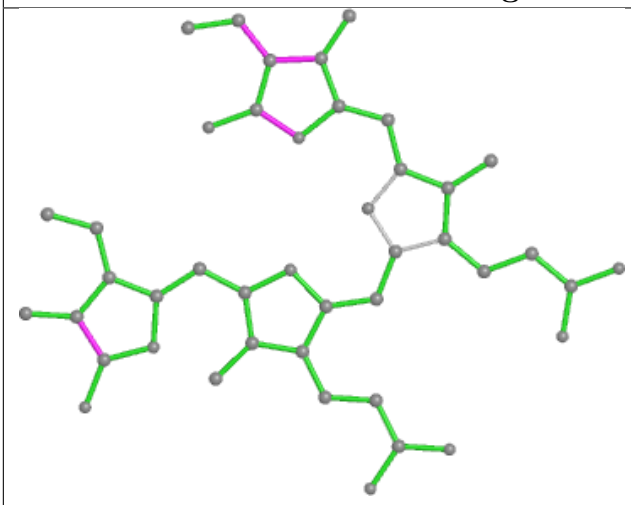


Rings

Ligand PEB hM 1001



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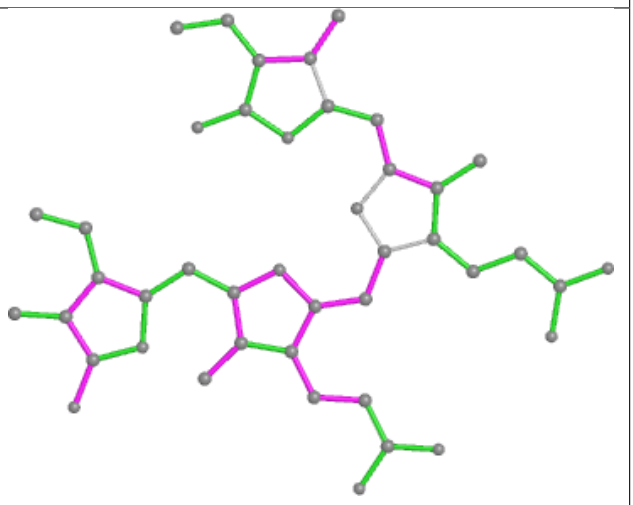
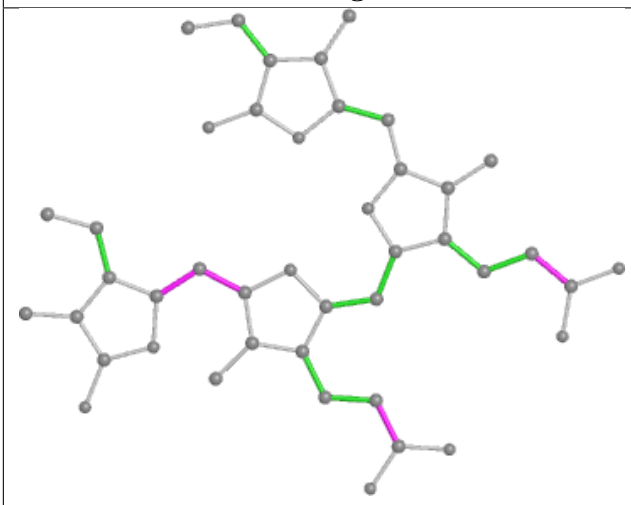


Bond angles



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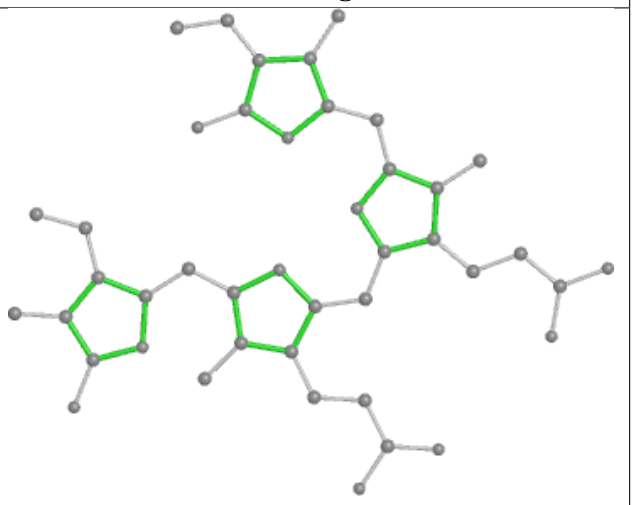
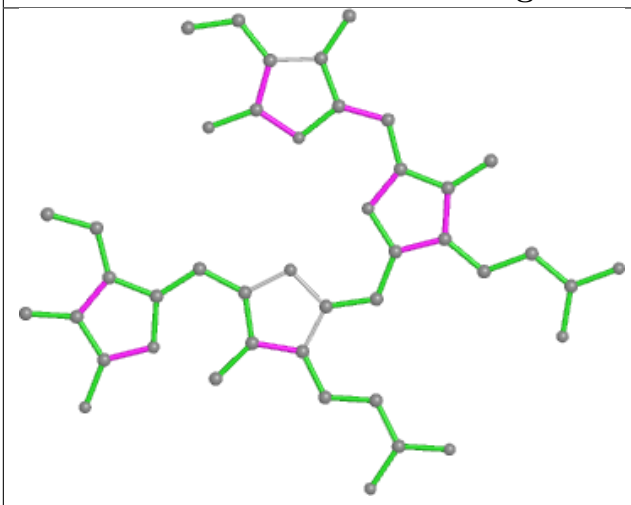
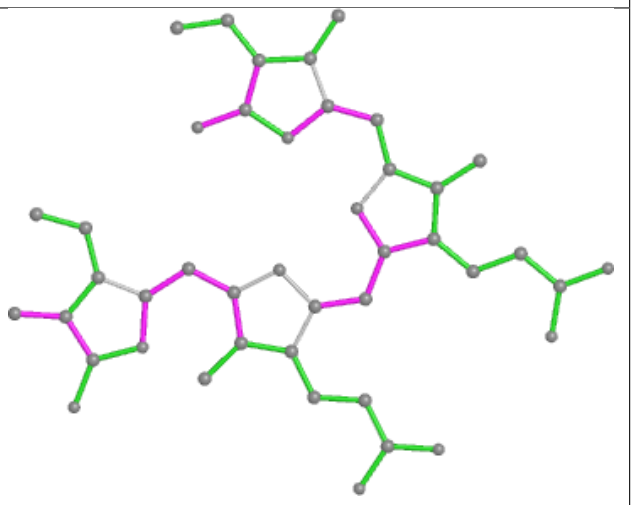


Rings

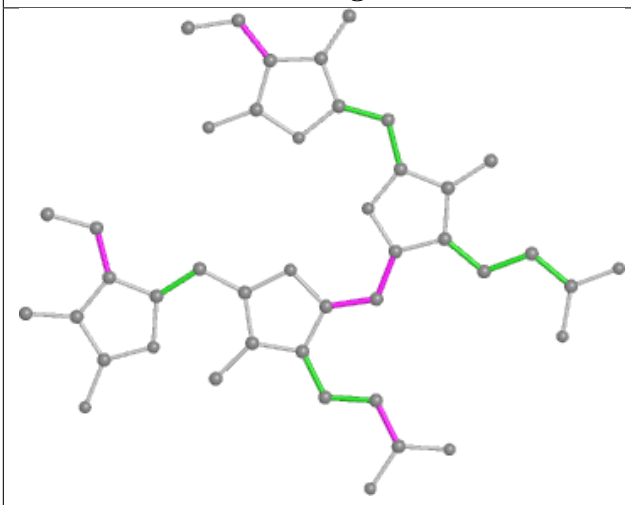
Ligand PUB dx 407



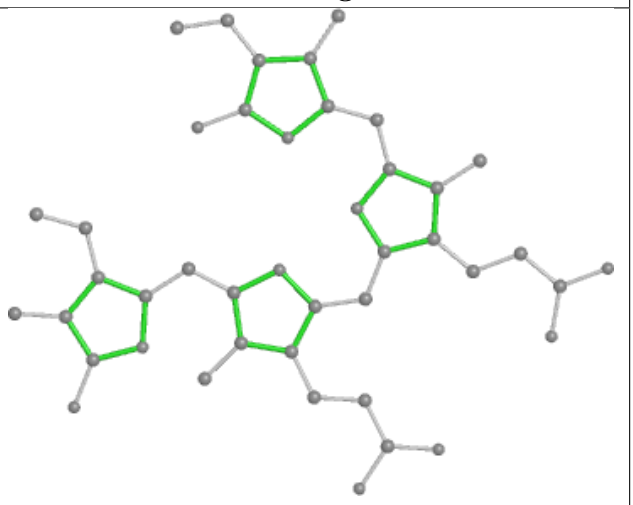
Bond lengths



Bond angles

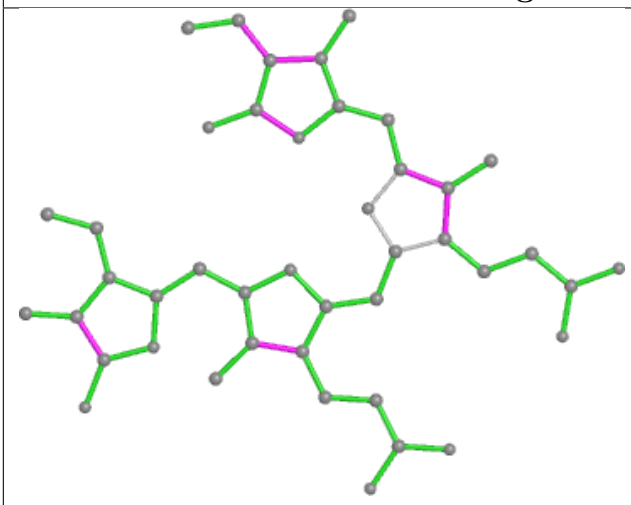


Torsions



Rings

Ligand PEB cY 202



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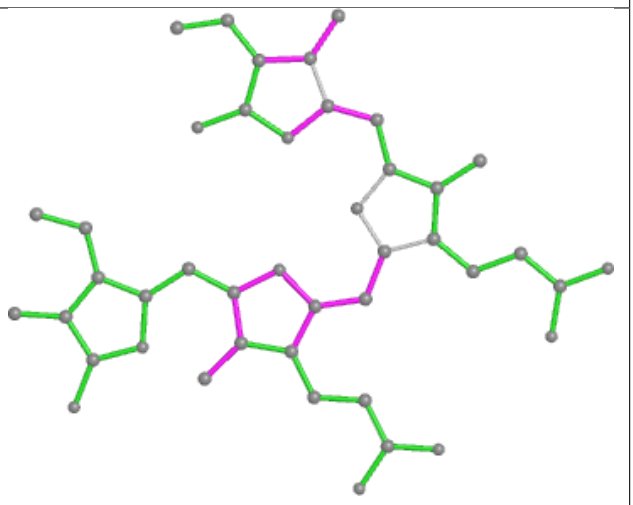

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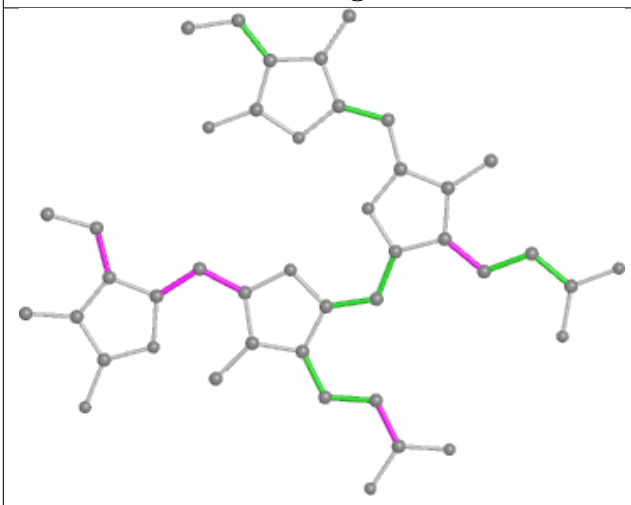

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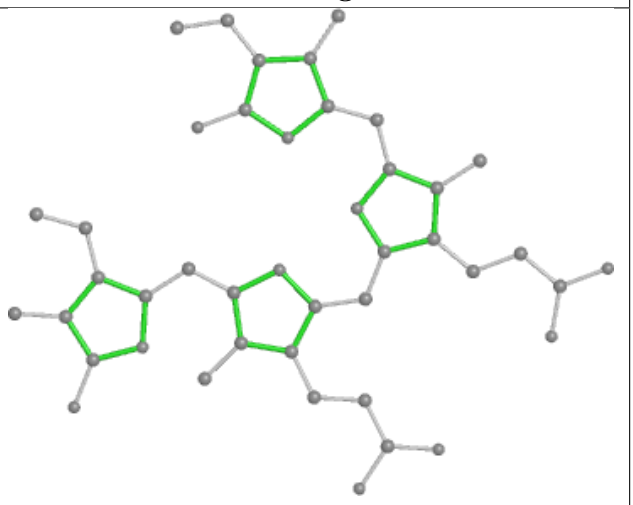
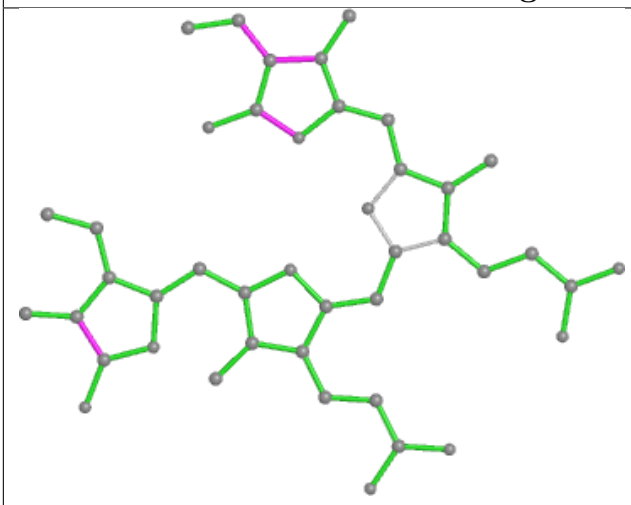


Rings

Ligand PEB go 201



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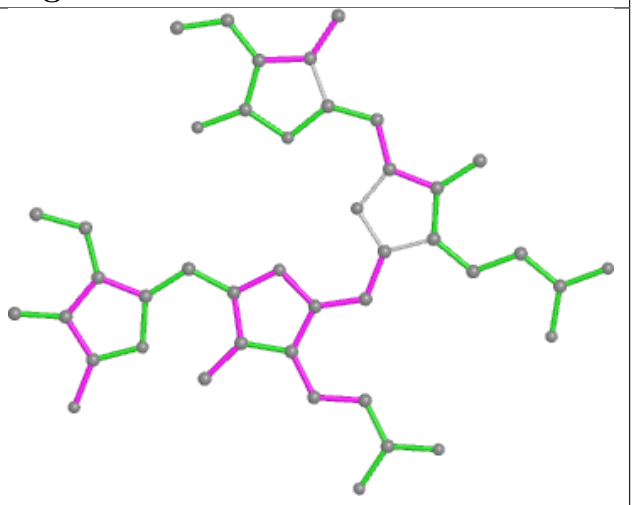

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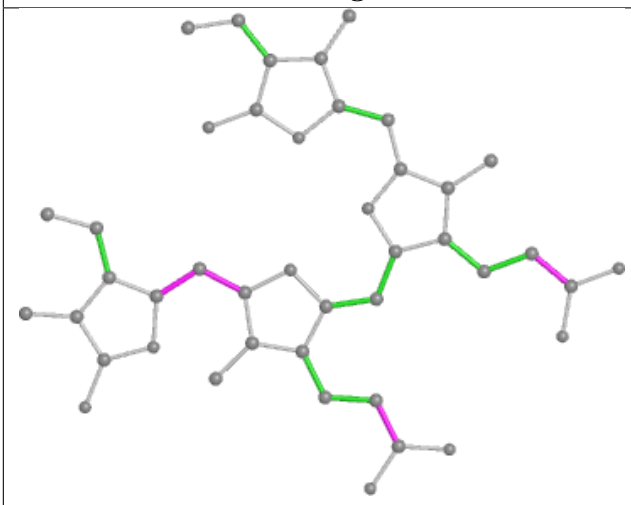

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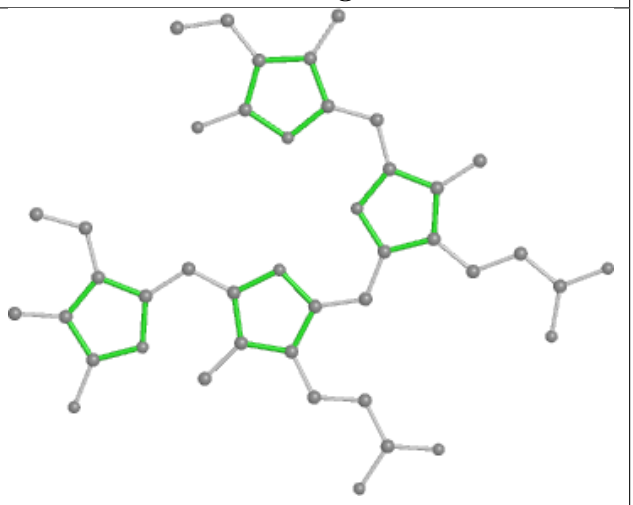
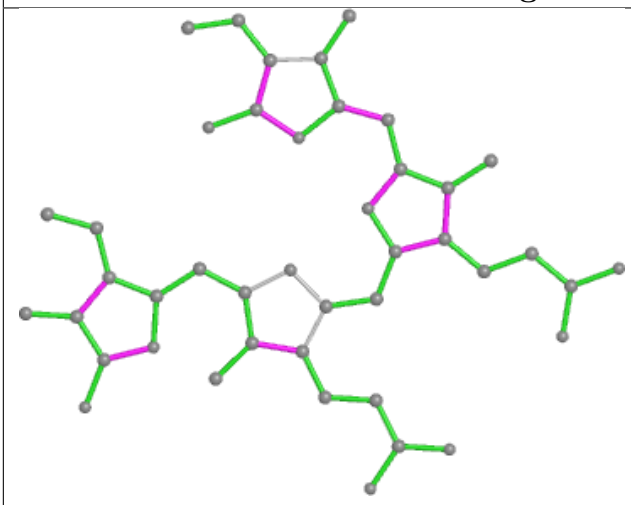


Rings

Ligand PUB t3 203



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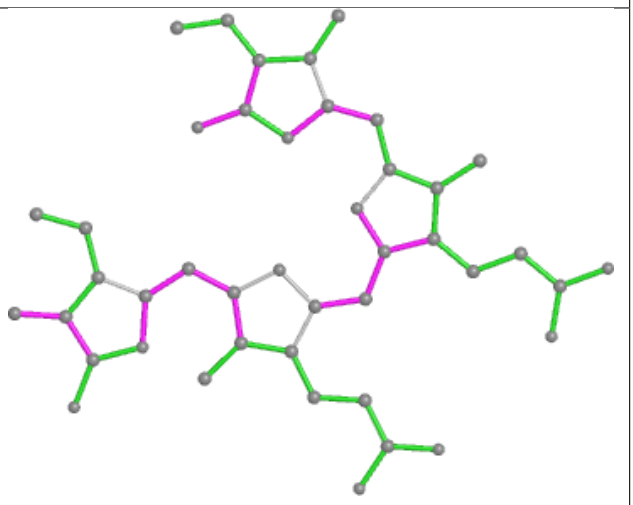

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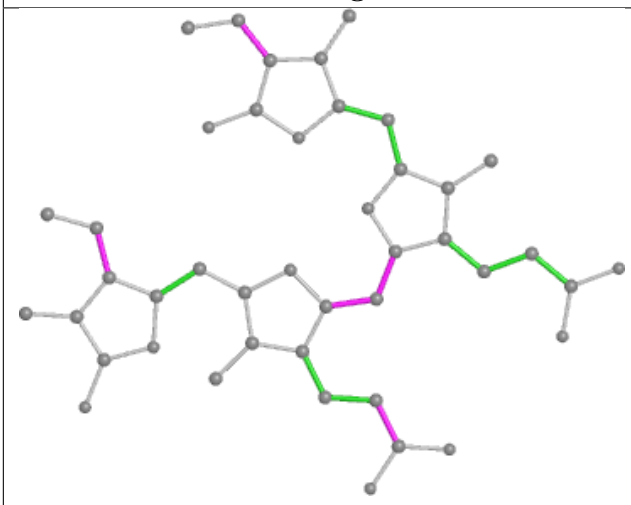

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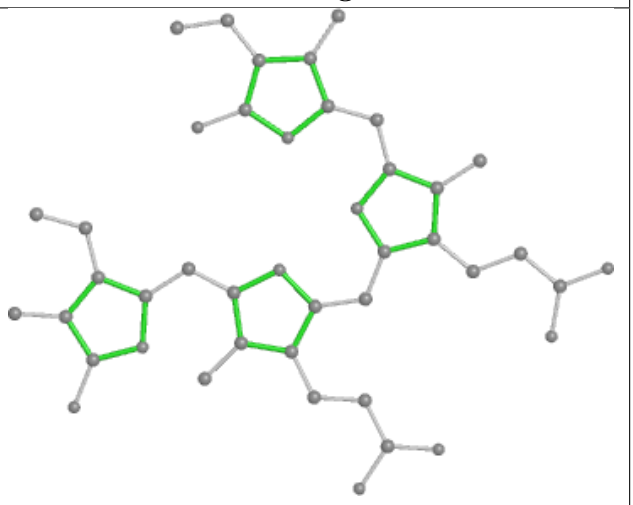
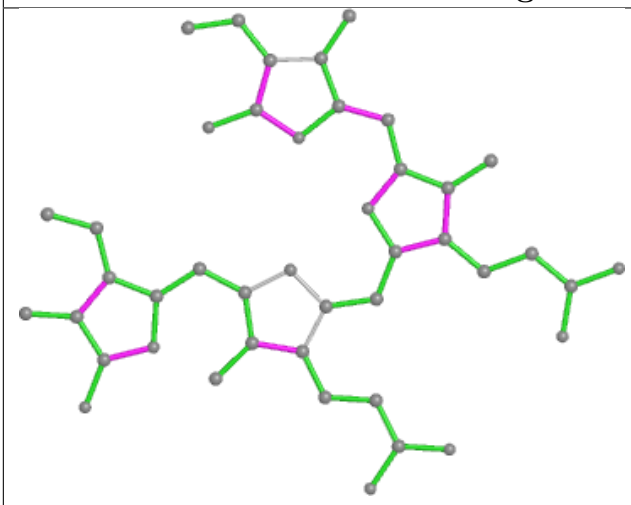


Rings

Ligand PUB n6 203



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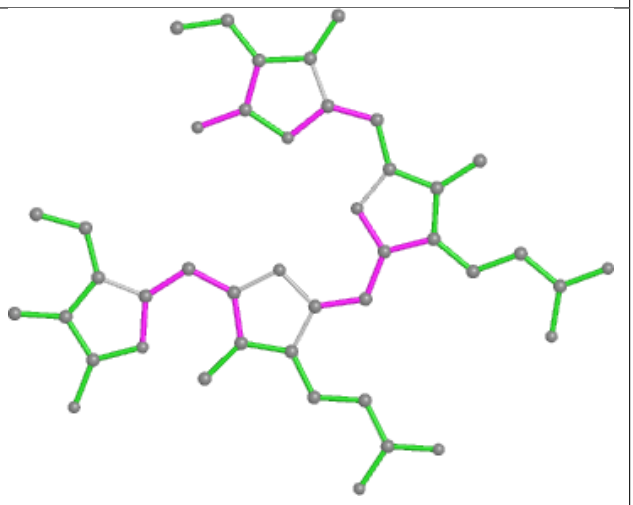

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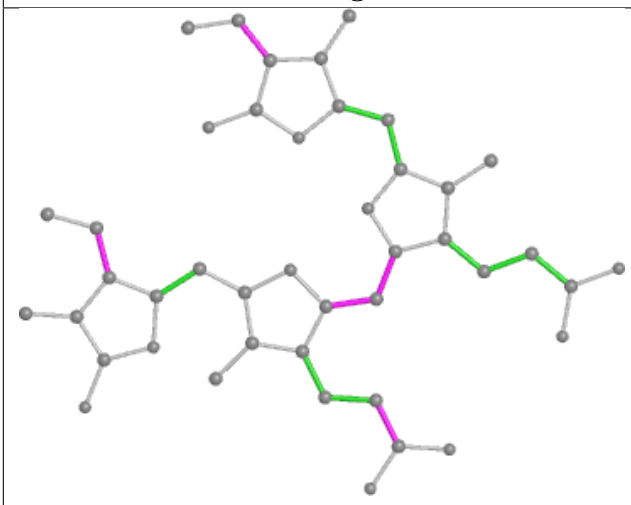

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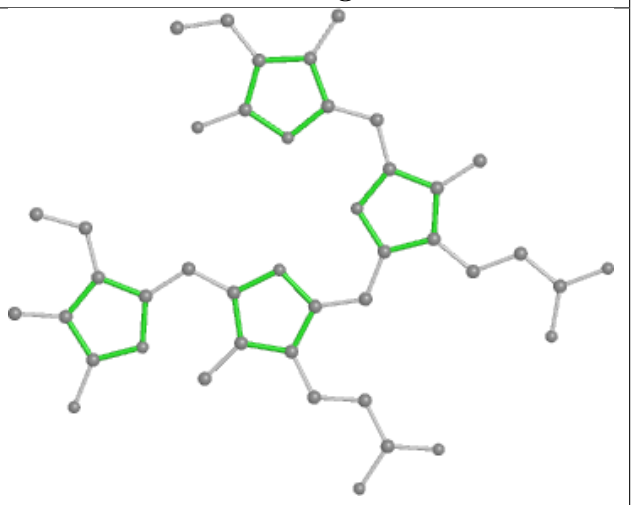
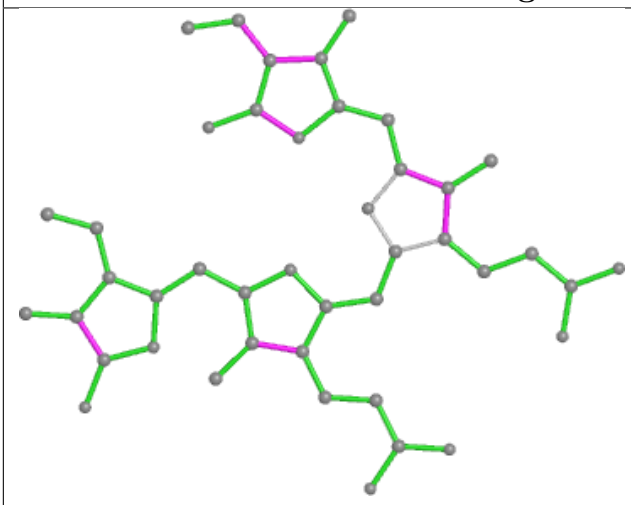


Rings

Ligand PEB L9 202



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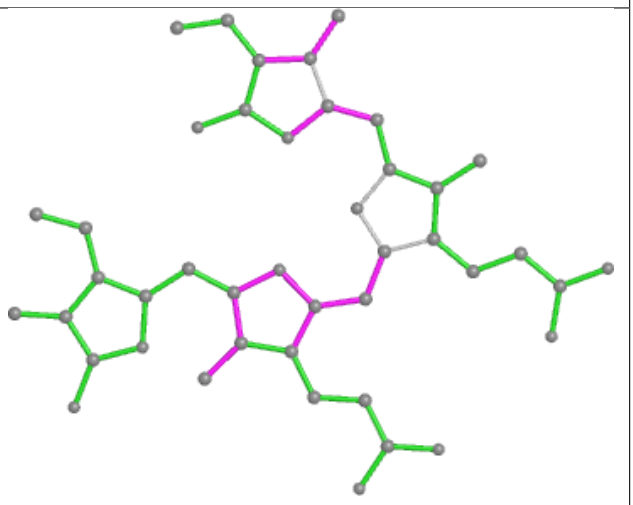

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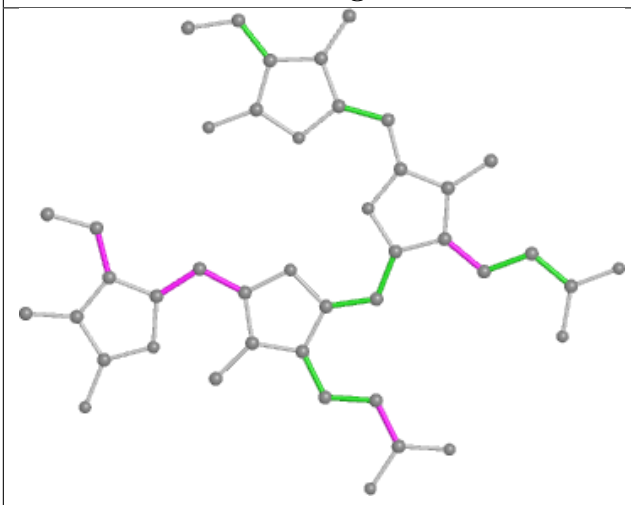

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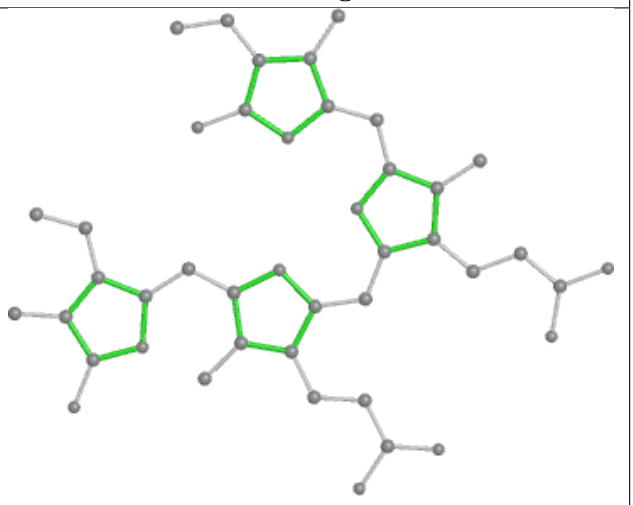
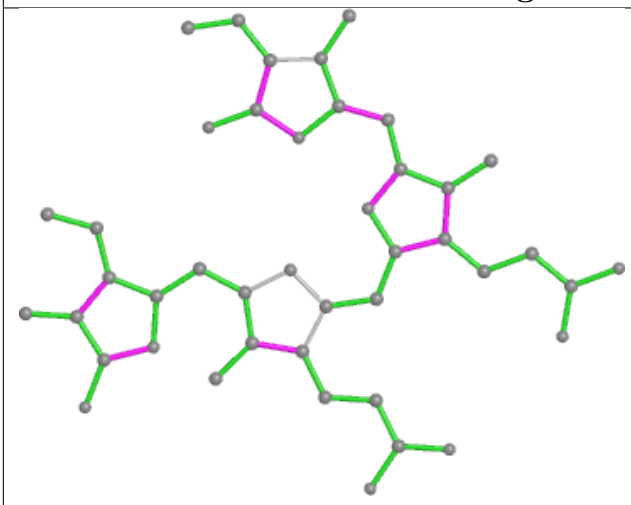


Rings

Ligand PUB d8 304



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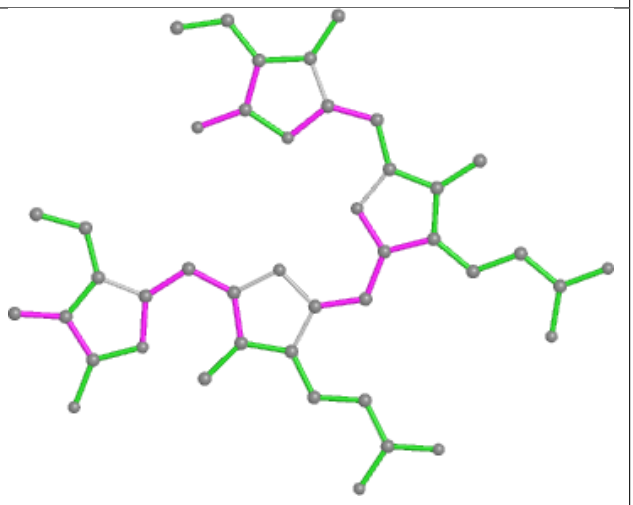

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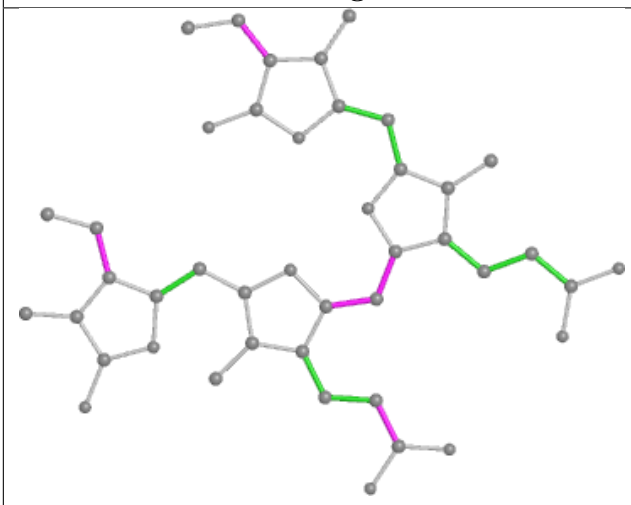

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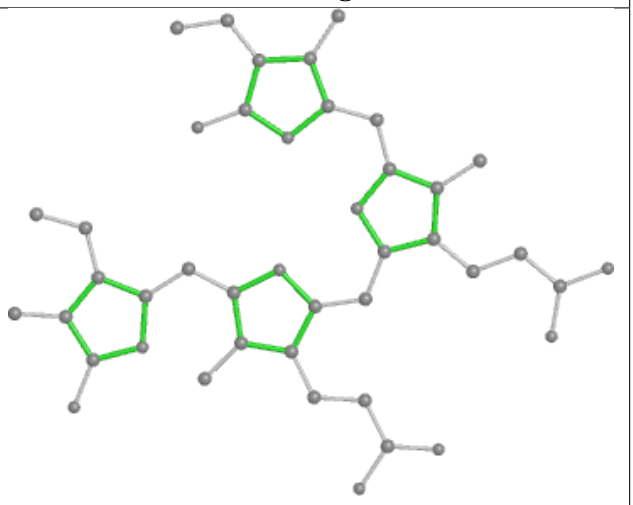

Rings

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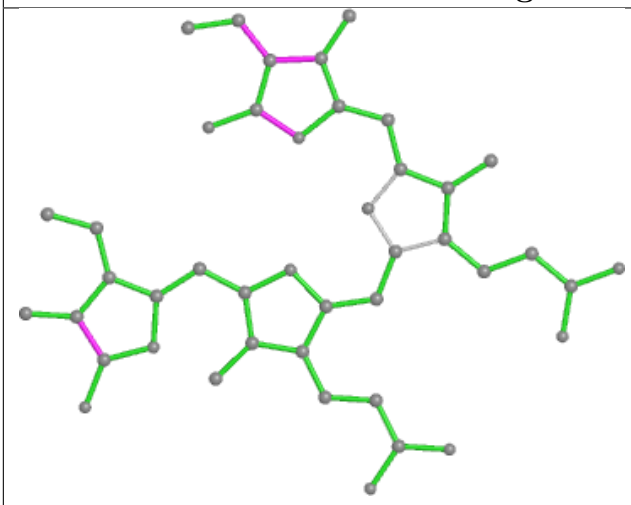

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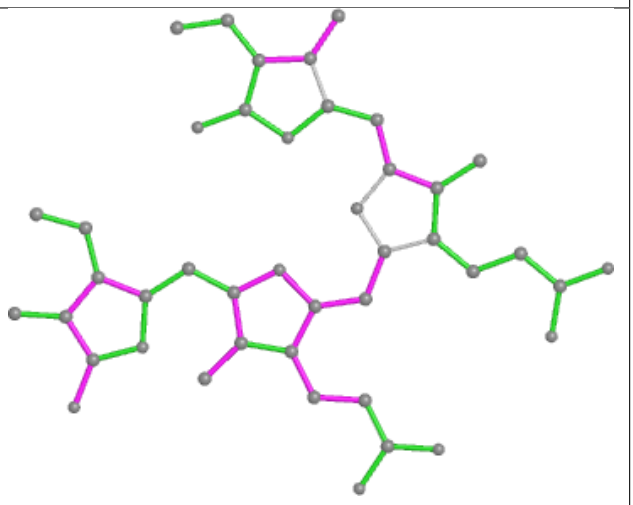

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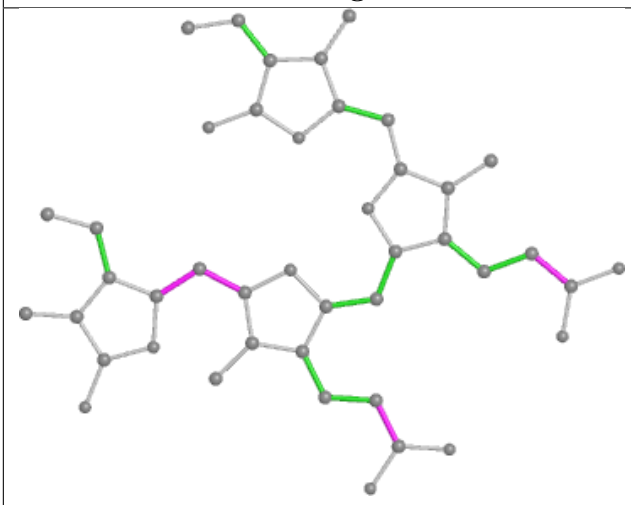

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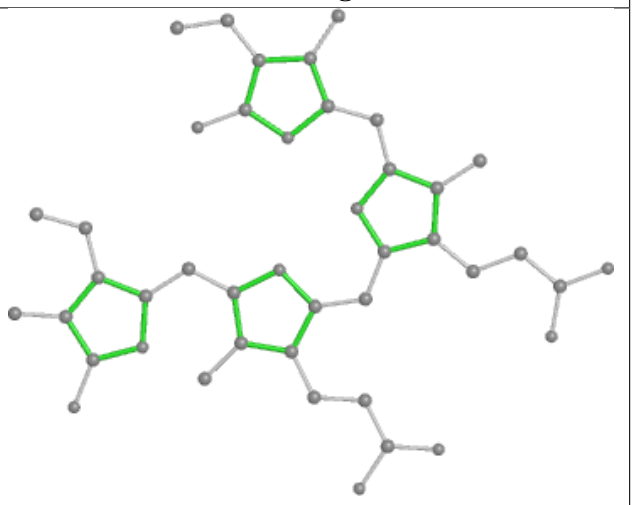
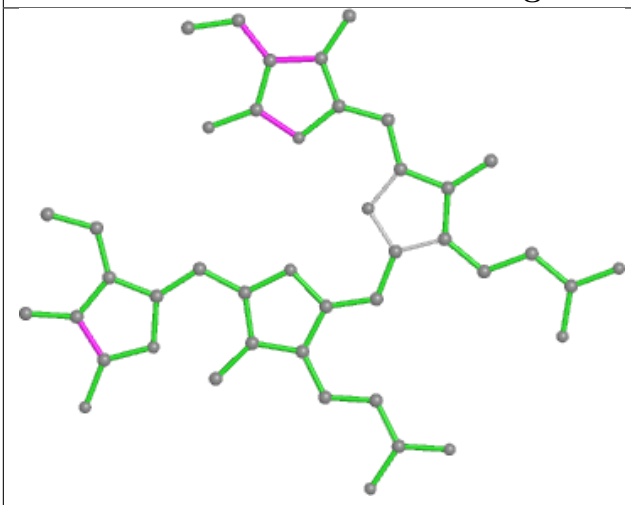


Rings

Ligand PEB l5 201



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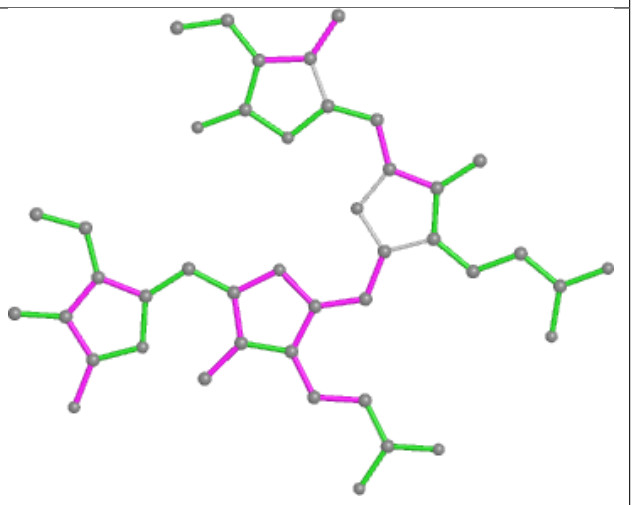

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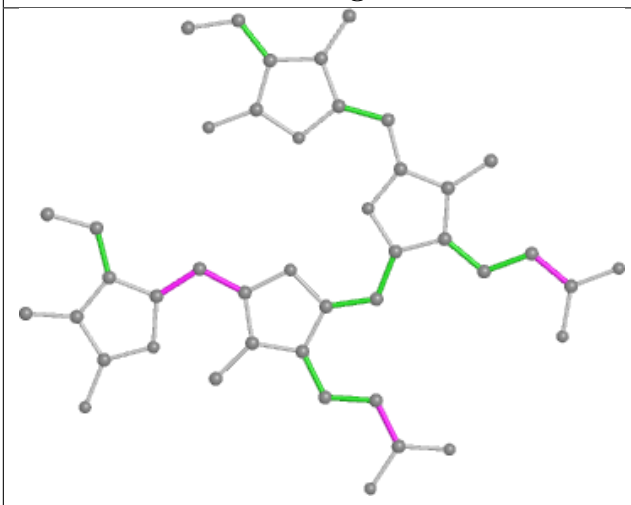

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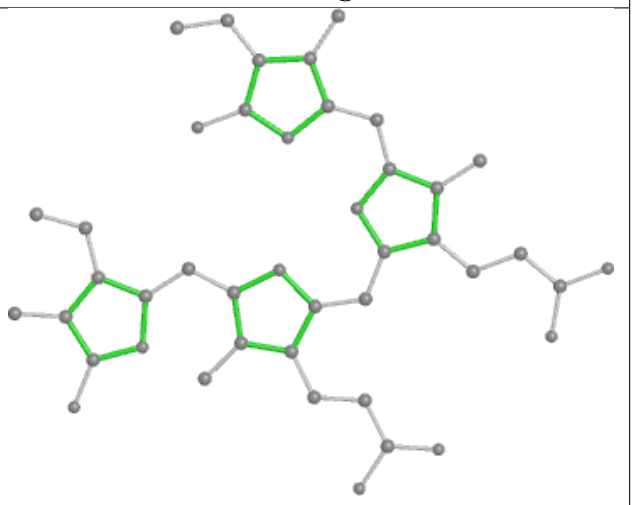
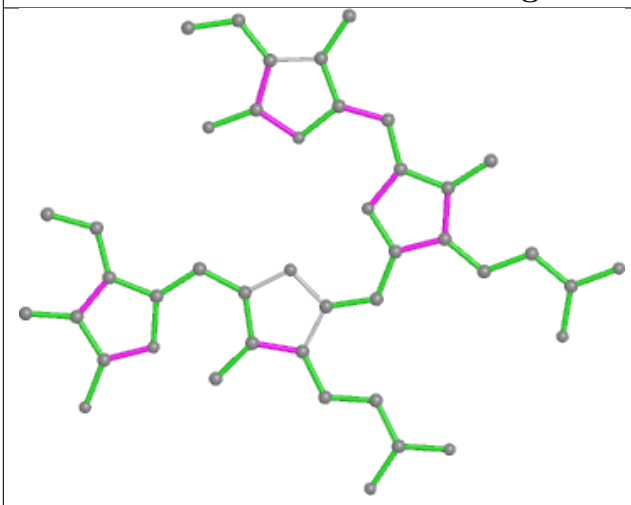


Rings

Ligand PUB lx 201



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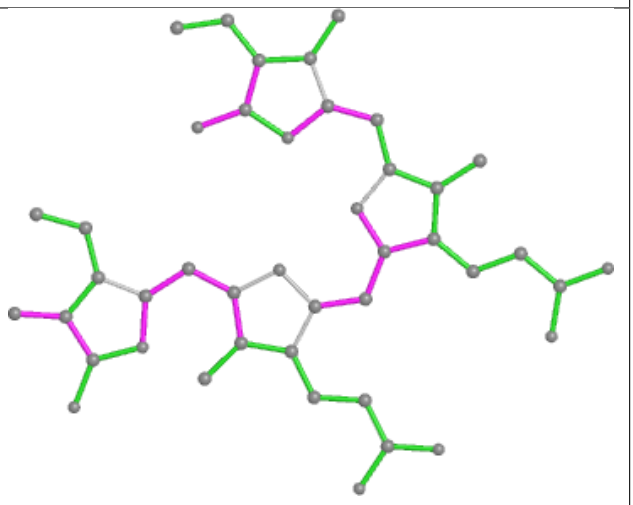

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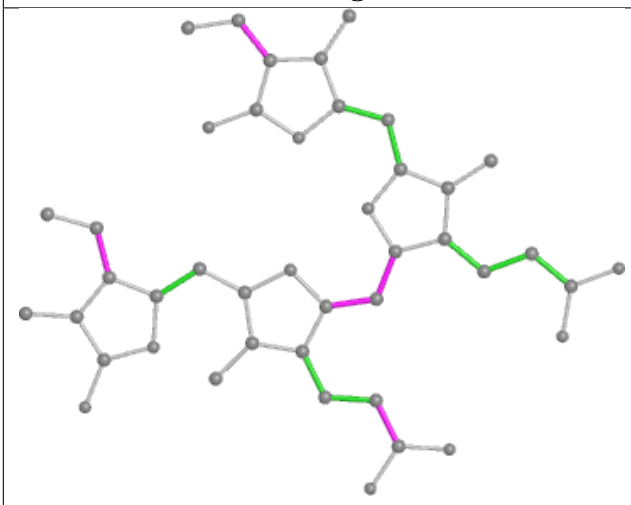

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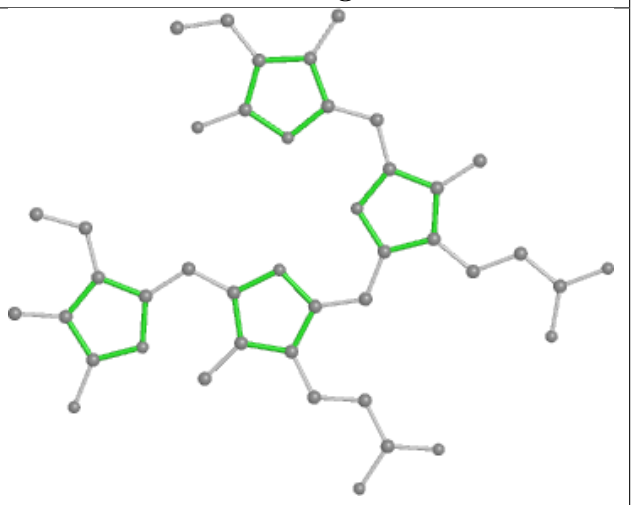

Rings

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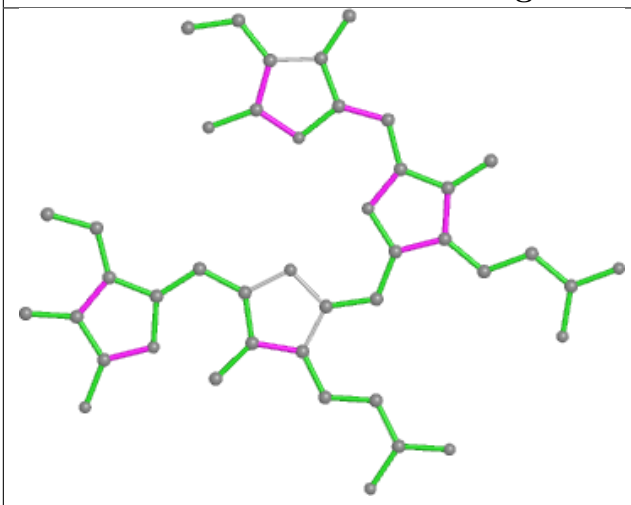

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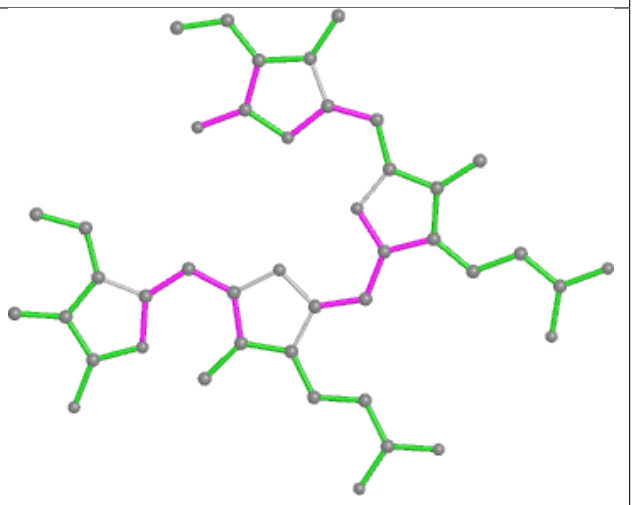

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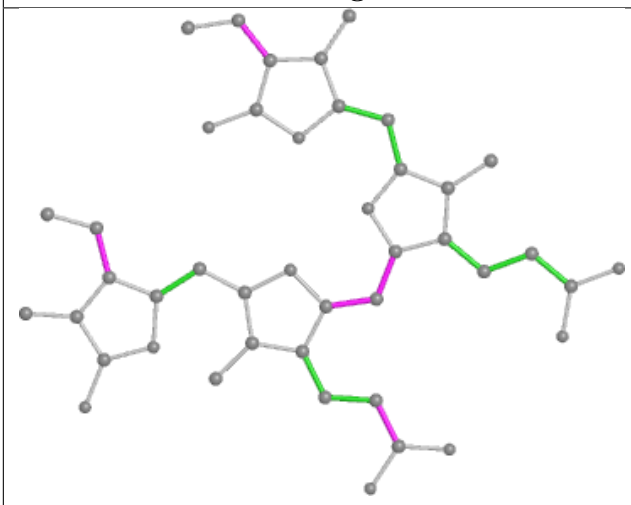

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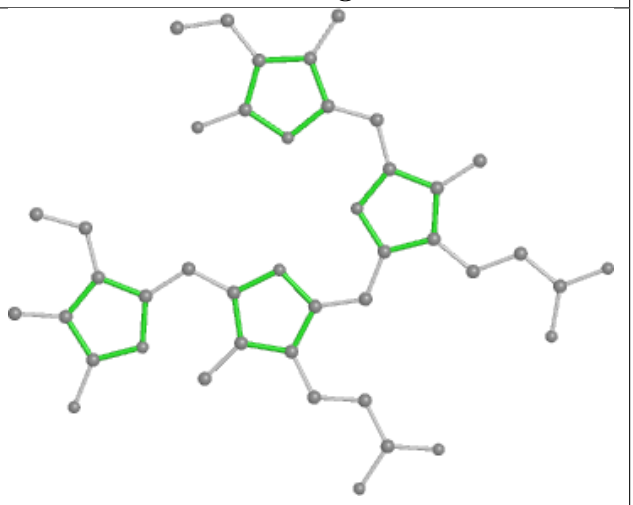
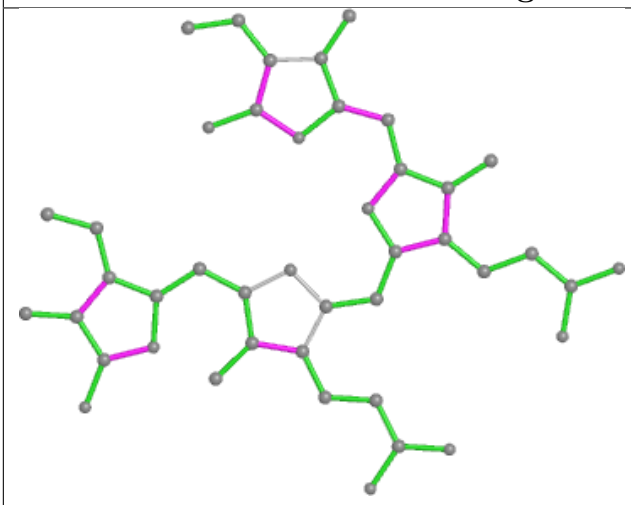


Rings

Ligand PUB cL 203



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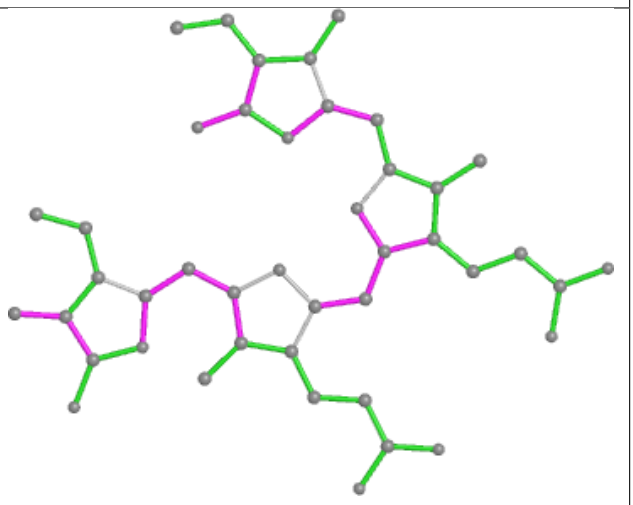
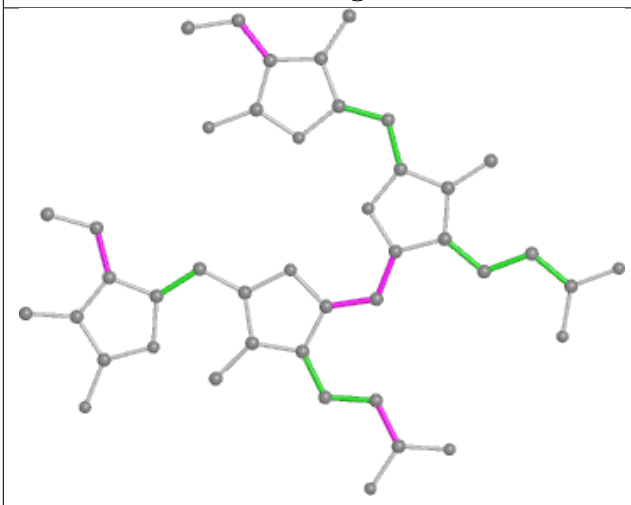


Bond angles



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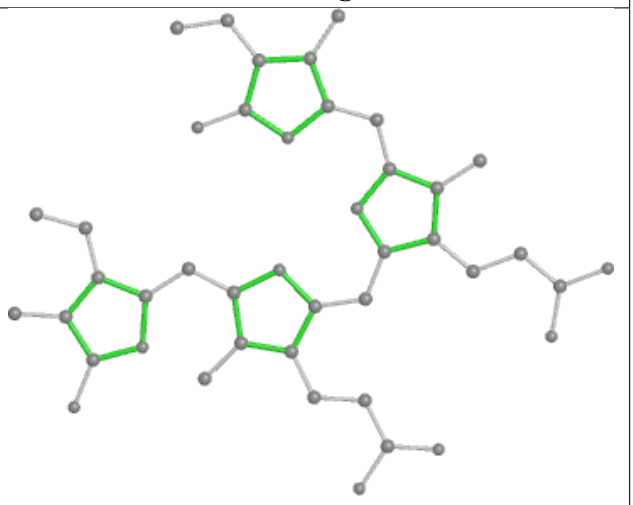
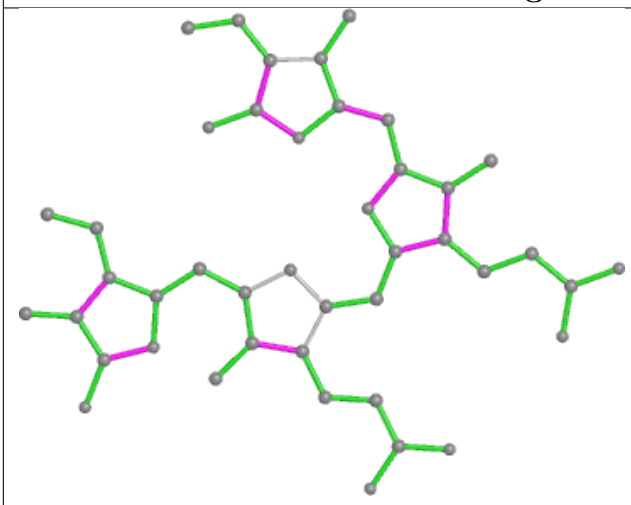


Rings

Ligand PUB lj 202



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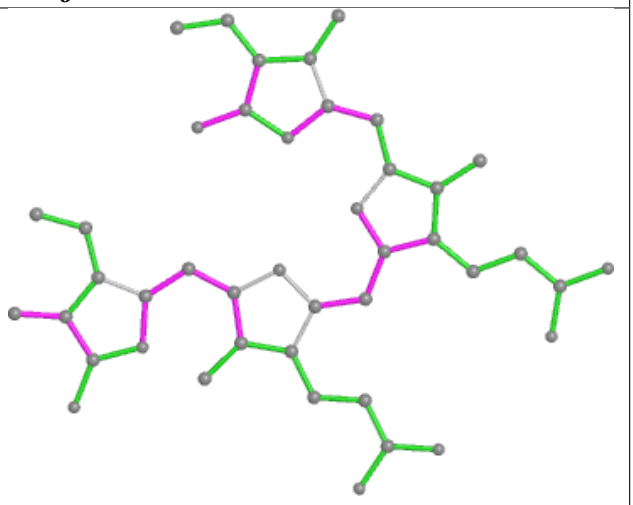
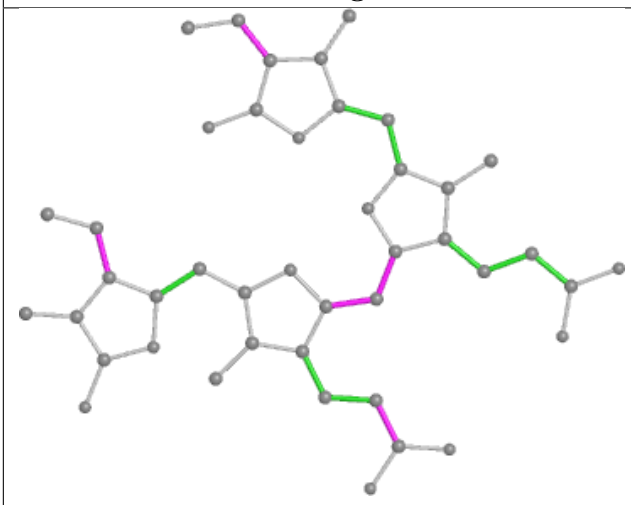


Bond angles



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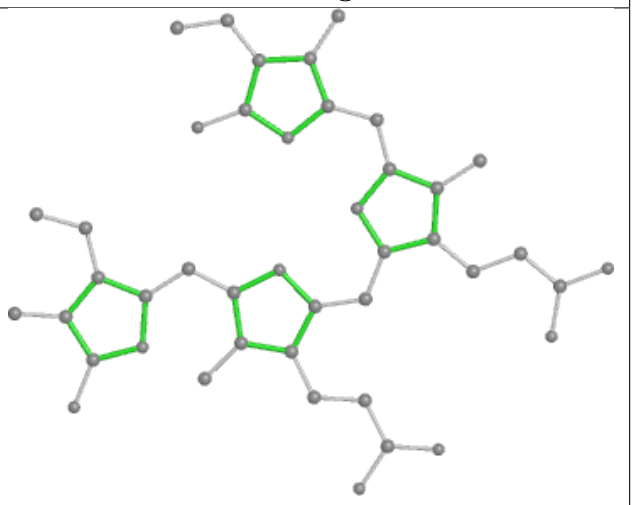
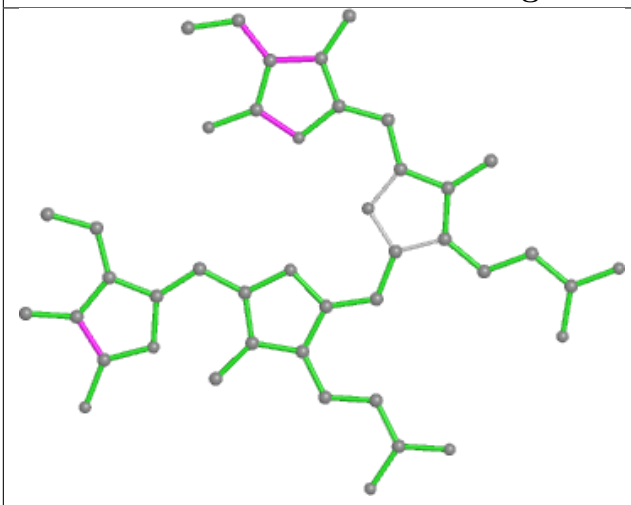


Rings

Ligand PEB s6 201



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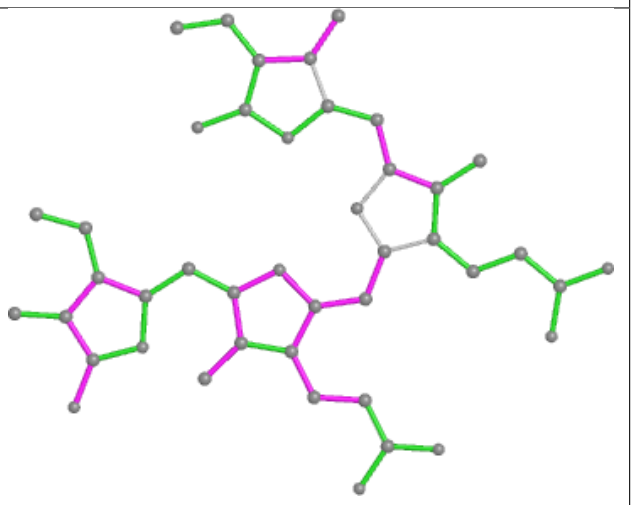
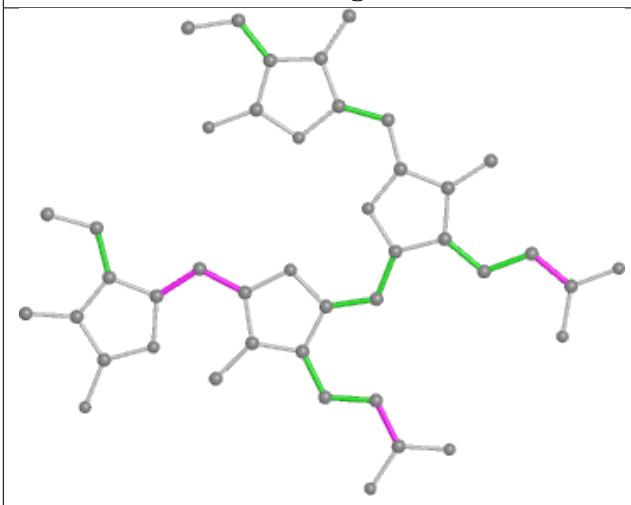
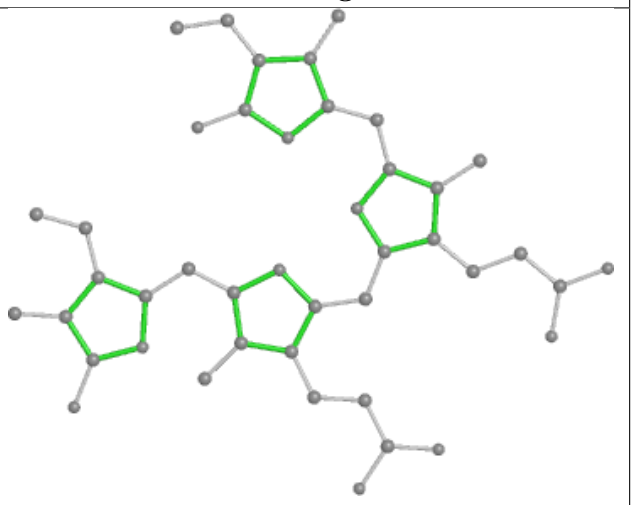


Bond angles

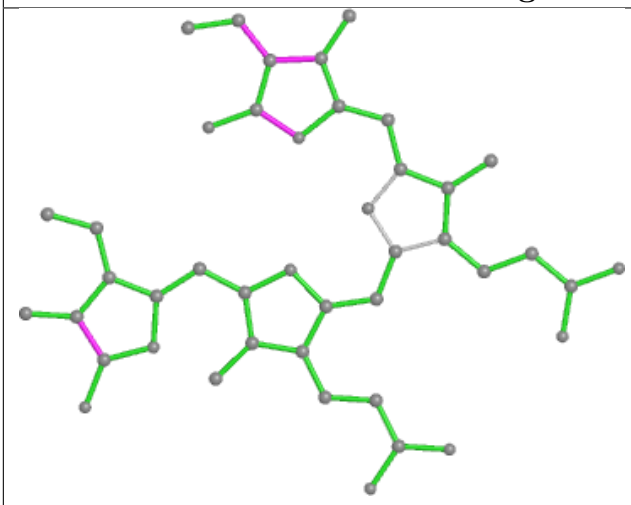


Torsions



Rings

Ligand PEB dJ 201



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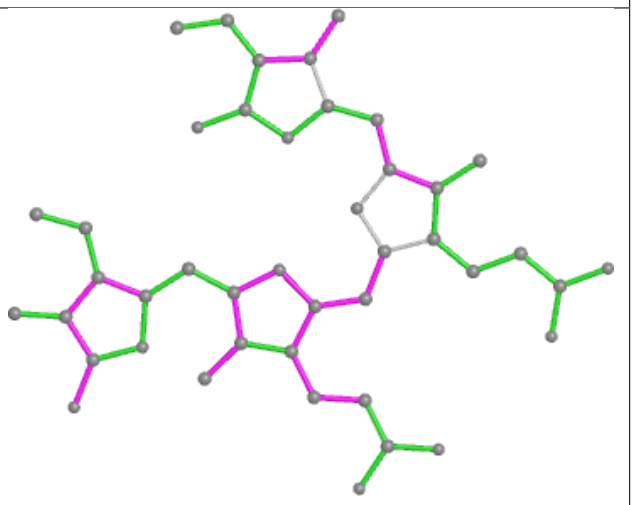

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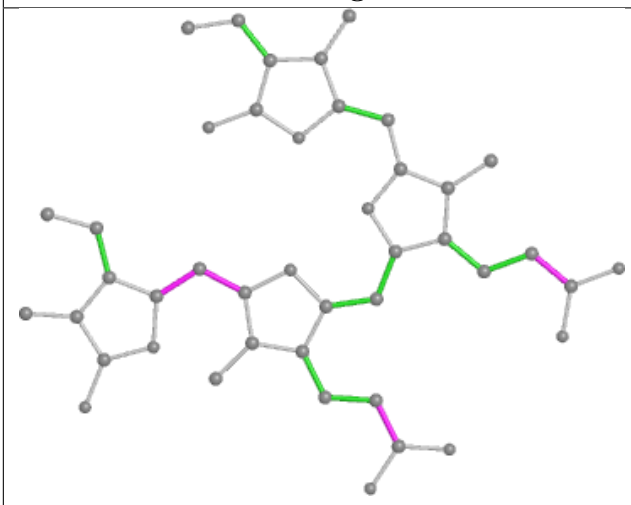

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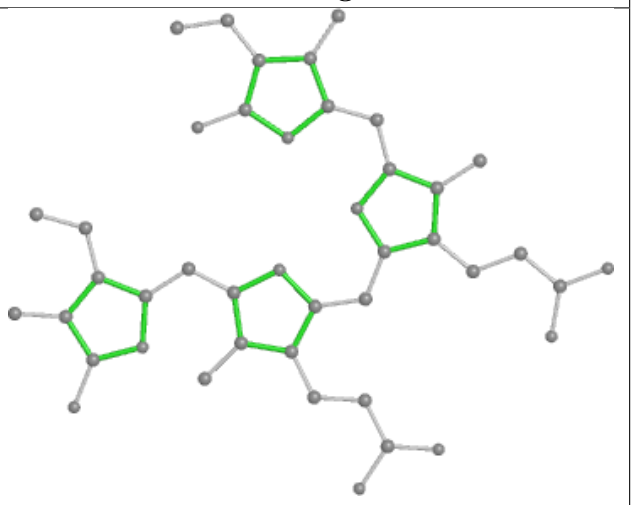
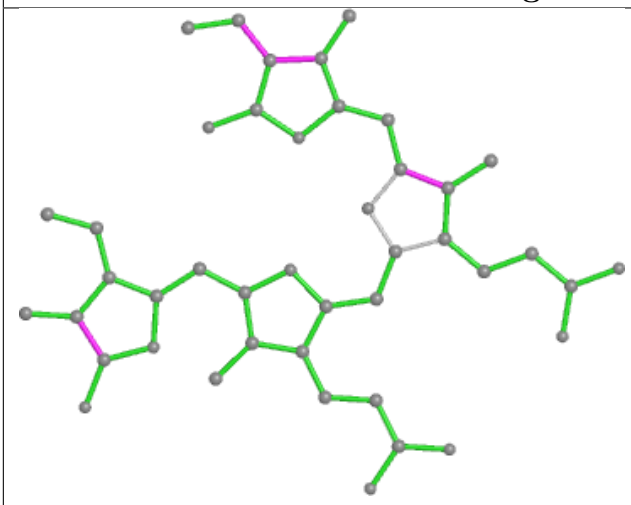


Rings

Ligand PEB gj 202



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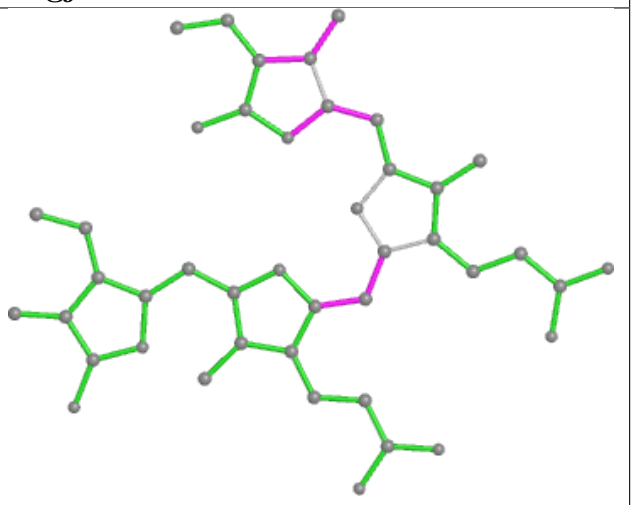

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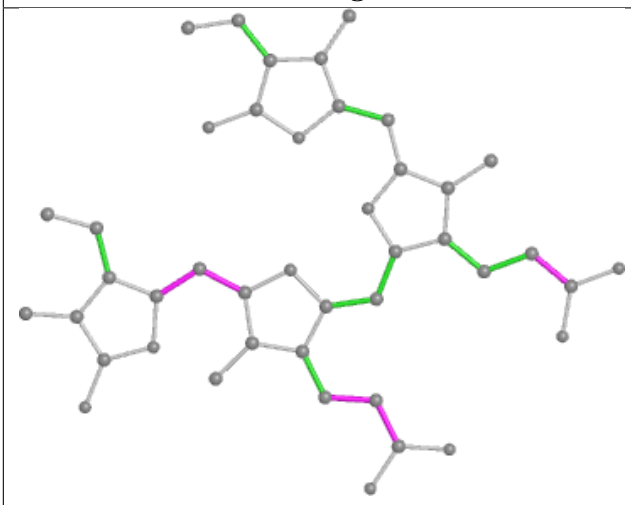

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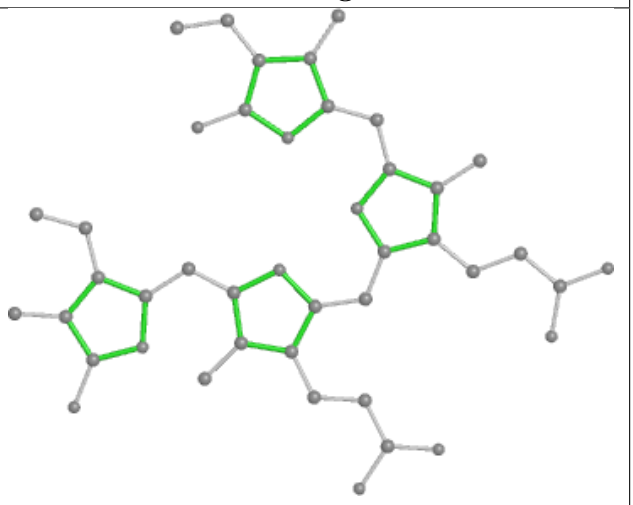
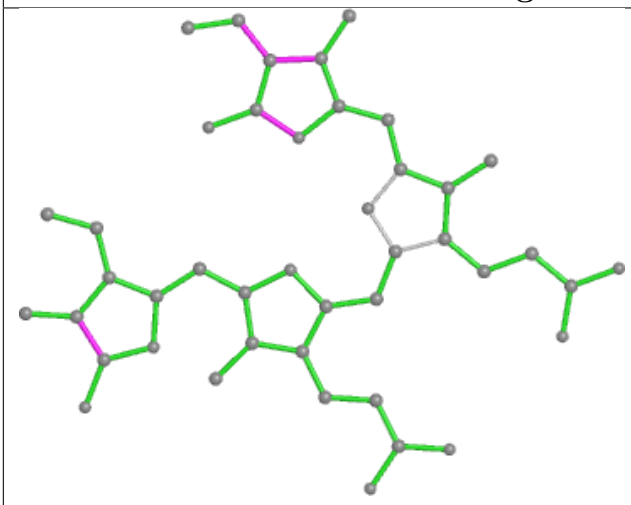


Rings

Ligand PEB P3 201



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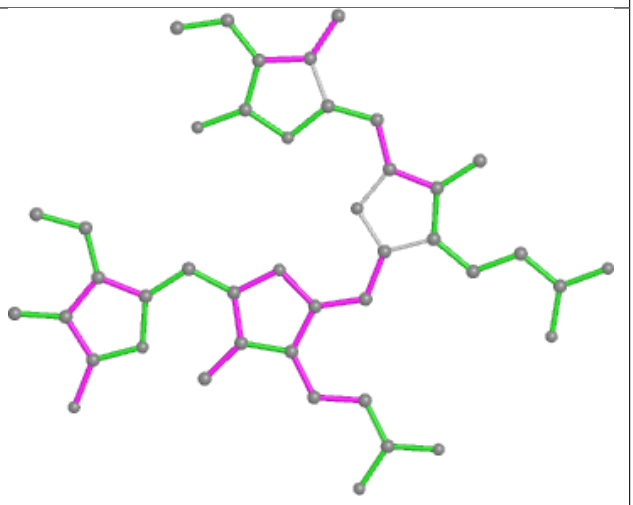

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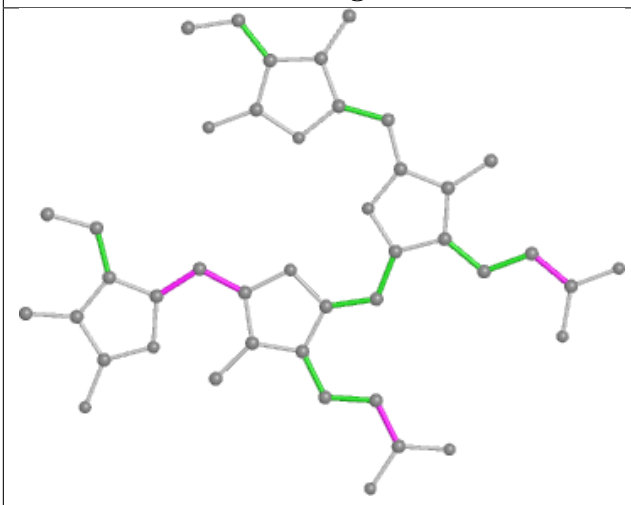

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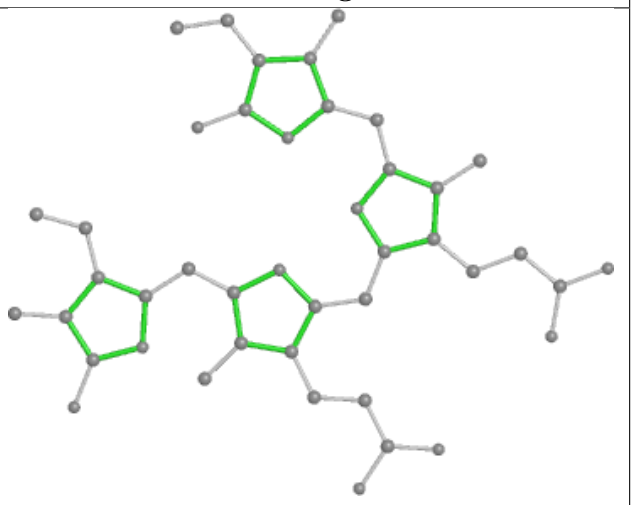
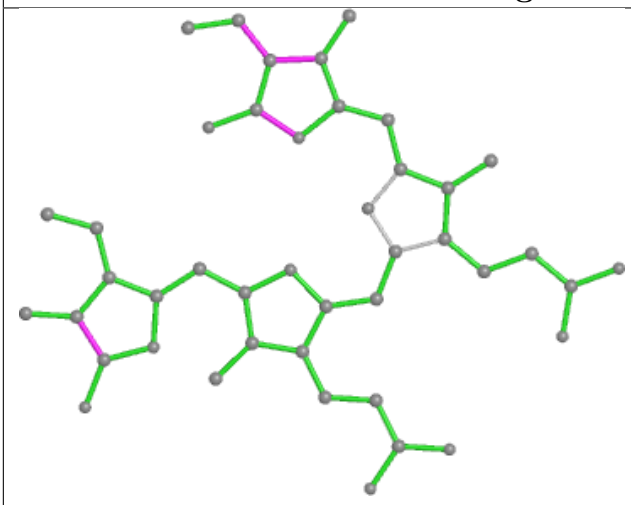


Rings

Ligand PEB C6 201



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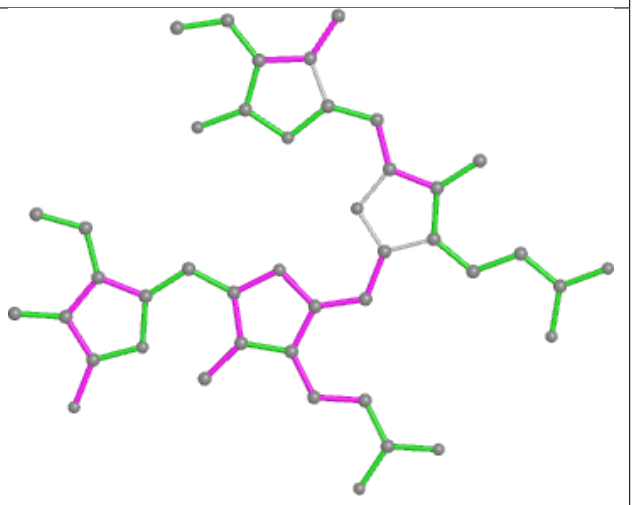

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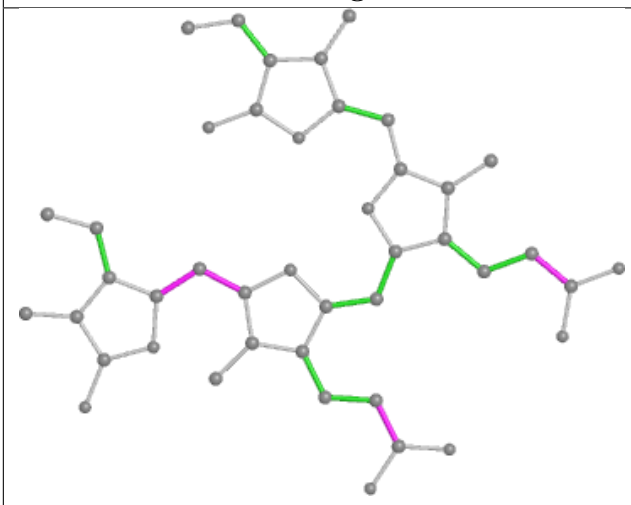

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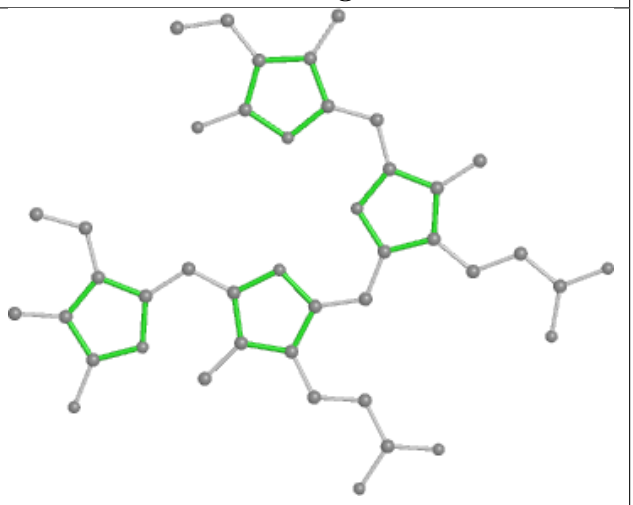
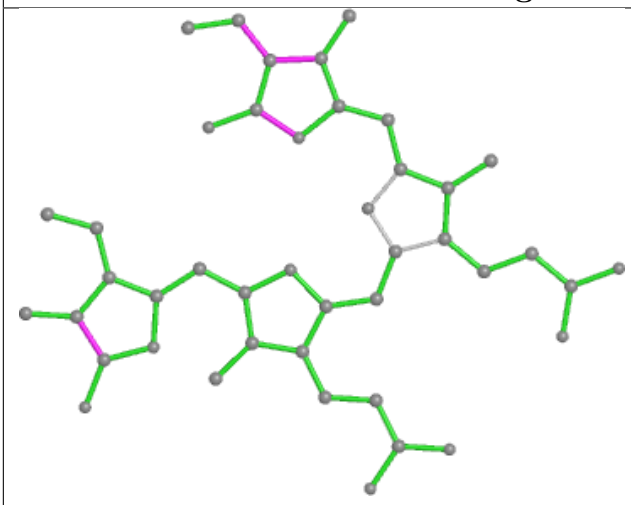


Rings

Ligand PEB A8 202



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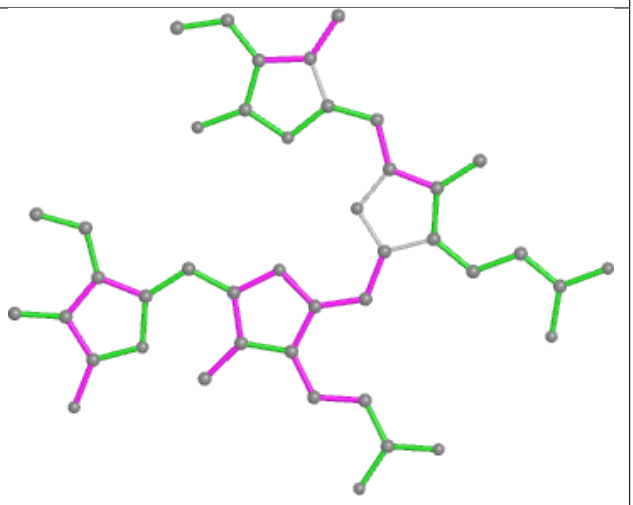

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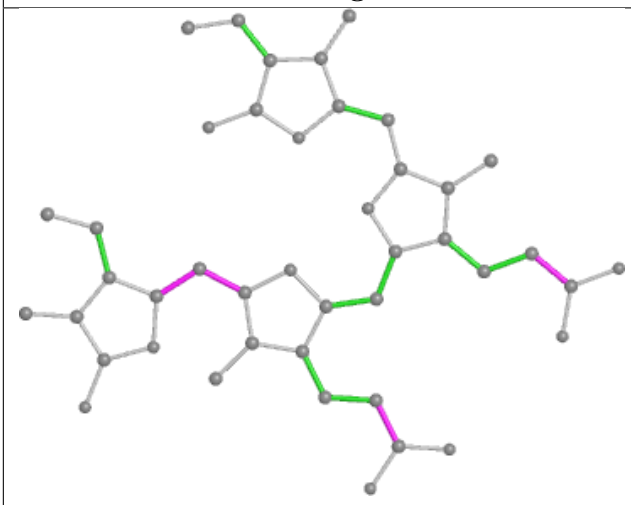

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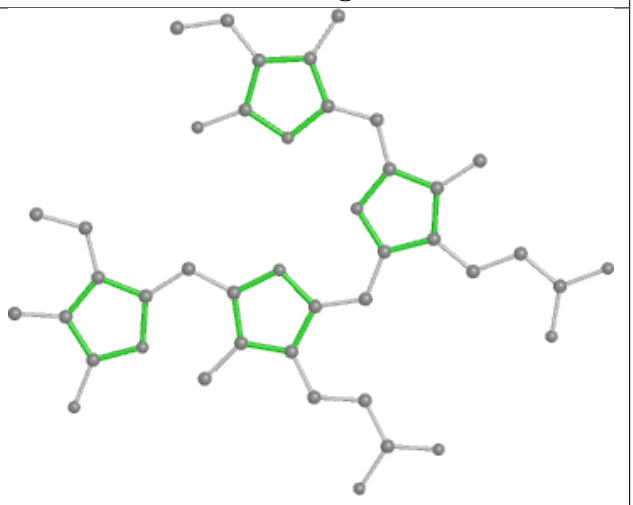
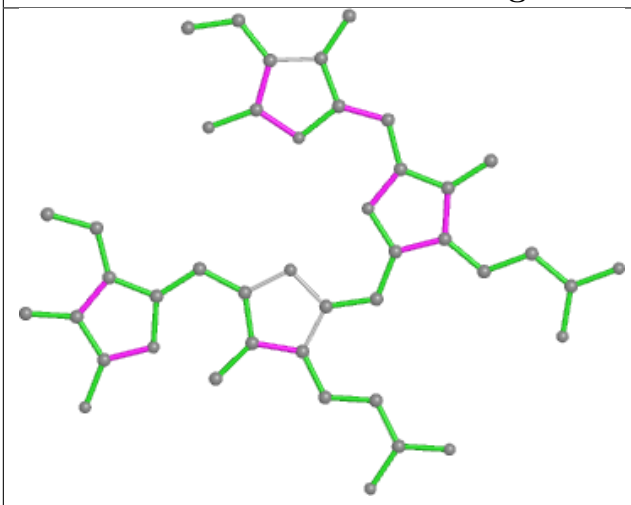


Rings

Ligand PUB iC 1003



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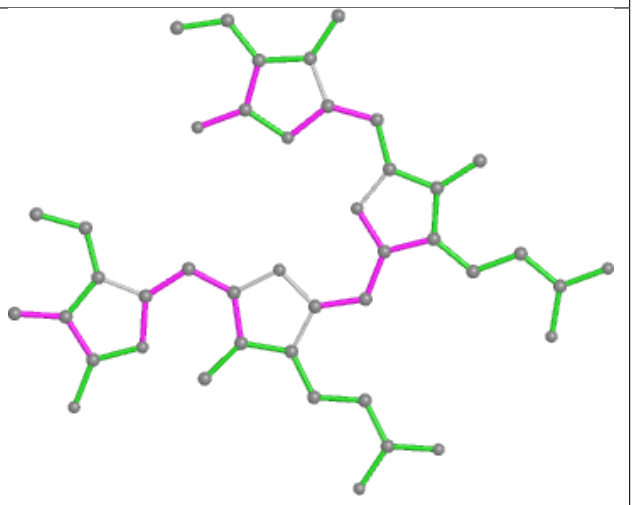

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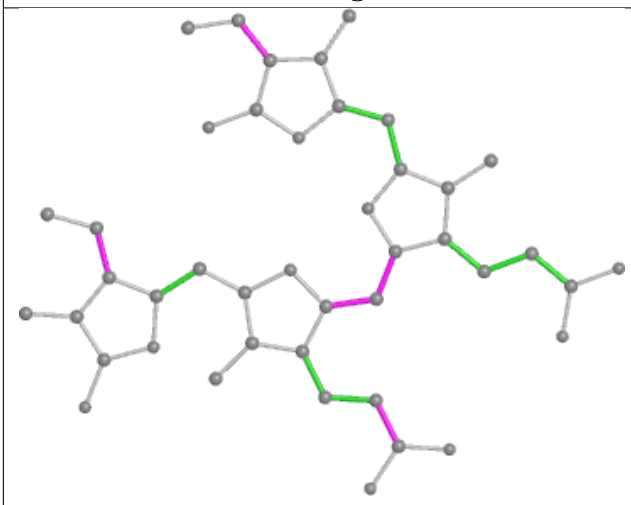

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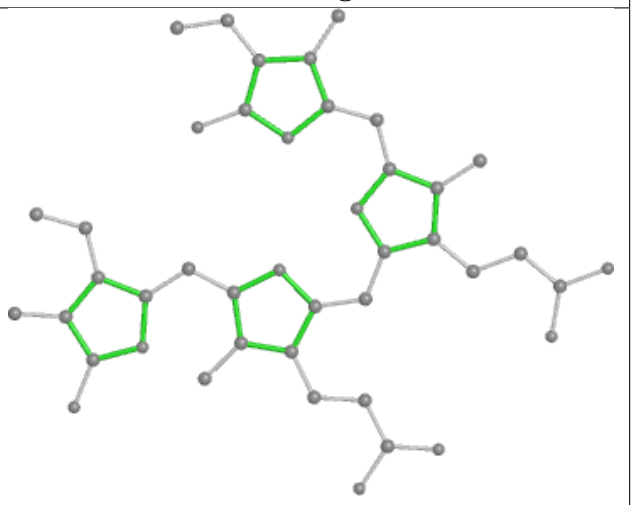

Rings

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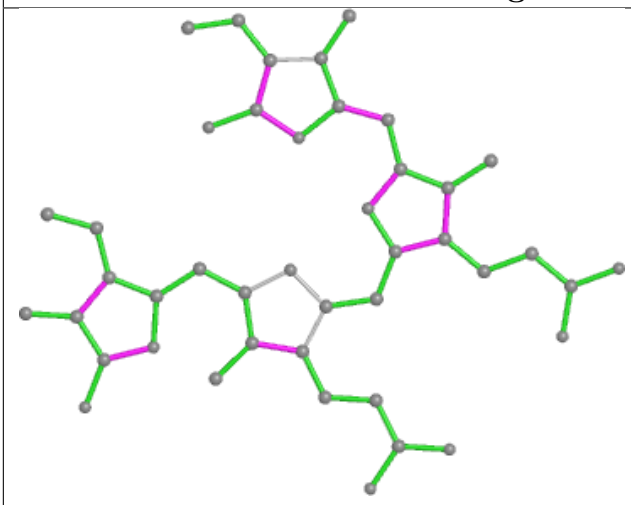

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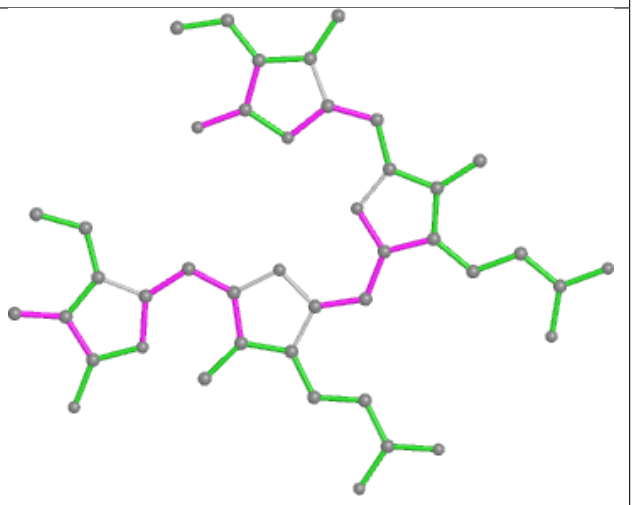

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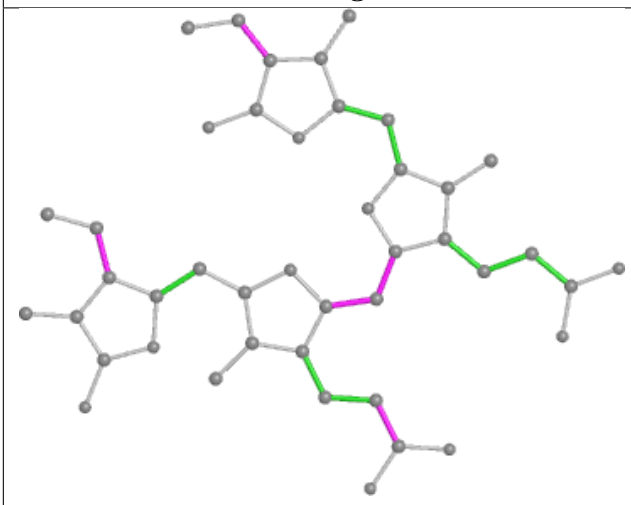

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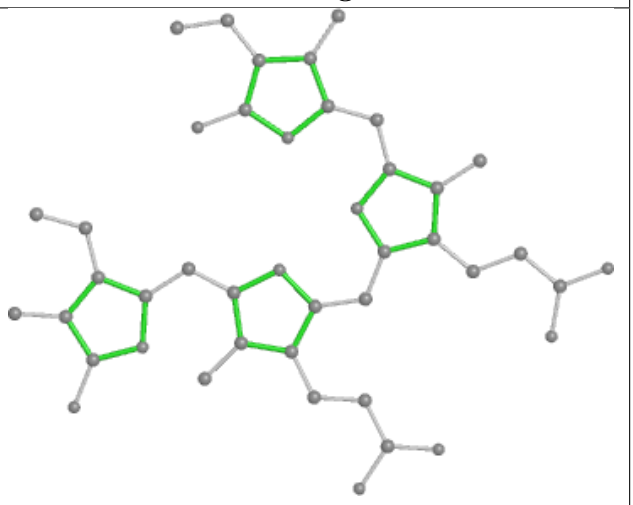
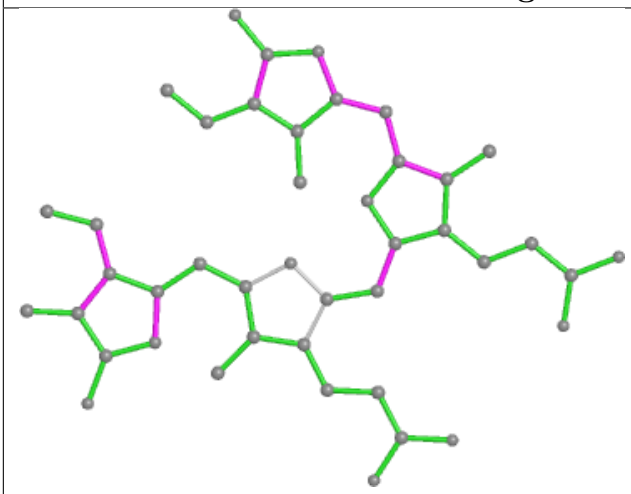


Rings

Ligand PVN e8 303



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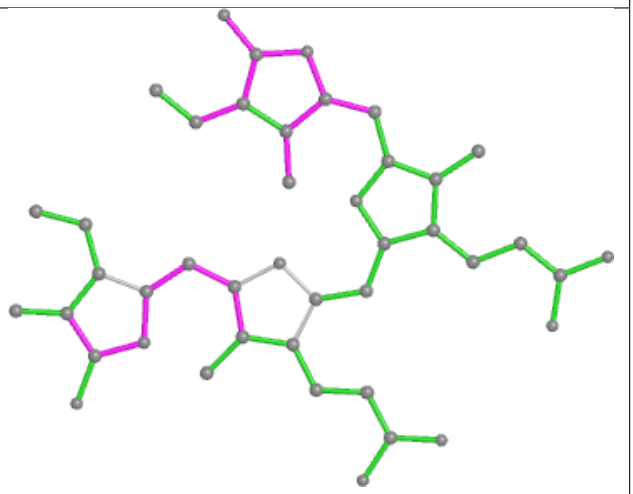

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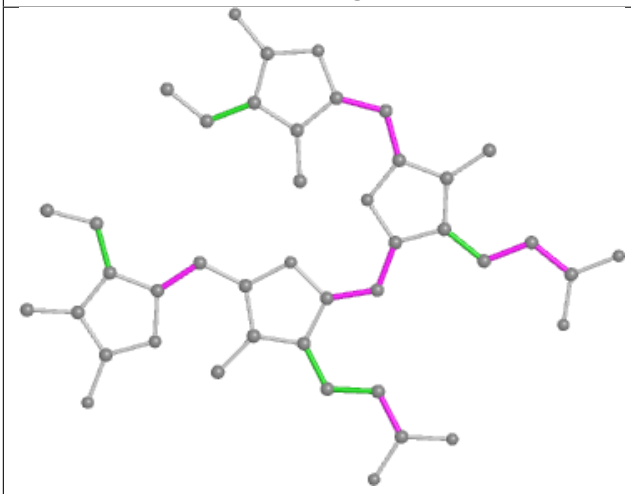

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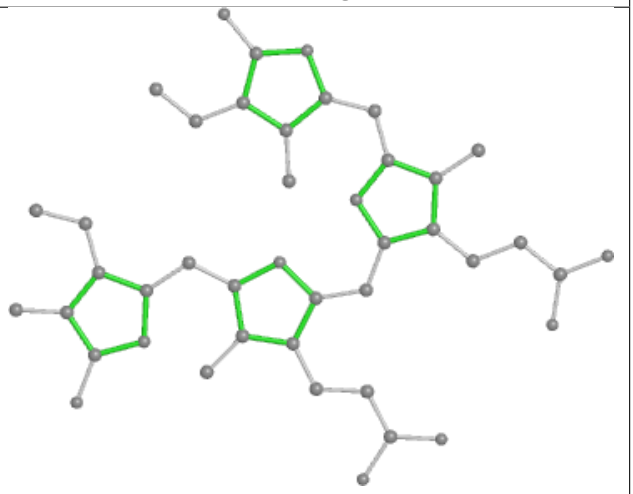
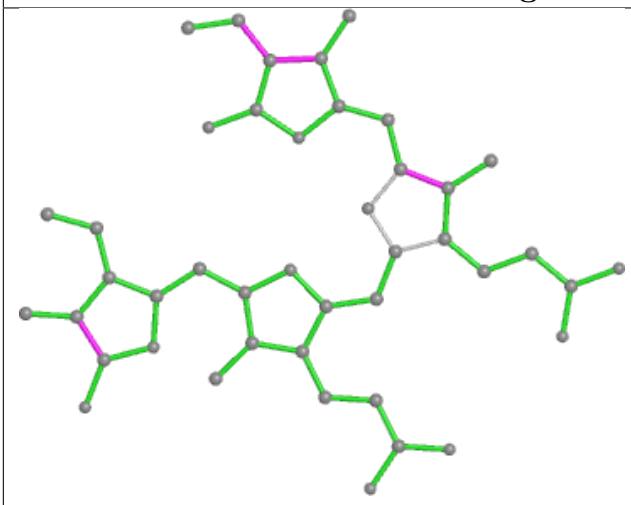


Rings

Ligand PEB g7 202



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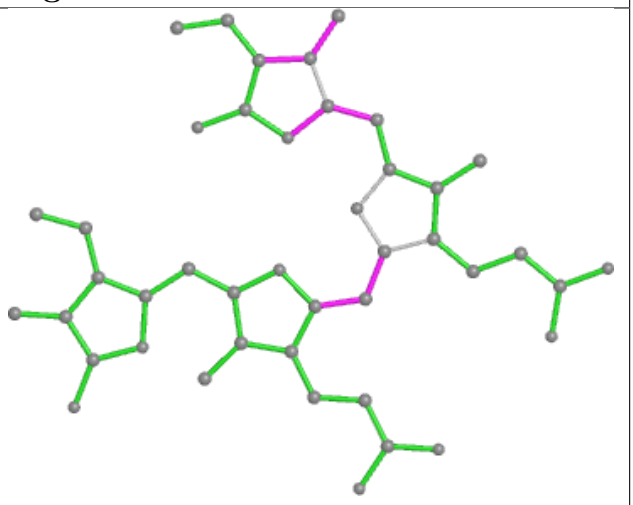

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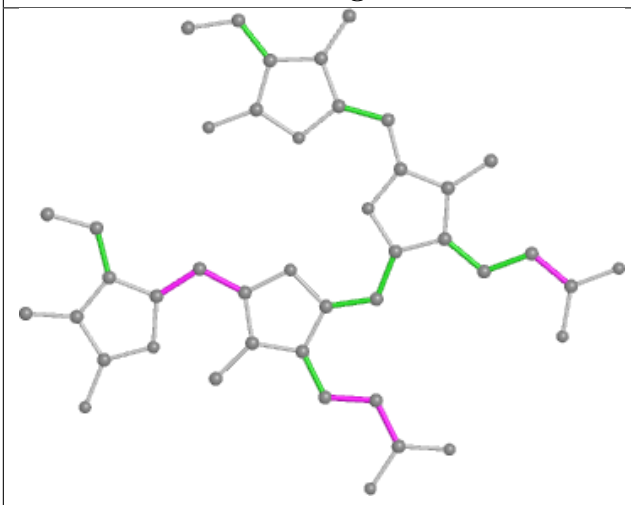

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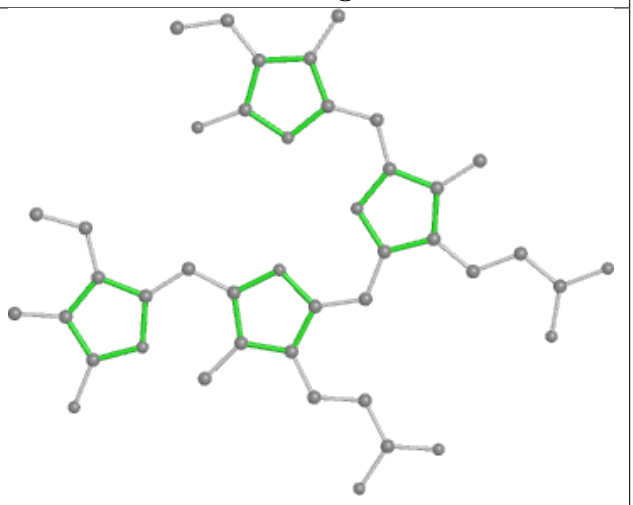
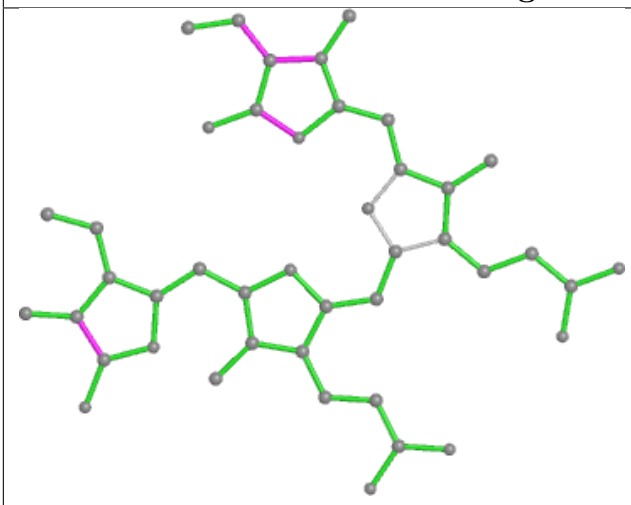


Rings

Ligand PEB L6 201



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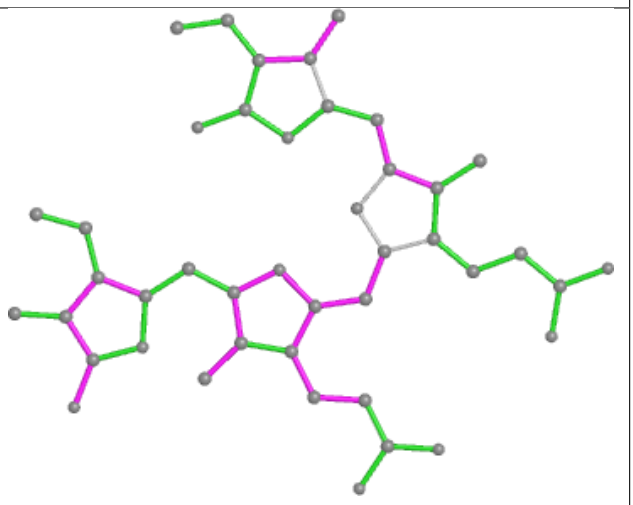

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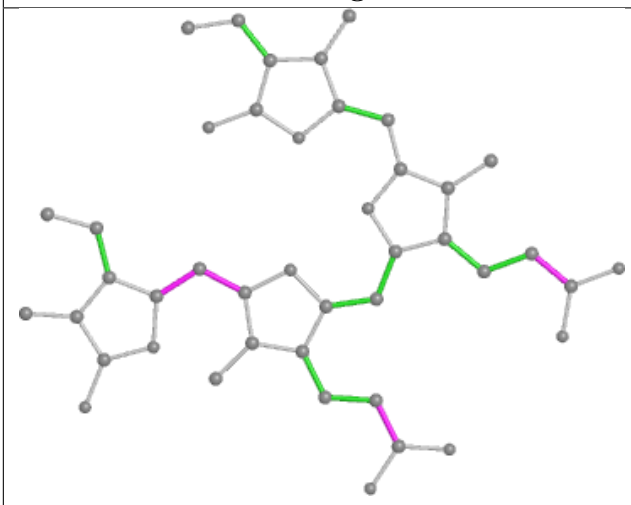

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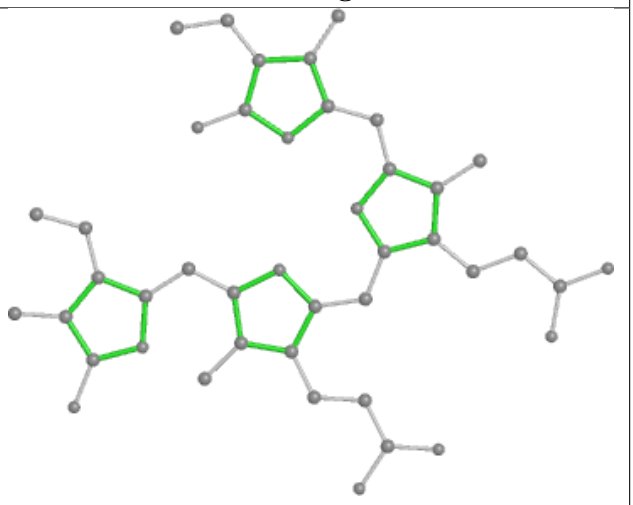
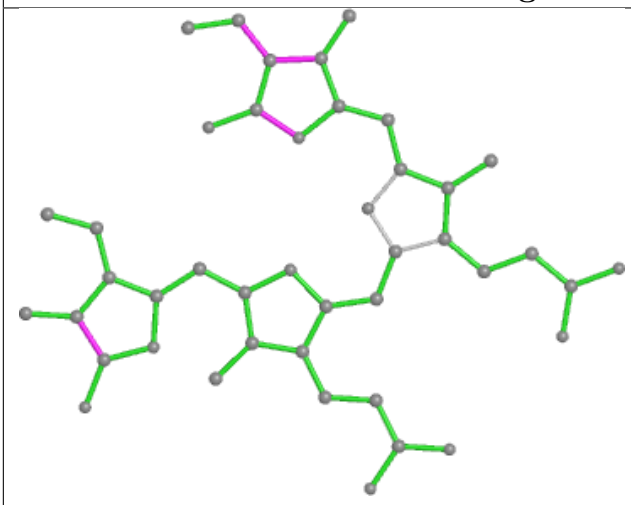


Rings

Ligand PEB S5 201



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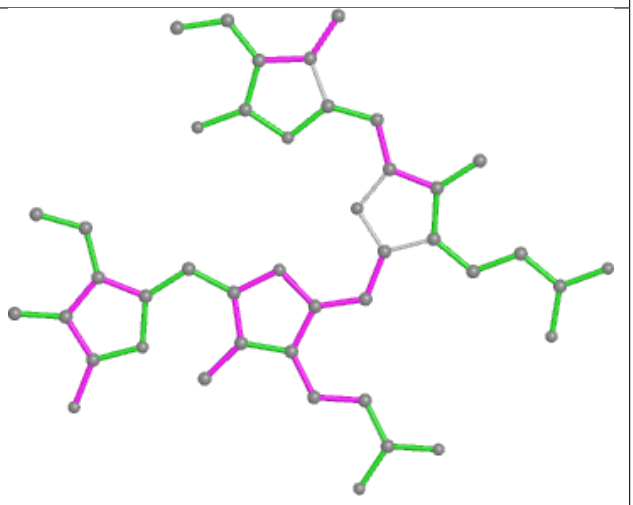

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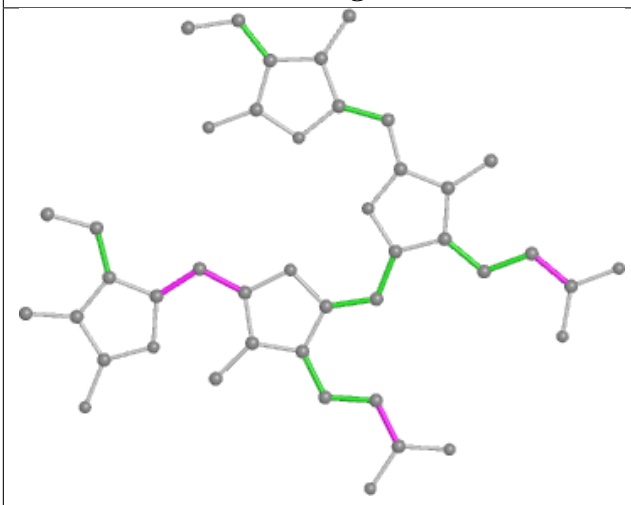

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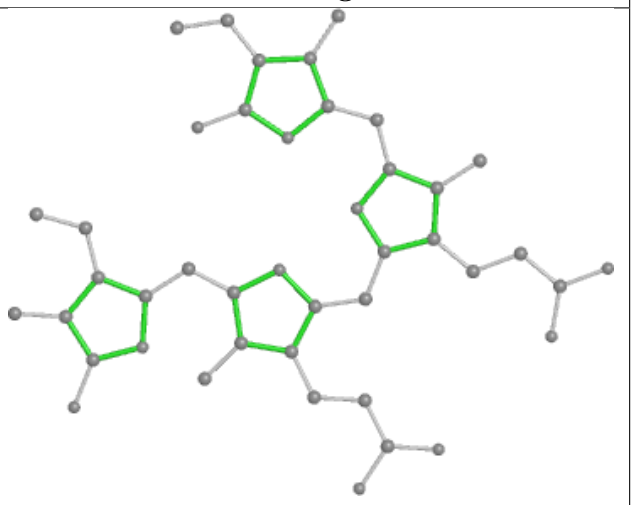
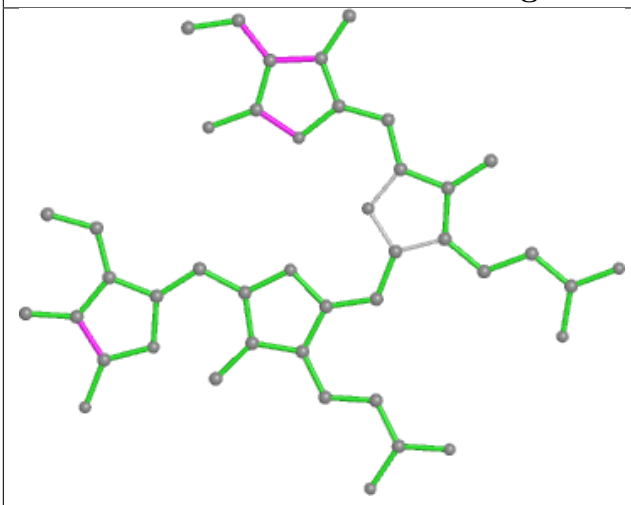


Rings

Ligand PEB e9 303



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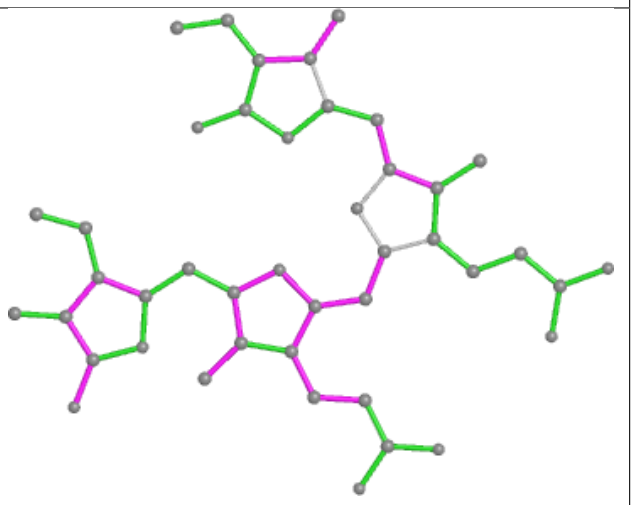

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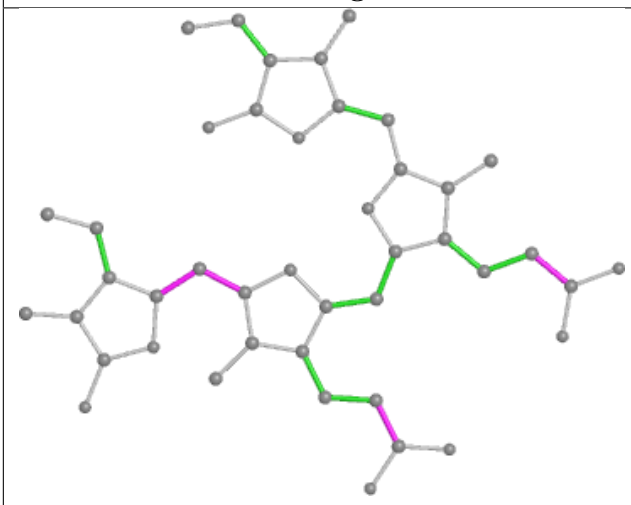

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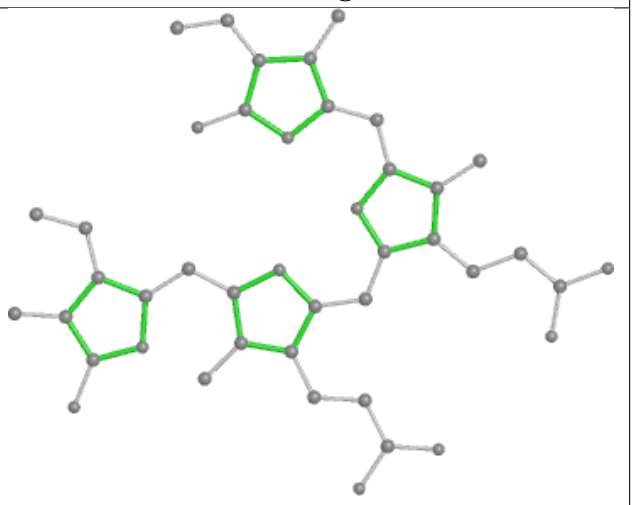
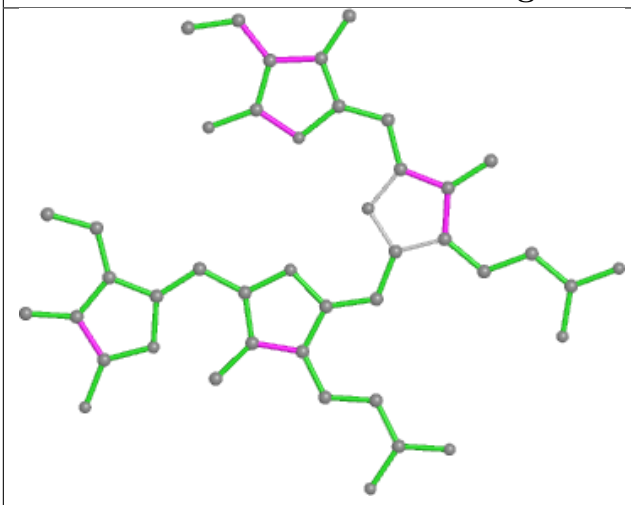


Rings

Ligand PEB F5 202



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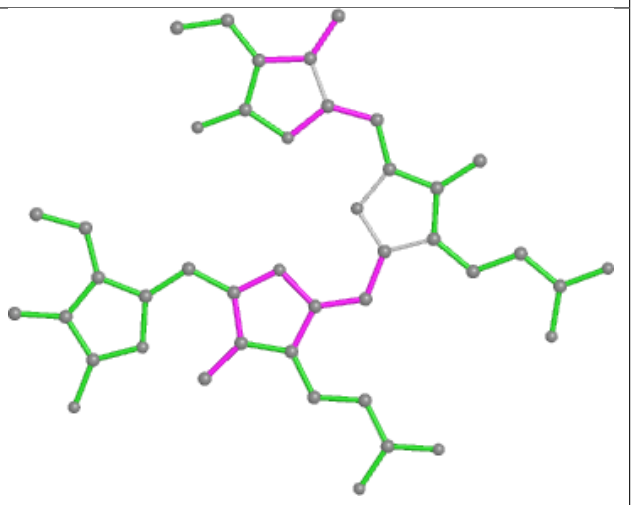

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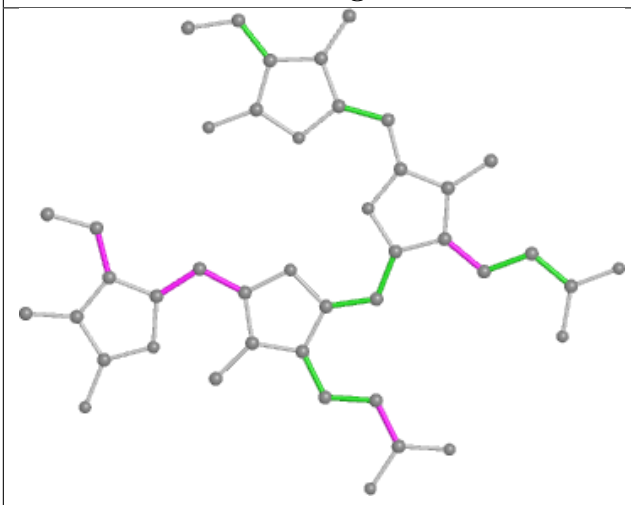
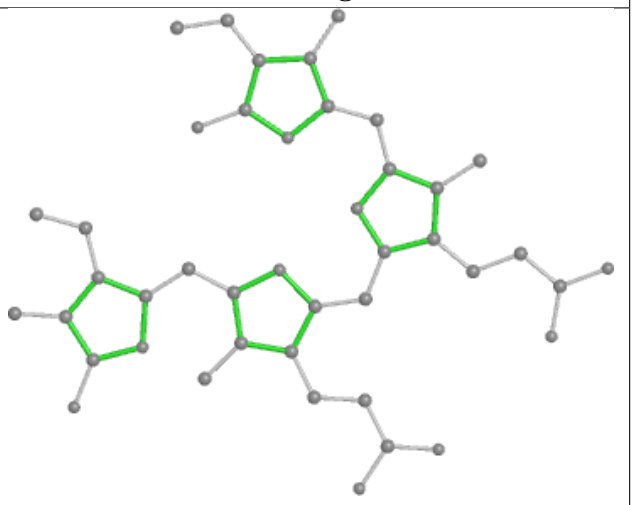
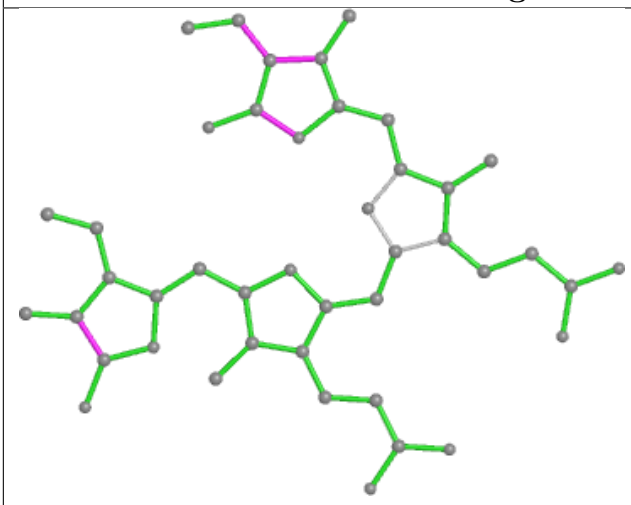


Torsions



Rings

Ligand PEB lm 1001



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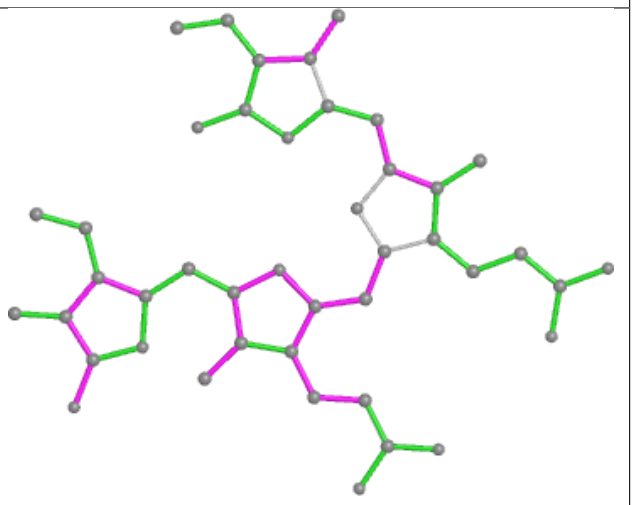

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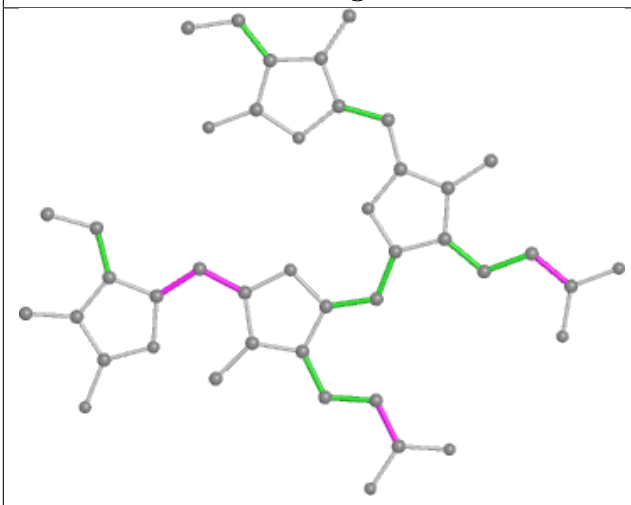

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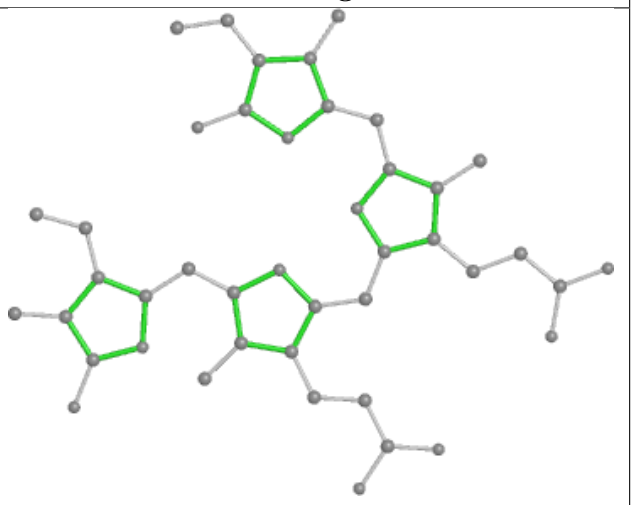
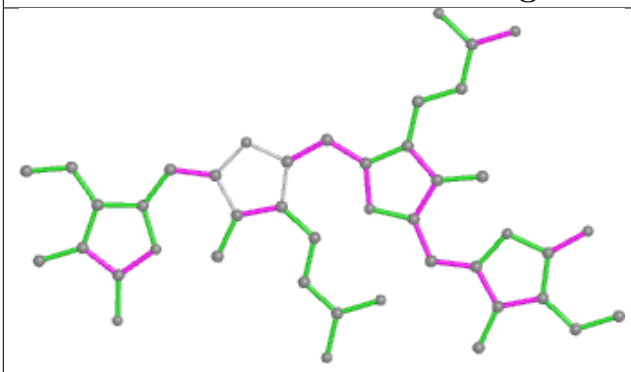


Rings

Ligand CYC I1 201



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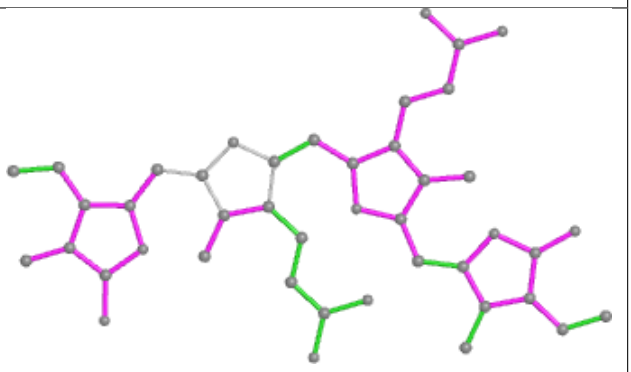

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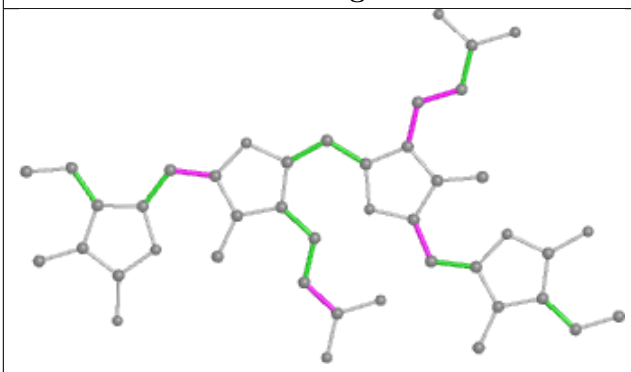

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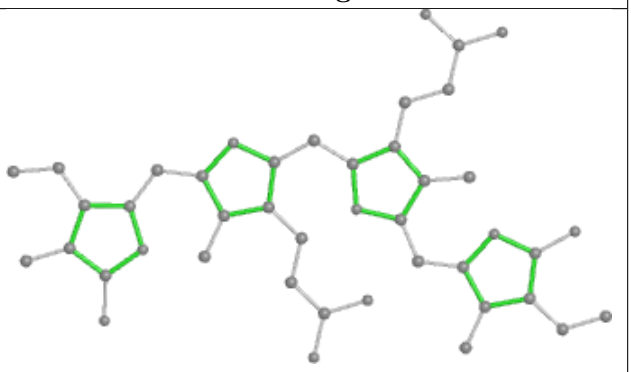
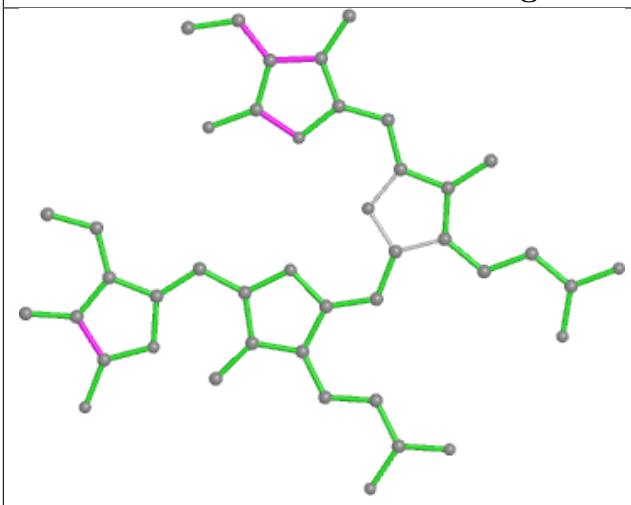


Rings

Ligand PEB cx 201



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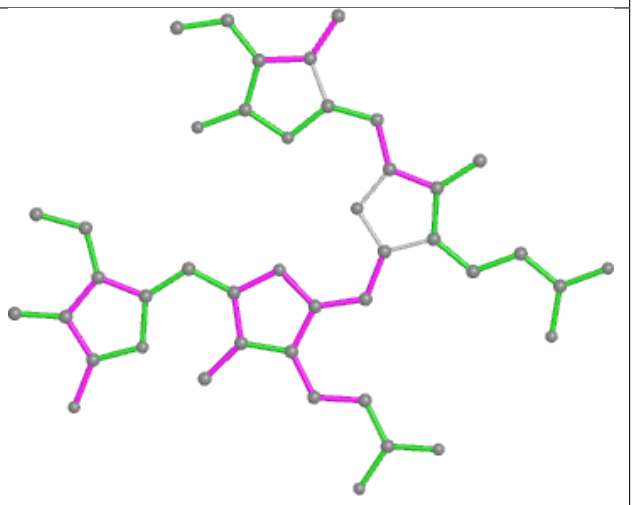

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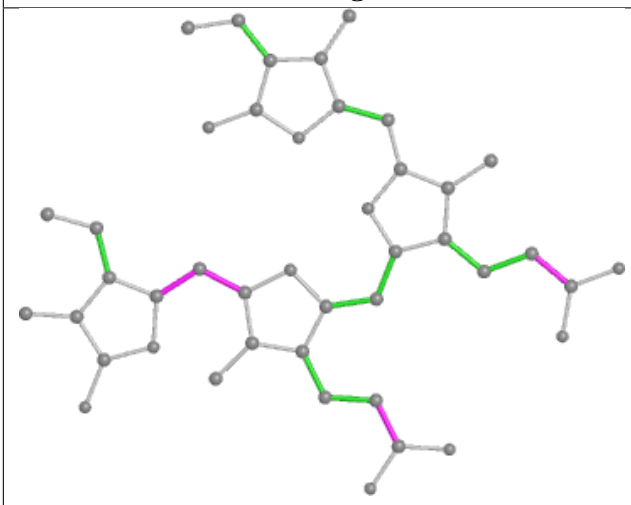

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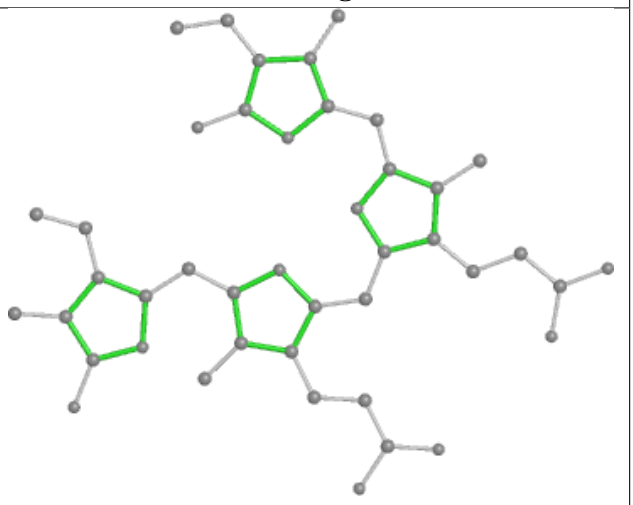
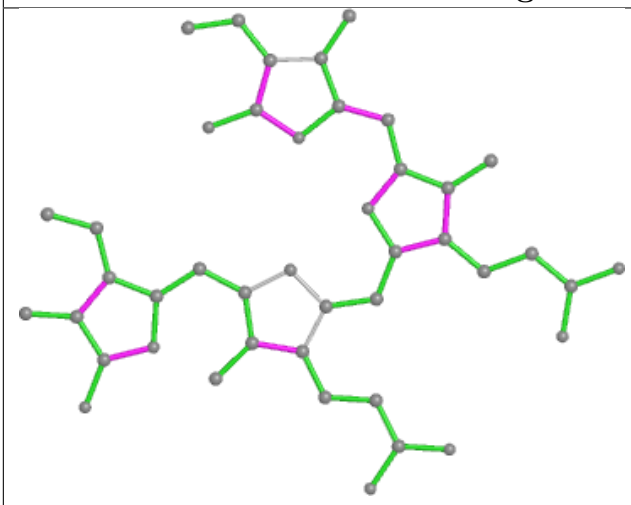


Rings

Ligand PUB p8 203



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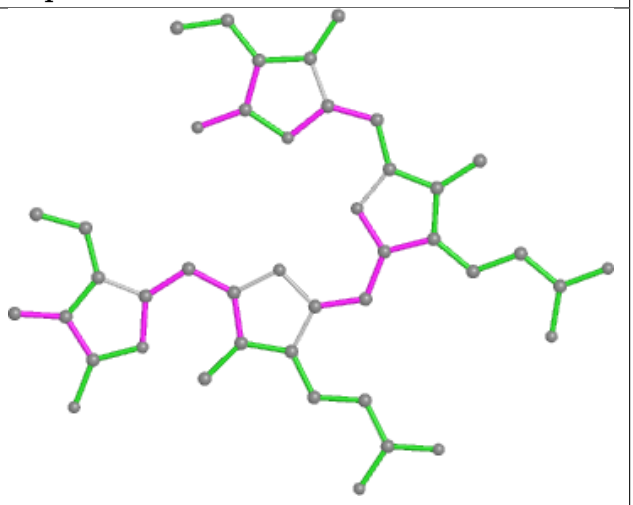

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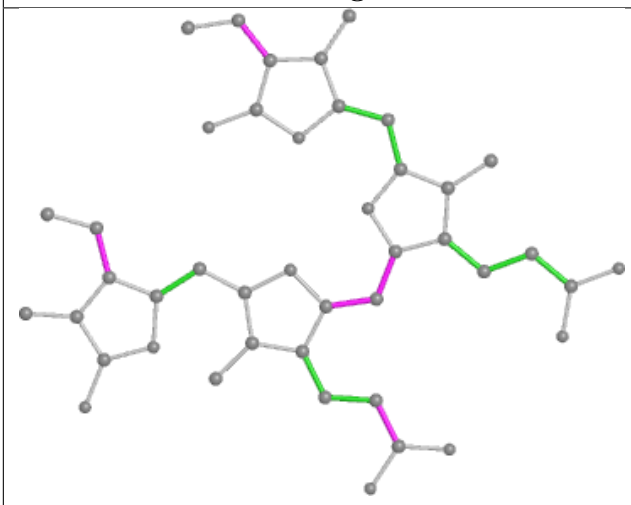

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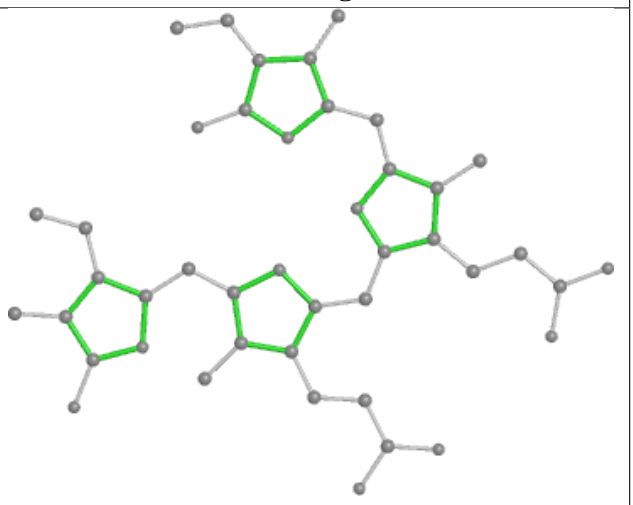
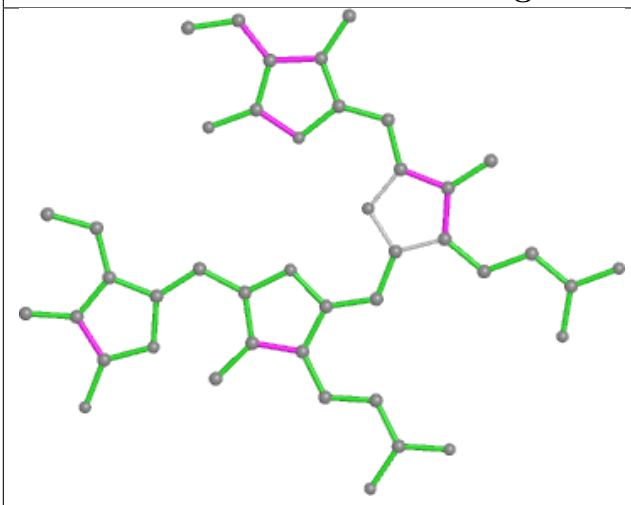


Rings

Ligand PEB hR 202



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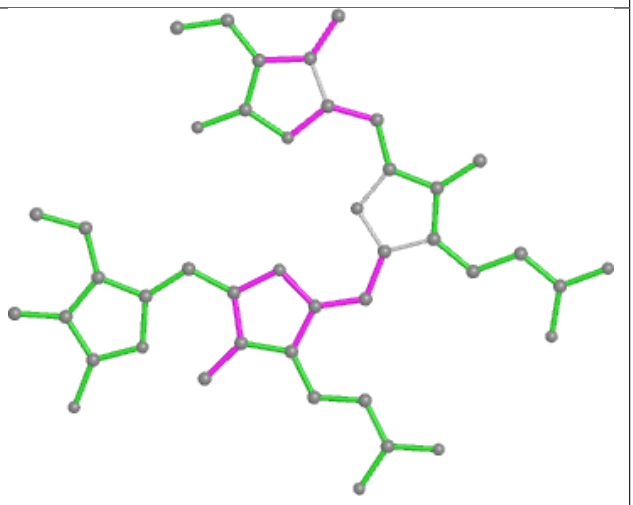

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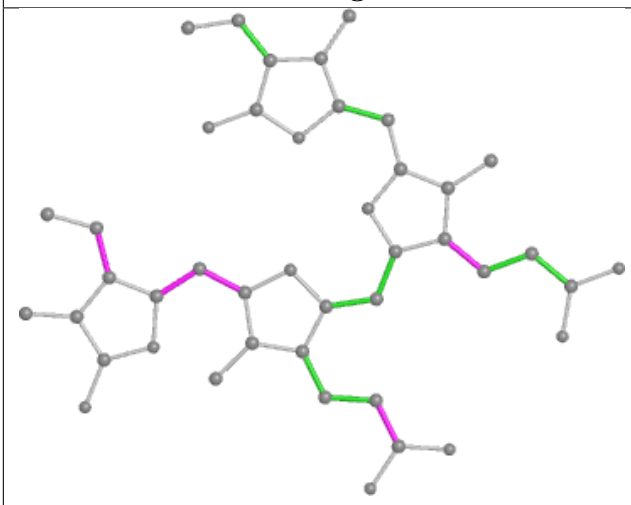

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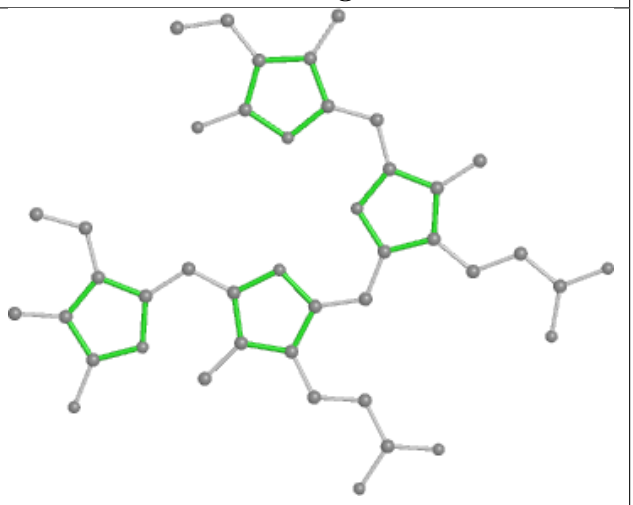
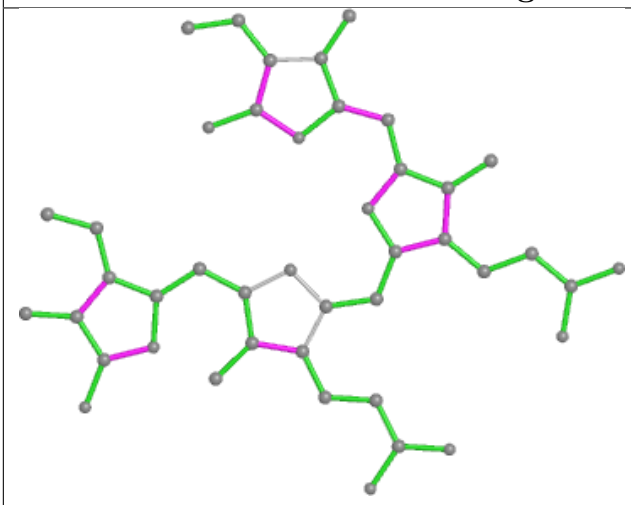


Rings

Ligand PUB gy 305



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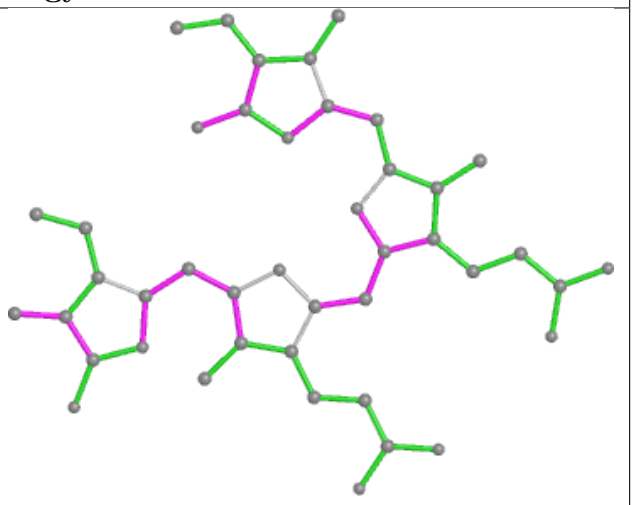

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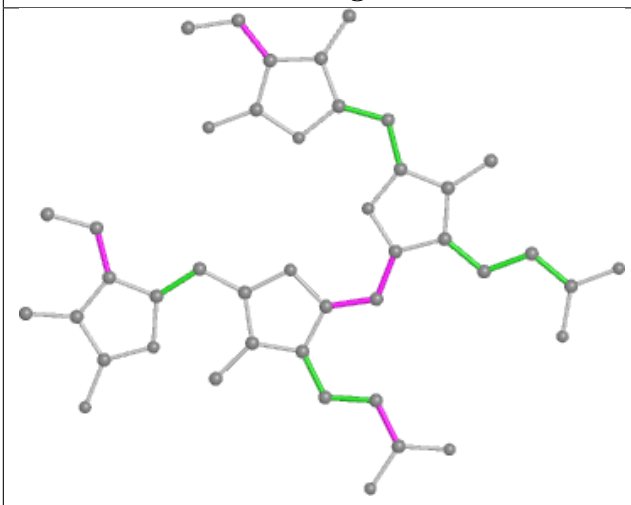

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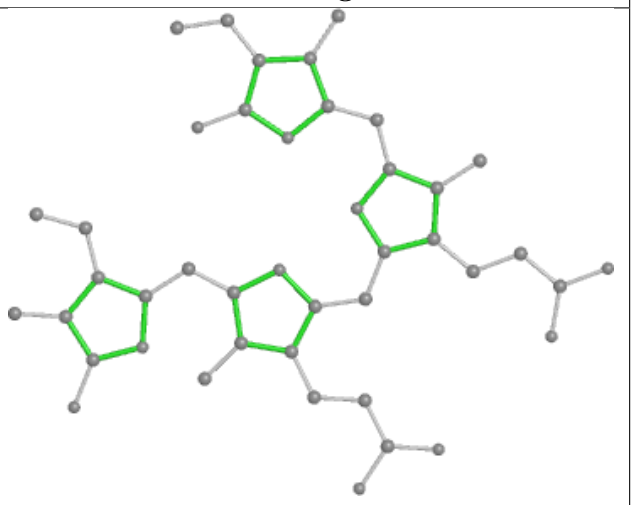

Rings

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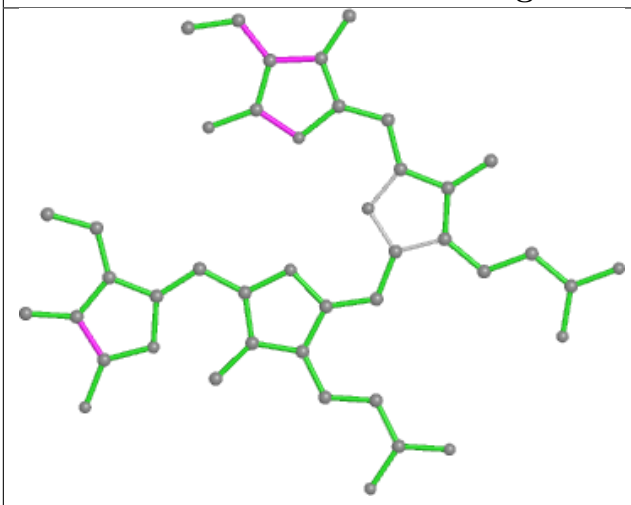

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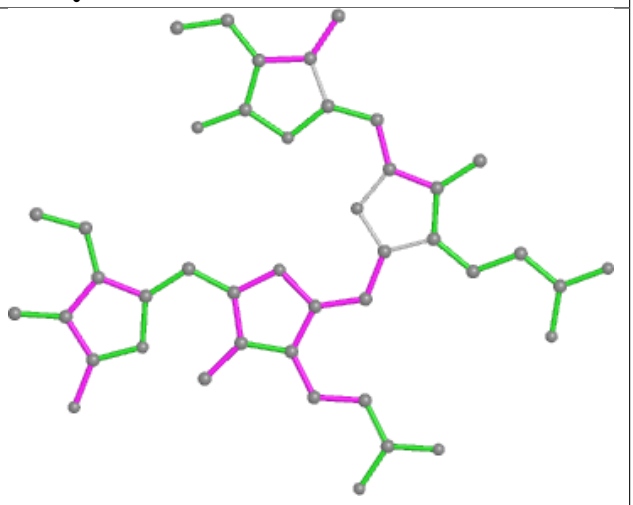

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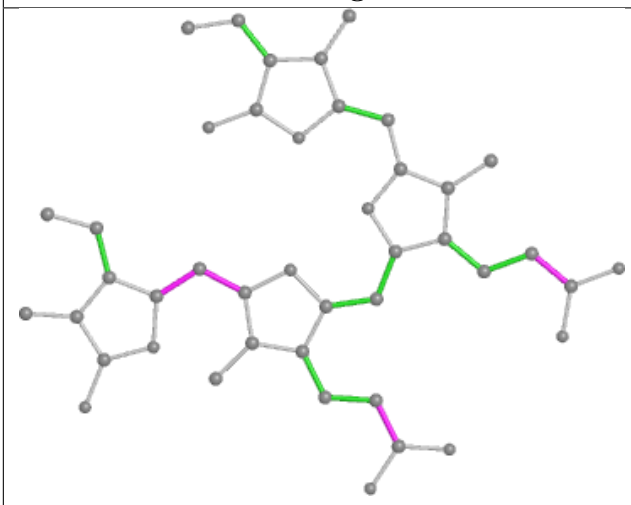

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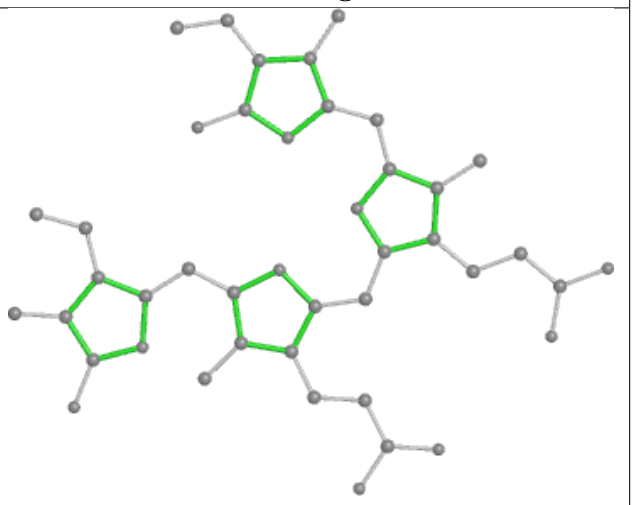
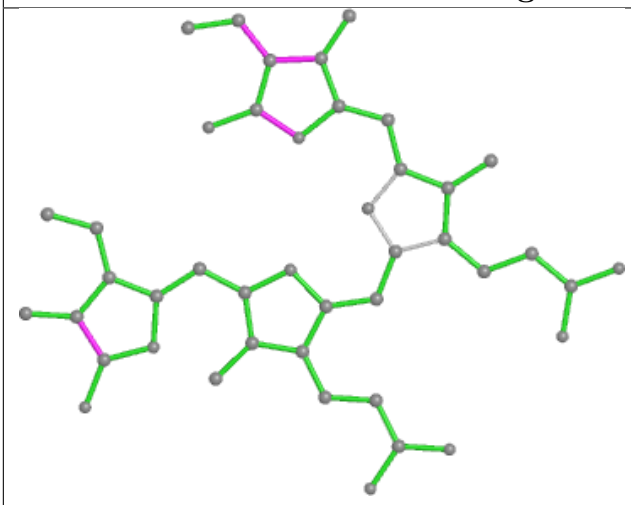


Rings

Ligand PEB eV 201



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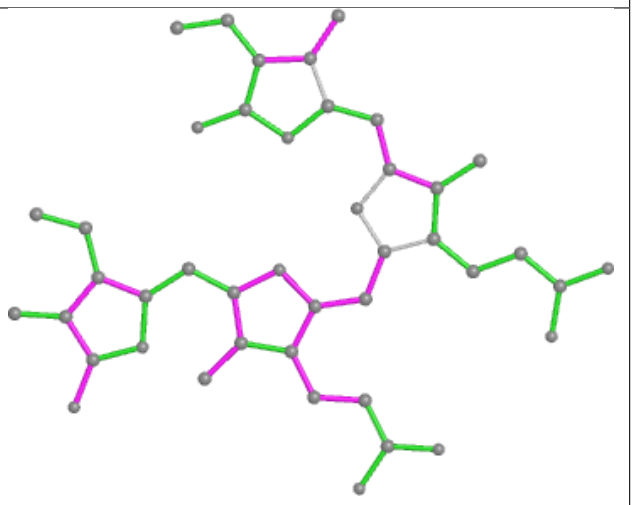

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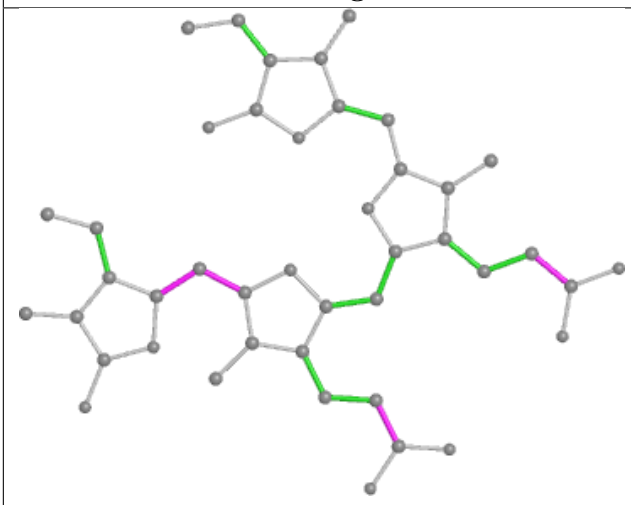

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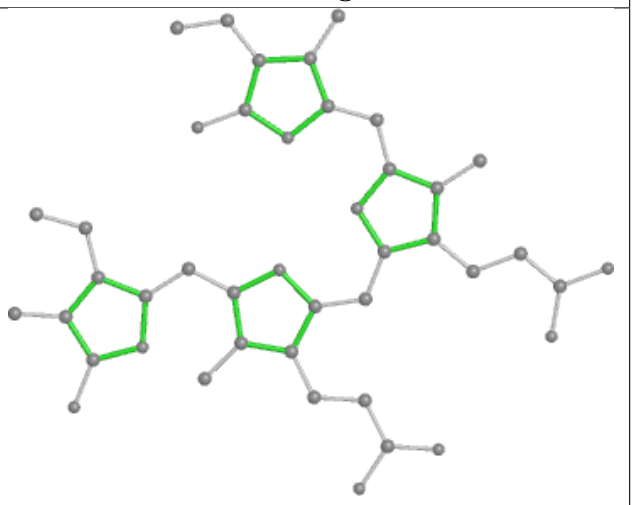

Rings

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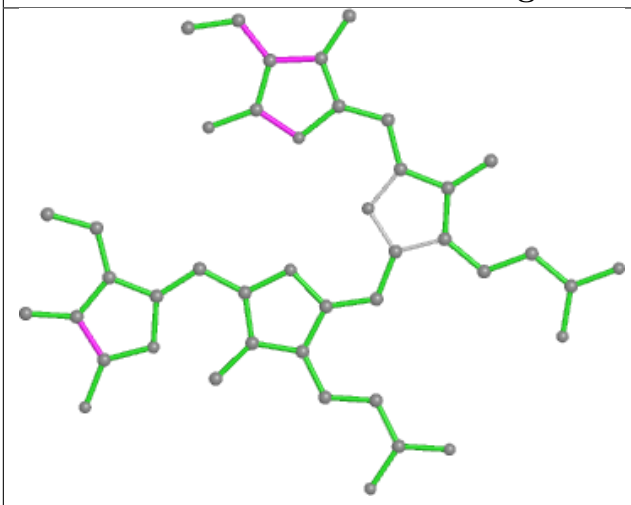

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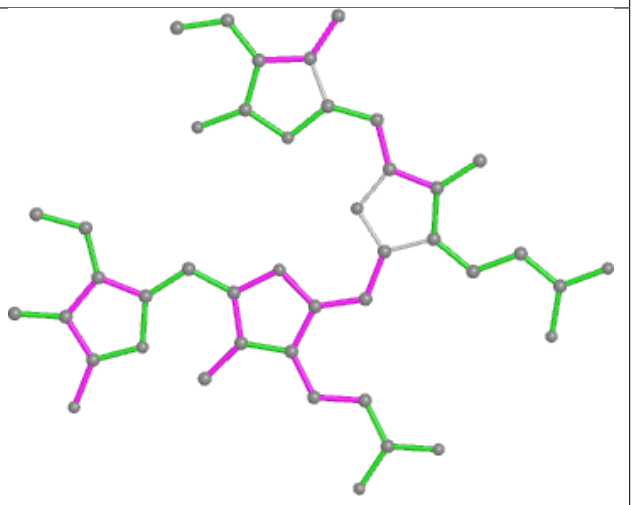

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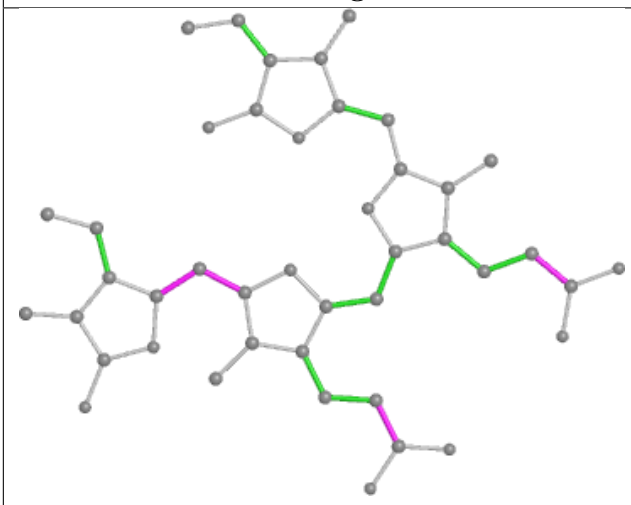

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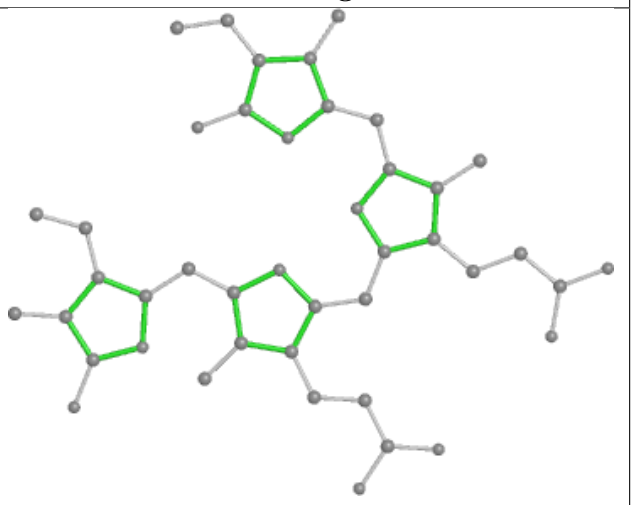
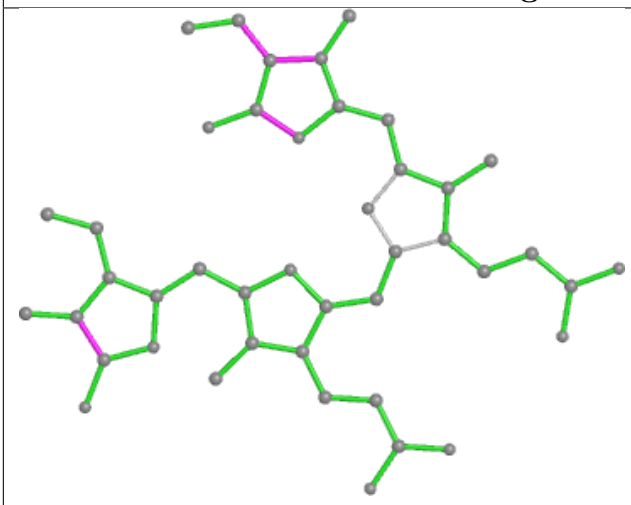


Rings

Ligand PEB ck 201



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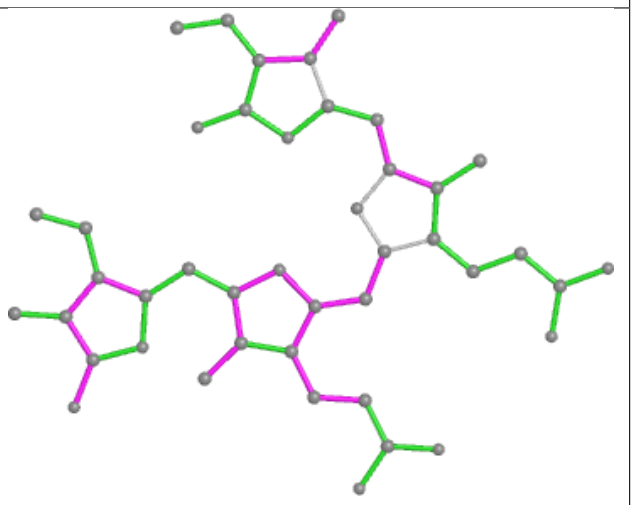

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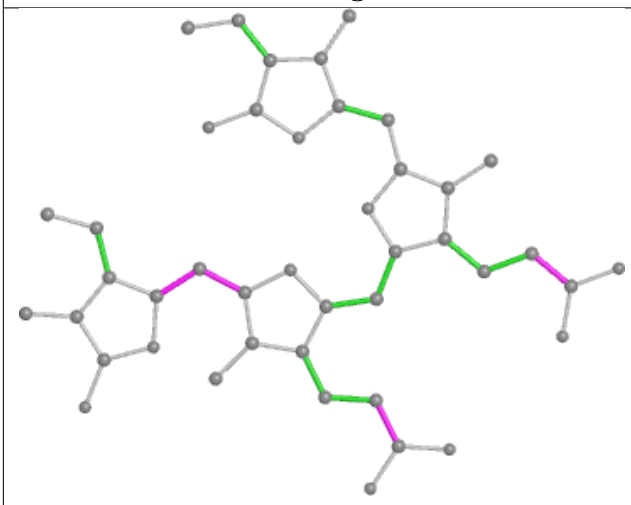

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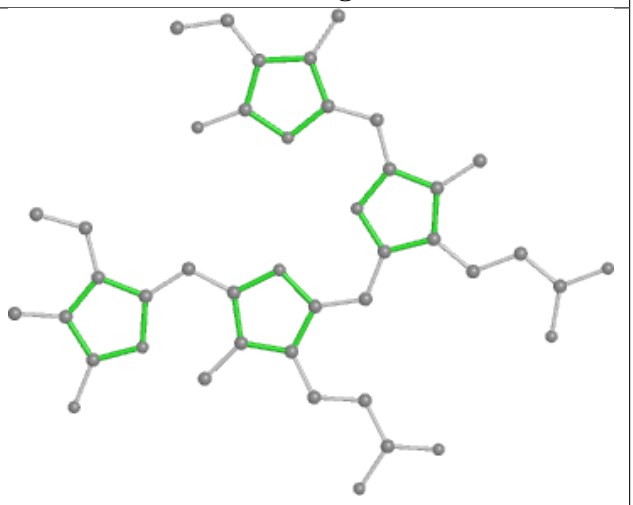
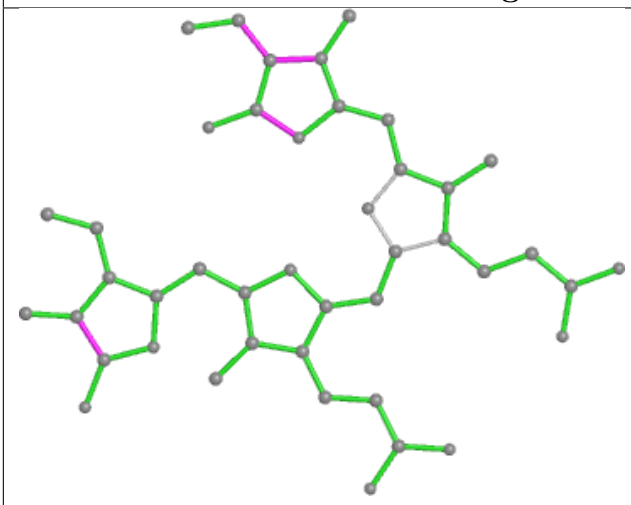


Rings

Ligand PEB dM 1002



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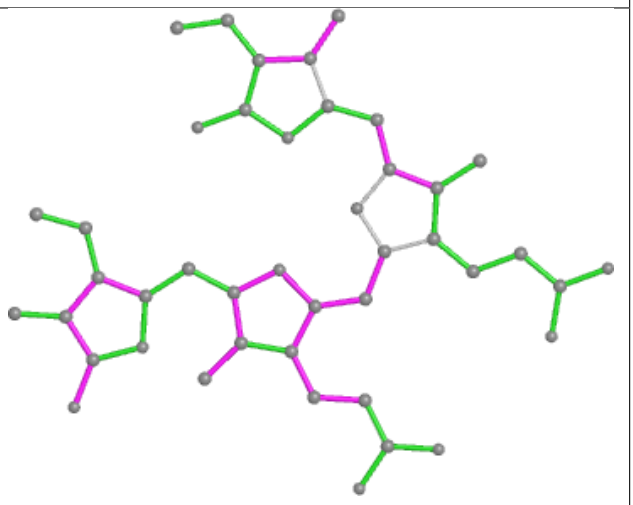

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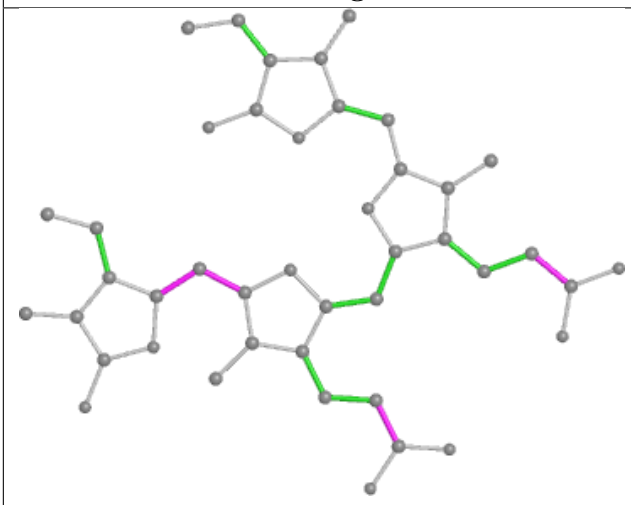

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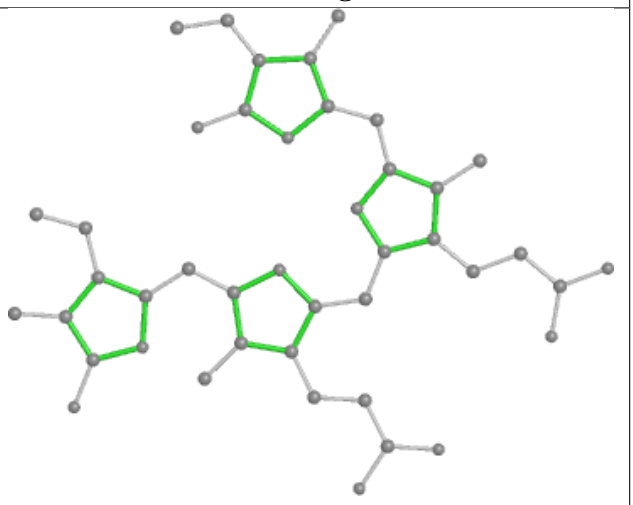
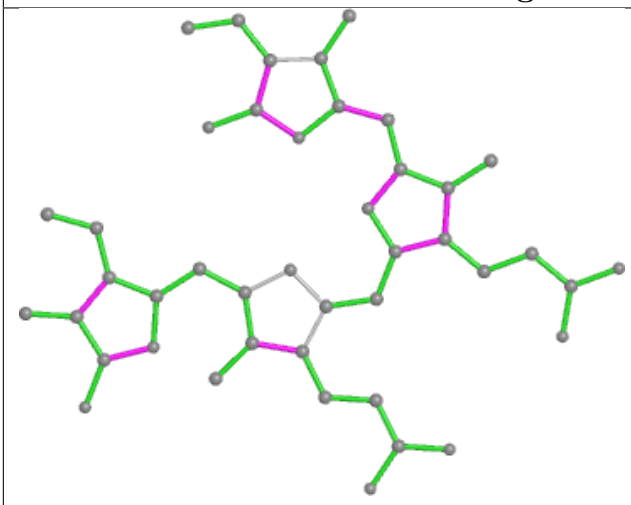


Rings

Ligand PUB p7 202



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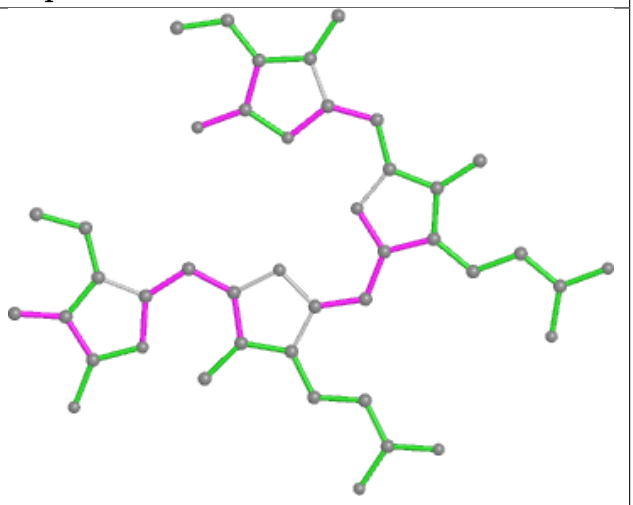

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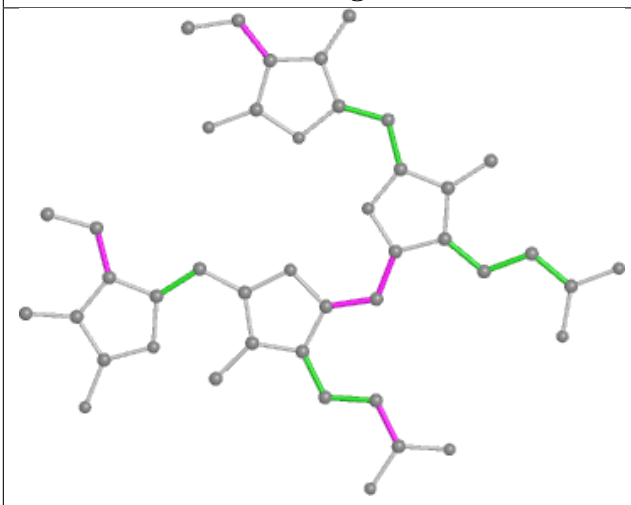

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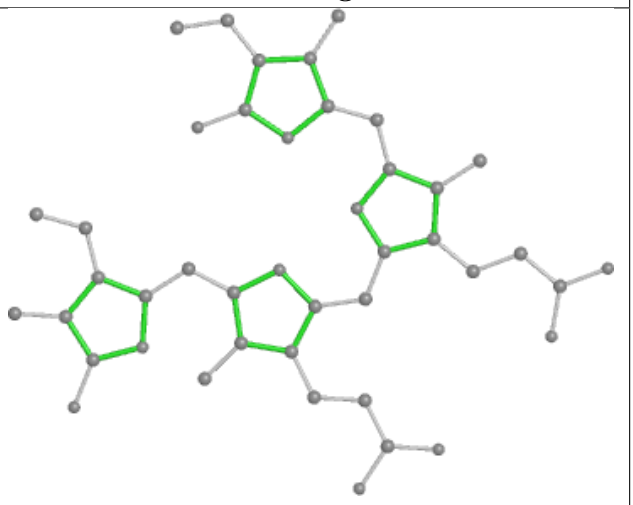
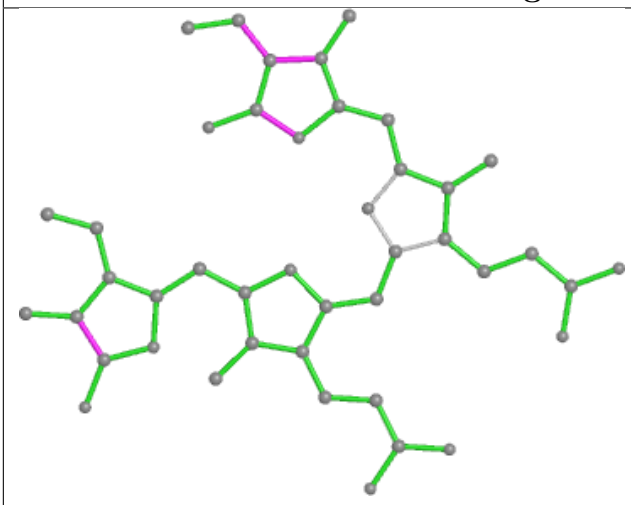


Rings

Ligand PEB l3 201



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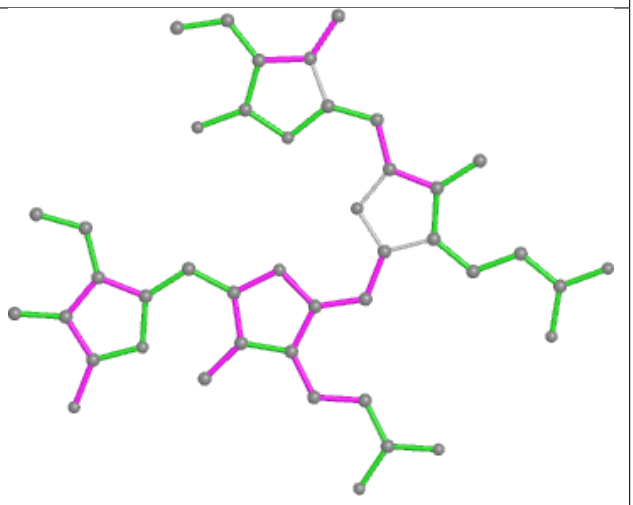

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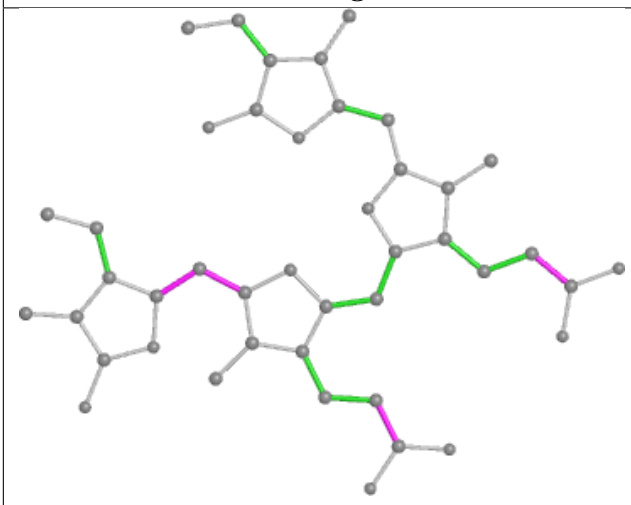

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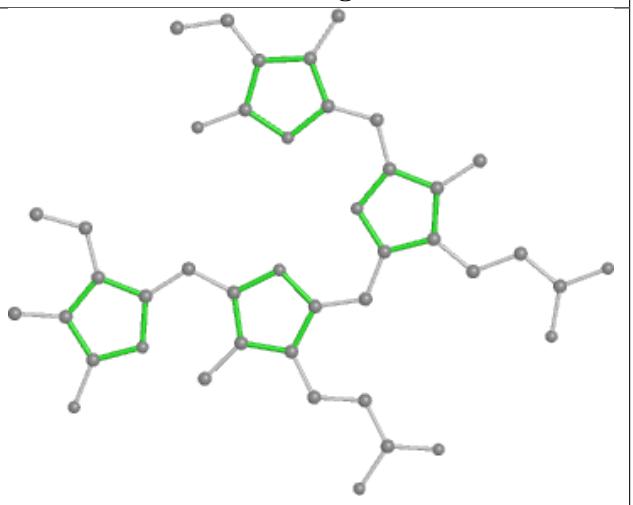
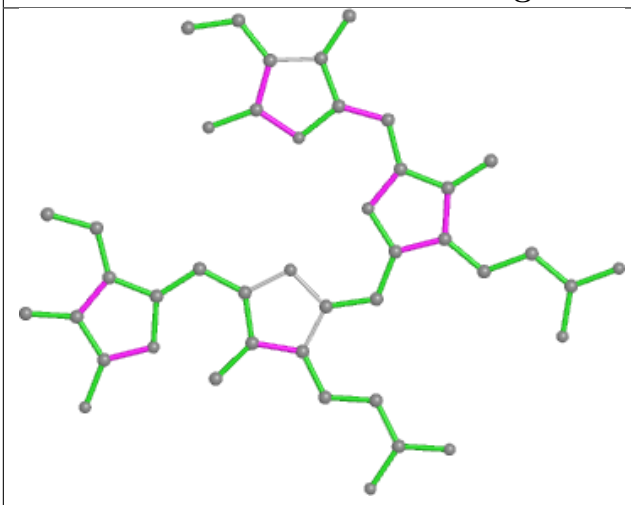
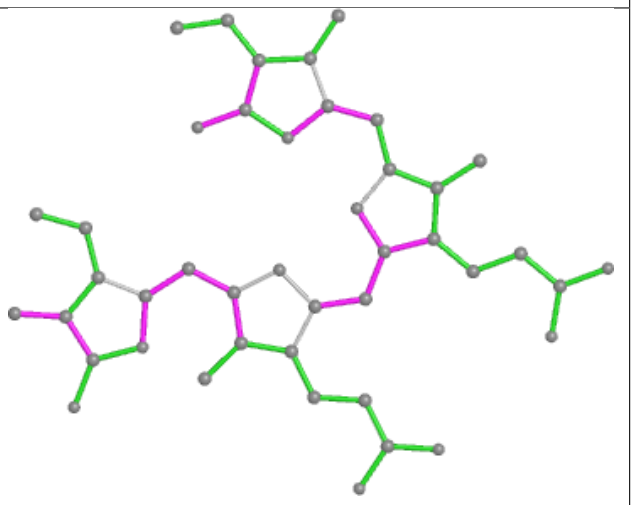


Rings

Ligand PUB B9 203



Bond lengths



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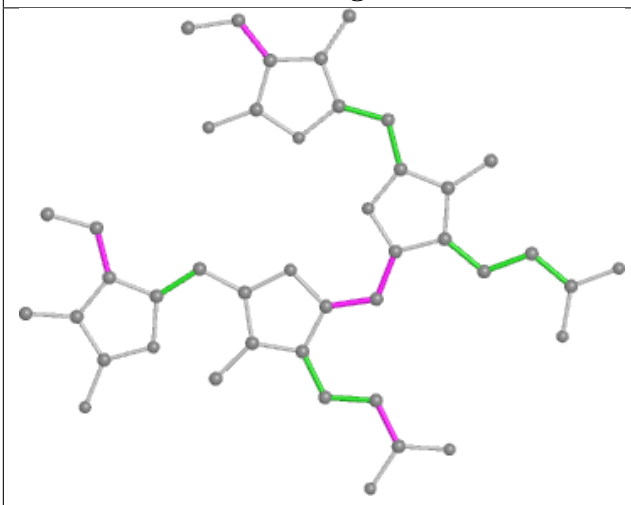
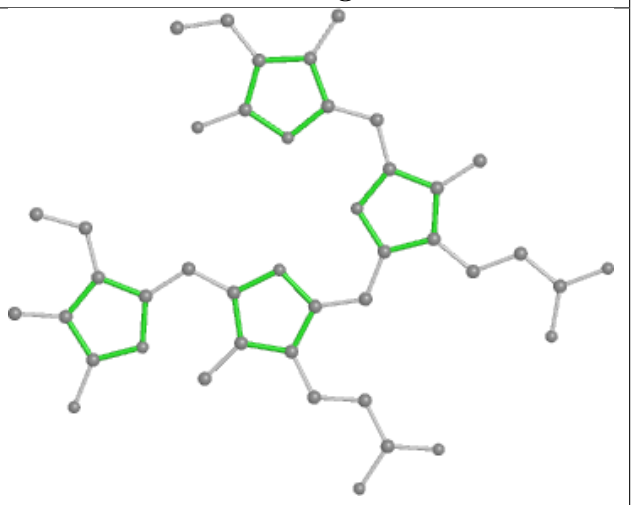
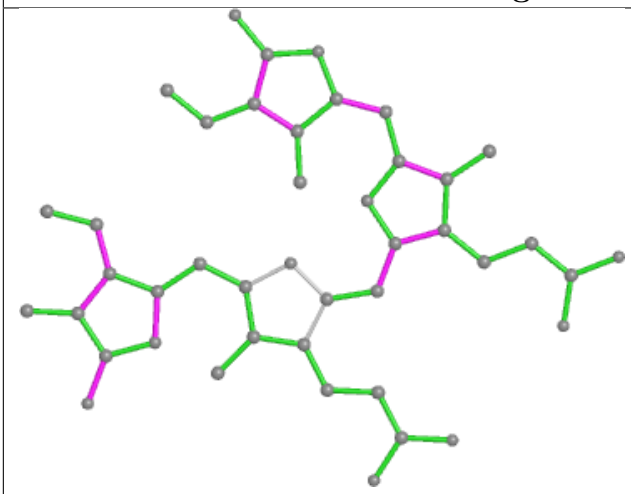


Torsions



Rings

Ligand PVN C2 303



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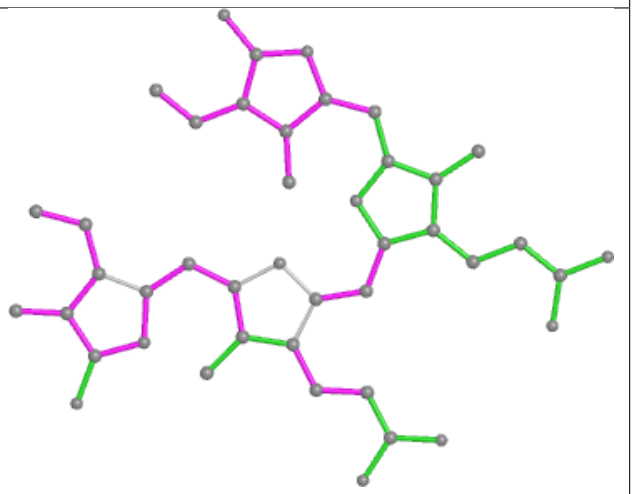

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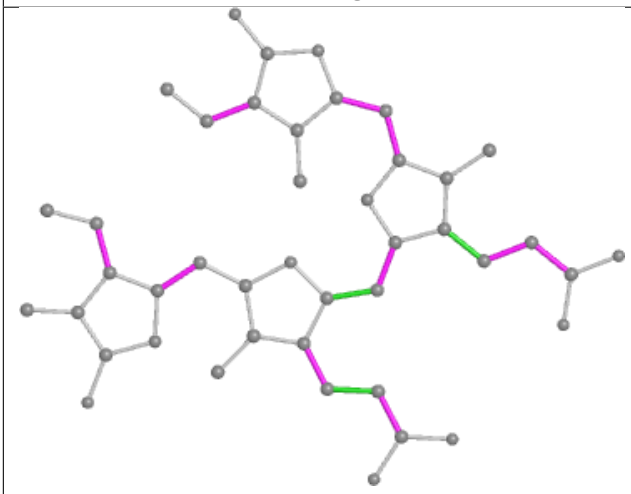

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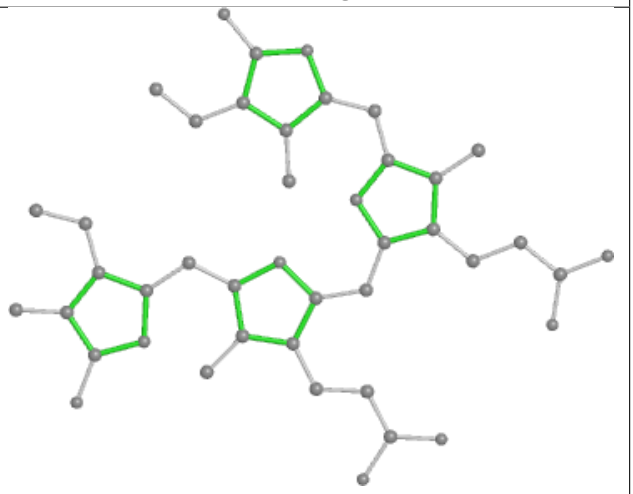
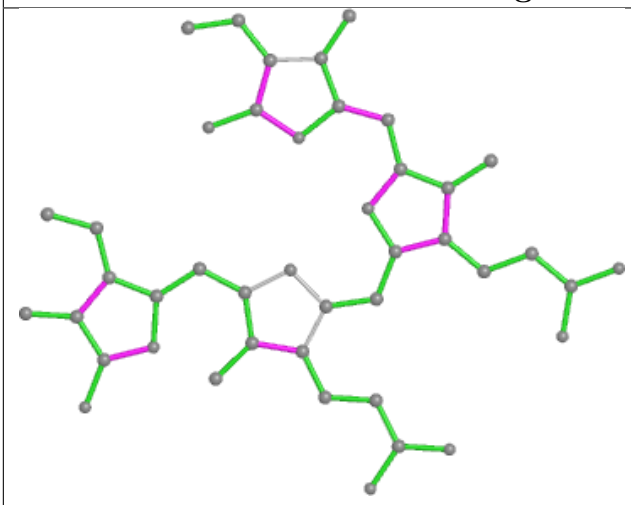


Rings

Ligand PUB jI 1003



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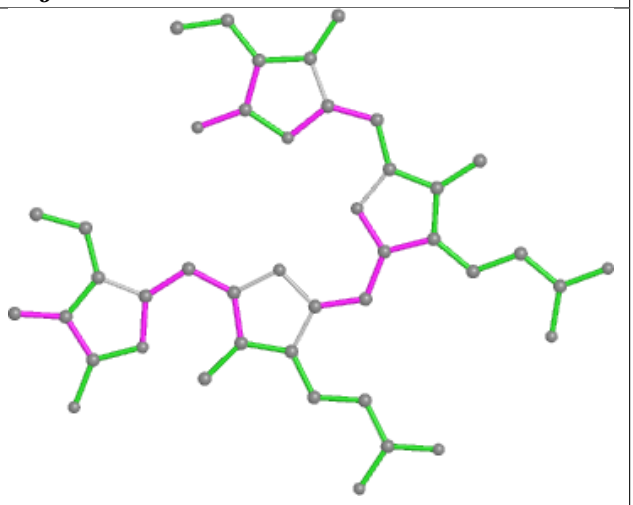

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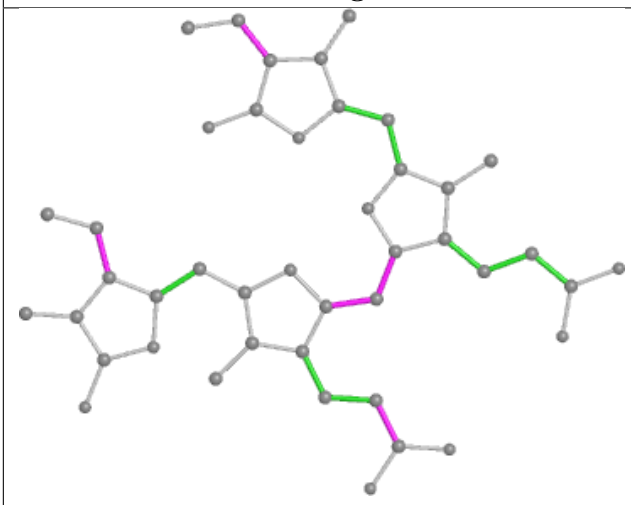

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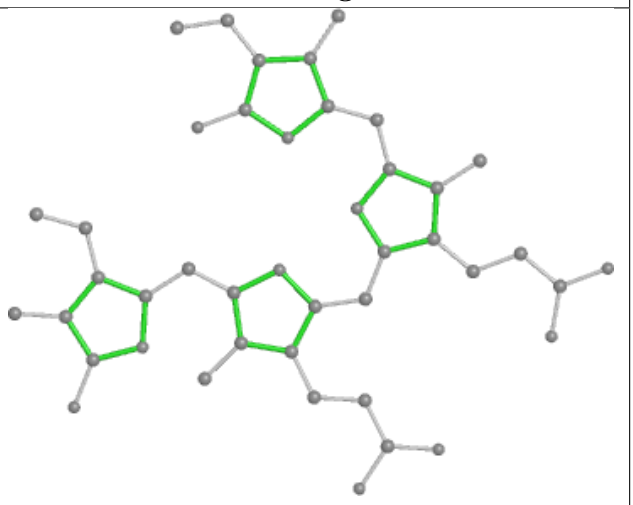
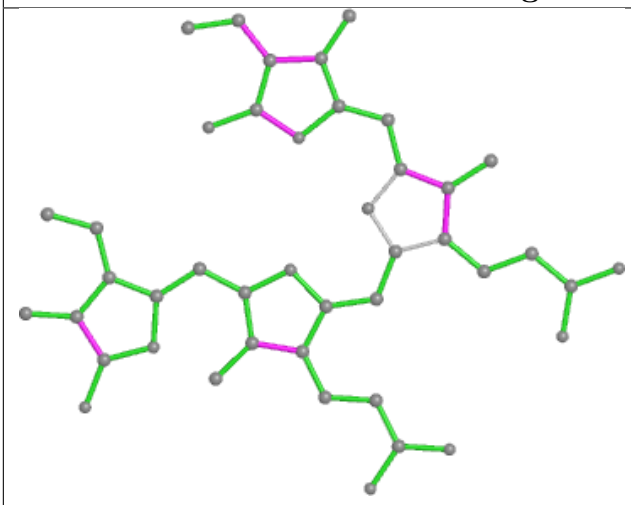


Rings

Ligand PEB r3 202



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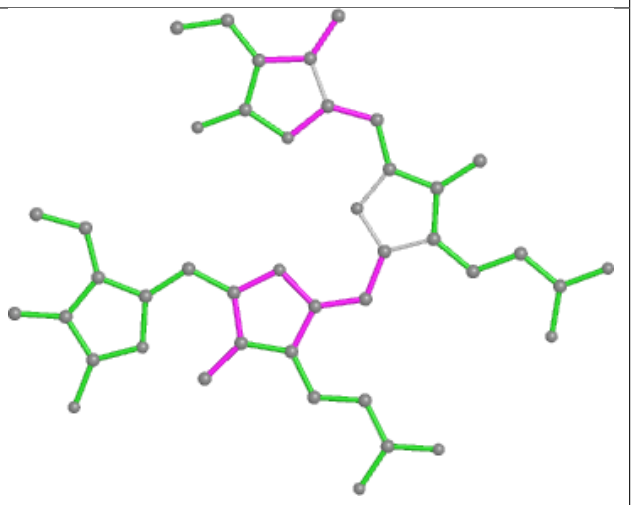

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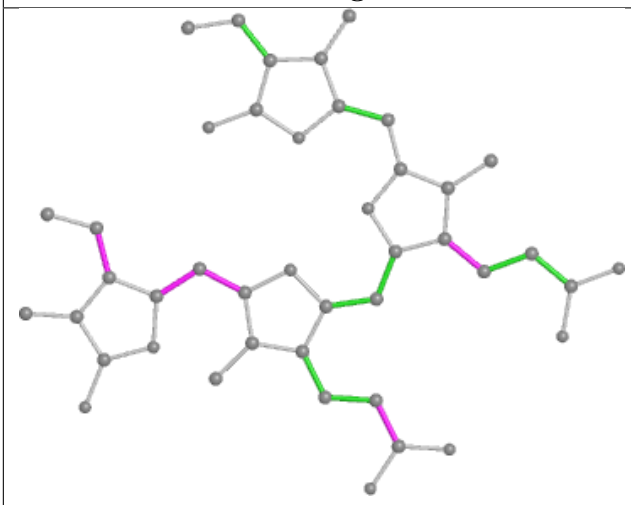

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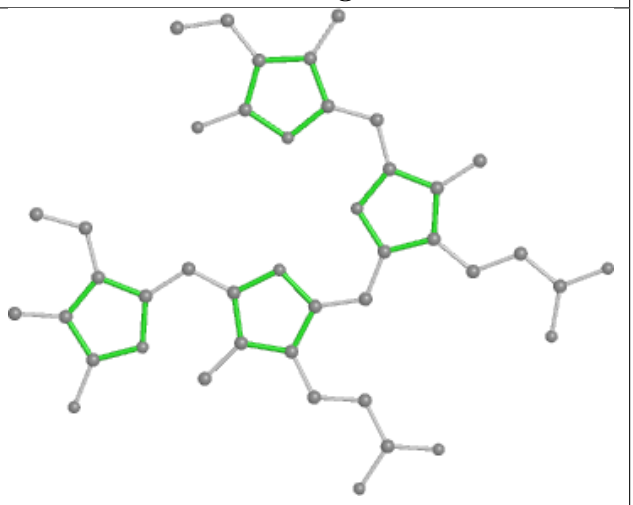
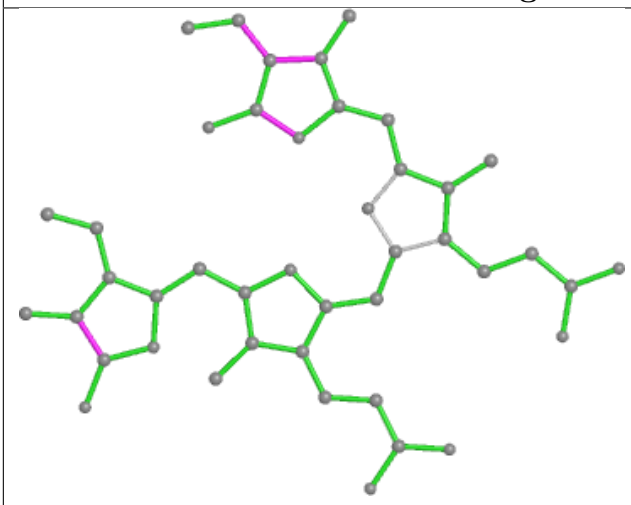


Rings

Ligand PEB bz 202



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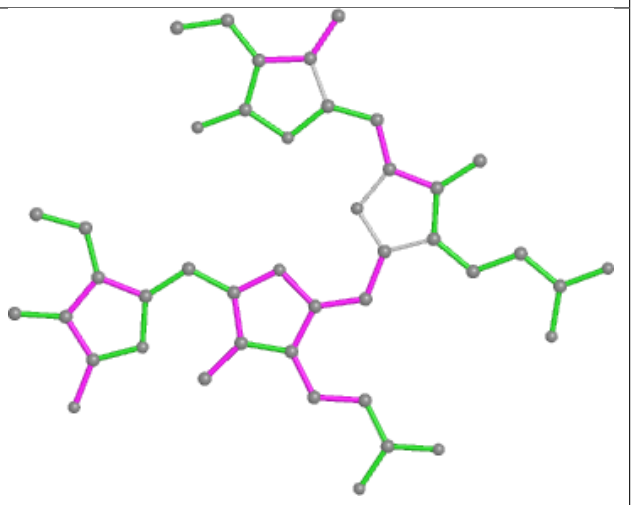

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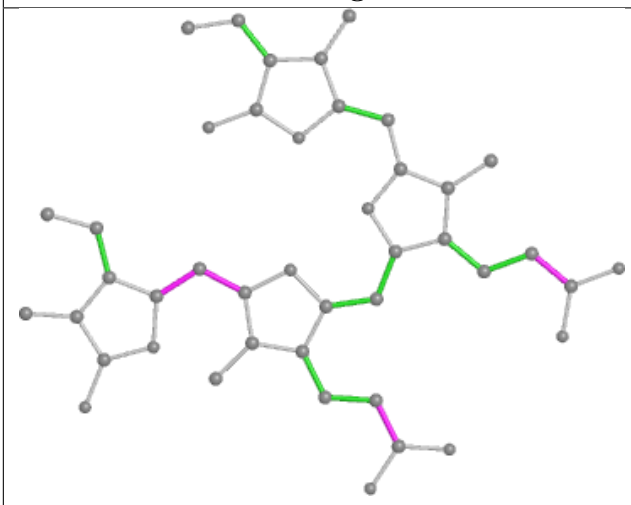

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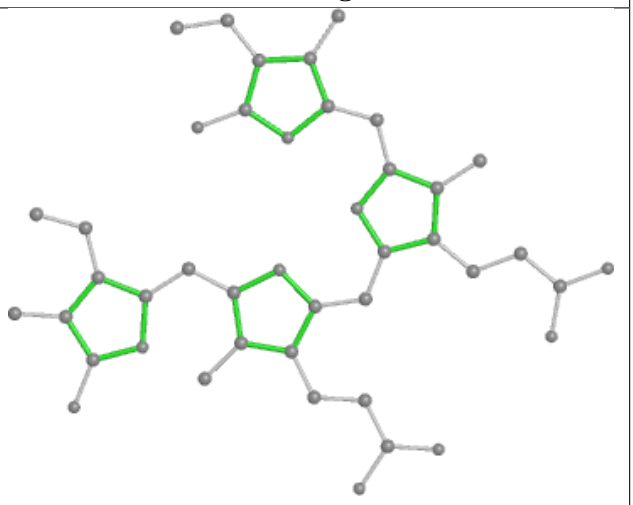
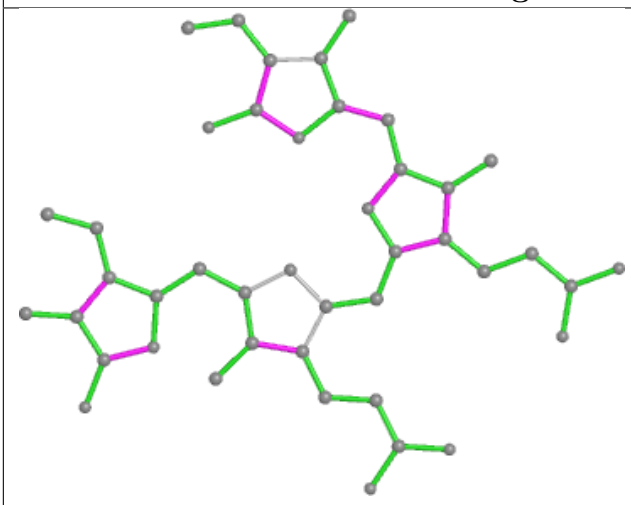


Rings

Ligand PUB hH 203



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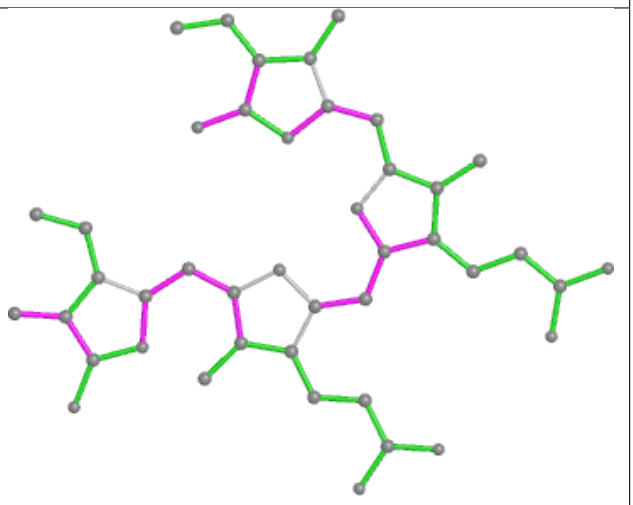

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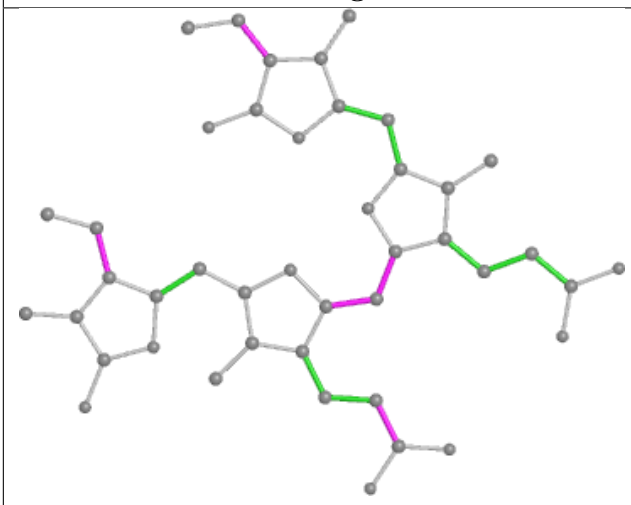

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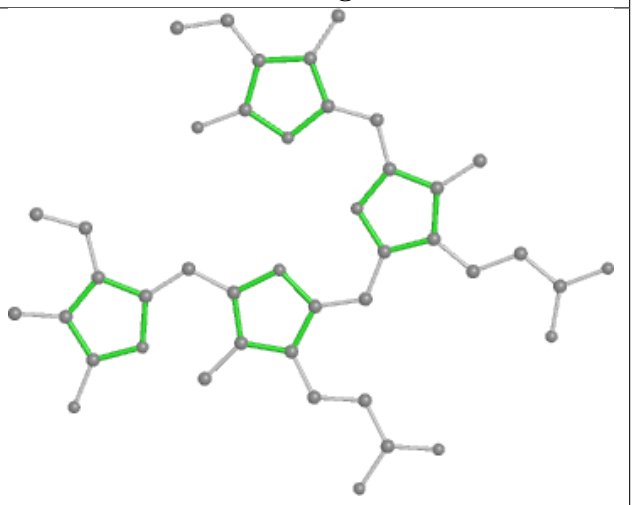
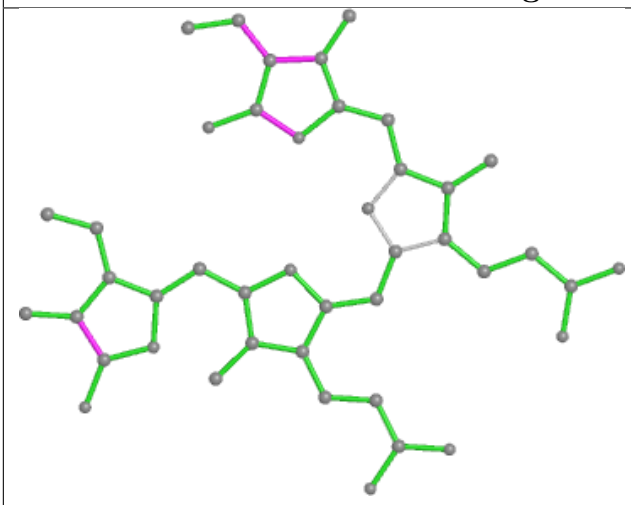


Rings

Ligand PEB fd 303



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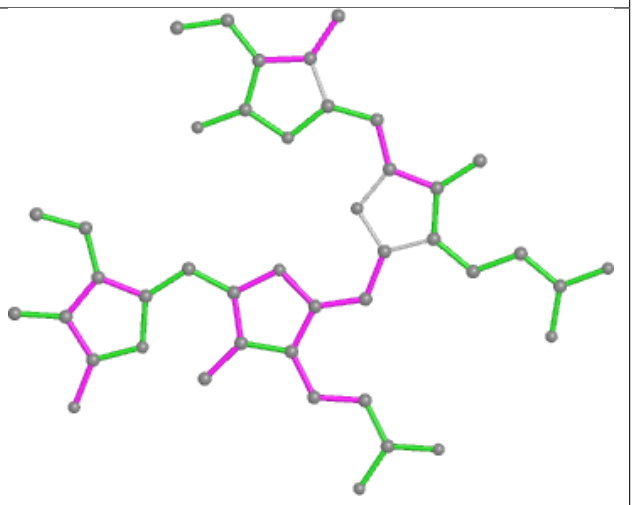

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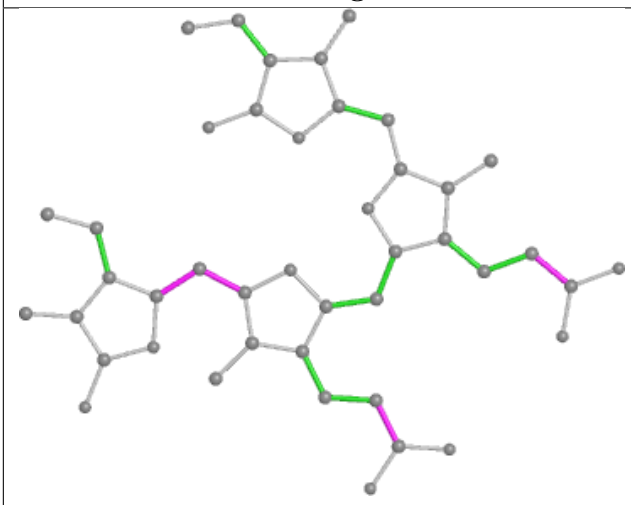

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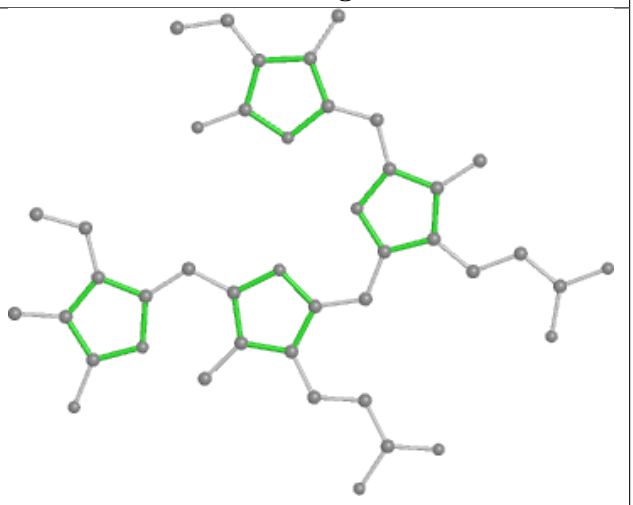

Rings

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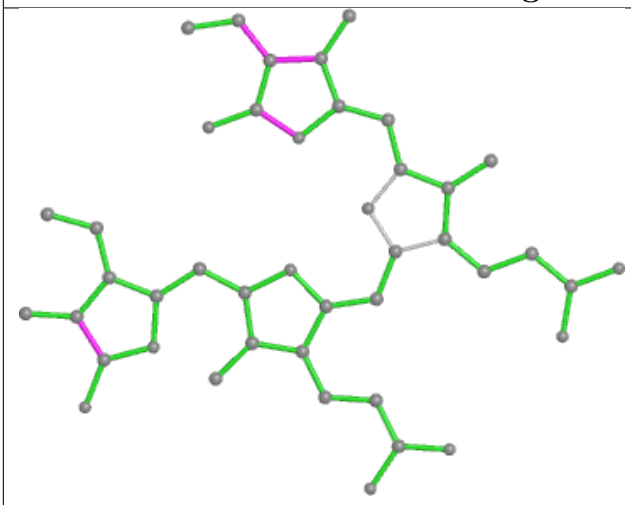

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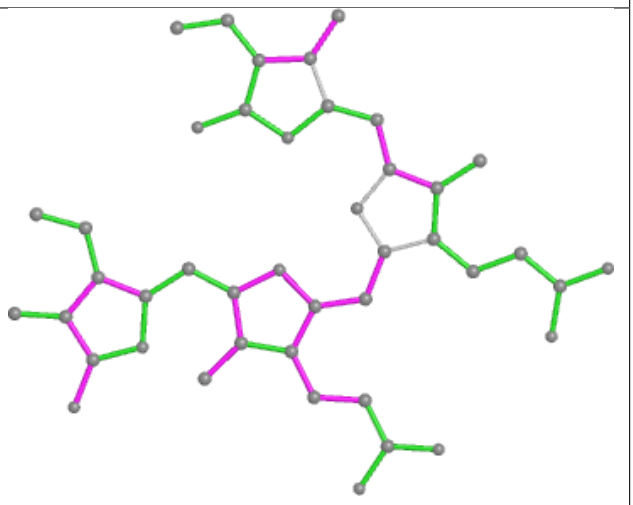

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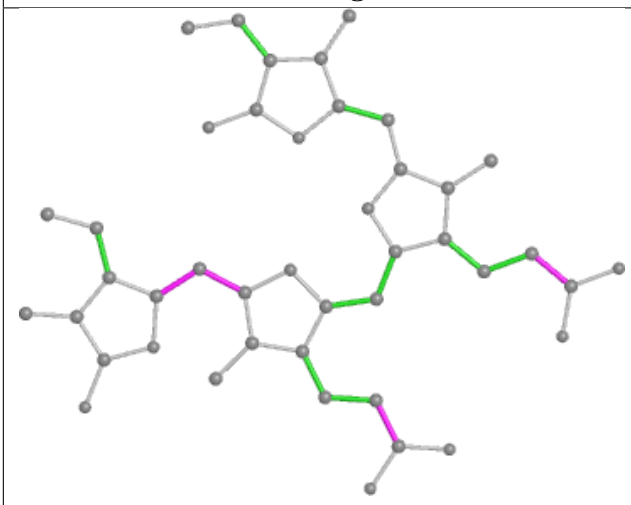

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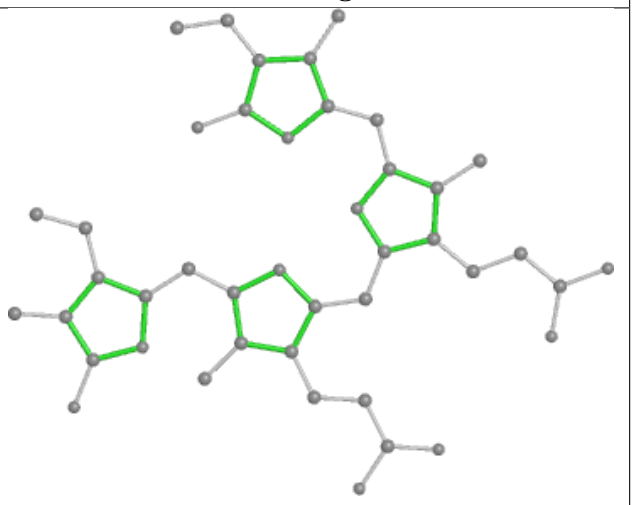
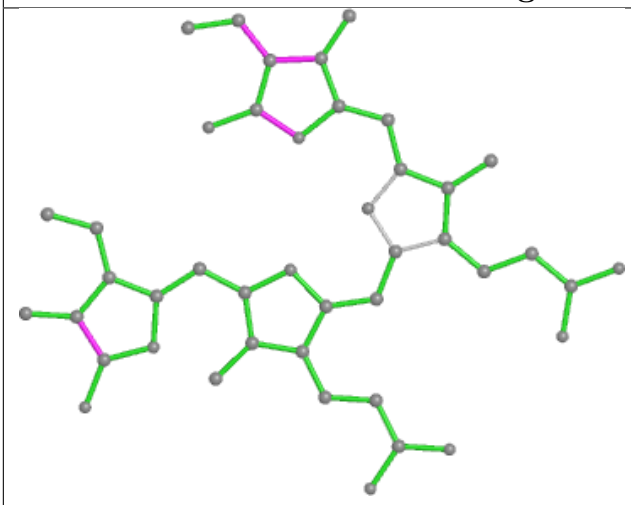


Rings

Ligand PEB du 203



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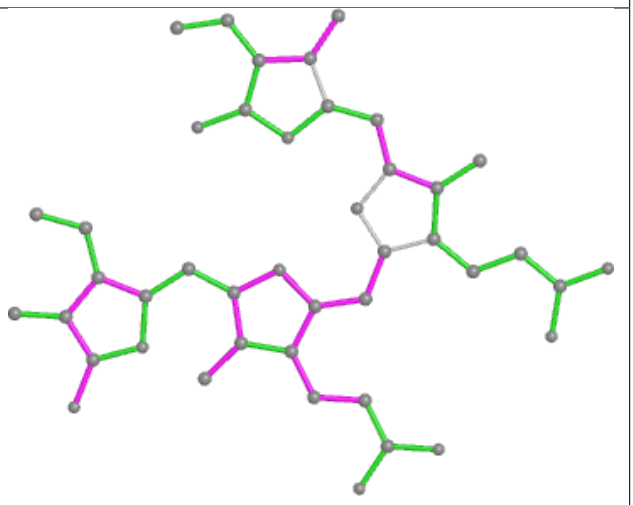

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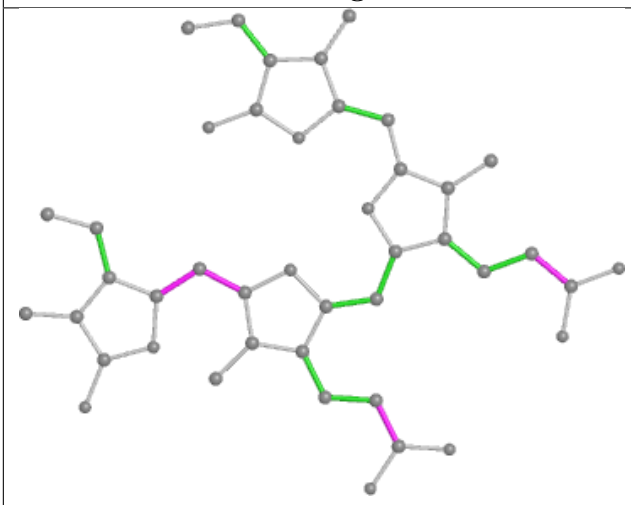

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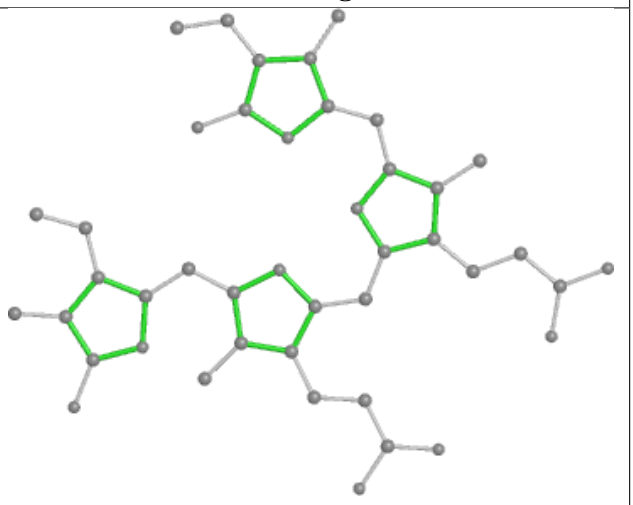
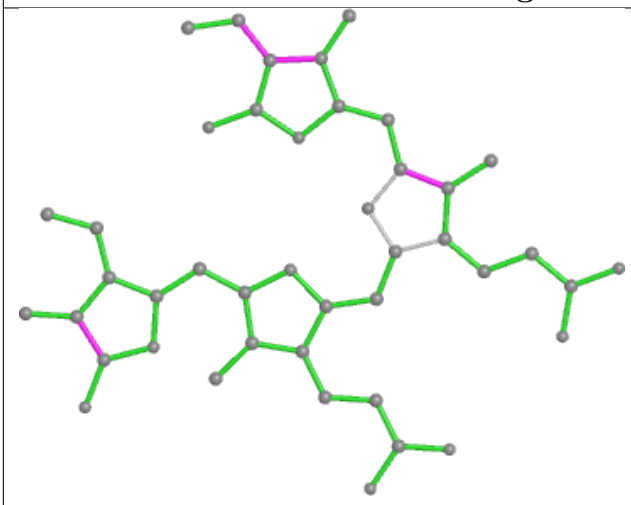


Rings

Ligand PEB cA 202



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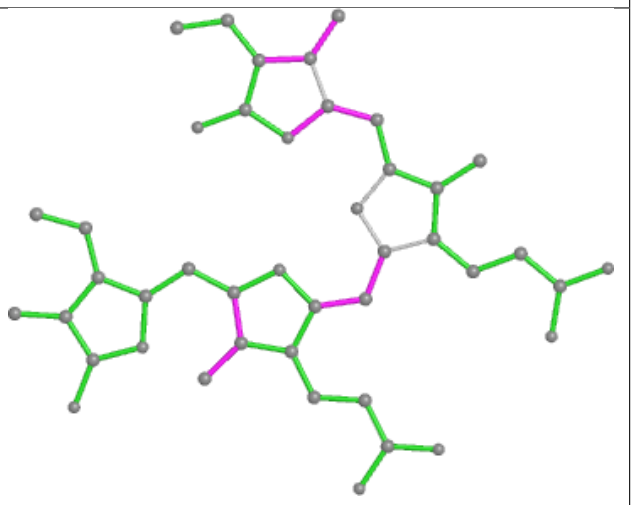

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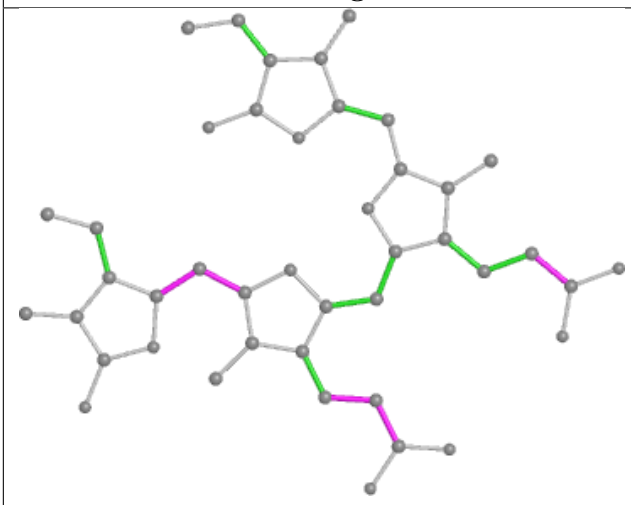

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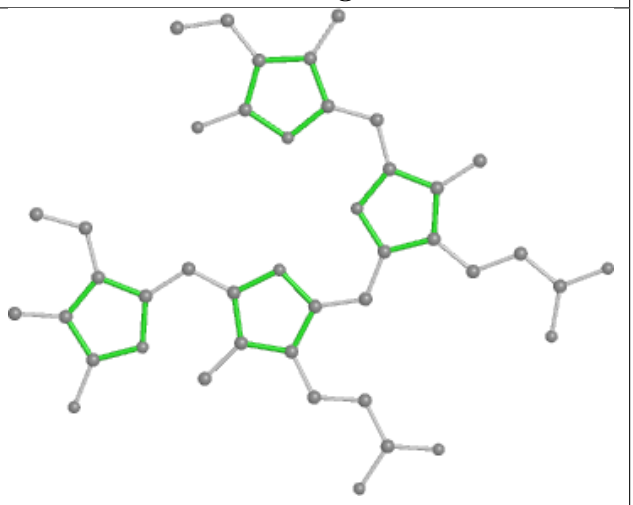
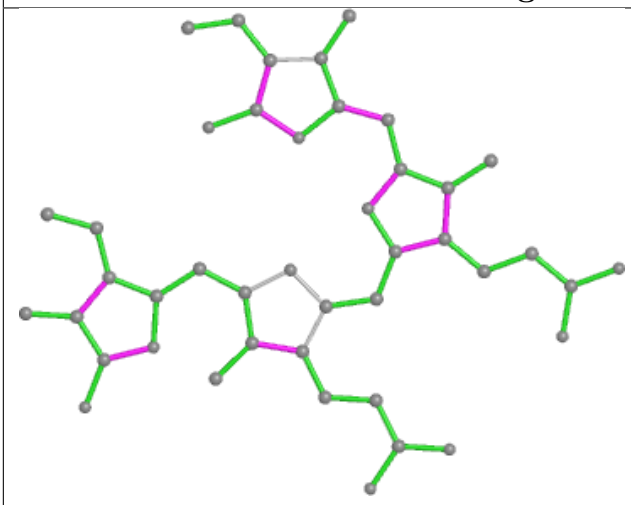


Rings

Ligand PUB ep 203



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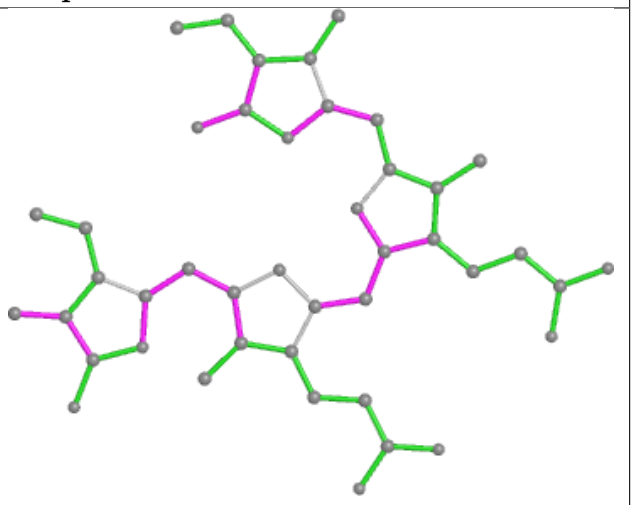

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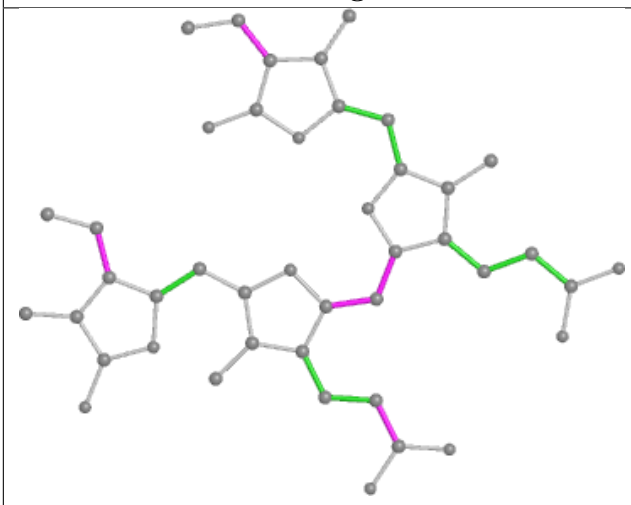

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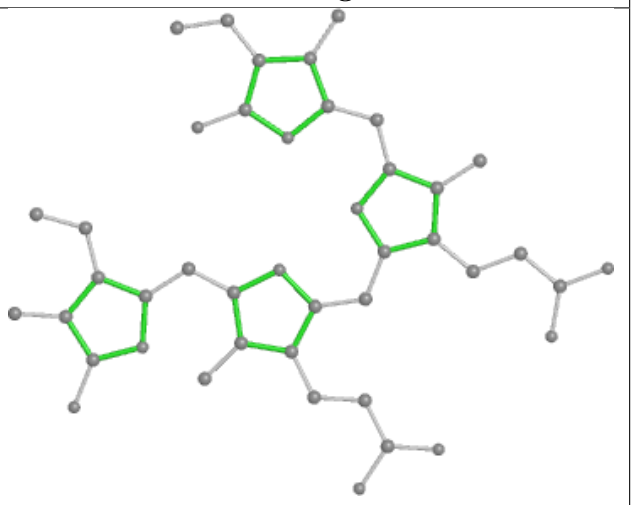
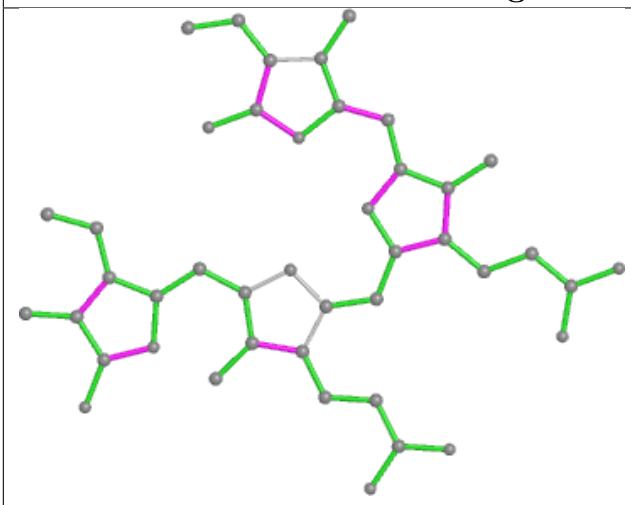


Rings

Ligand PUB iH 1002



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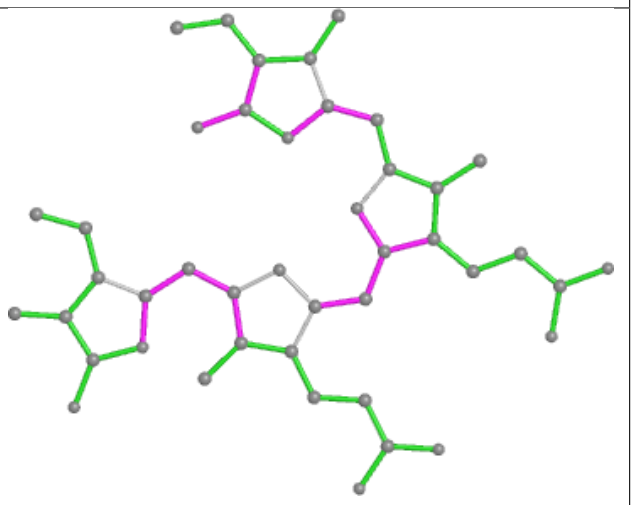
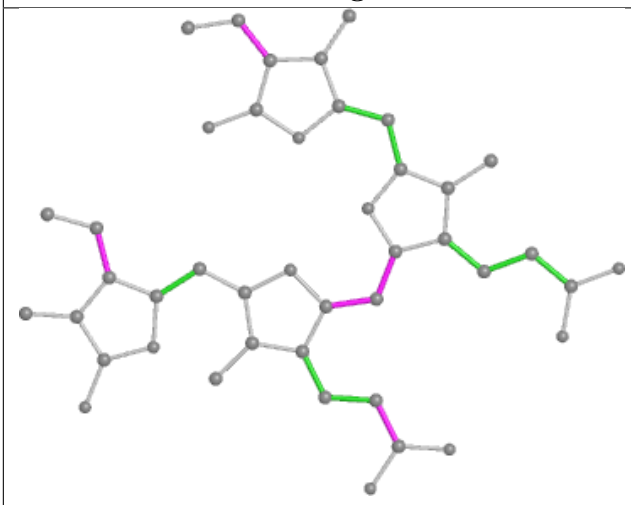


Bond angles



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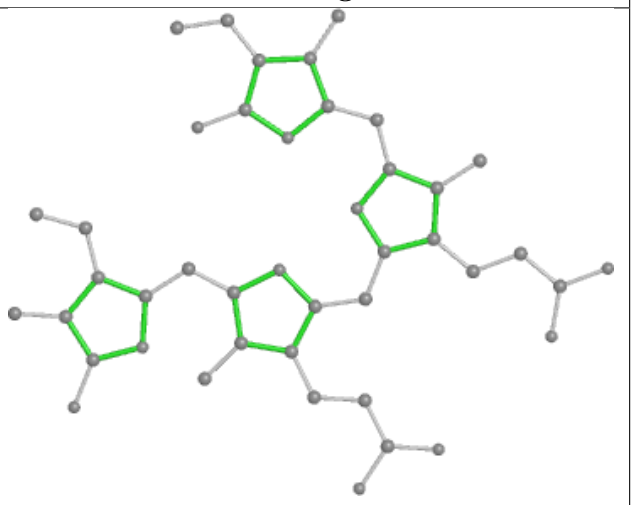
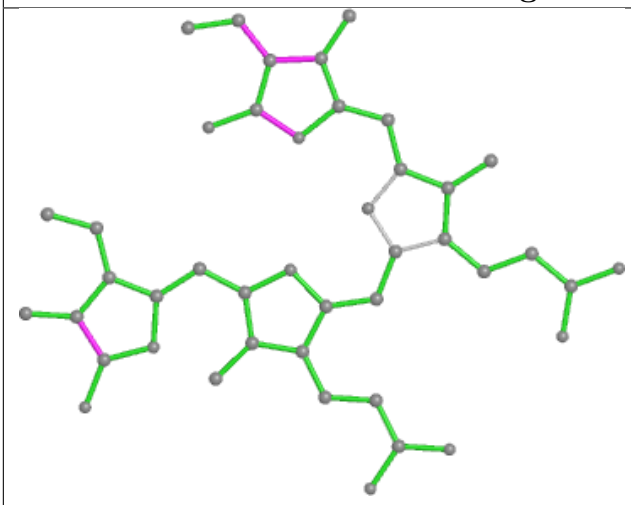


Rings

Ligand PEB en 201



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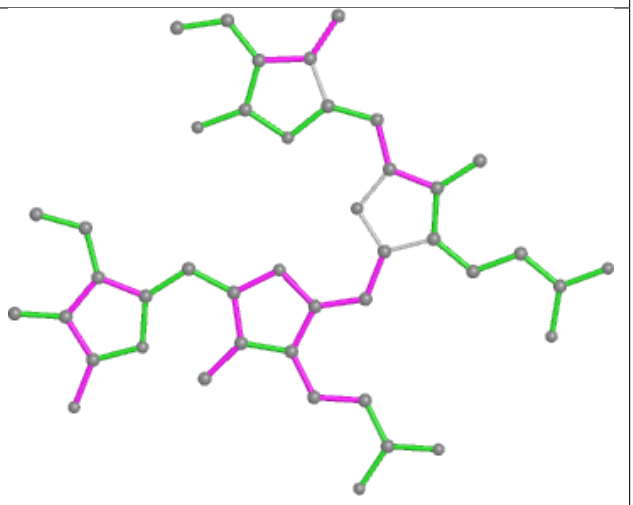

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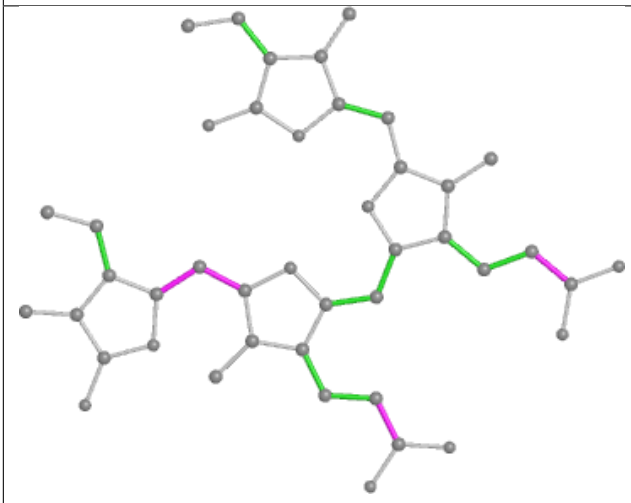

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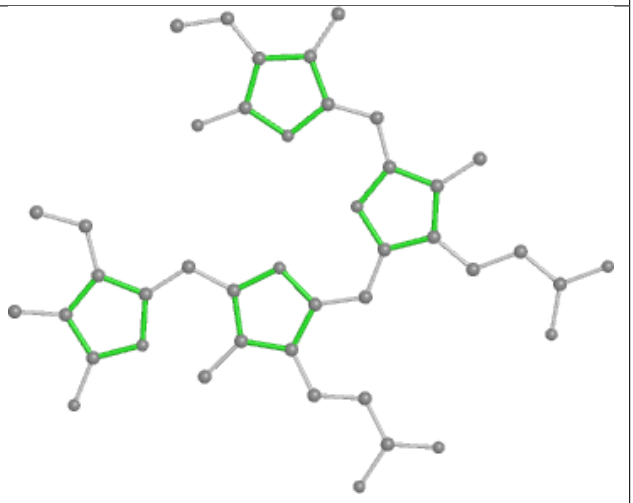
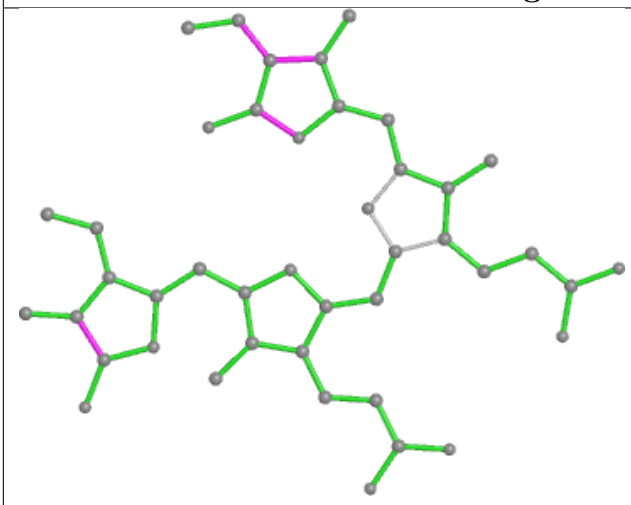


Rings

Ligand PEB ly 403



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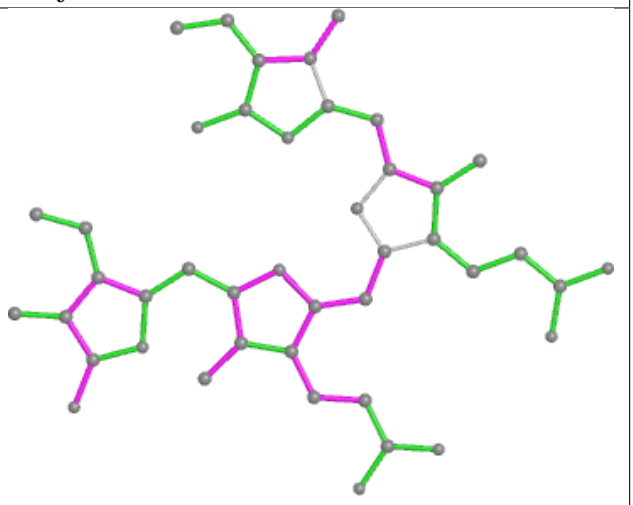
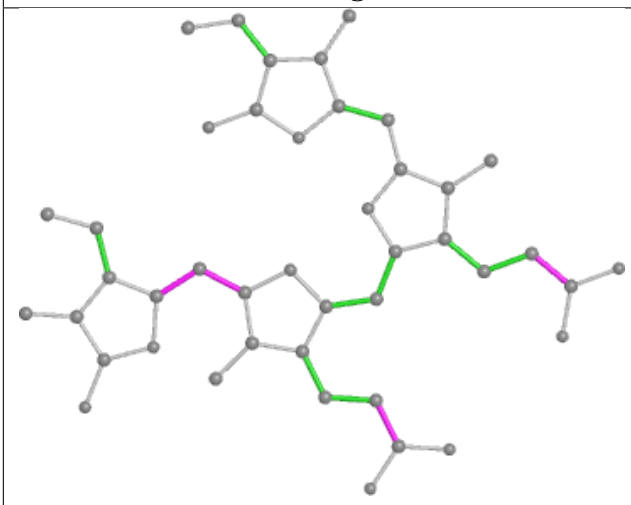
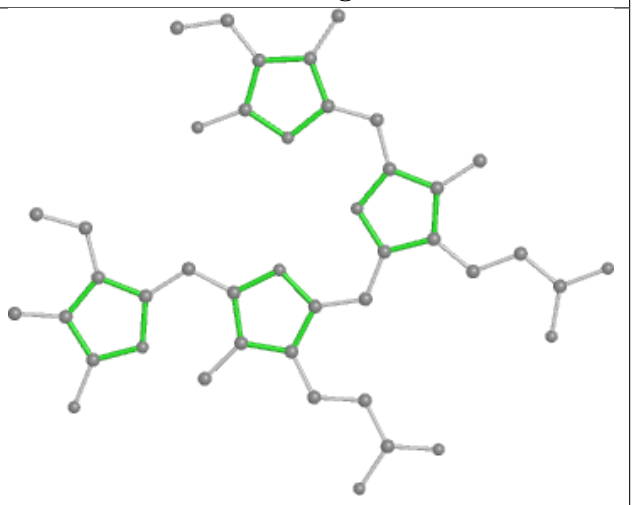


Bond angles

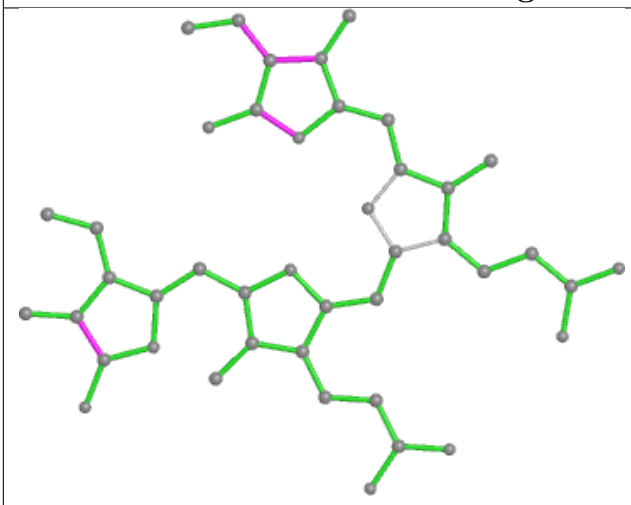


Torsions



Rings

Ligand PEB F2 202



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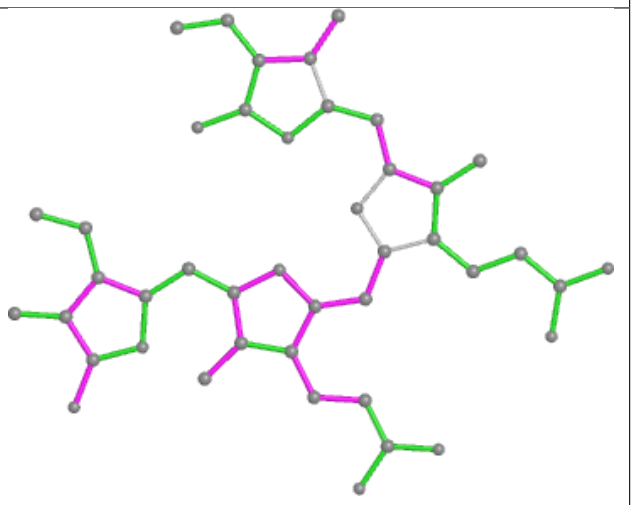

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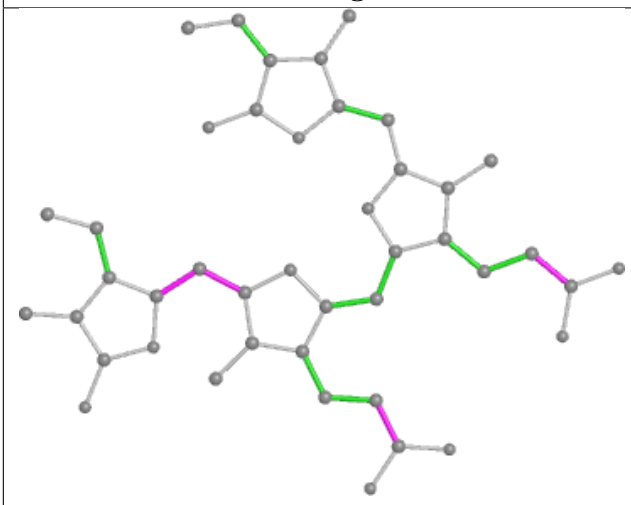

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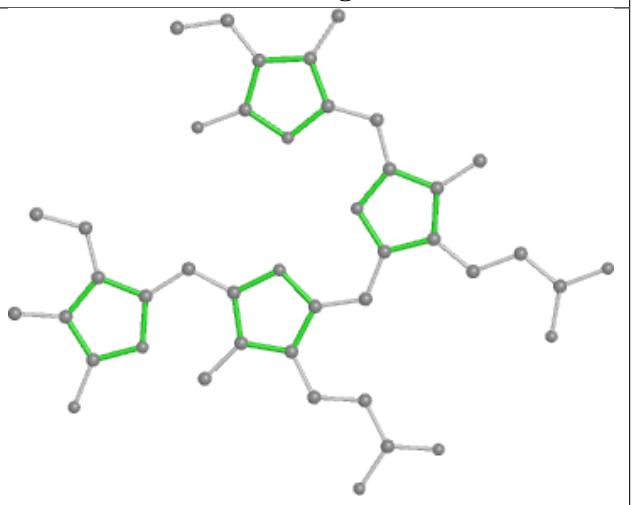
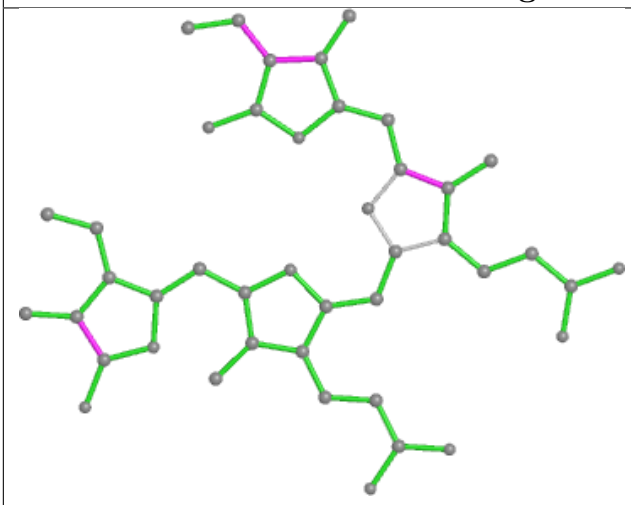


Rings

Ligand PEB h7 202



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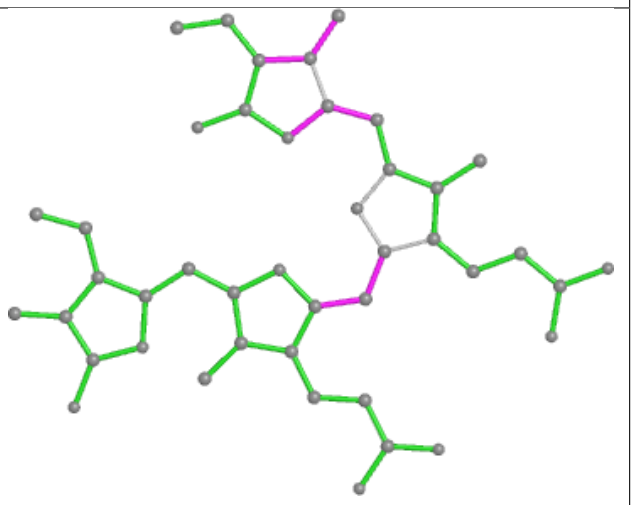

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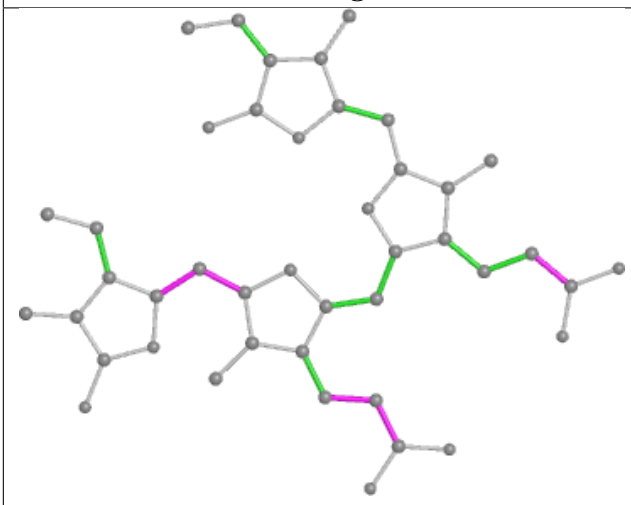

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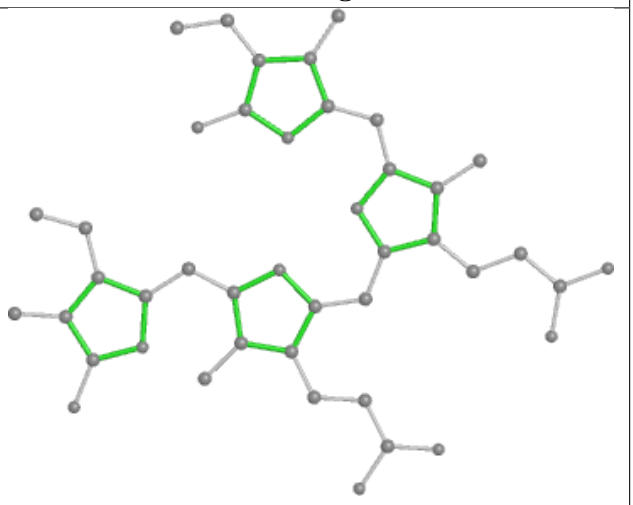
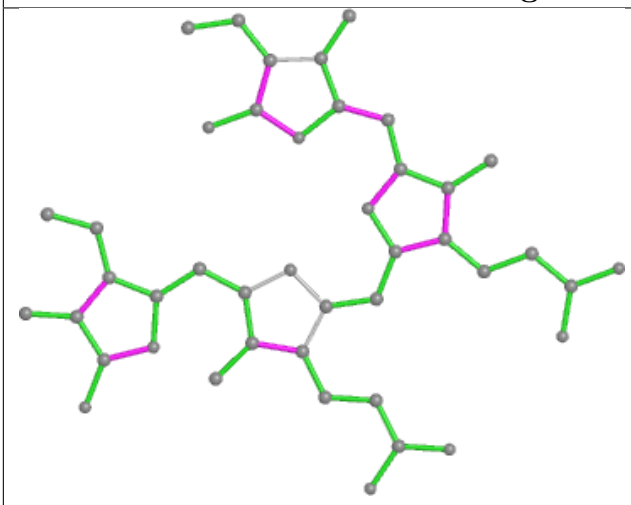


Rings

Ligand PUB lh 203



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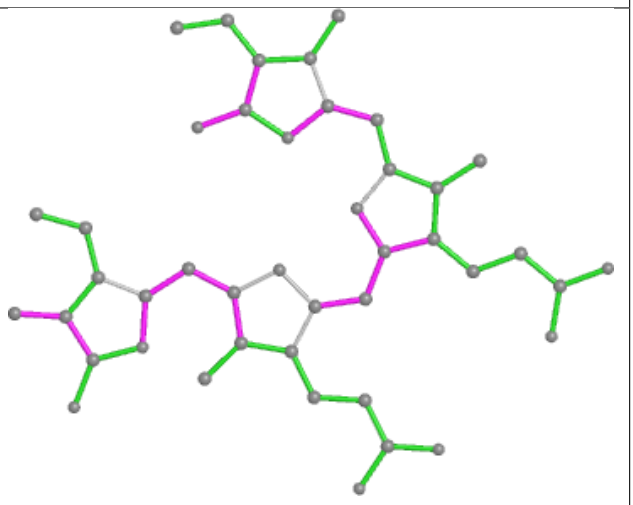
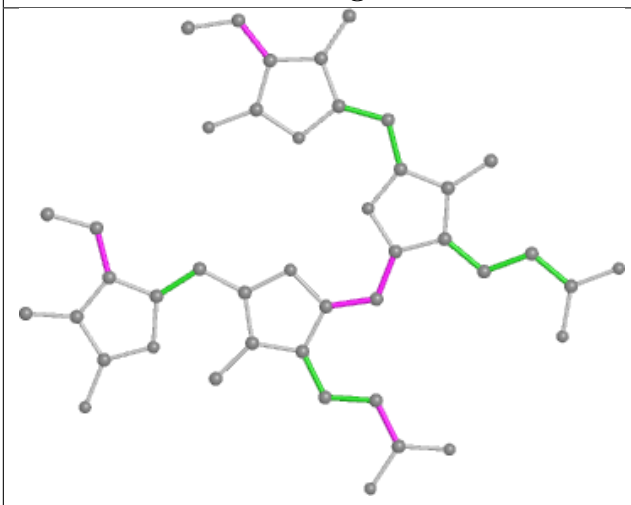


Bond angles



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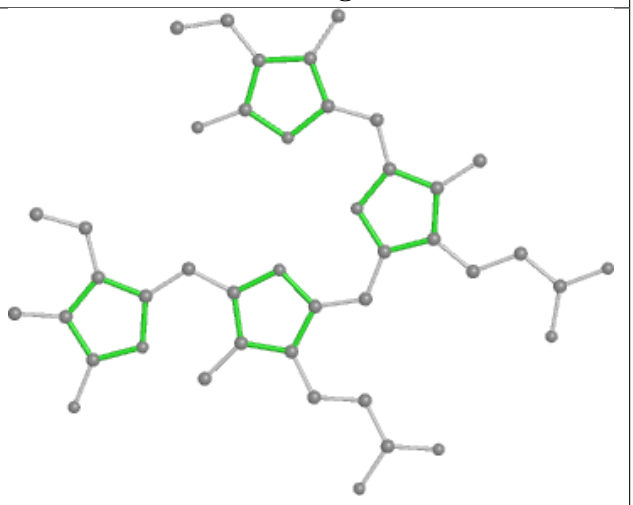
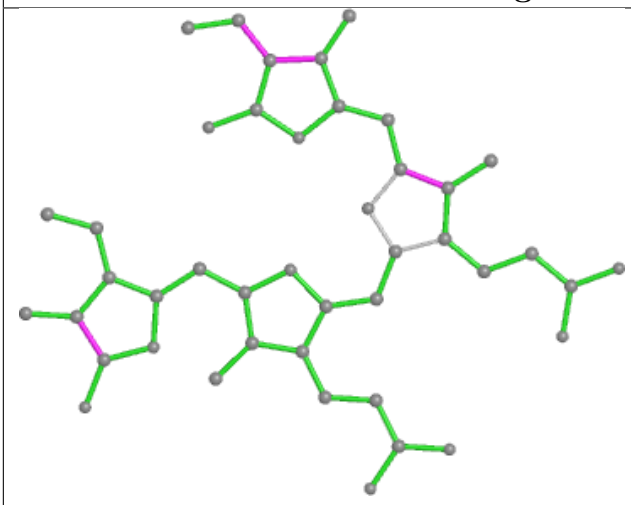


Rings

Ligand PEB hO 202



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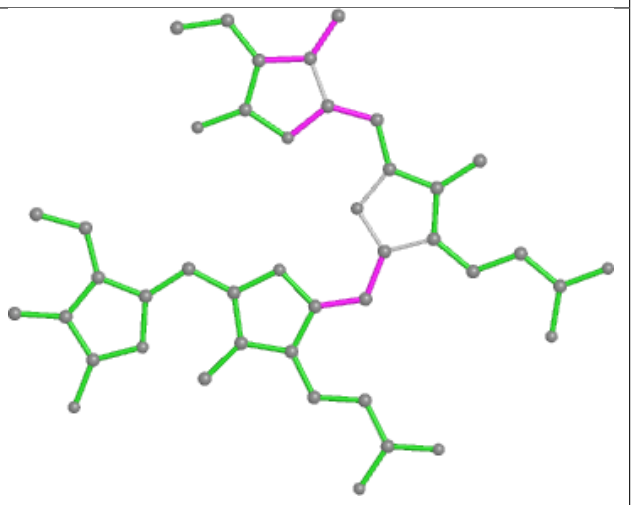

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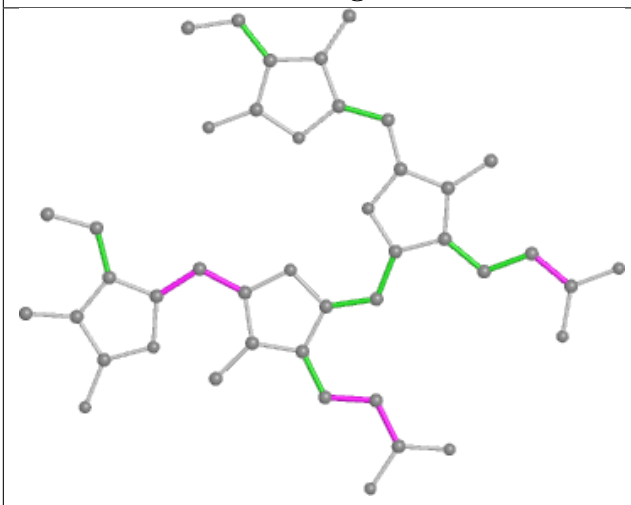

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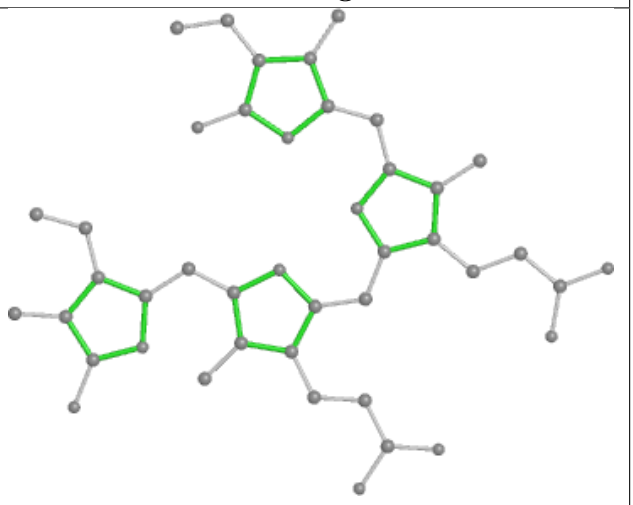

Rings

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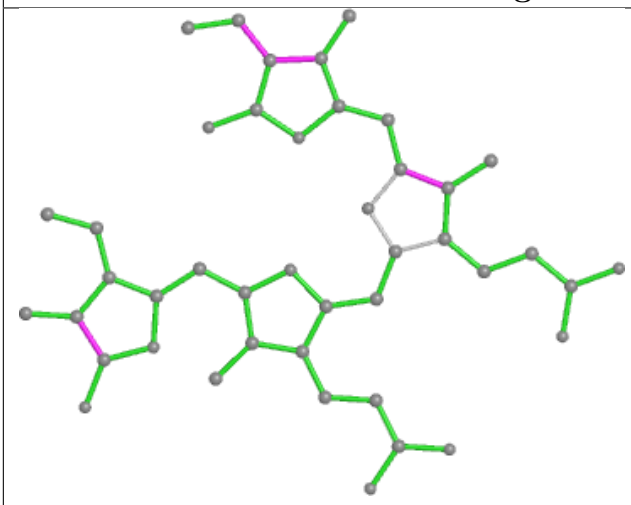

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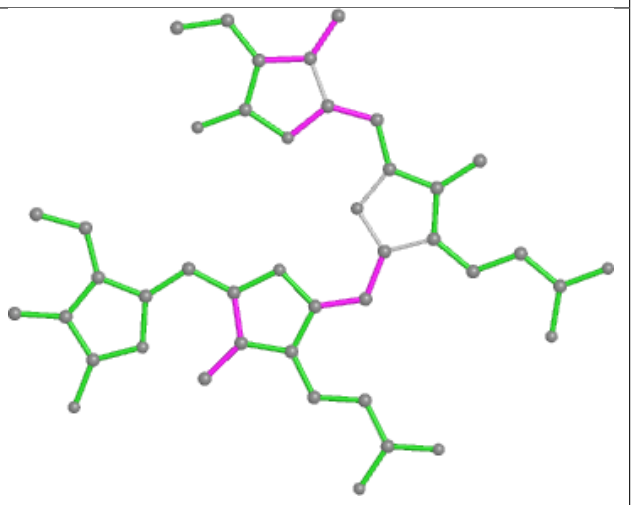

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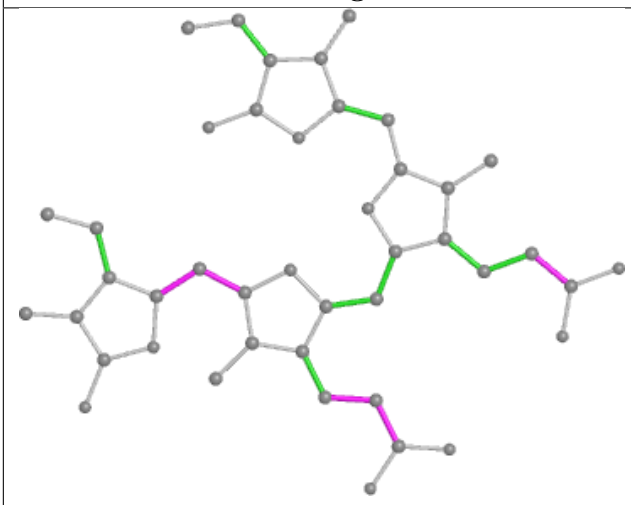

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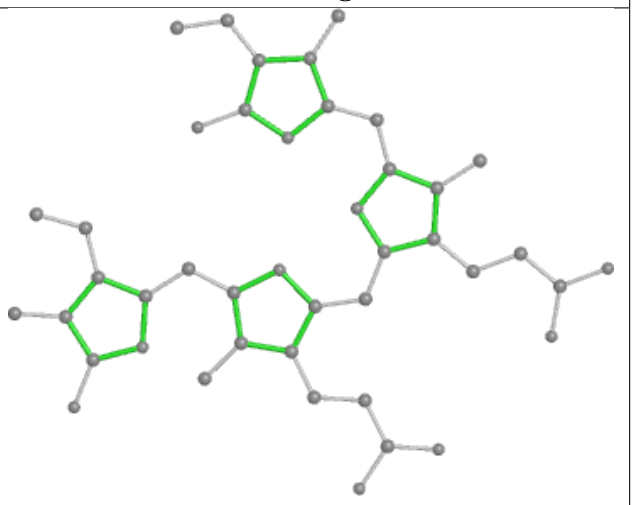
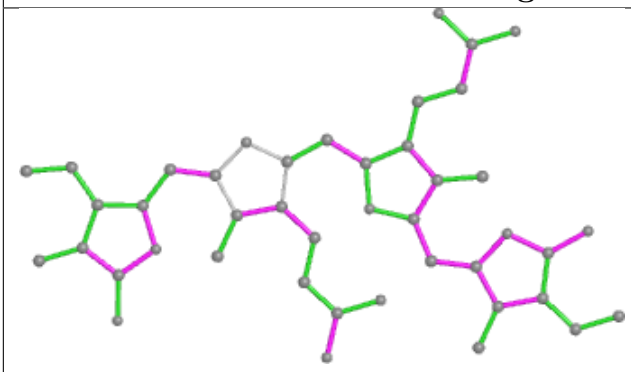


Rings

Ligand CYC a2 901



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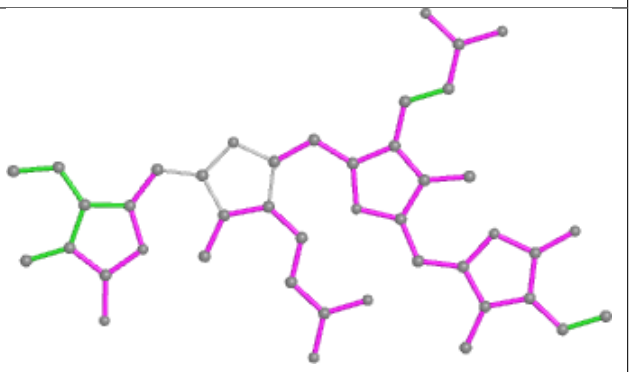

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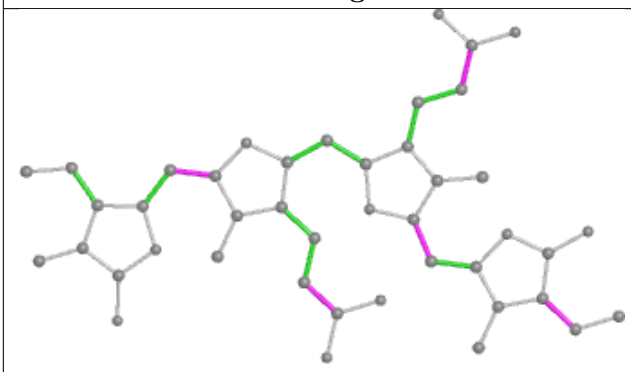

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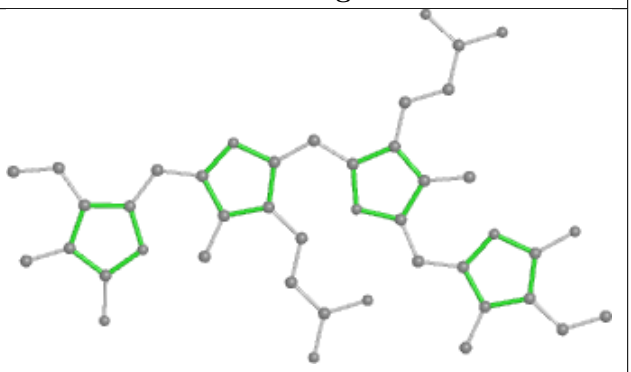

Rings

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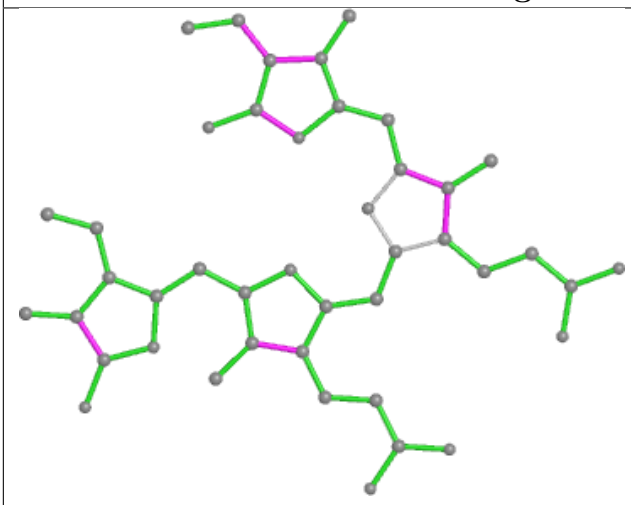

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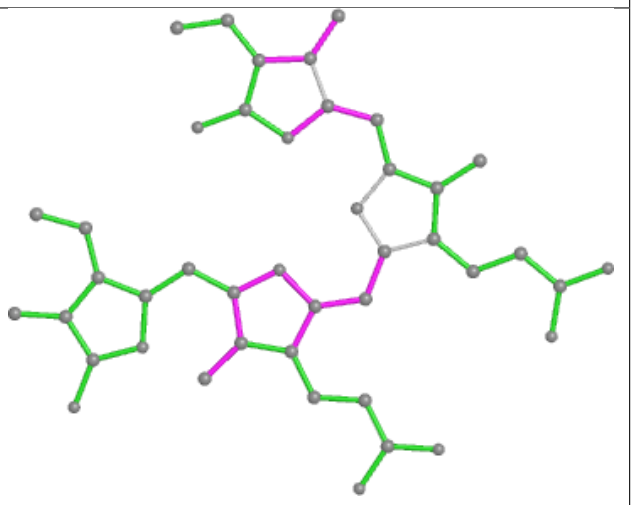

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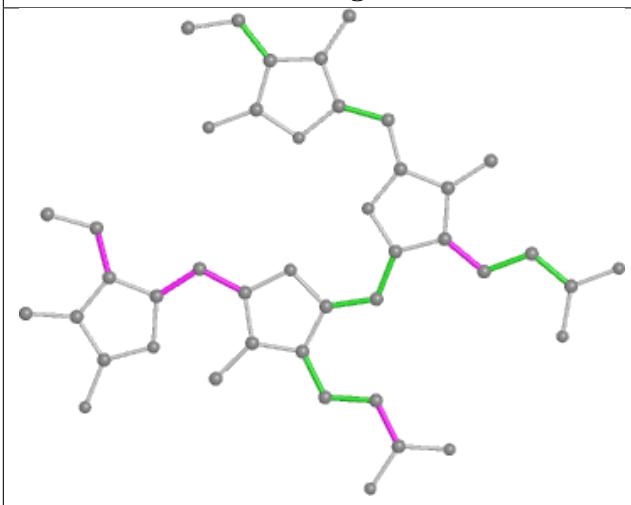

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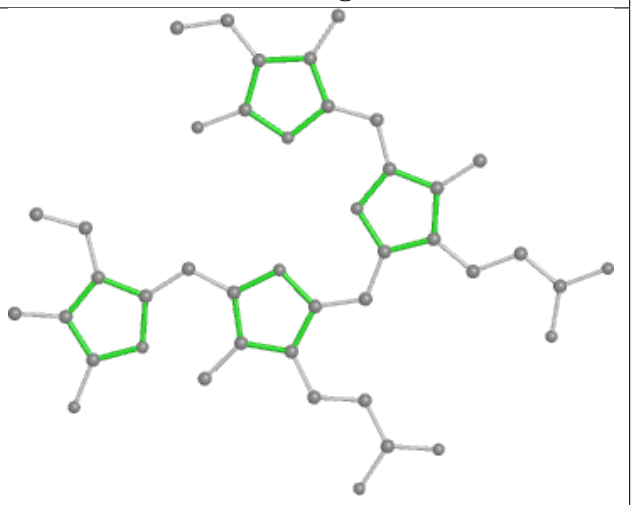
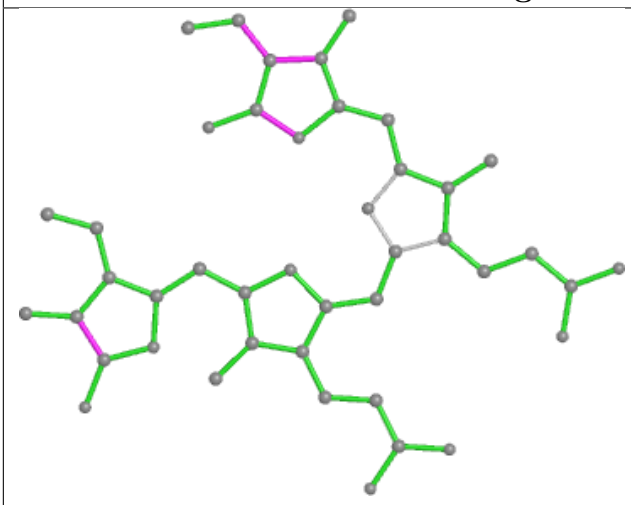


Rings

Ligand PEB N5 201



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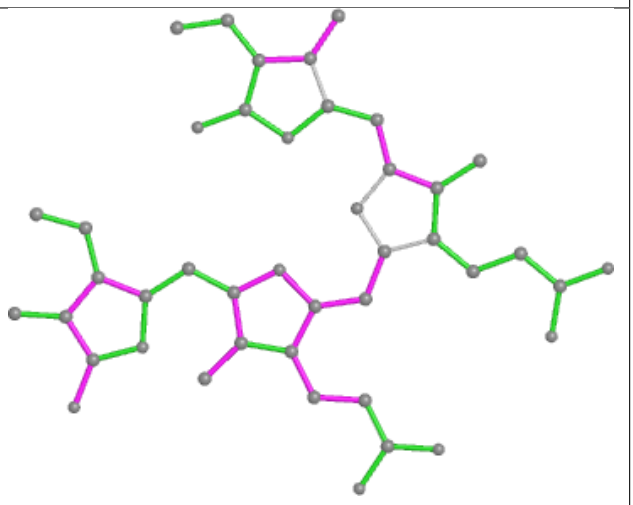
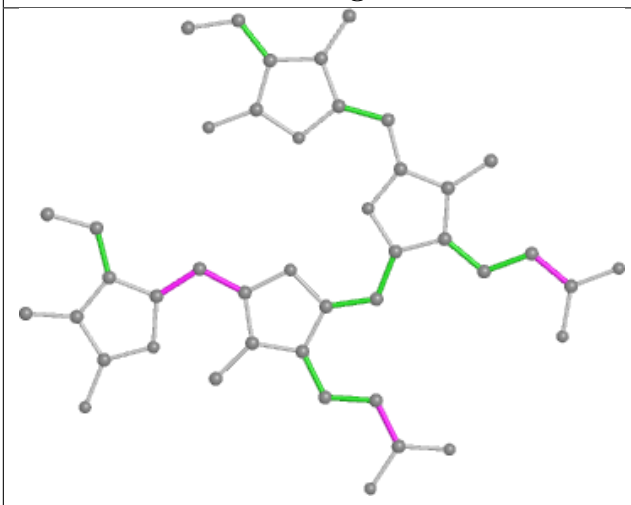


Bond angles



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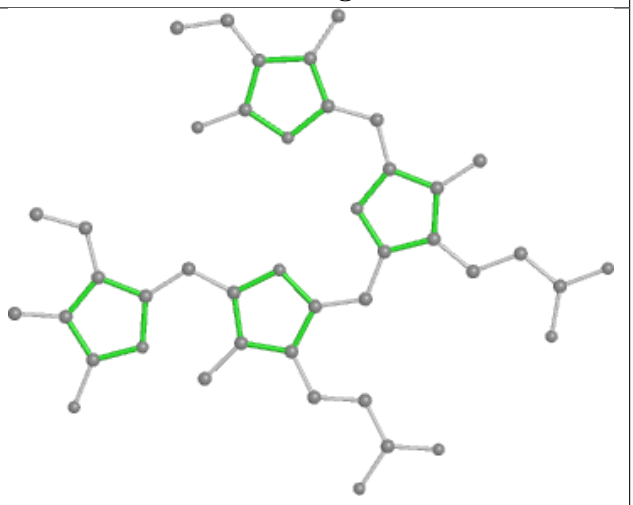
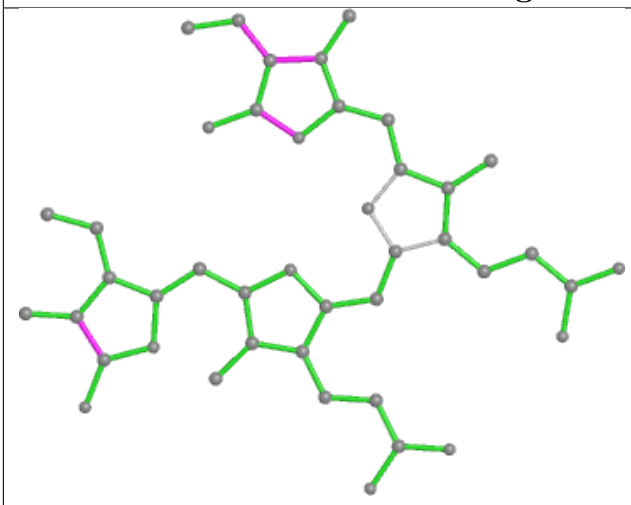


Rings

Ligand PEB V4 202



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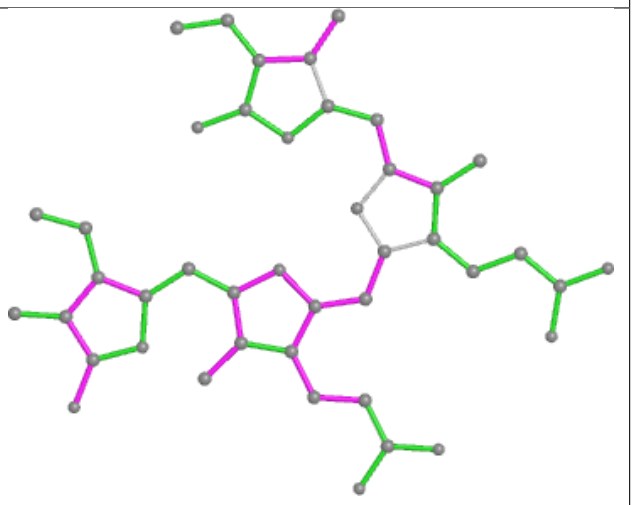

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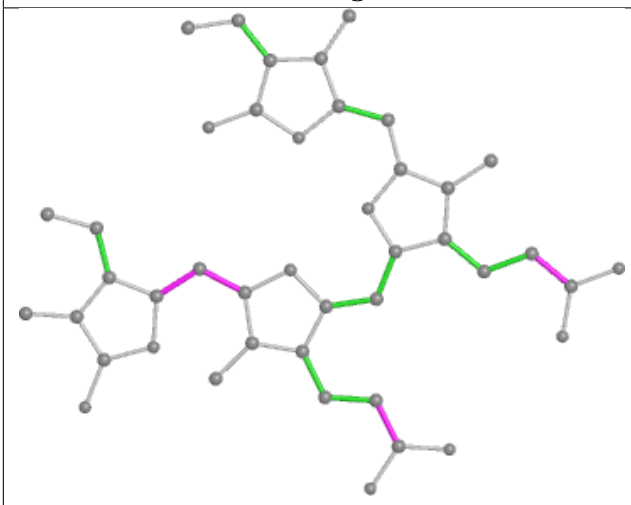

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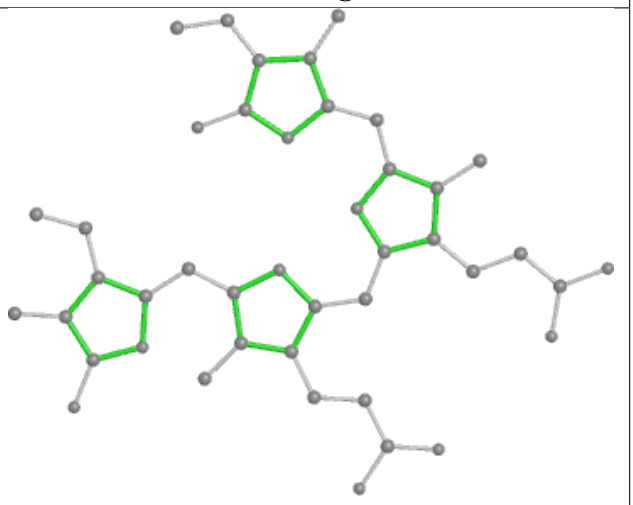
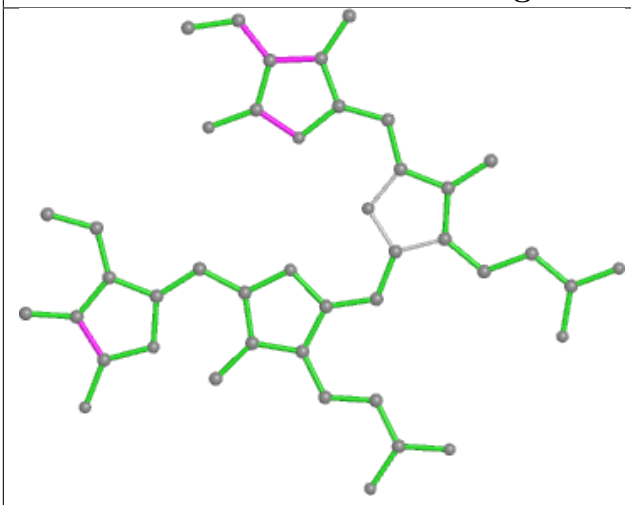


Rings

Ligand PEB m8 201



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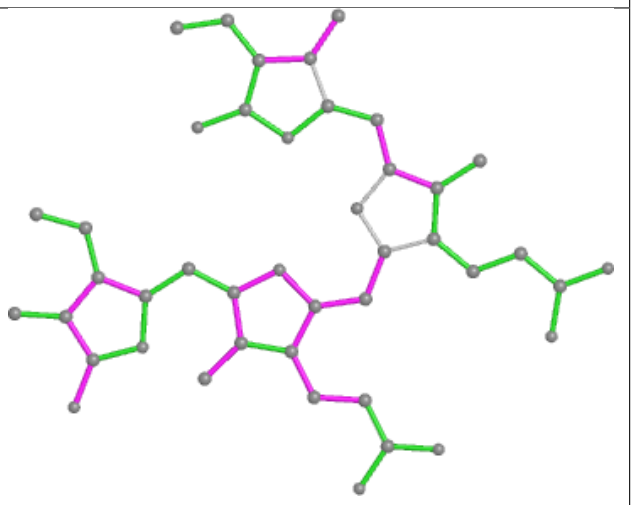

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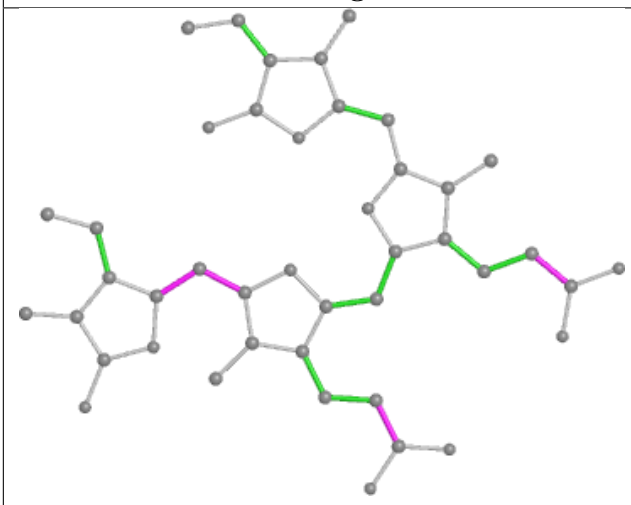

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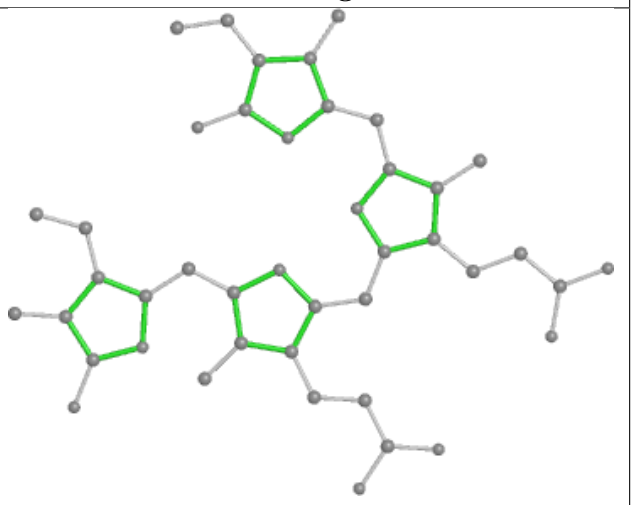

Rings

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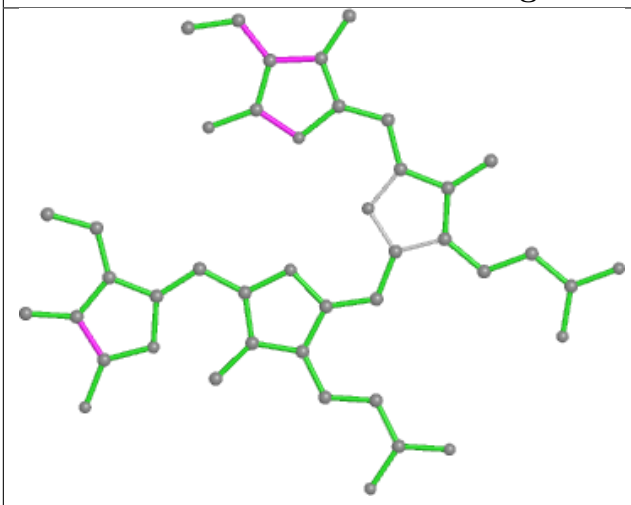

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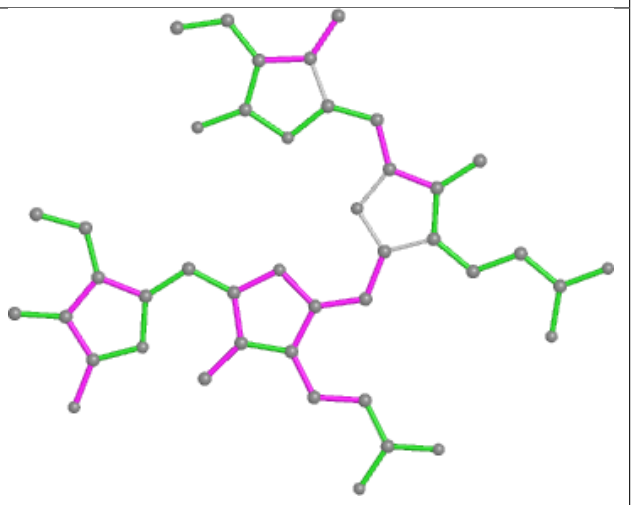

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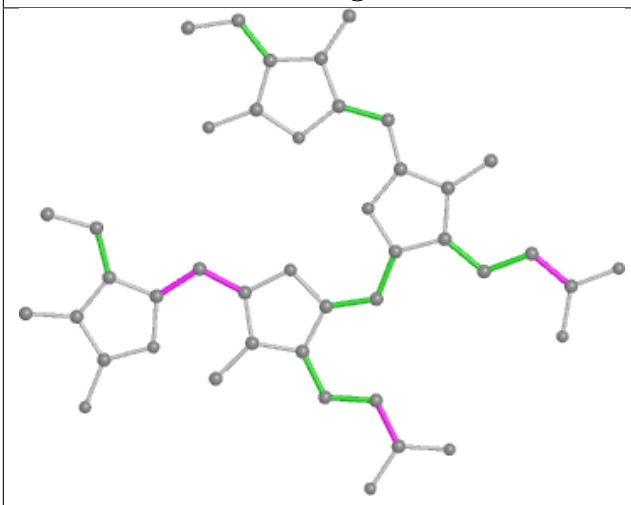

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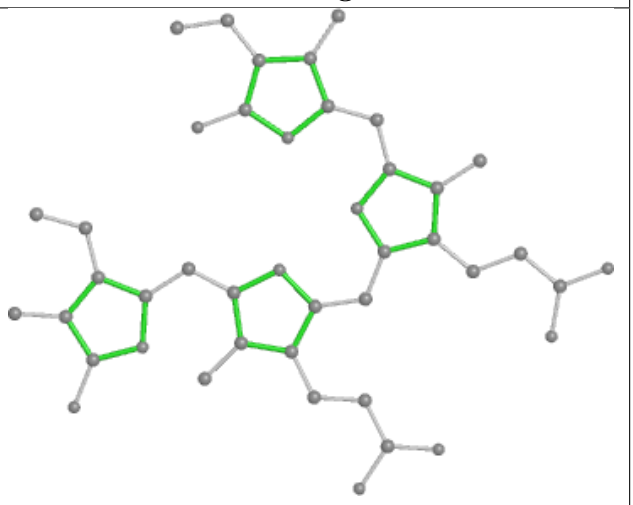
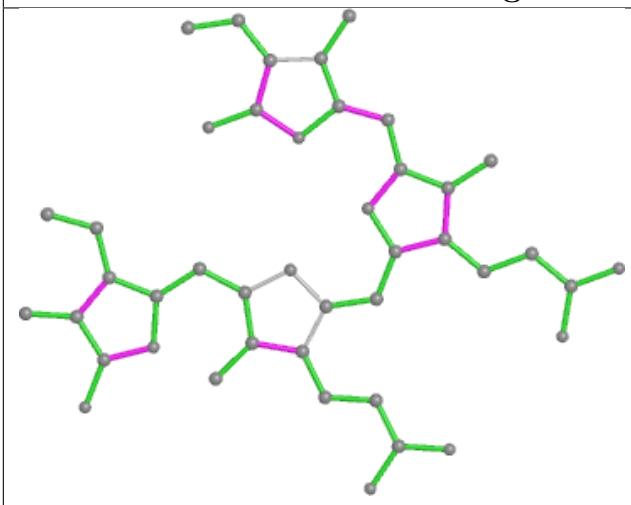


Rings

Ligand PUB kU 1003



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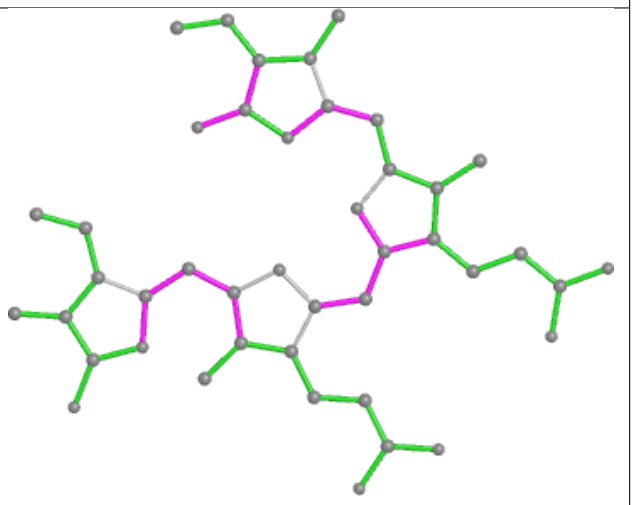

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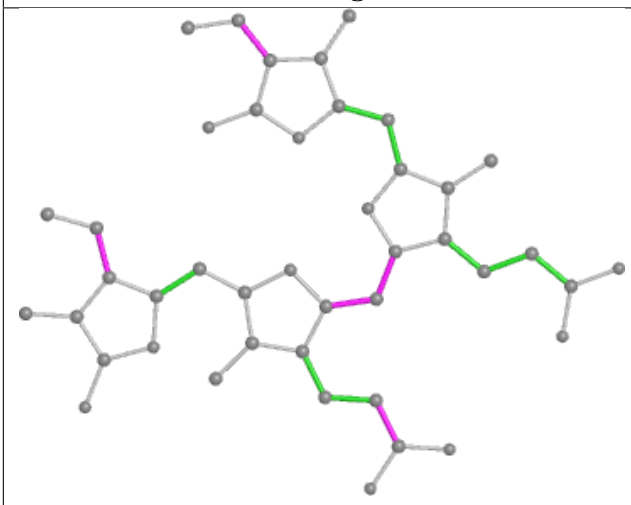

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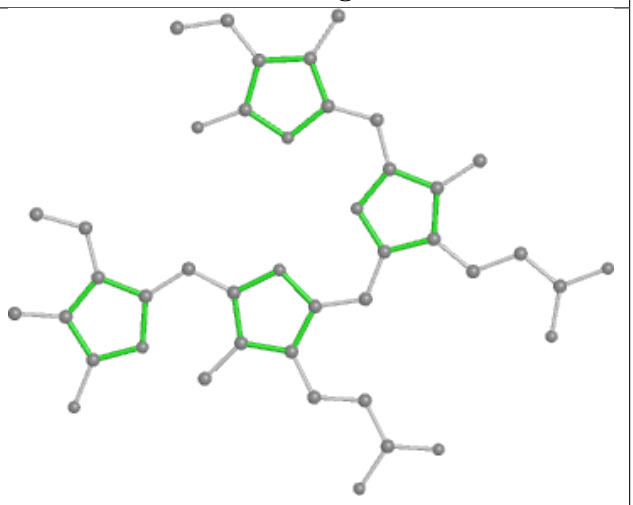
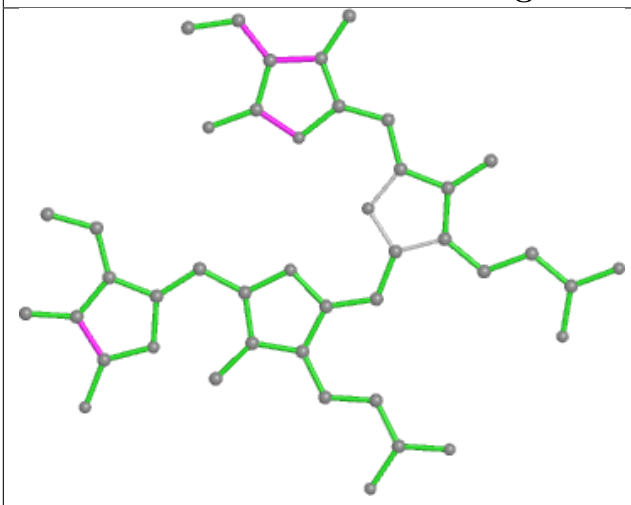


Rings

Ligand PEB Q4 203



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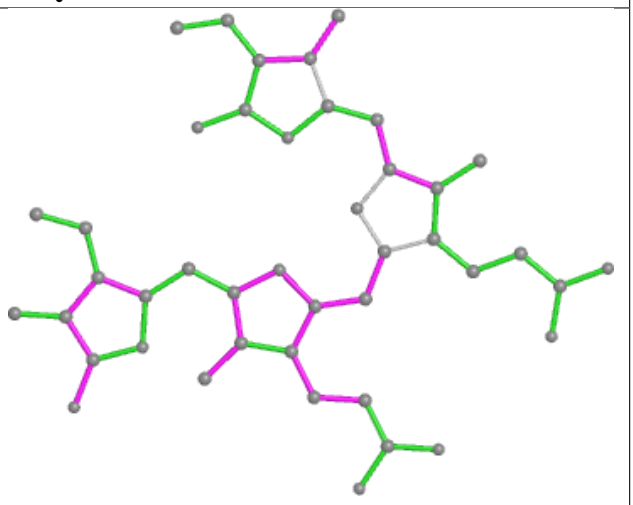

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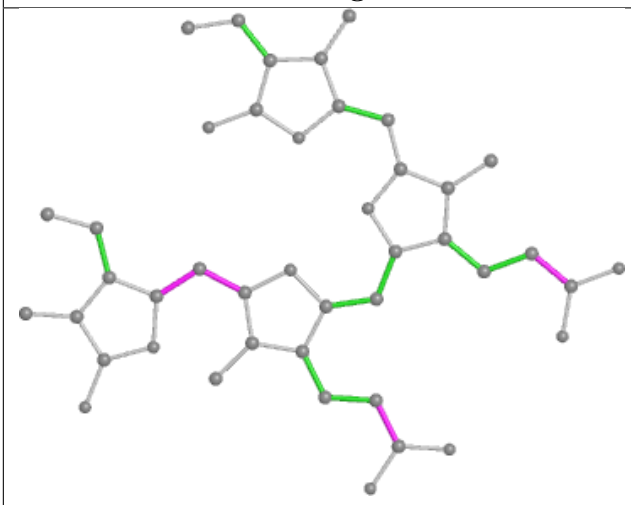
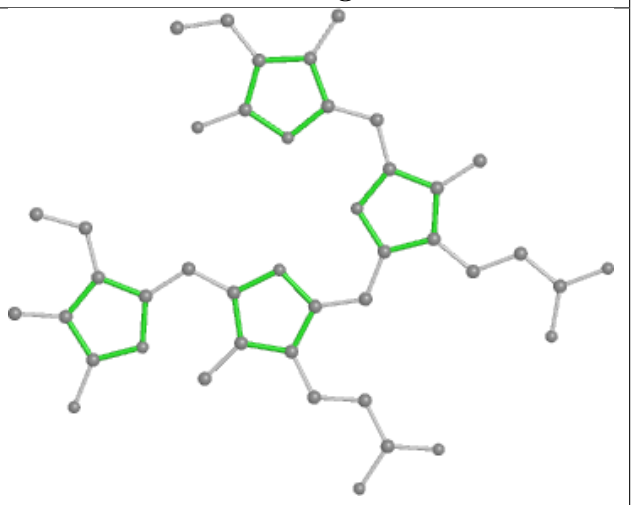
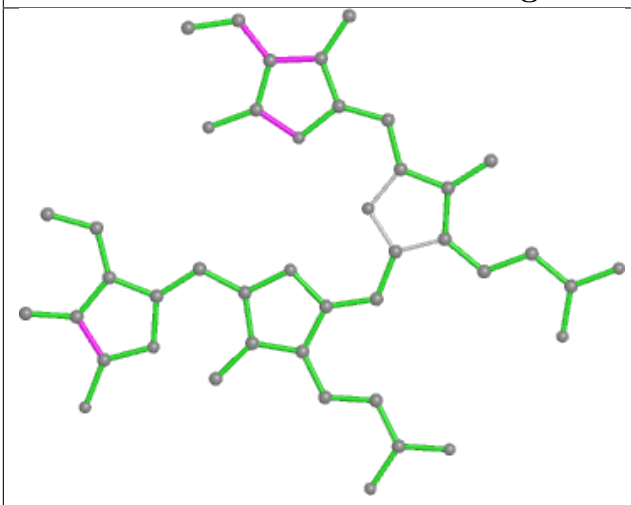


Torsions



Rings

Ligand PEB c5 202



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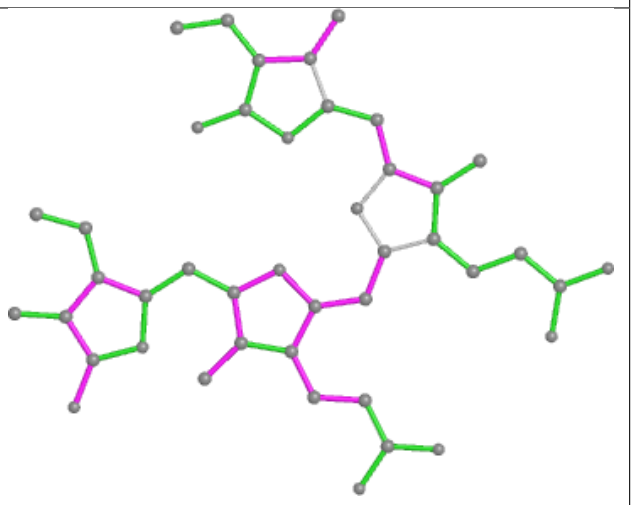
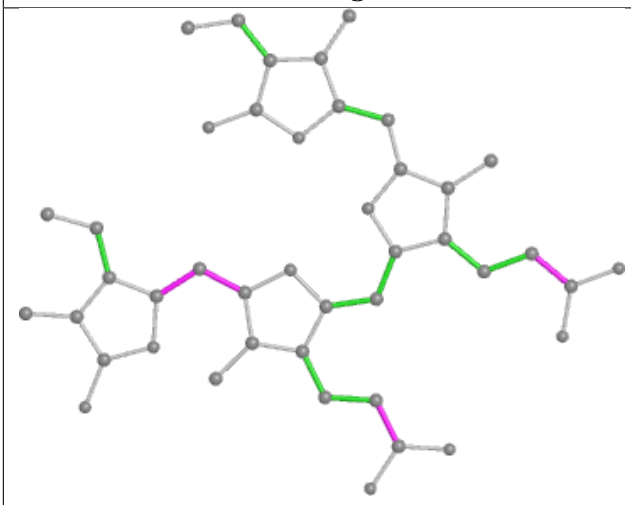


Bond angles



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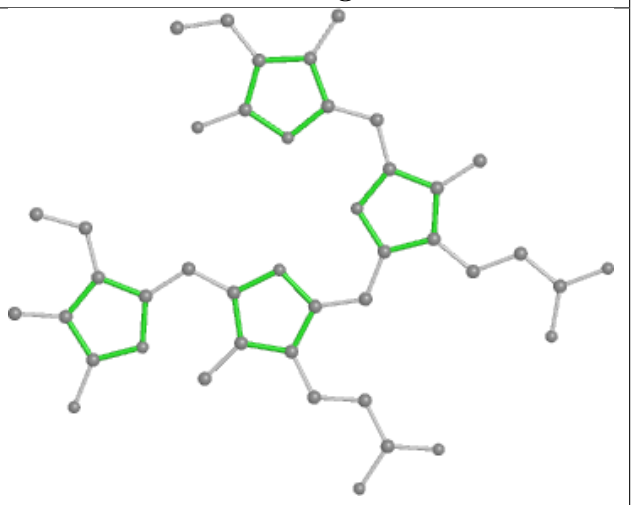
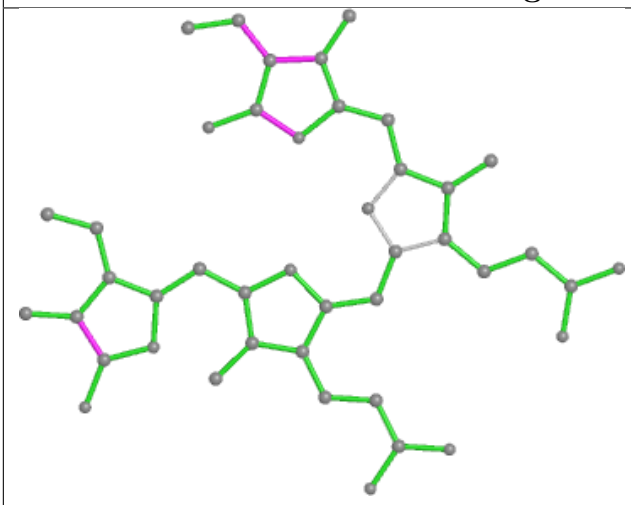


Rings

Ligand PEB i3 201



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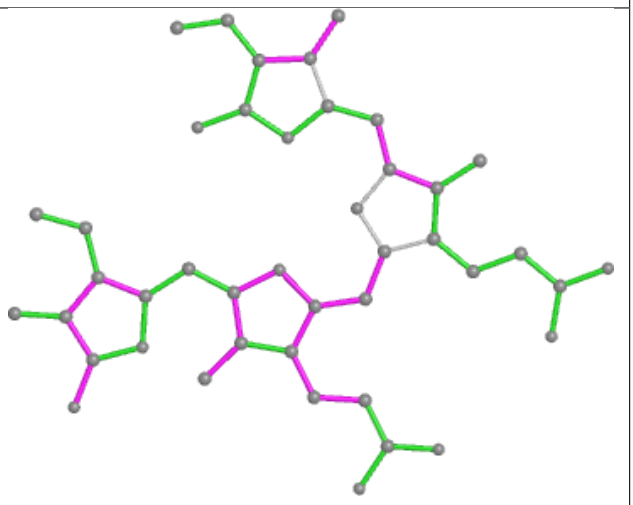

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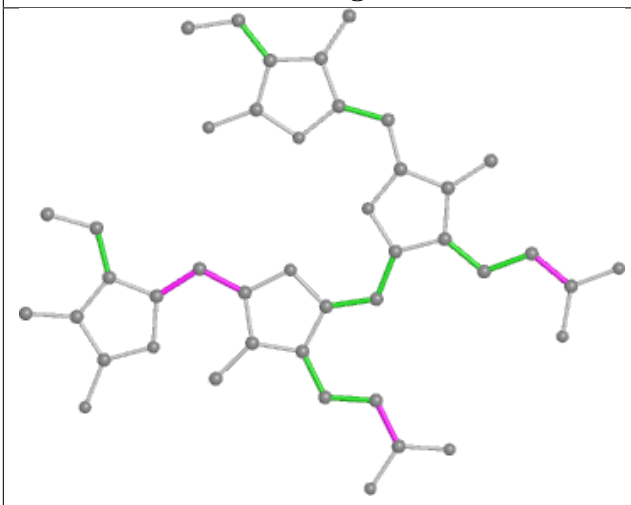

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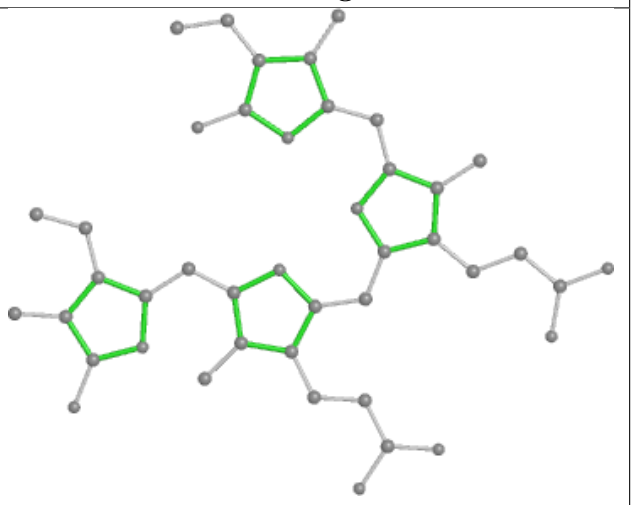
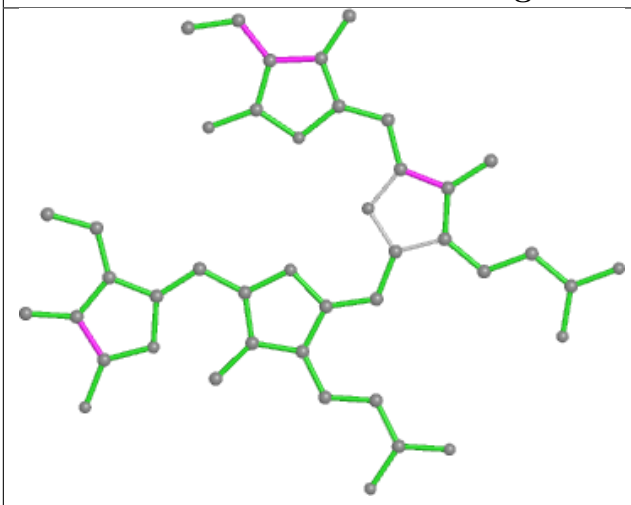


Rings

Ligand PEB bA 202



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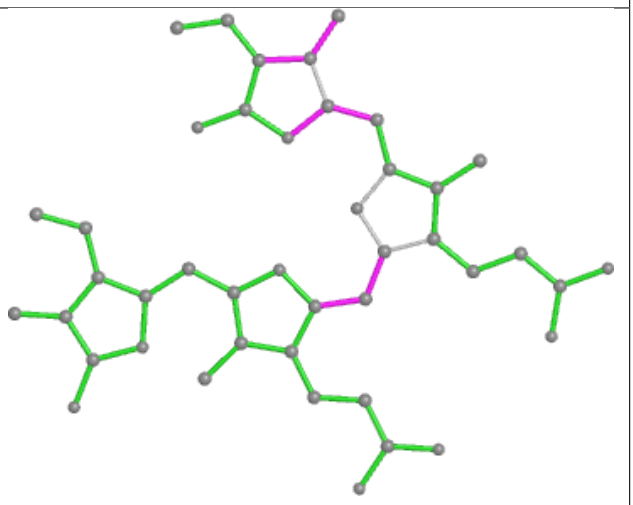

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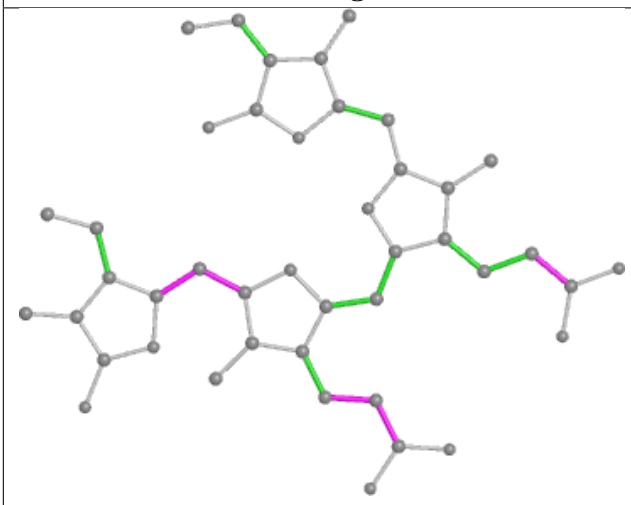

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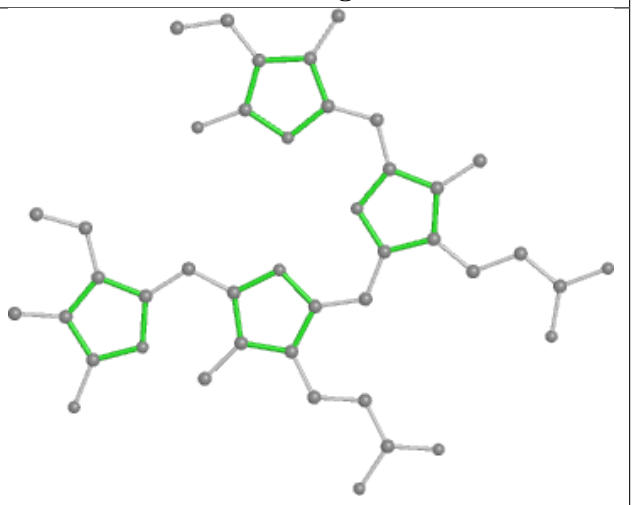
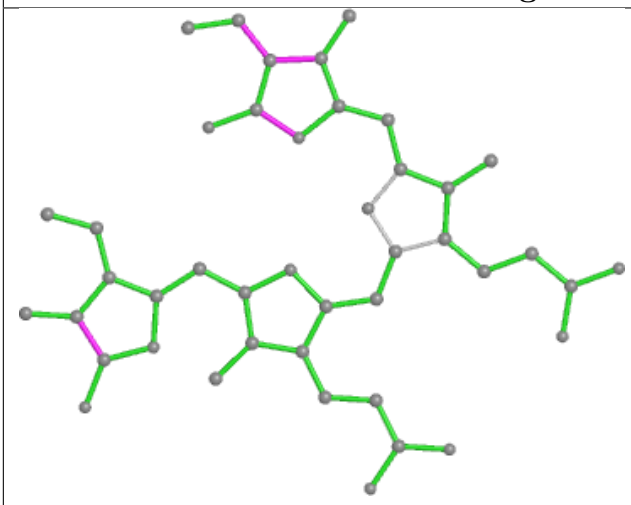


Rings

Ligand PEB v2 202



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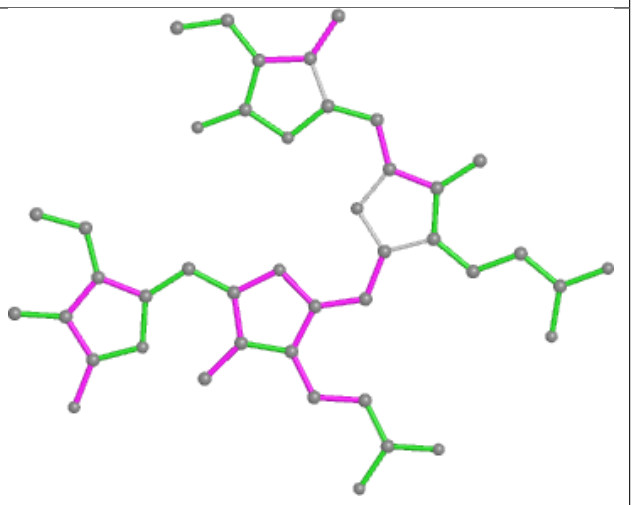

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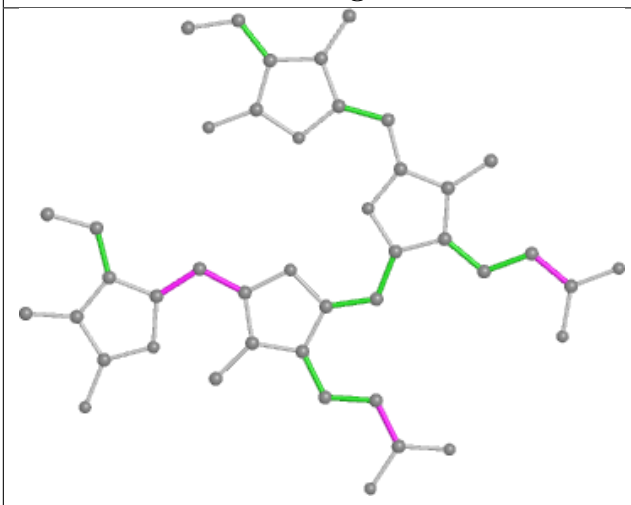

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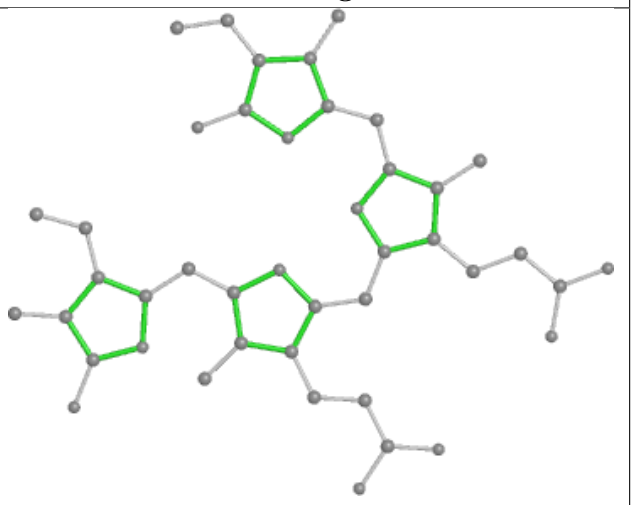
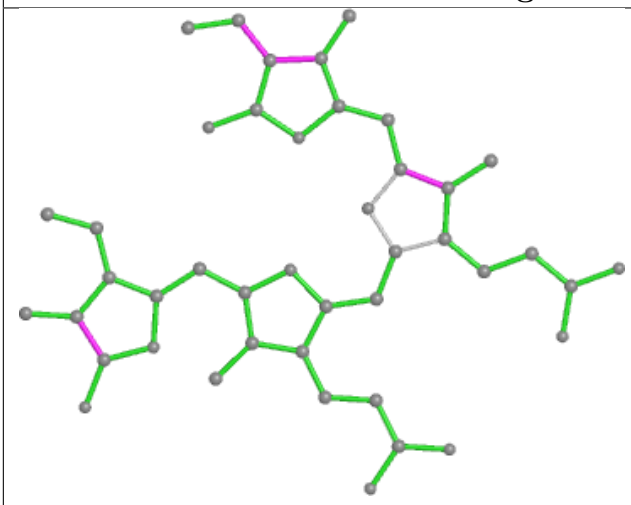


Rings

Ligand PEB cw 202



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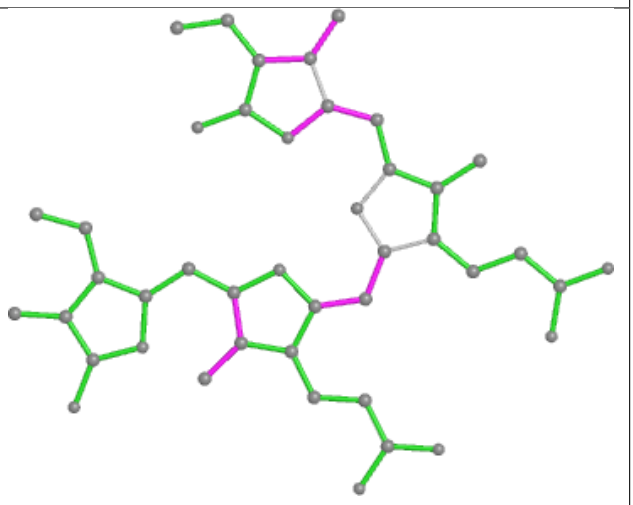

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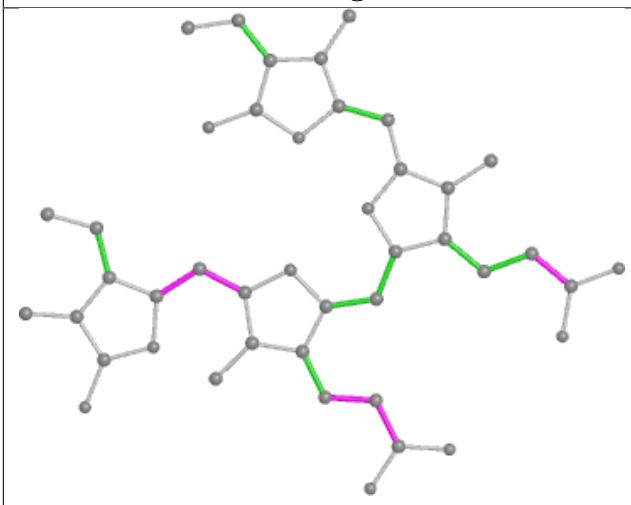

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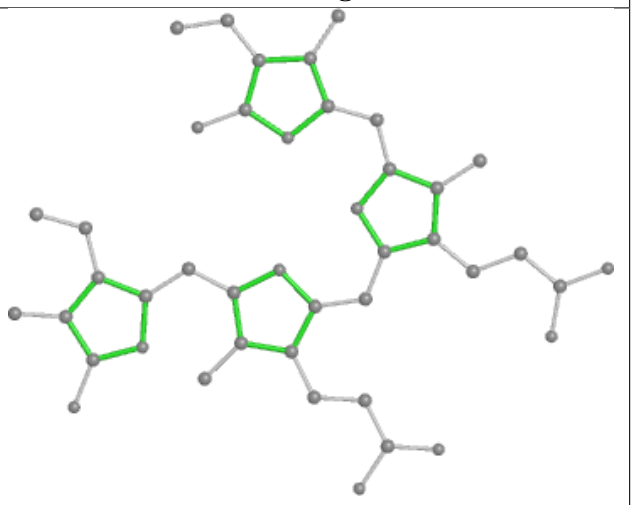
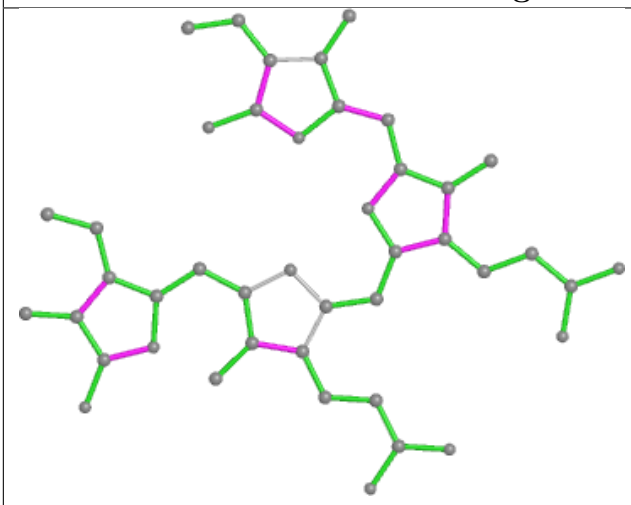


Rings

Ligand PUB bB 203



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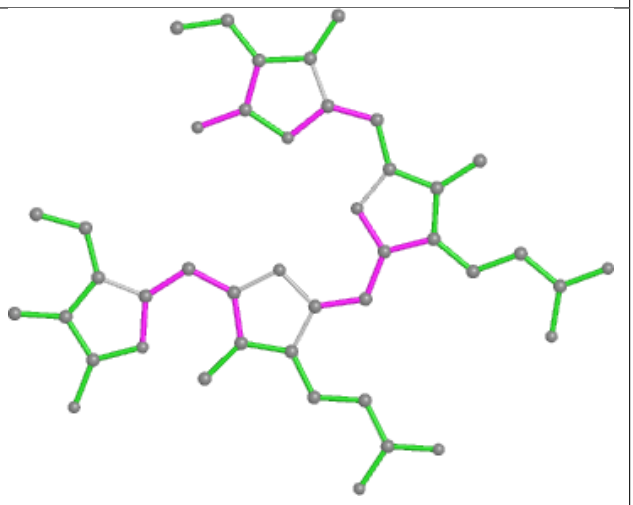

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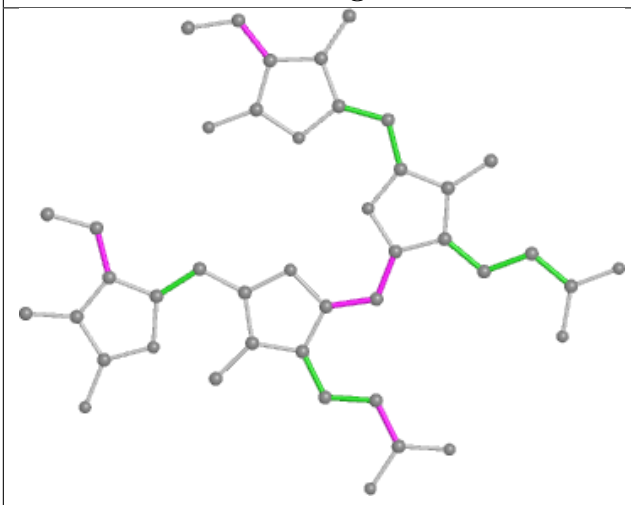

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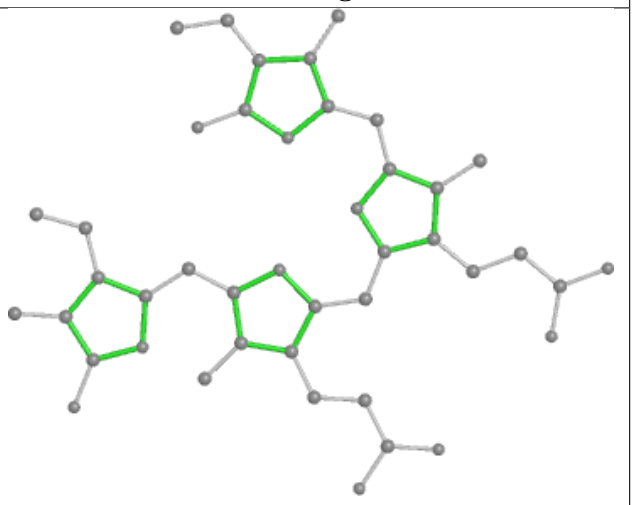
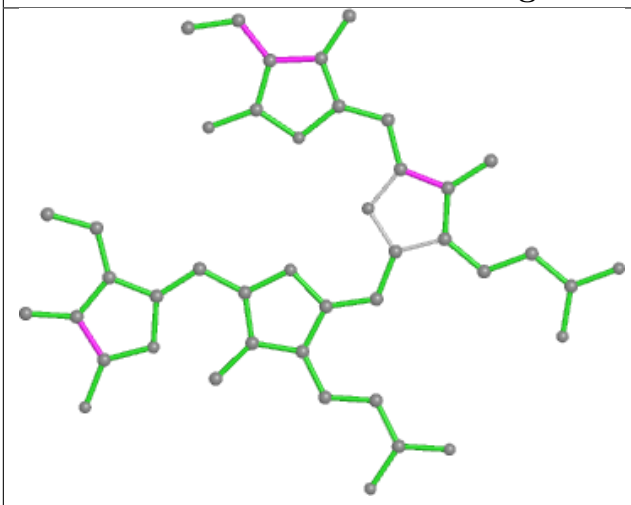


Rings

Ligand PEB eL 201



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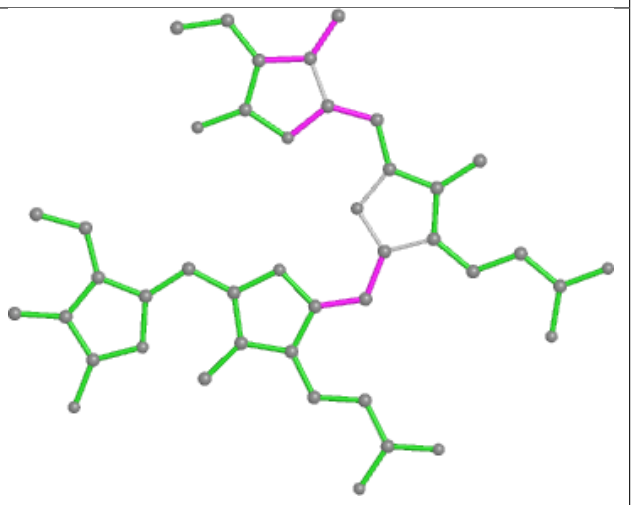

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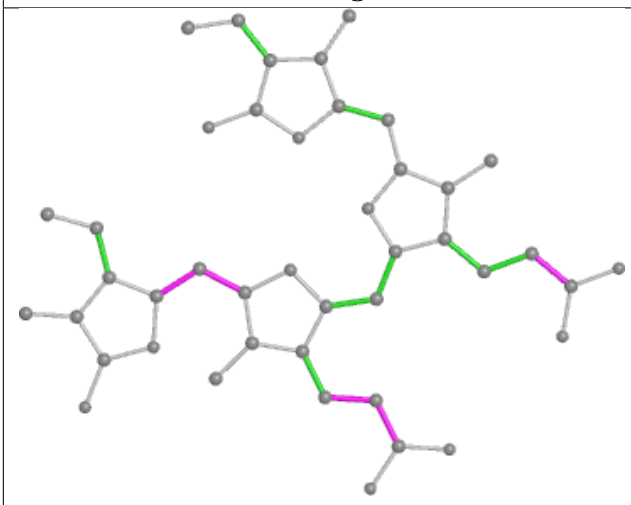

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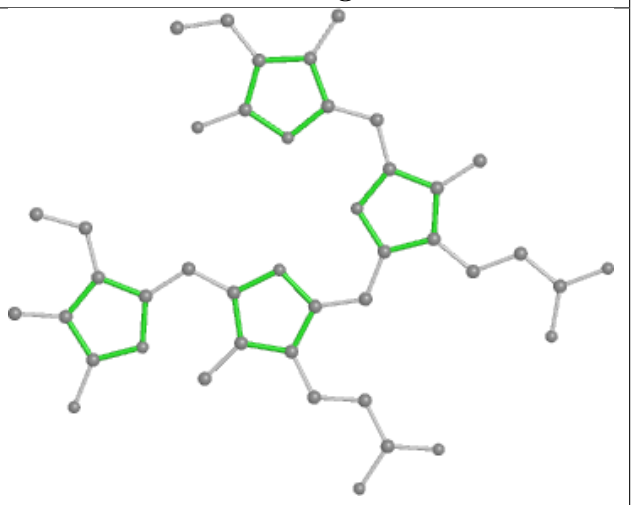
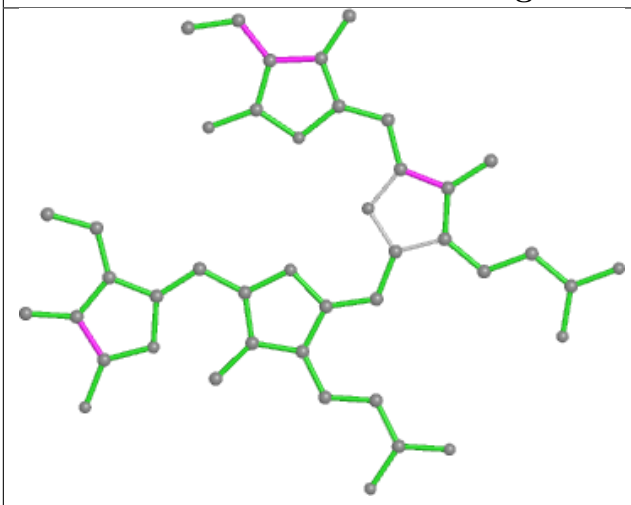


Rings

Ligand PEB Q9 202



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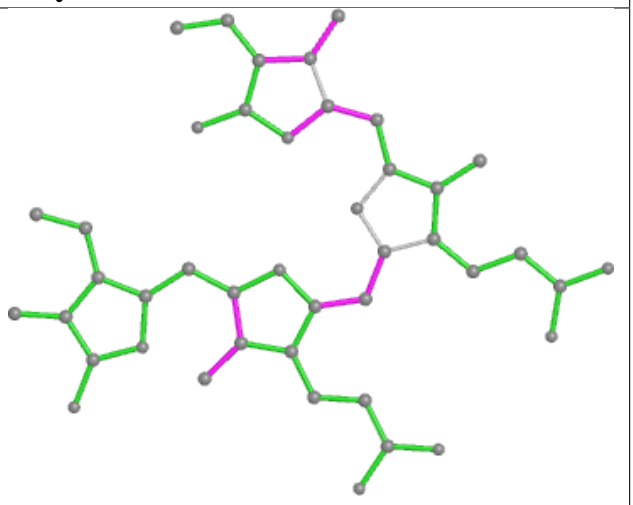

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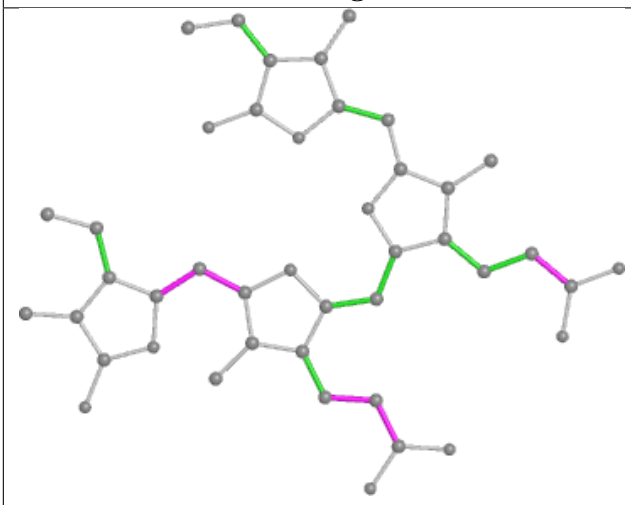

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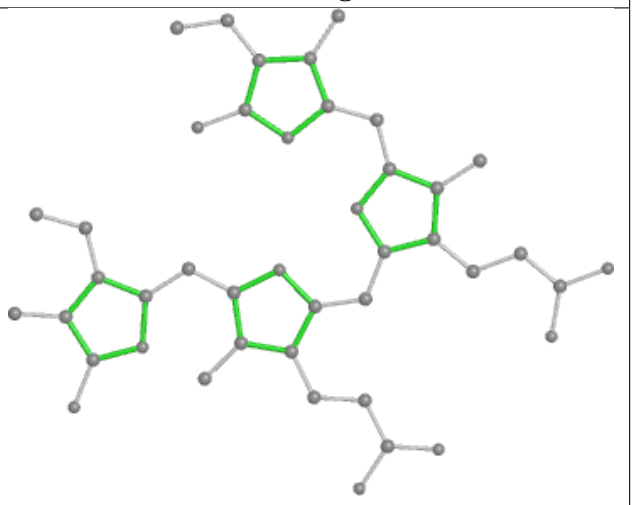
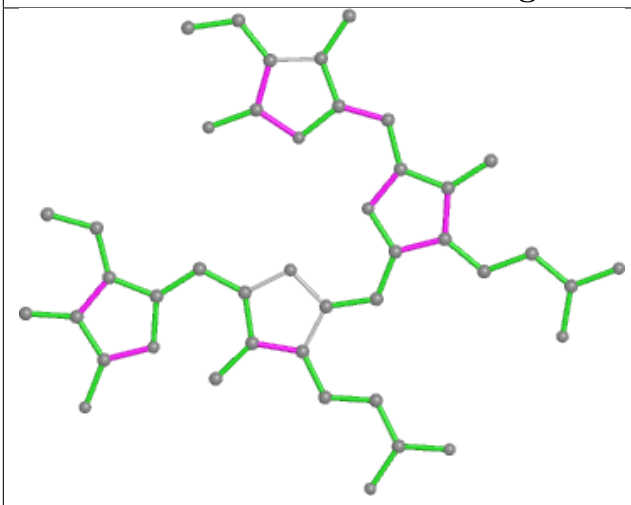


Rings

Ligand PUB e9 305



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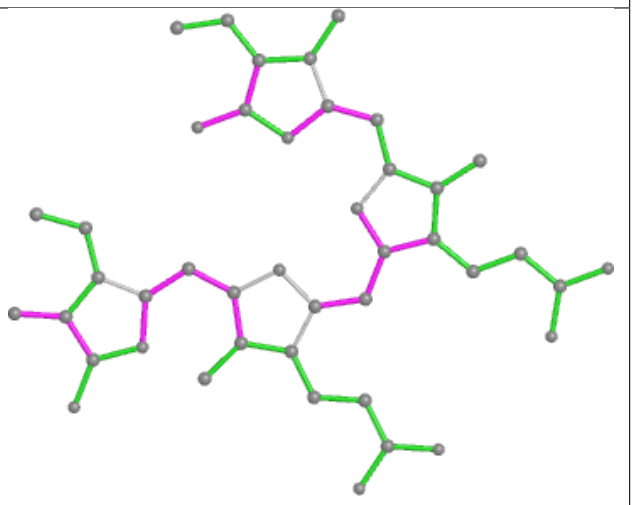

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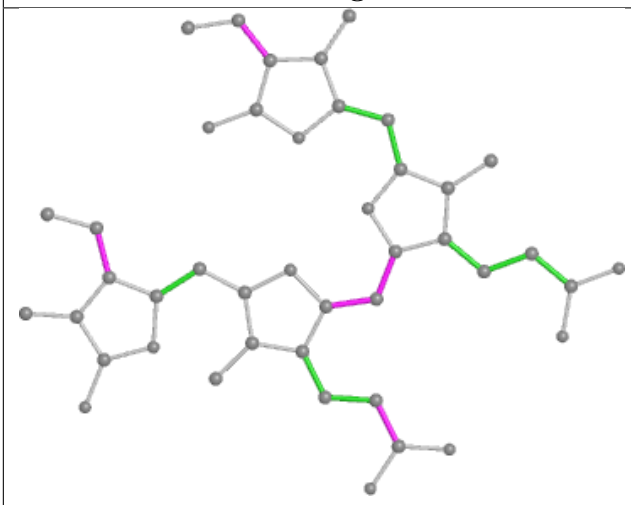

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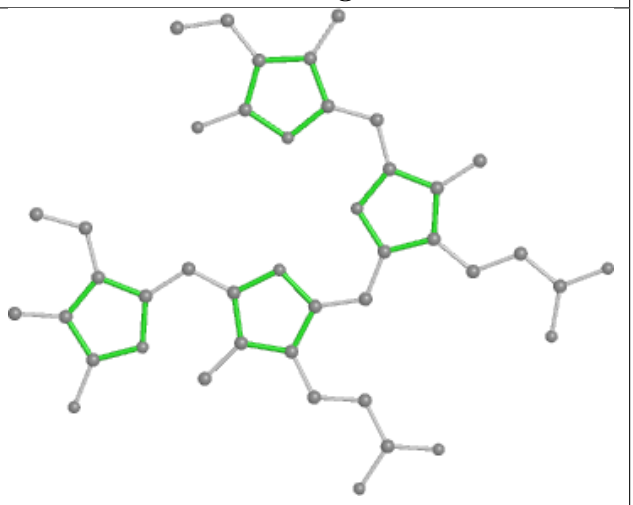
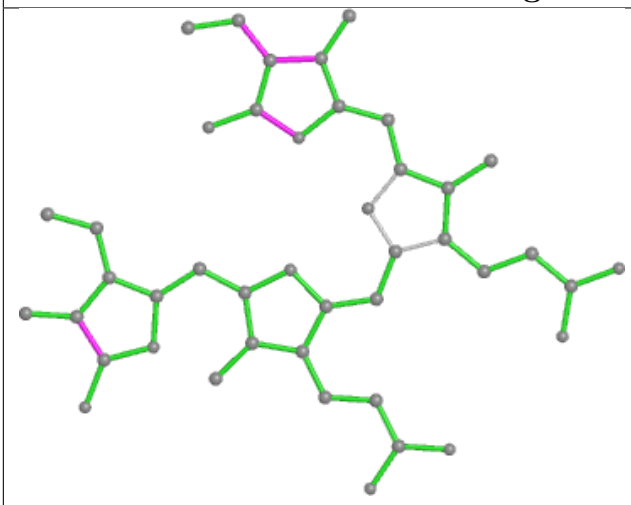


Rings

Ligand PEB f2 201



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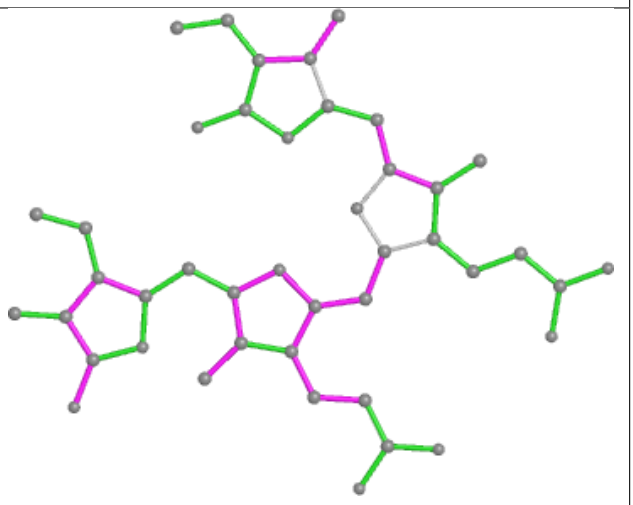

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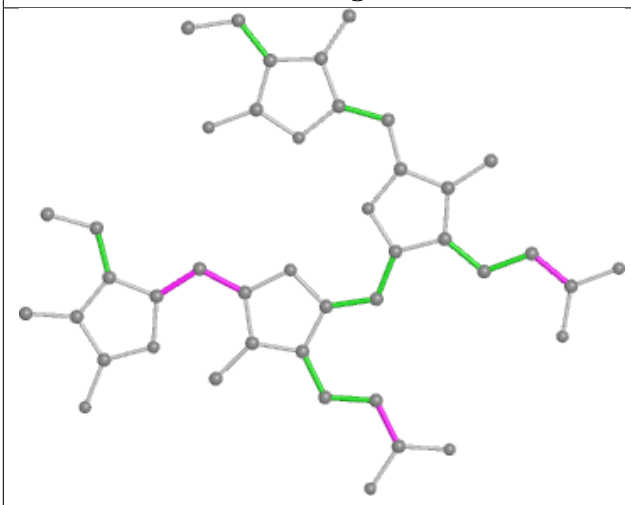

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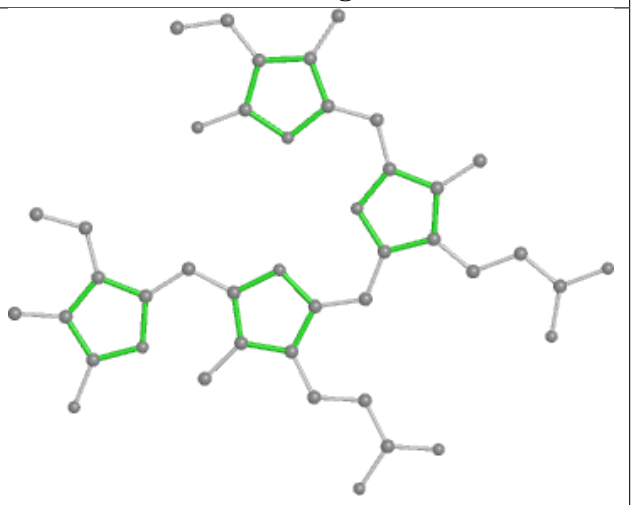

Rings

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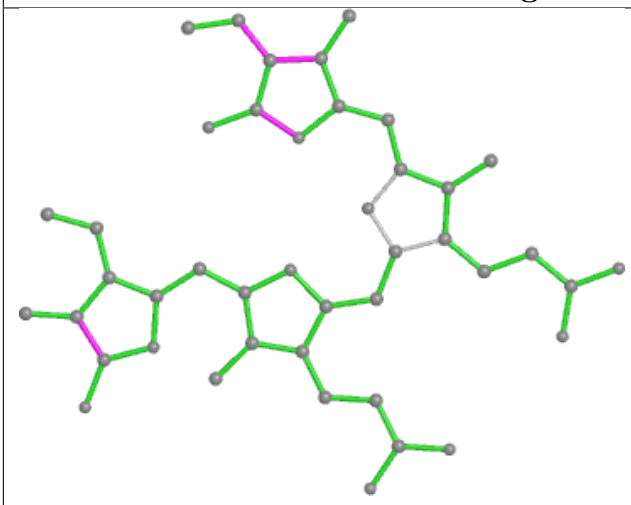

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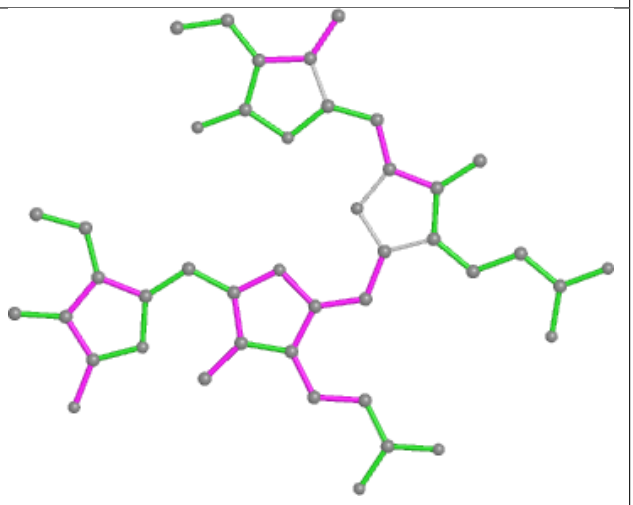

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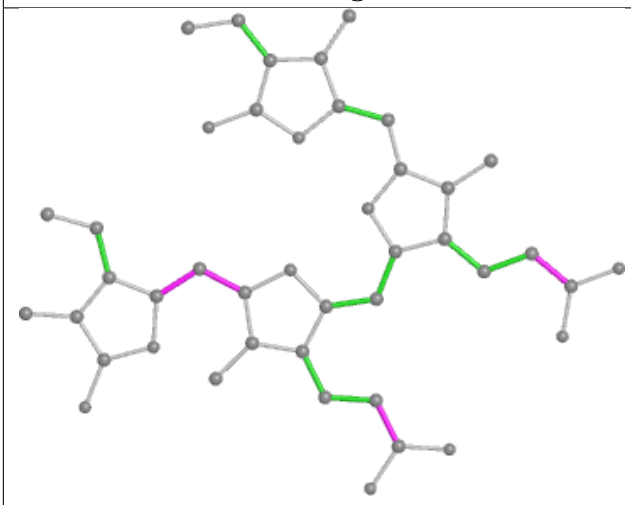

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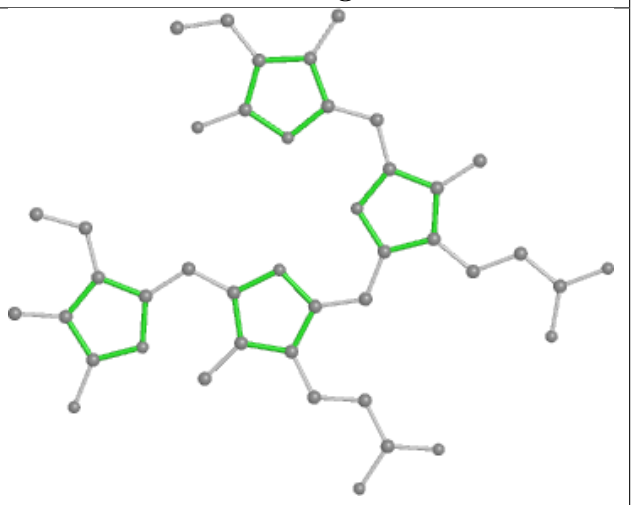
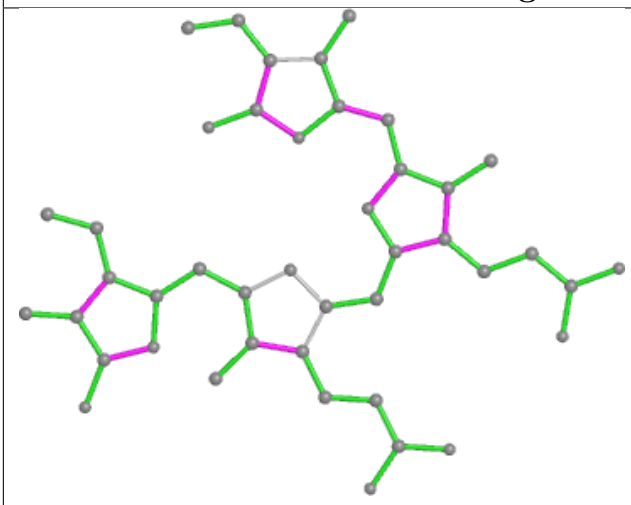


Rings

Ligand PUB co 202



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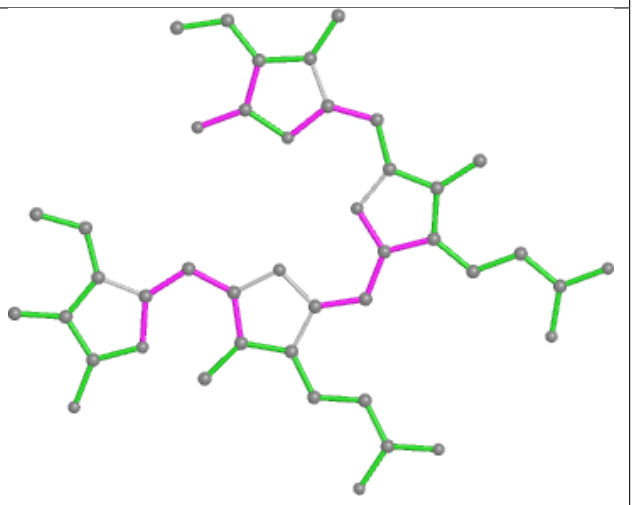

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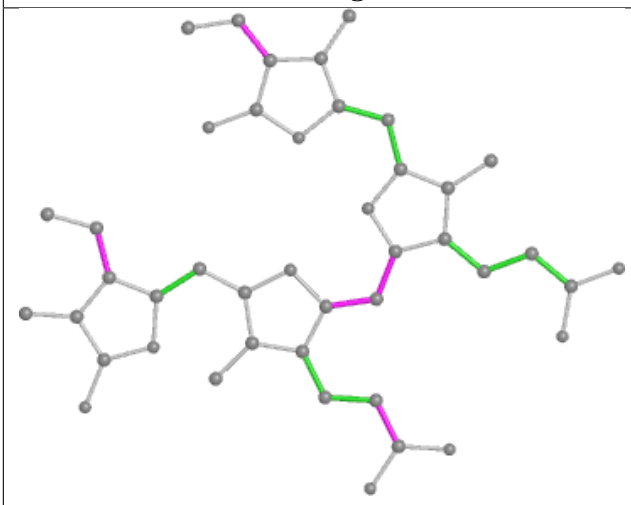

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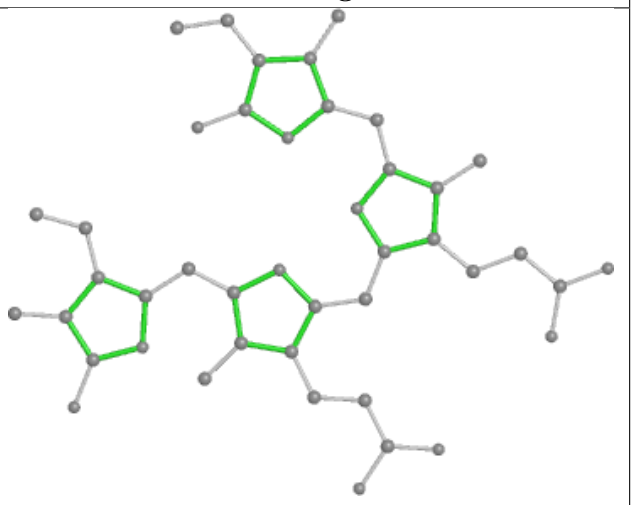
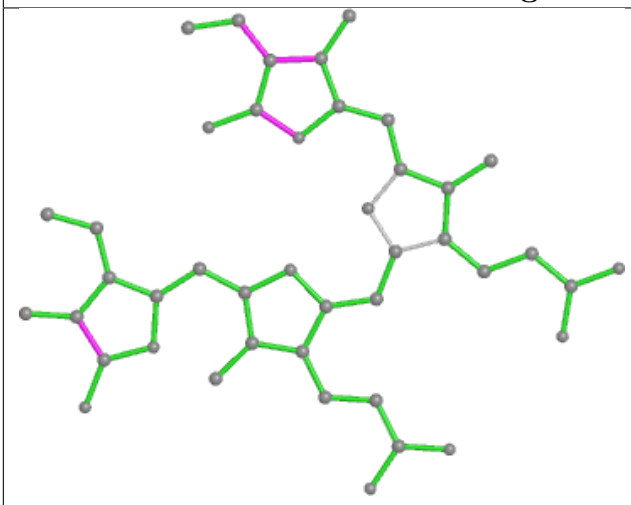


Rings

Ligand PEB eo 202



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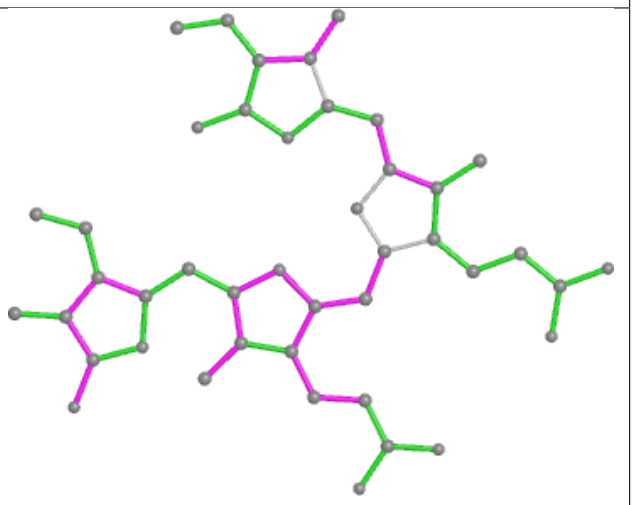

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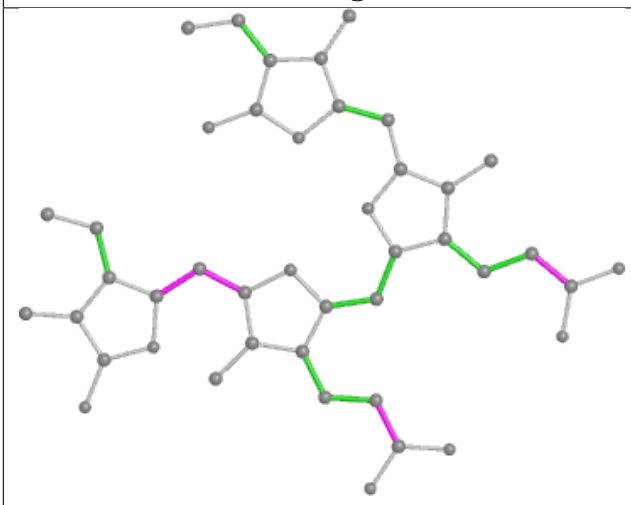

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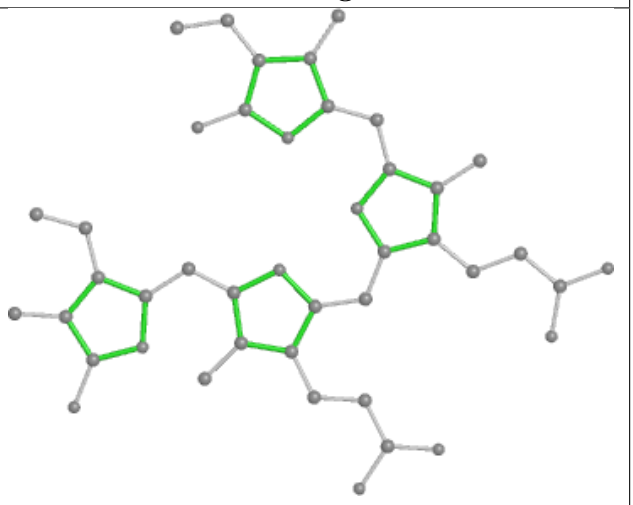
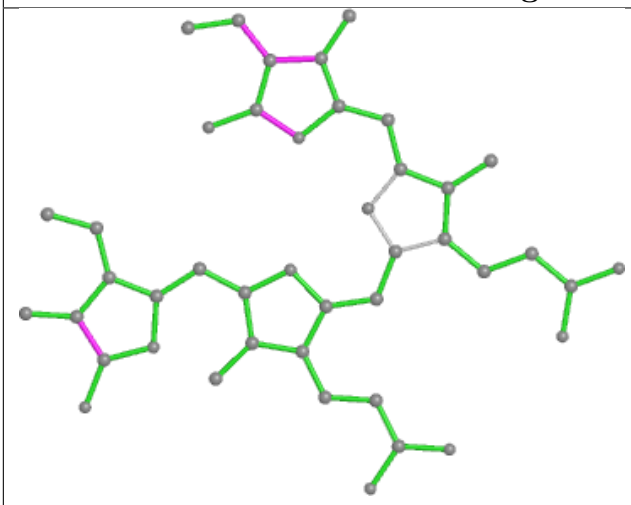


Rings

Ligand PEB az 201



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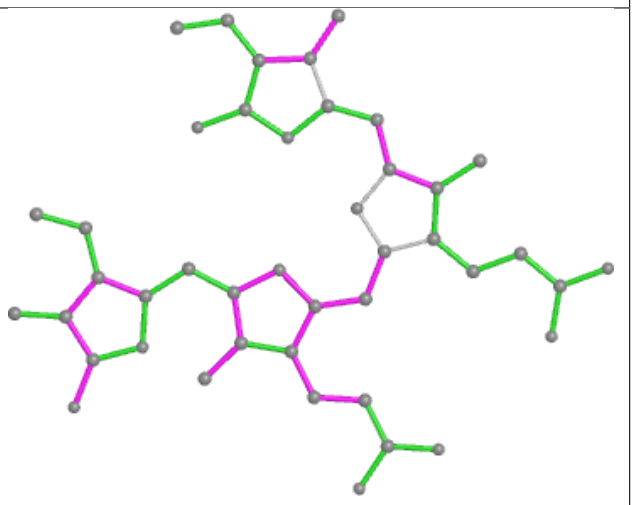

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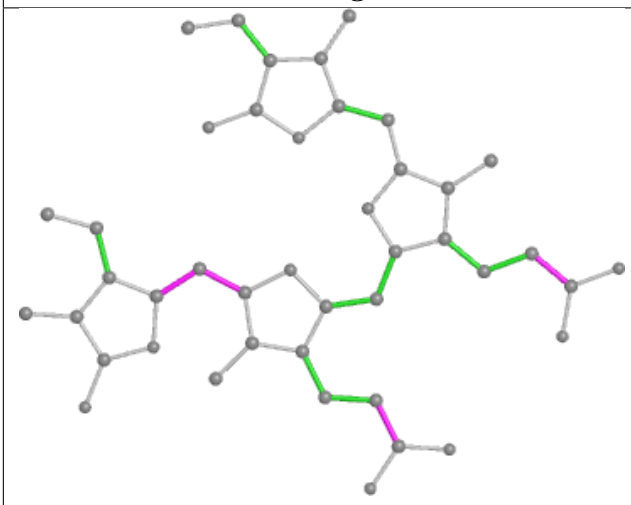
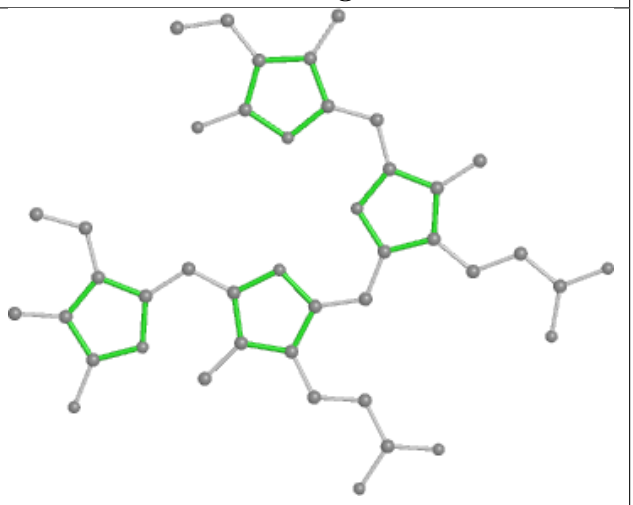
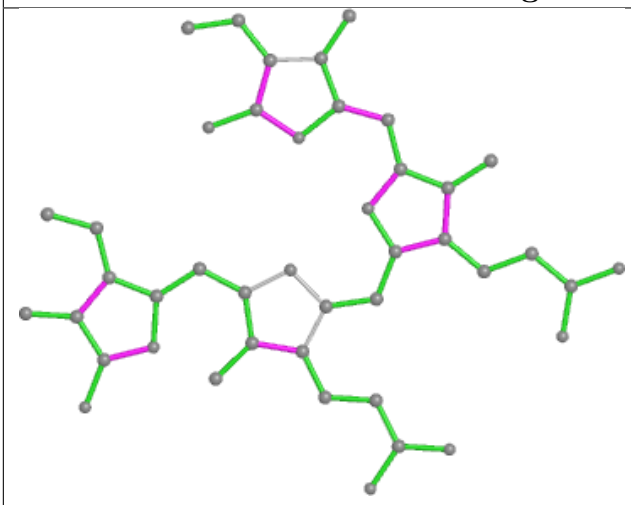


Torsions



Rings

Ligand PUB fo 203



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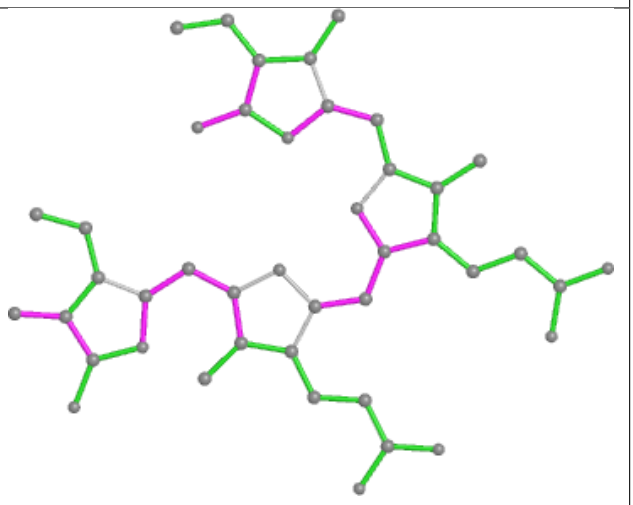

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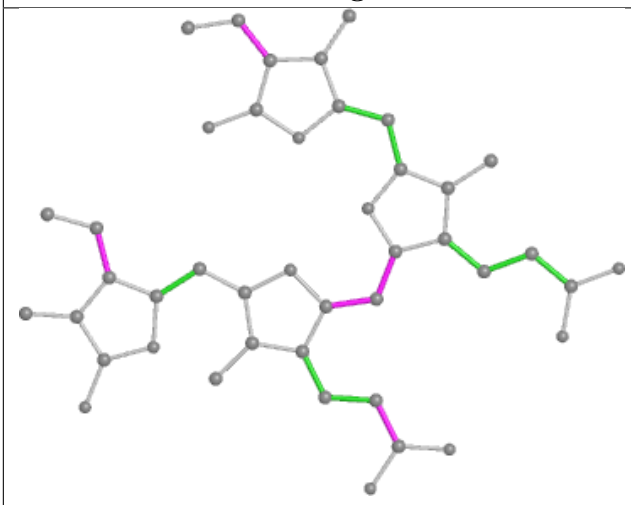

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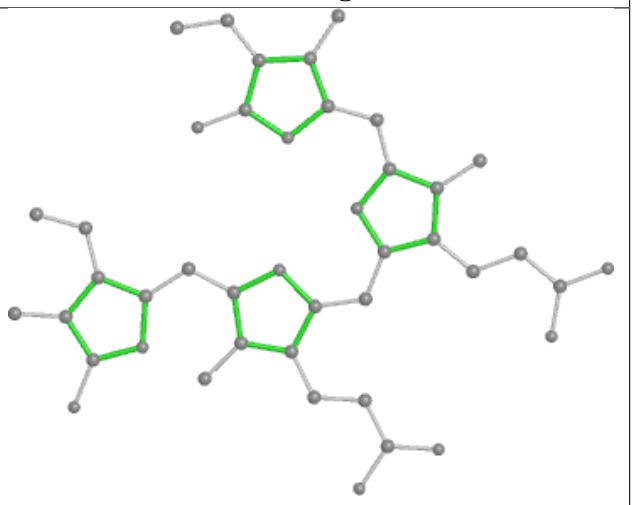
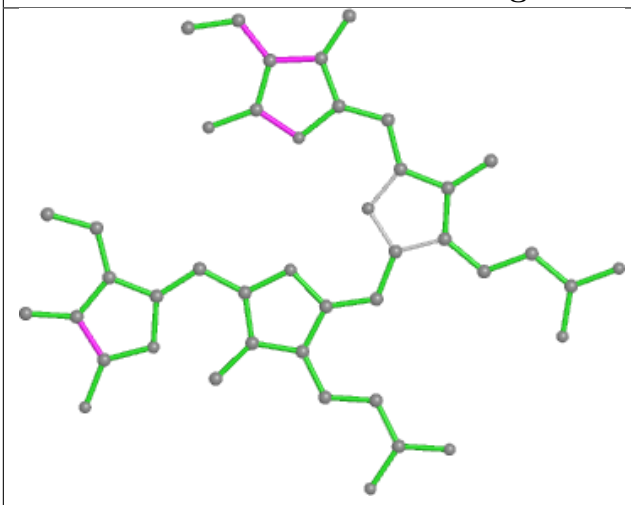


Rings

Ligand PEB b8 1002



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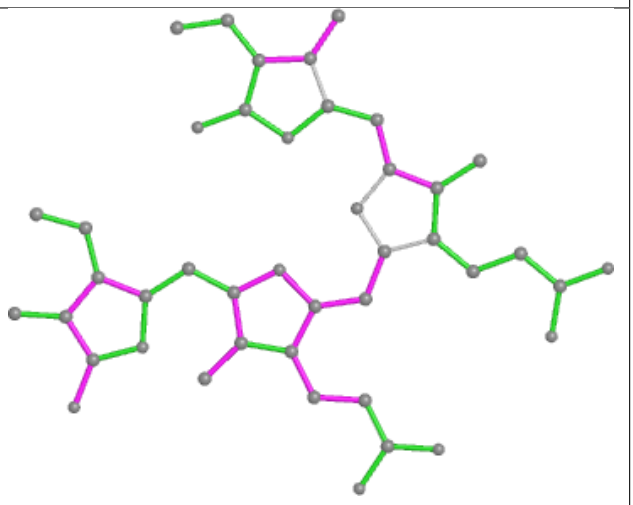

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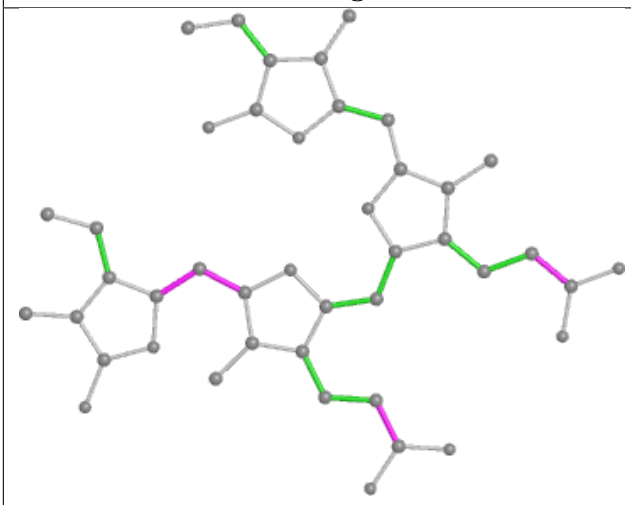

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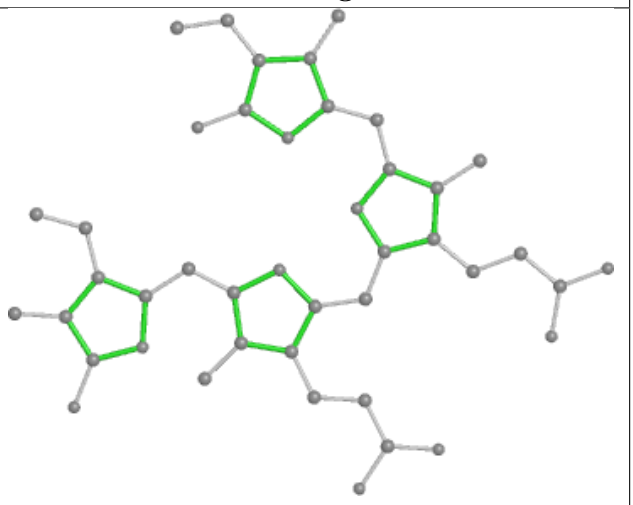

Rings

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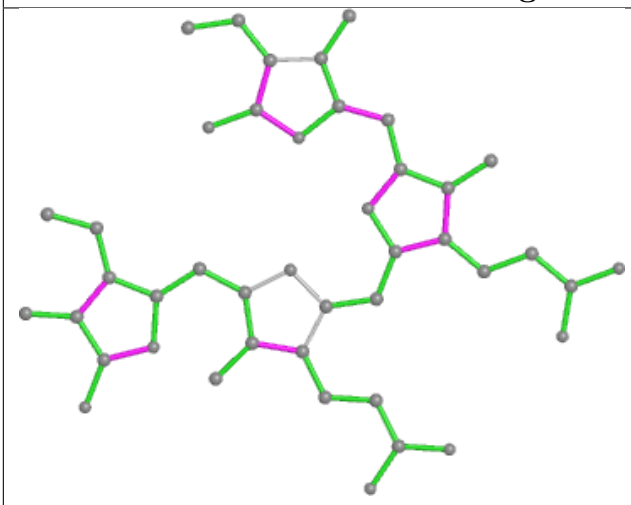

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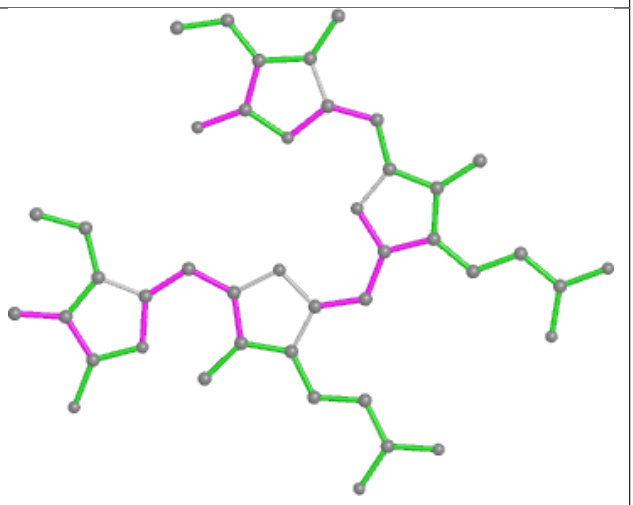

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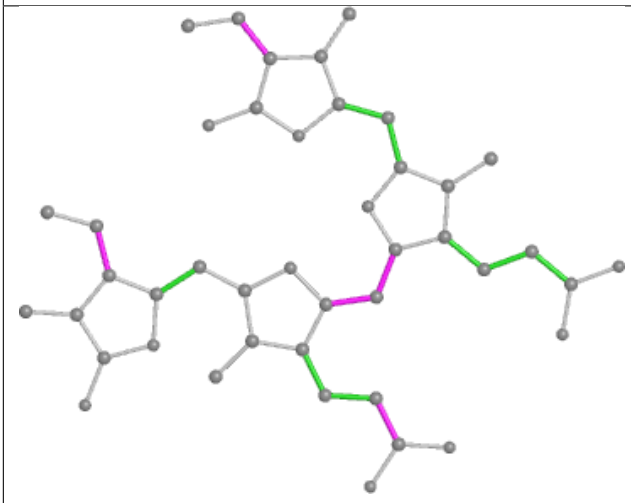

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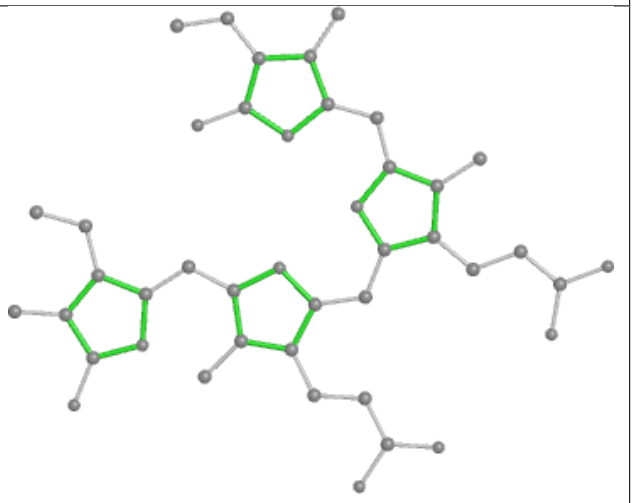
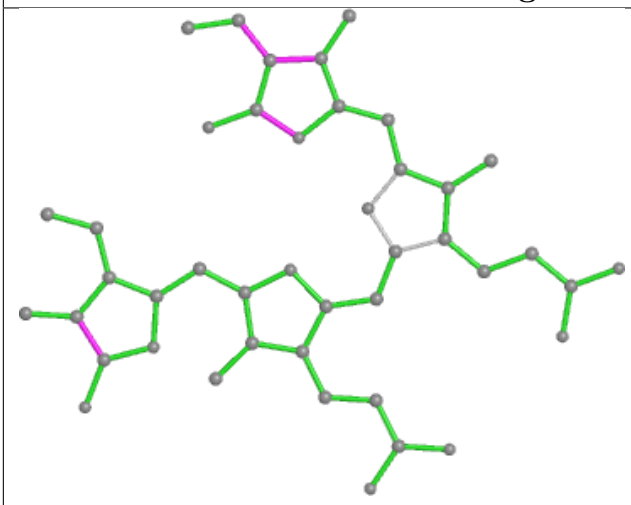


Rings

Ligand PEB do 201



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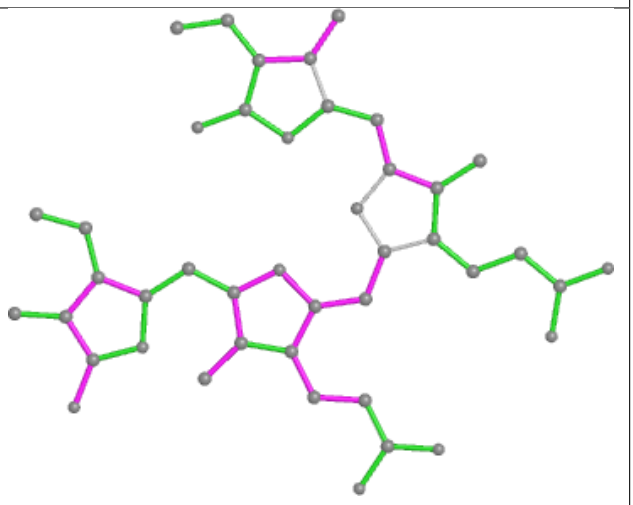

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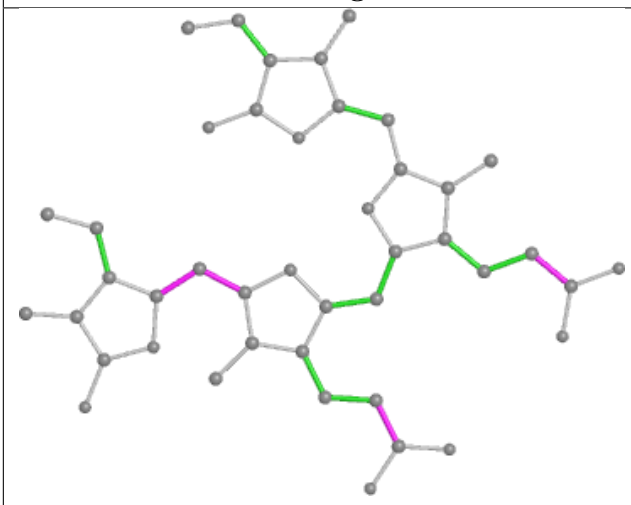

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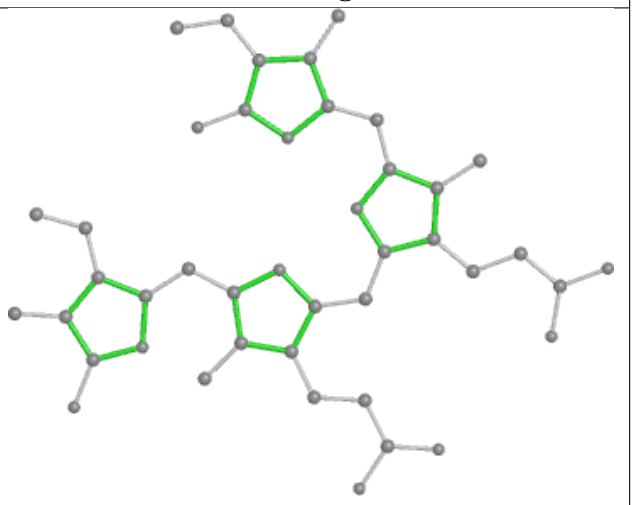

Rings

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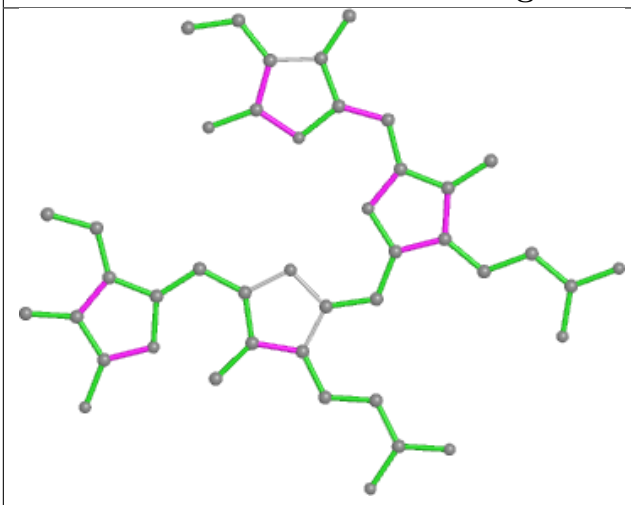

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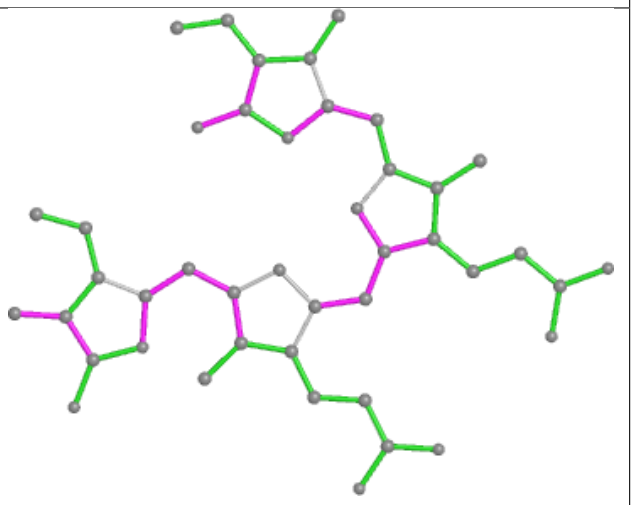

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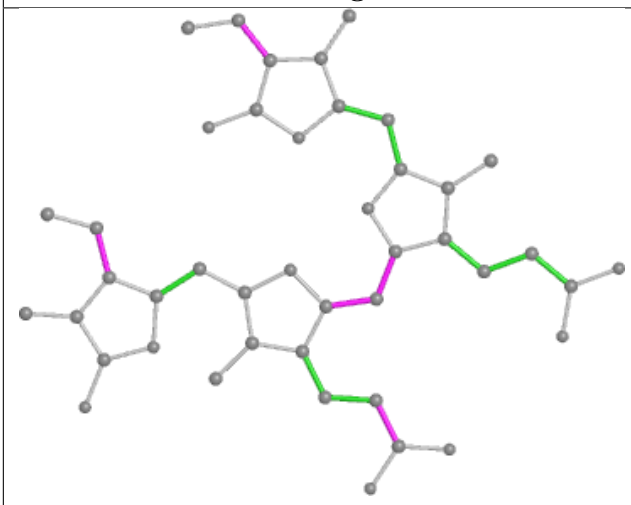

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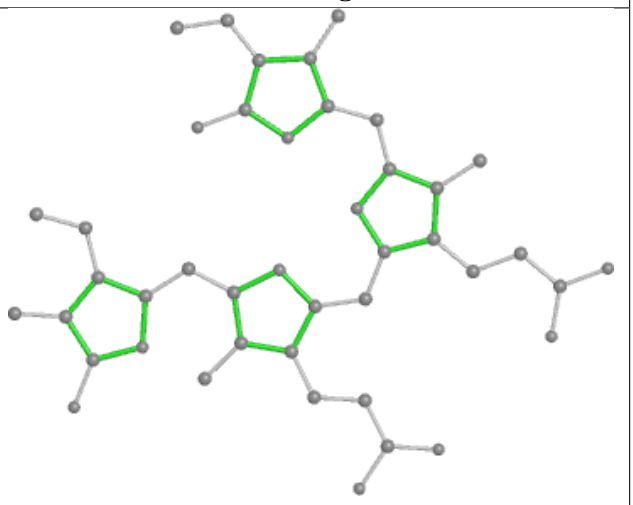

Rings

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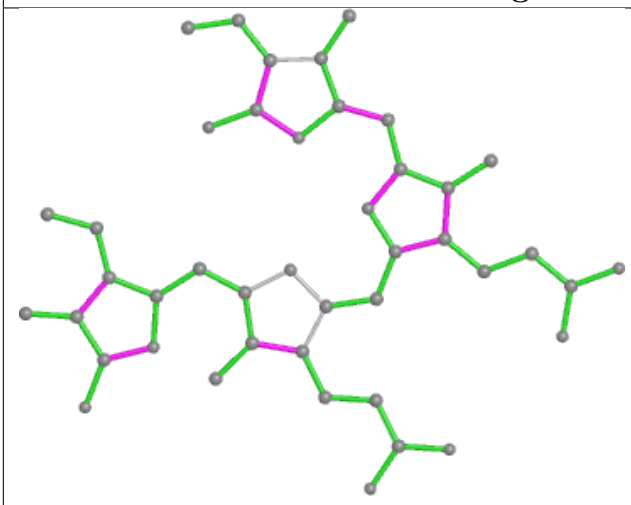

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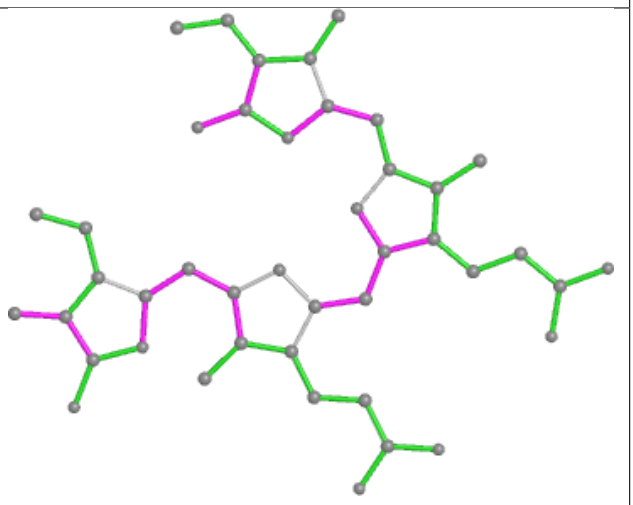

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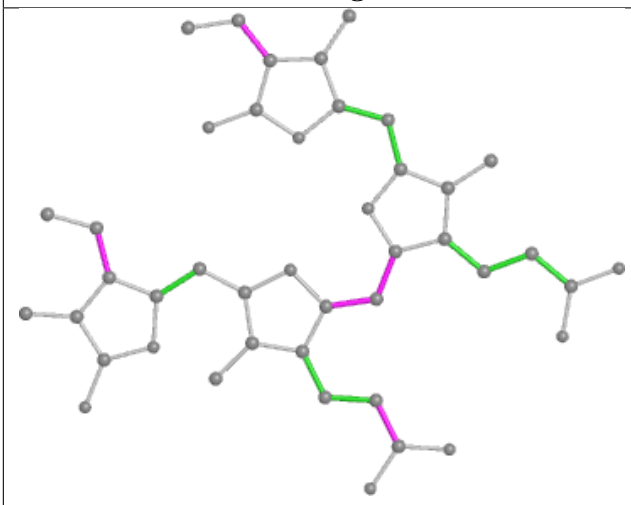

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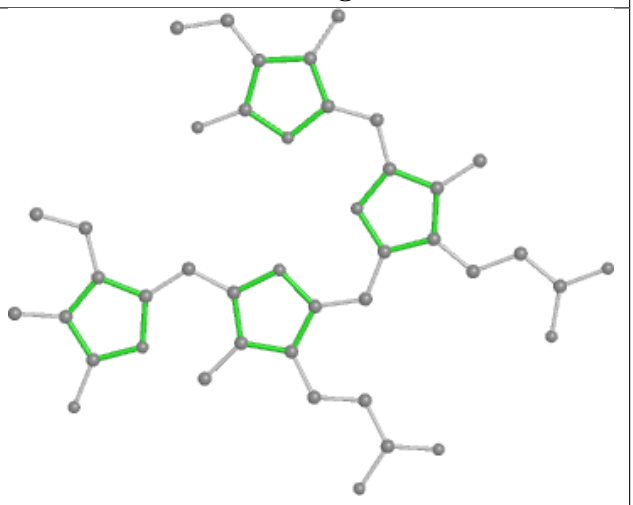
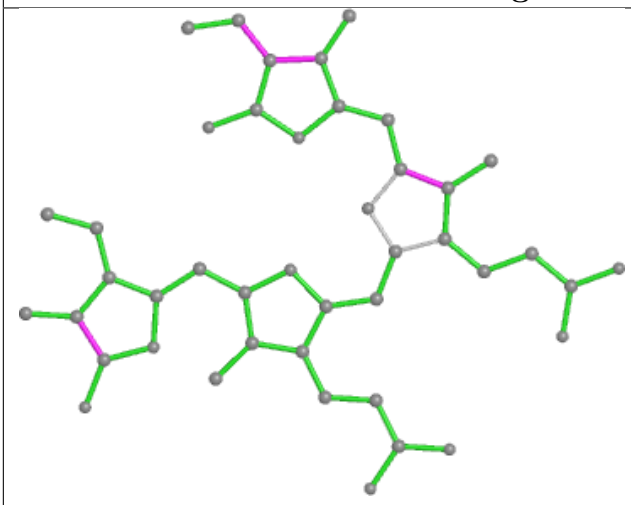


Rings

Ligand PEB e3 1002



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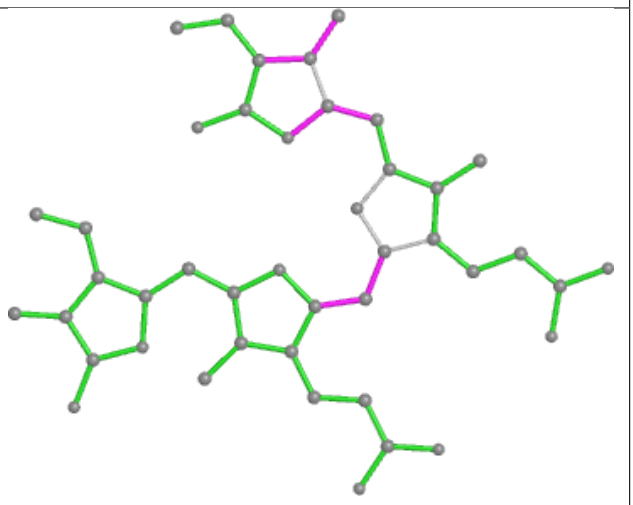

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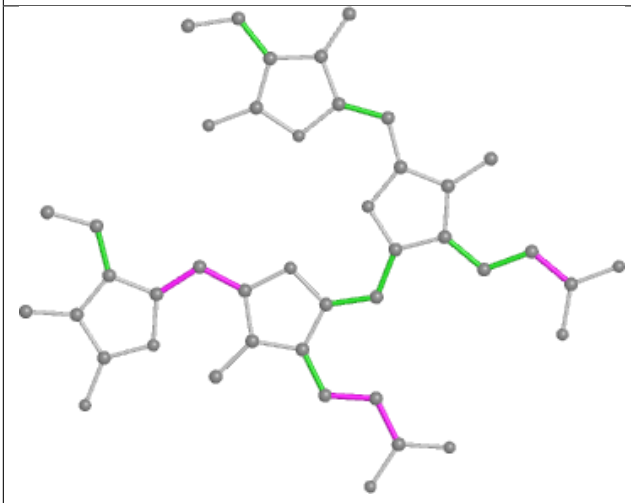

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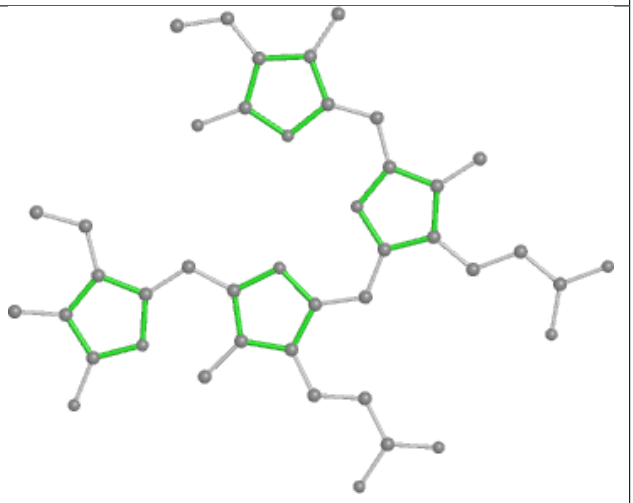

Rings

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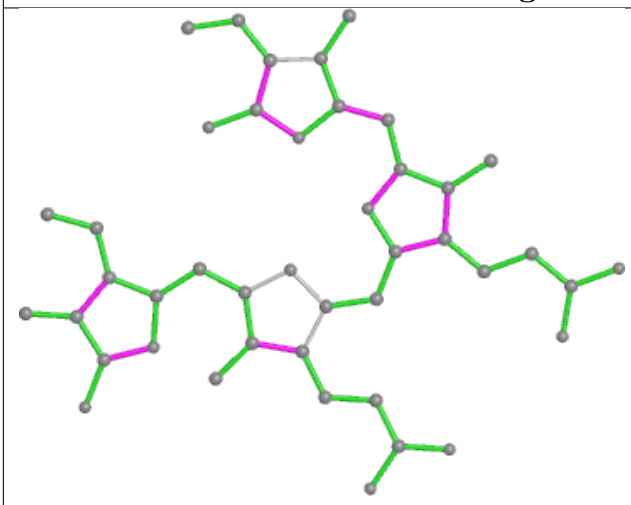

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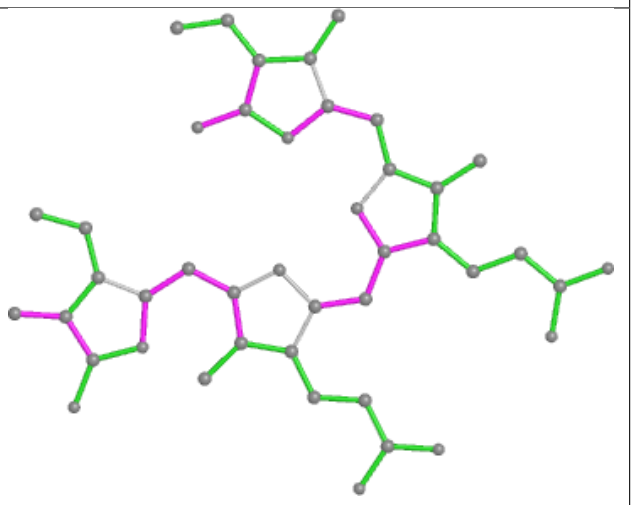

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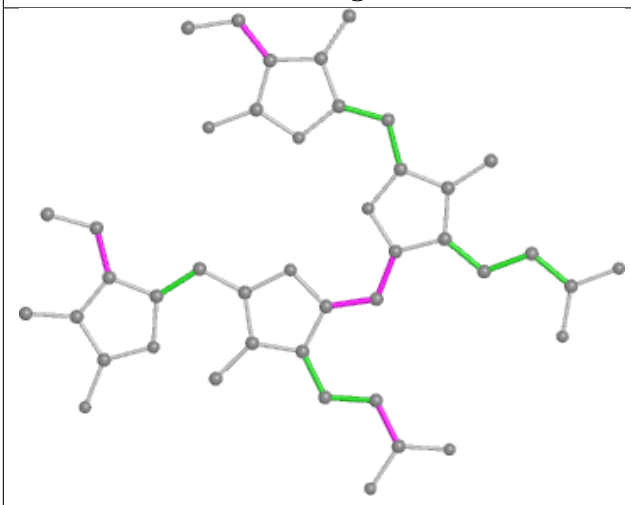

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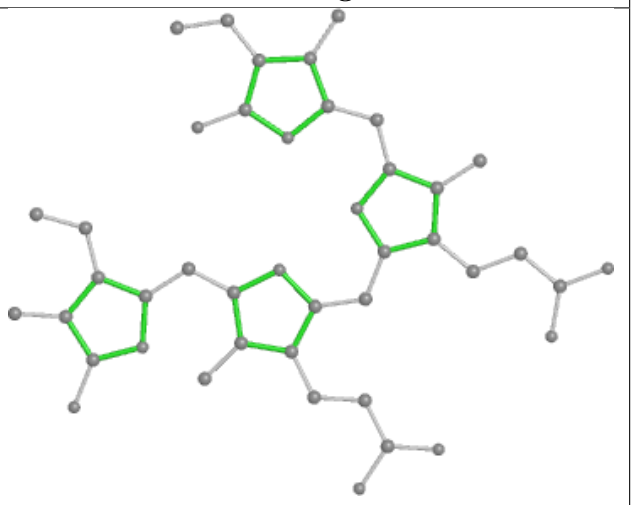
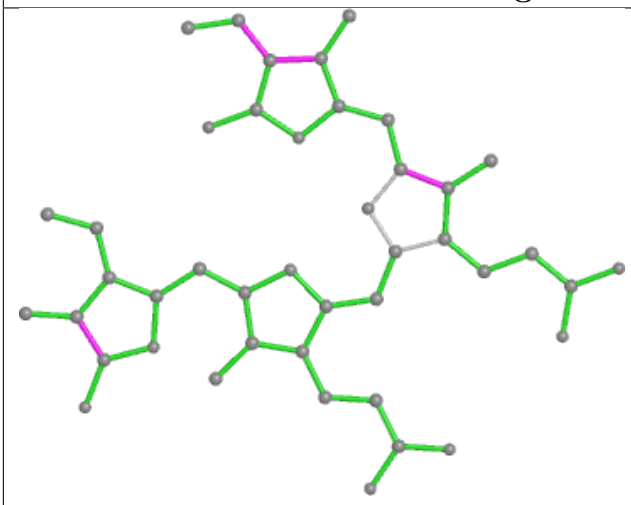


Rings

Ligand PEB H6 201



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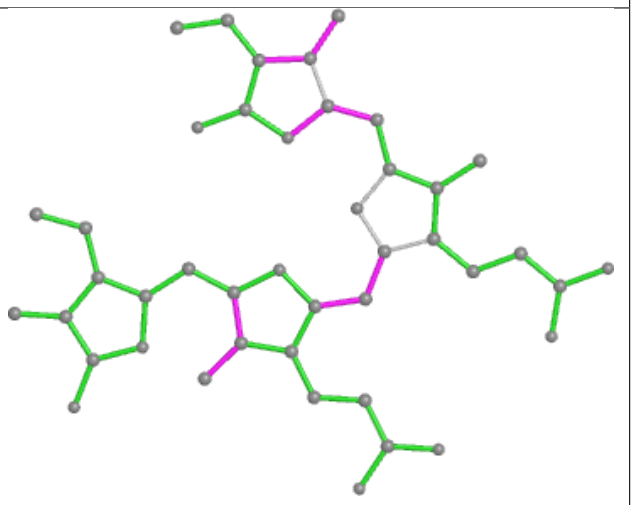

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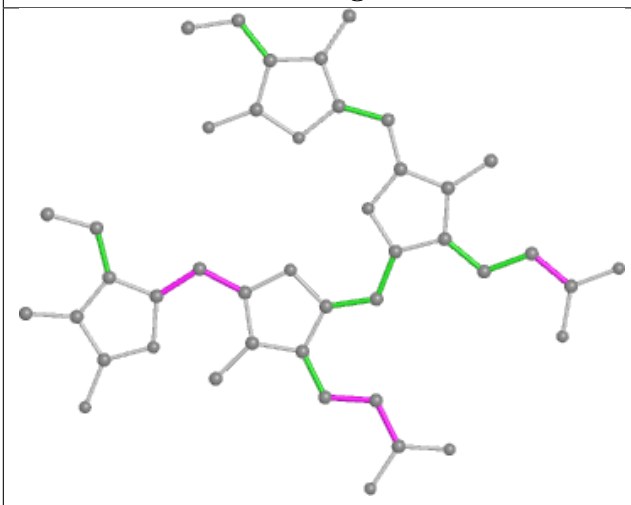

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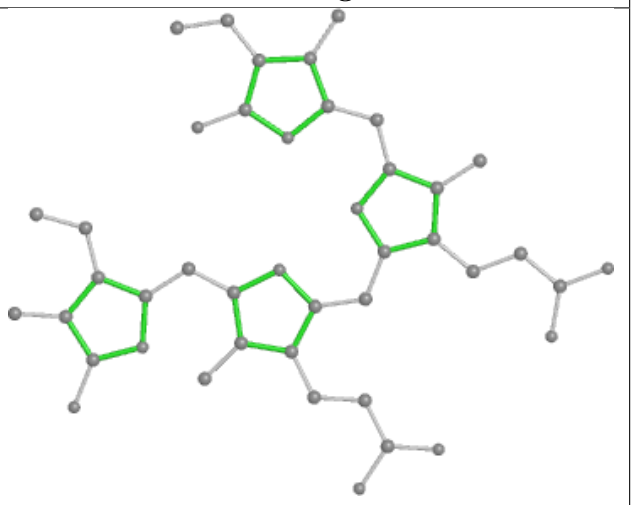

Rings

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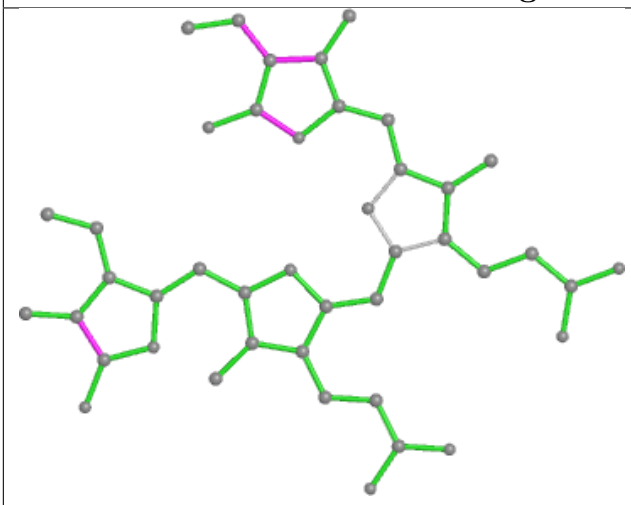

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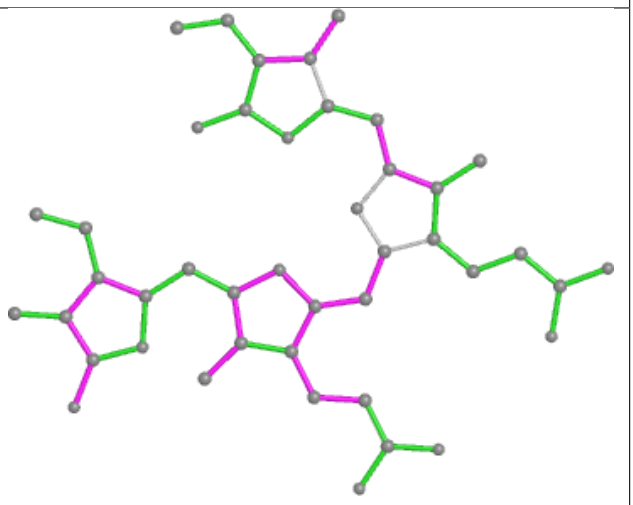

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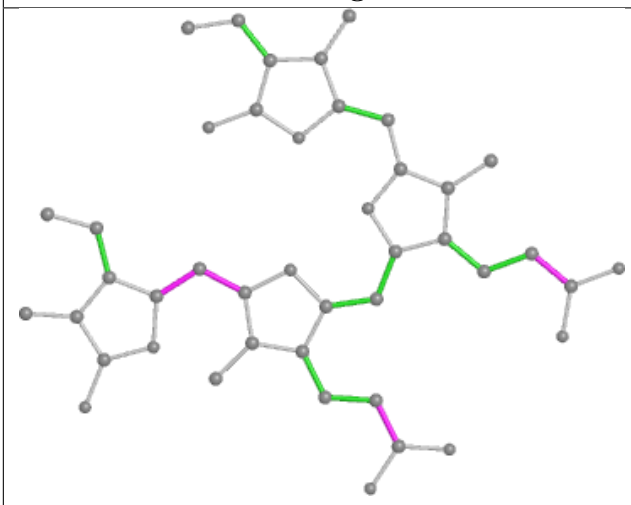

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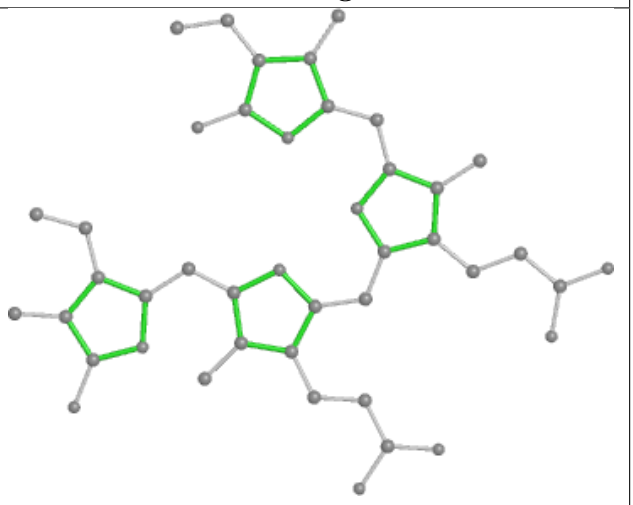
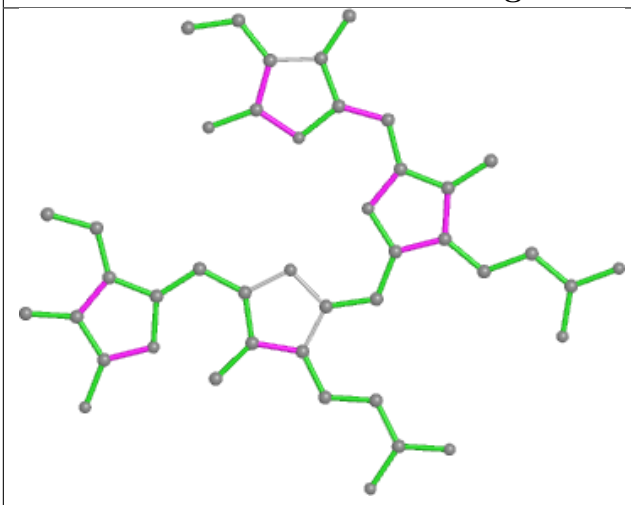


Rings

Ligand PUB Y5 1005



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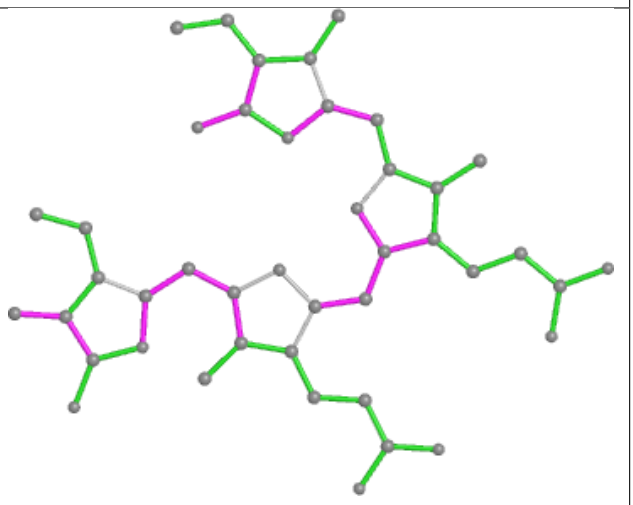

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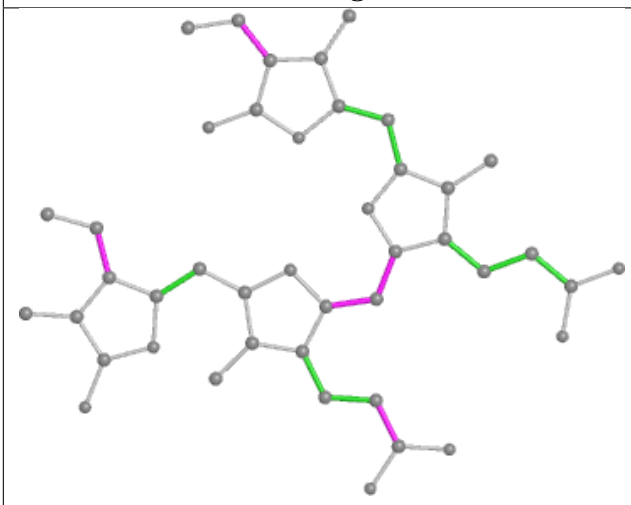

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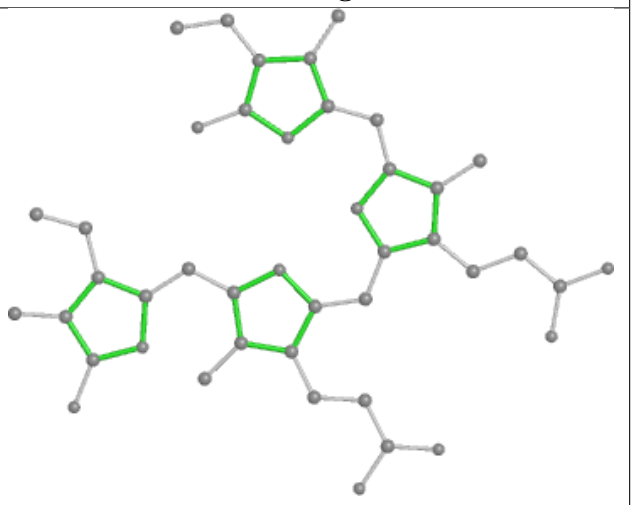

Rings

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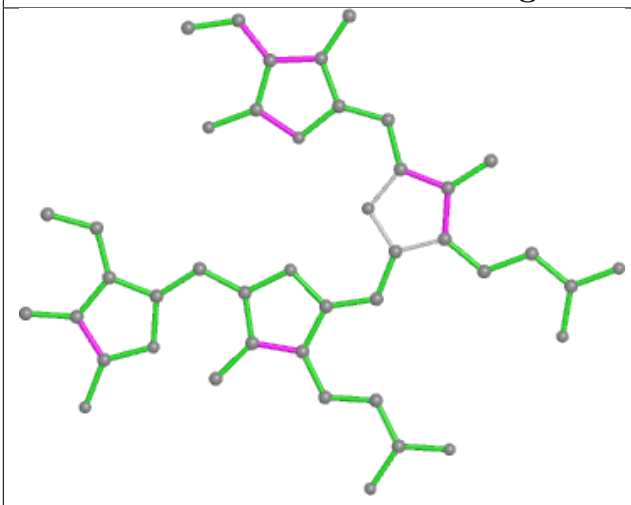

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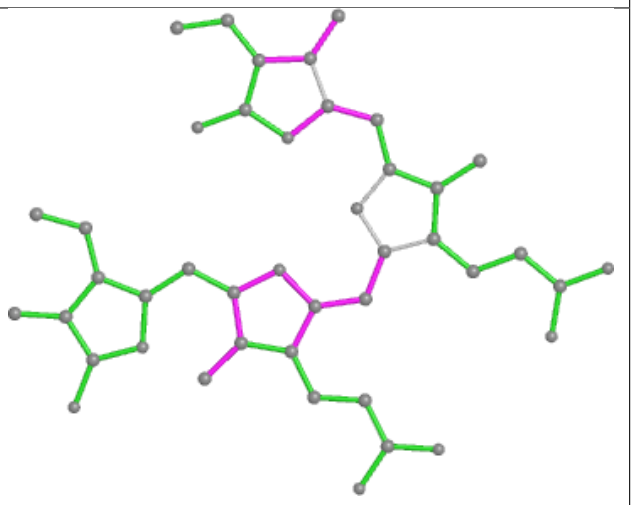

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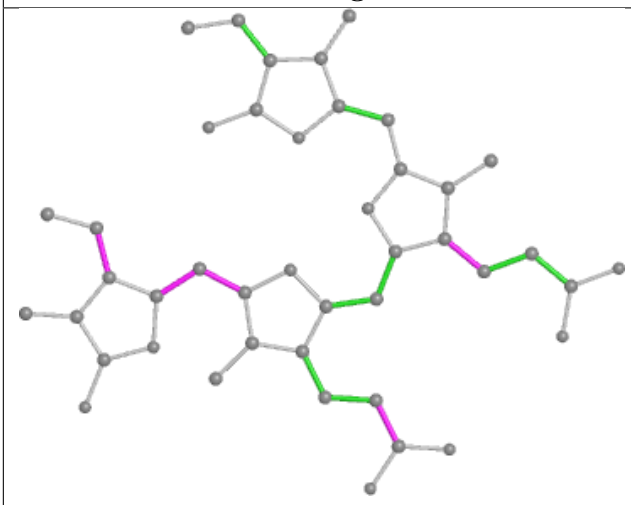

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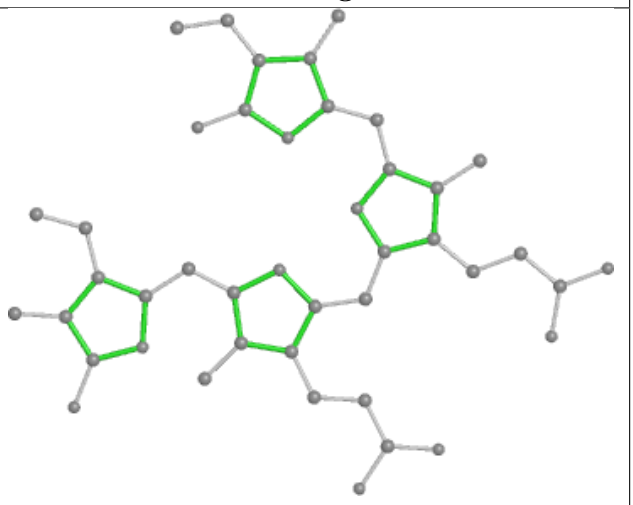
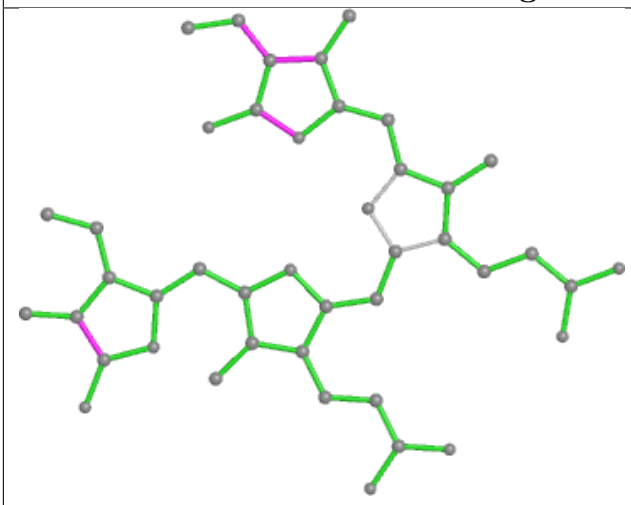


Rings

Ligand PEB k8 203



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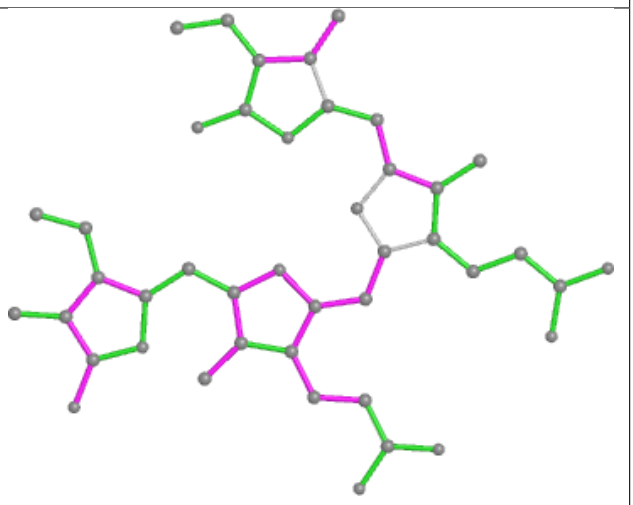
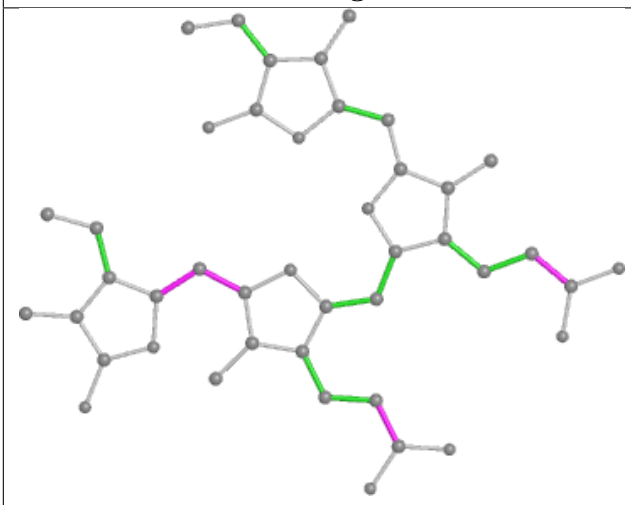
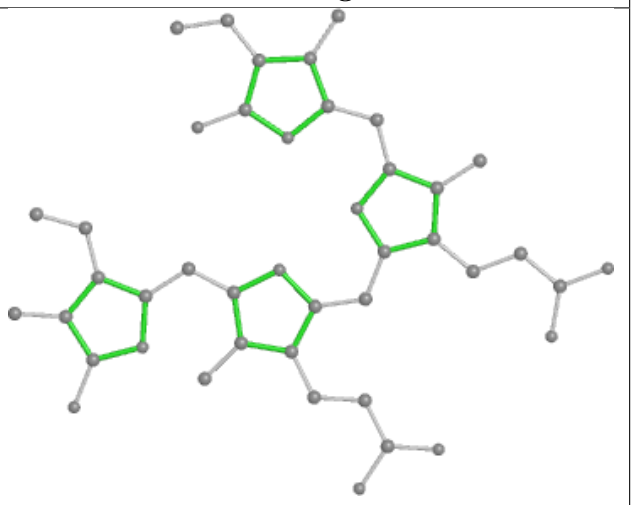


Bond angles

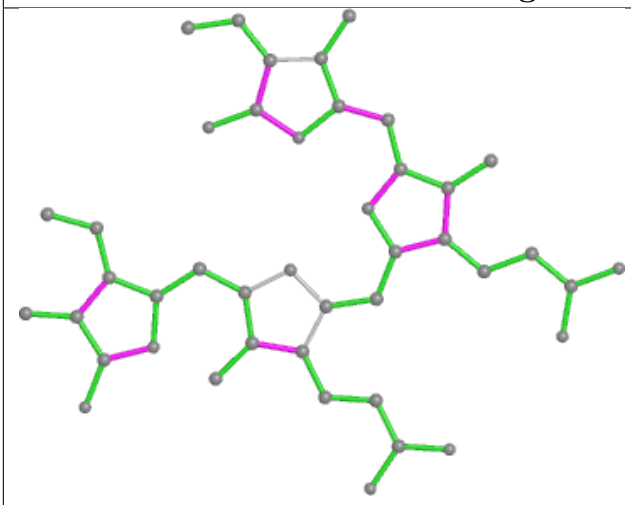


Torsions



Rings

Ligand PUB z6 203



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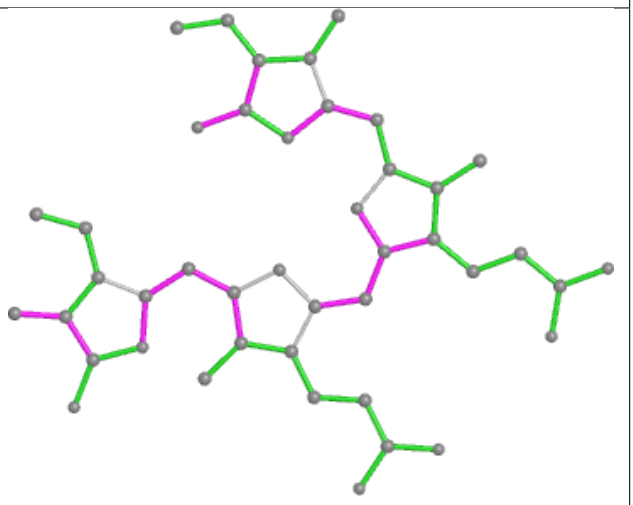

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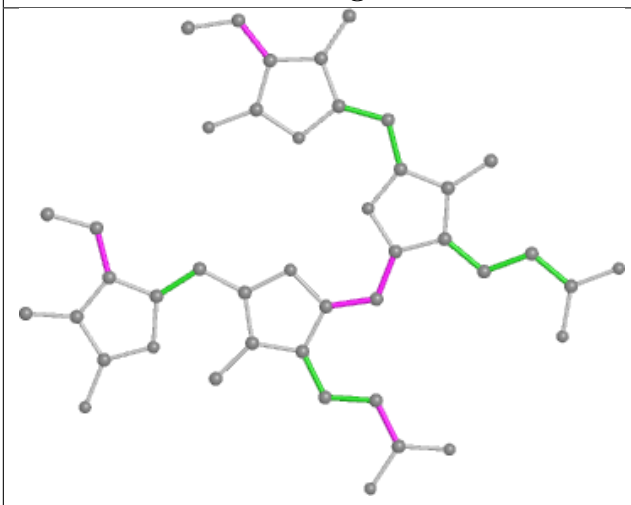

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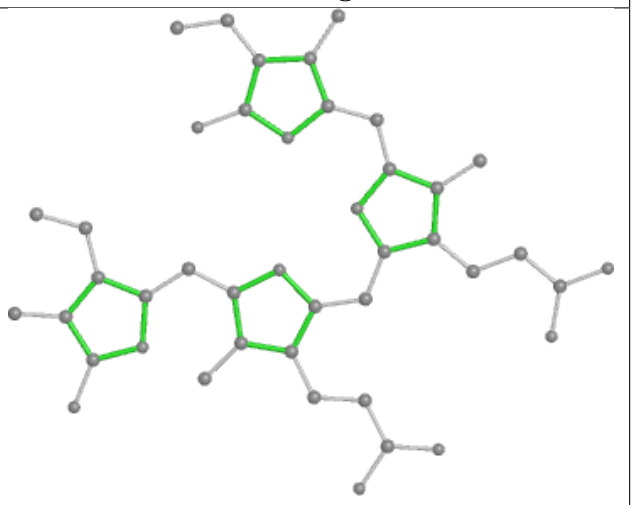
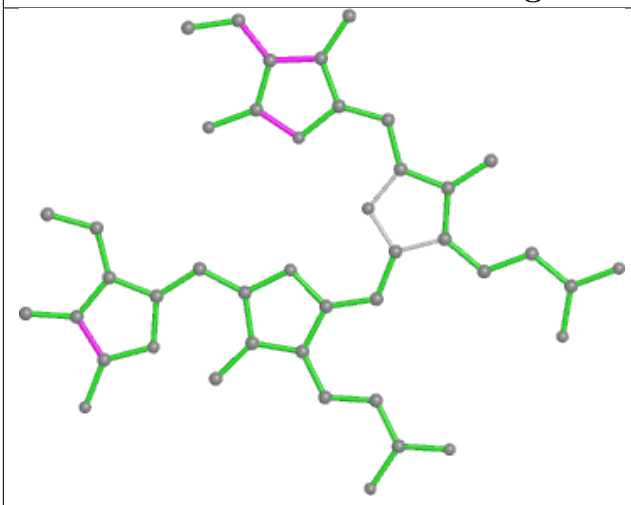


Rings

Ligand PEB fc 201



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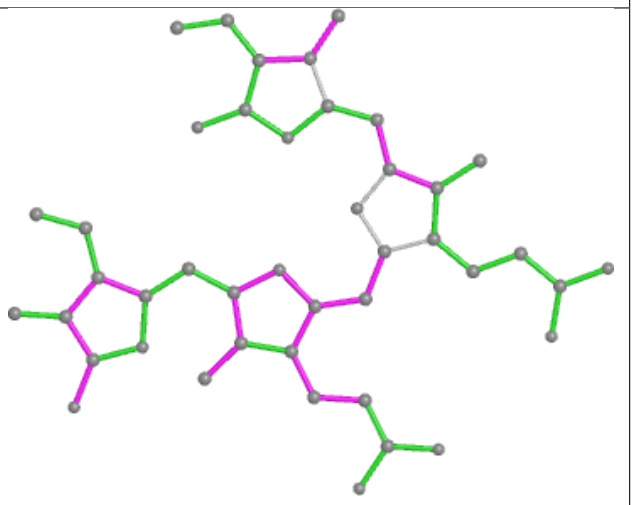

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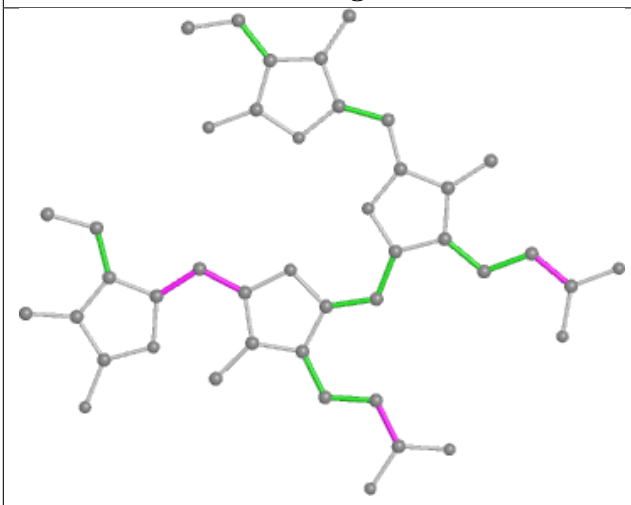

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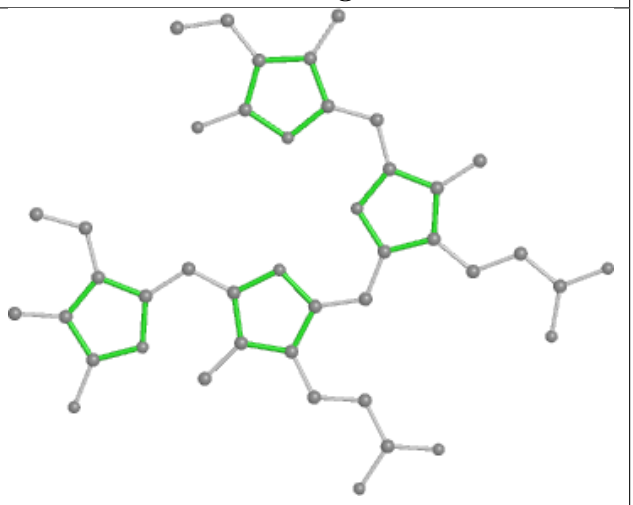
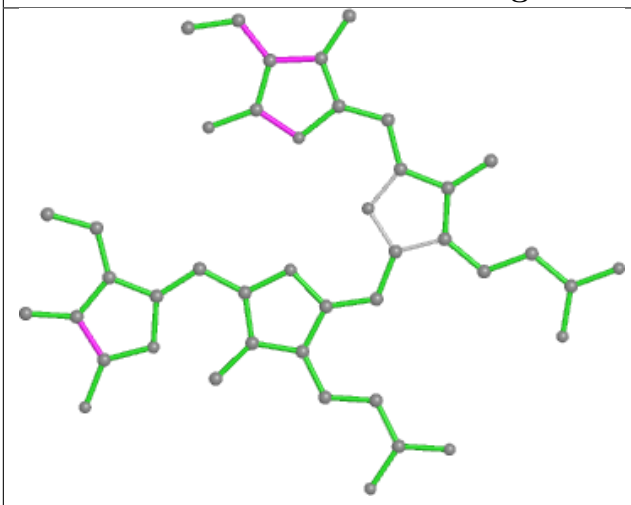


Rings

Ligand PEB eW 201



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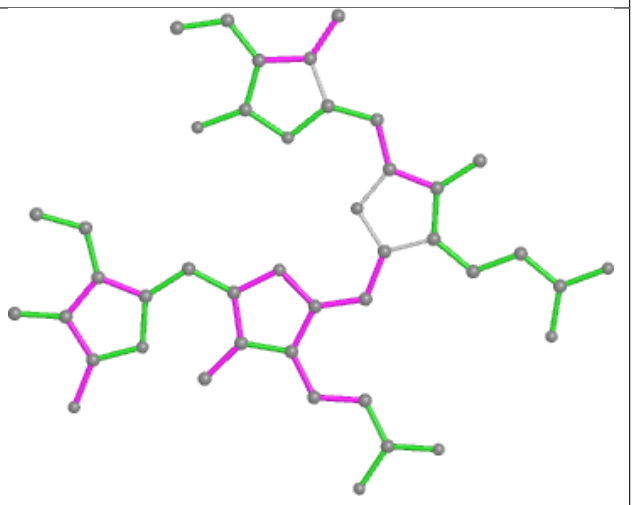

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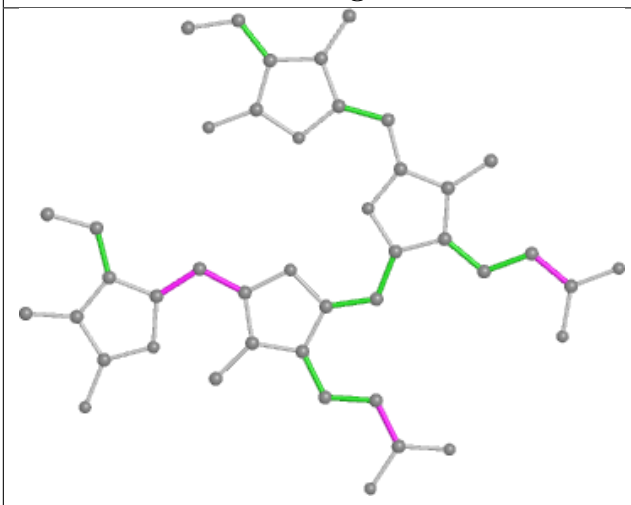

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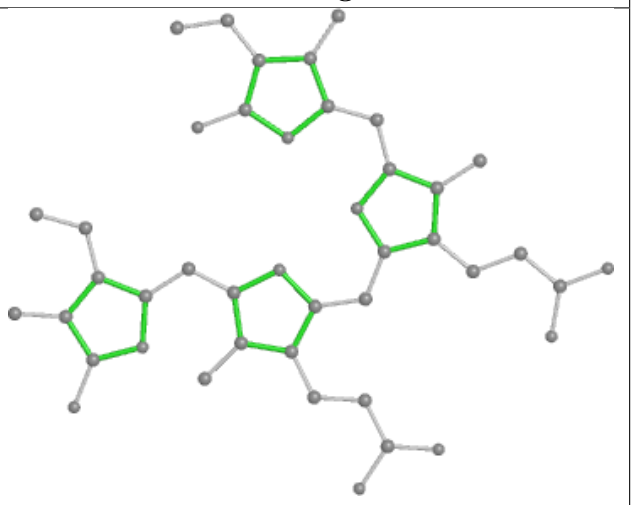

Rings

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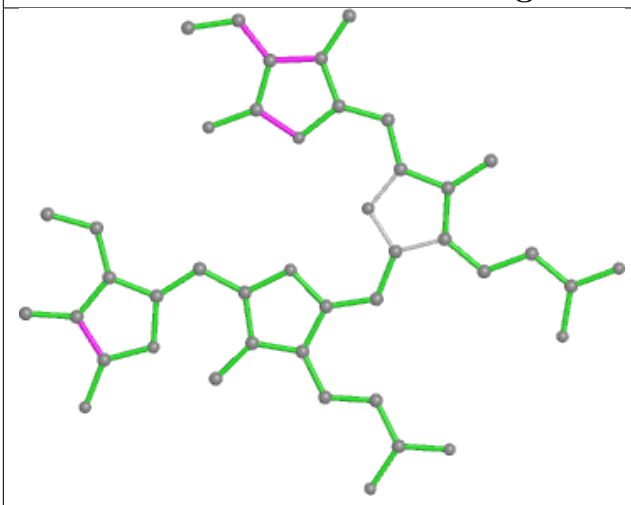

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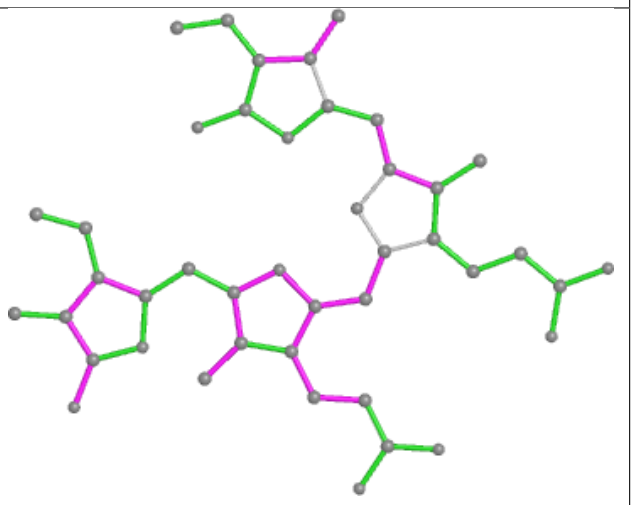

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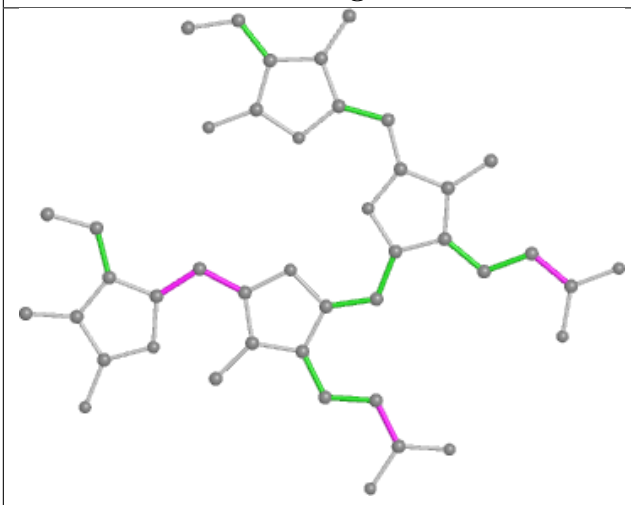

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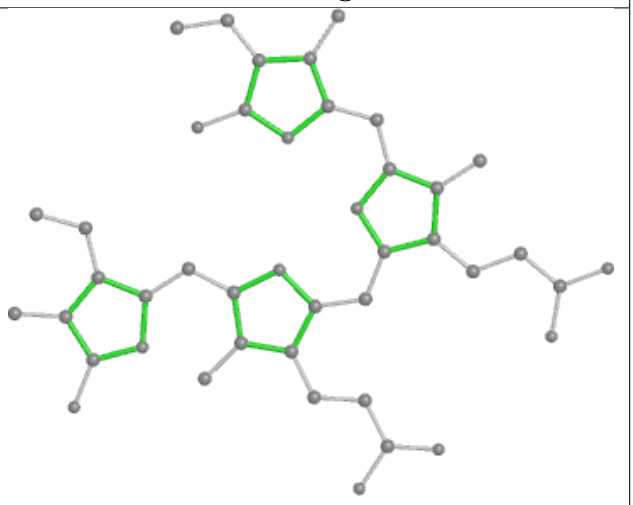
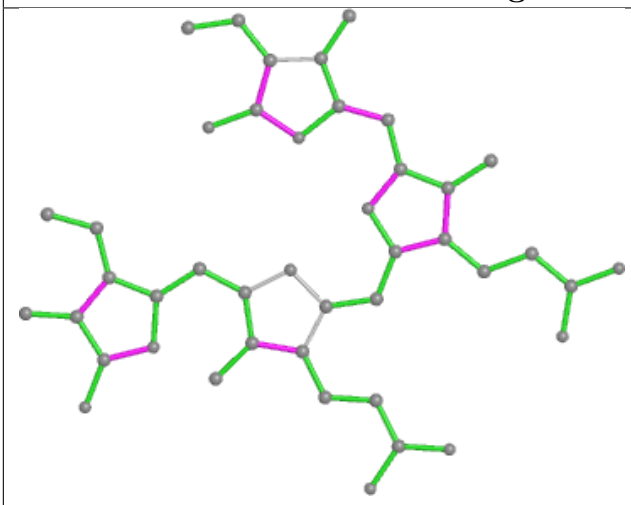


Rings

Ligand PUB iD 1003



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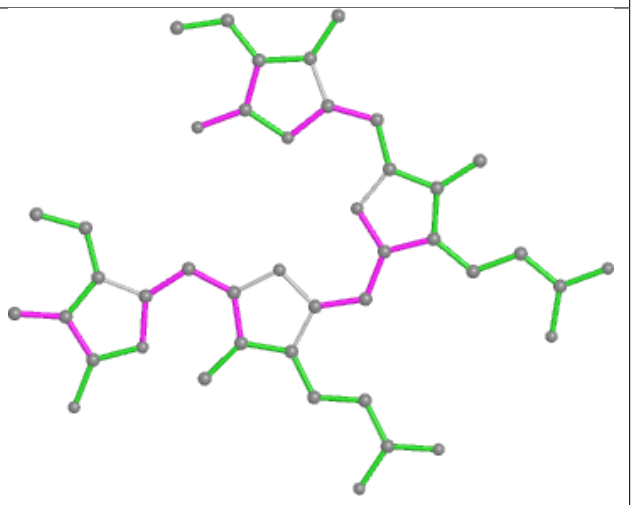

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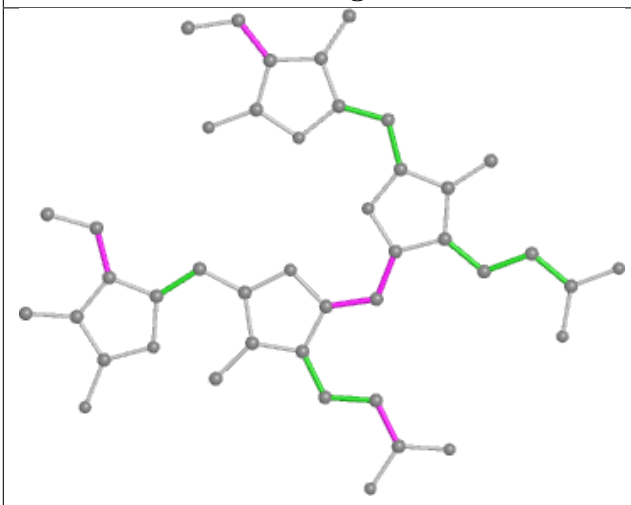

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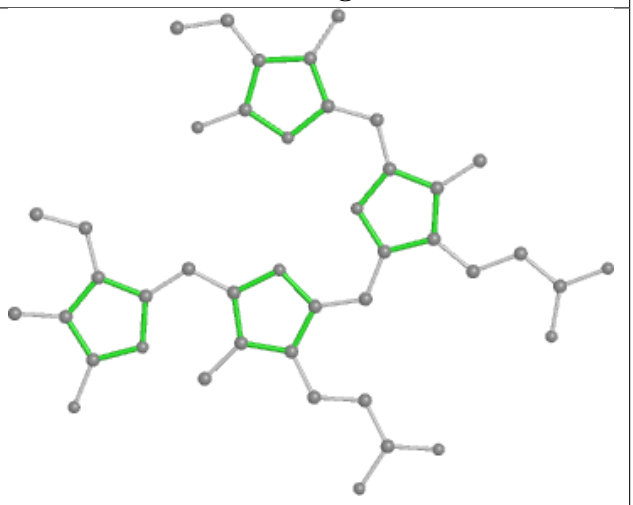

Rings

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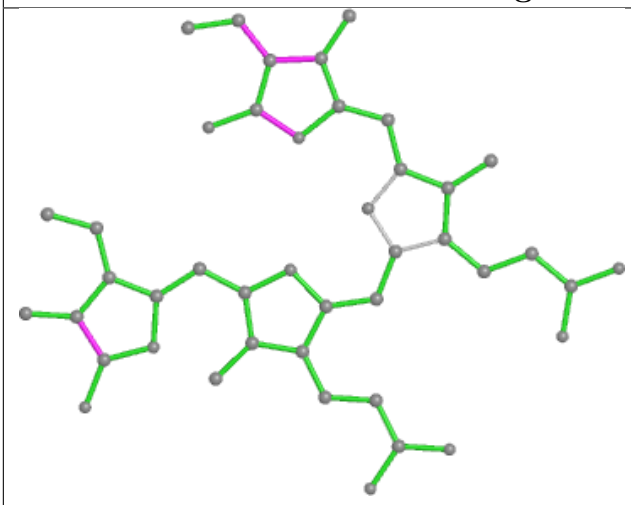

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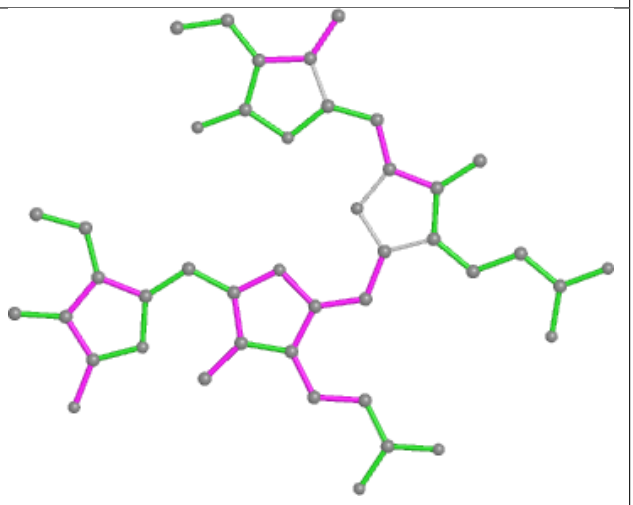

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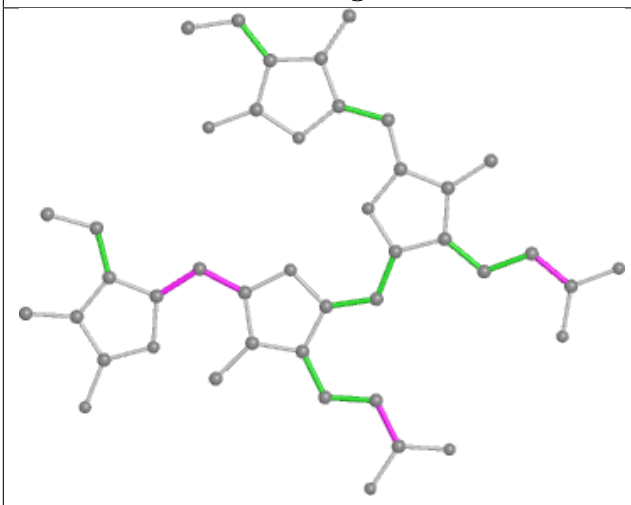

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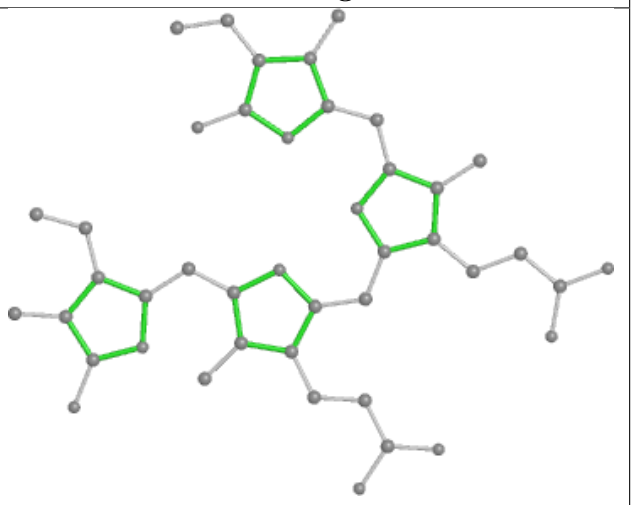

Rings

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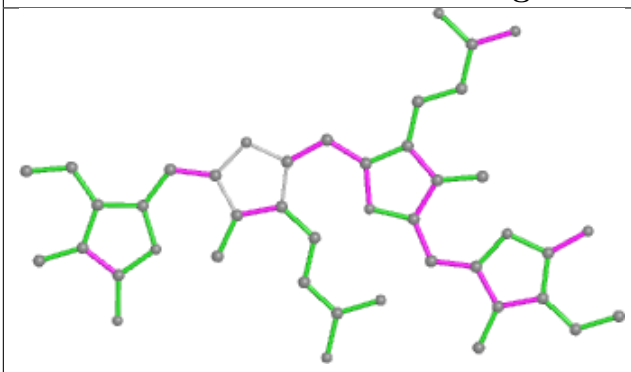

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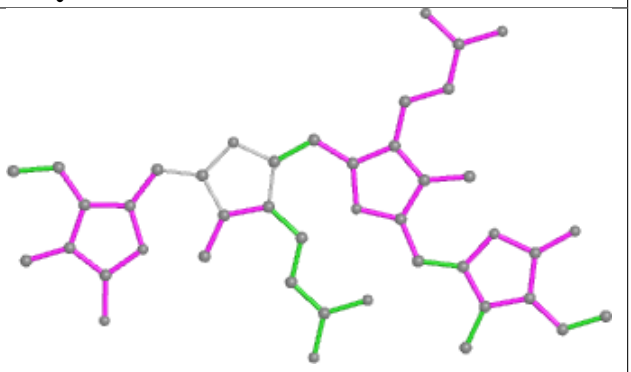

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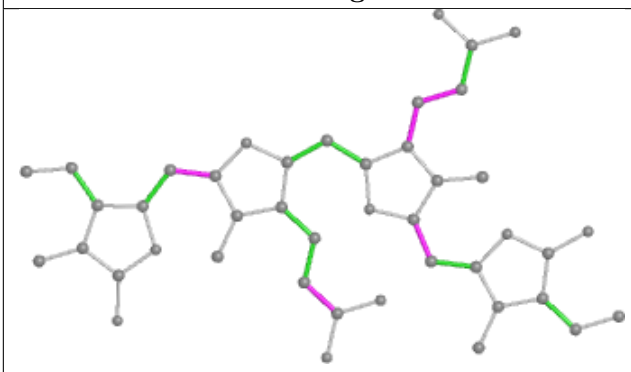

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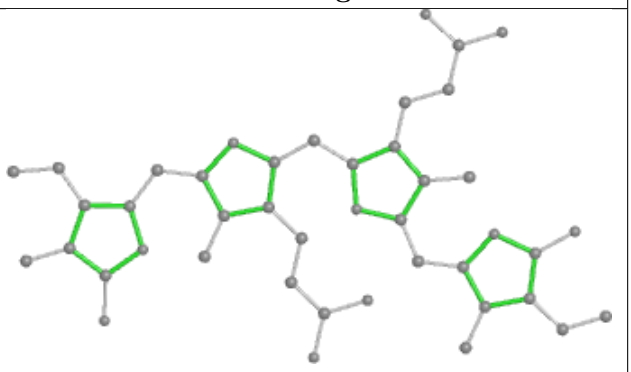
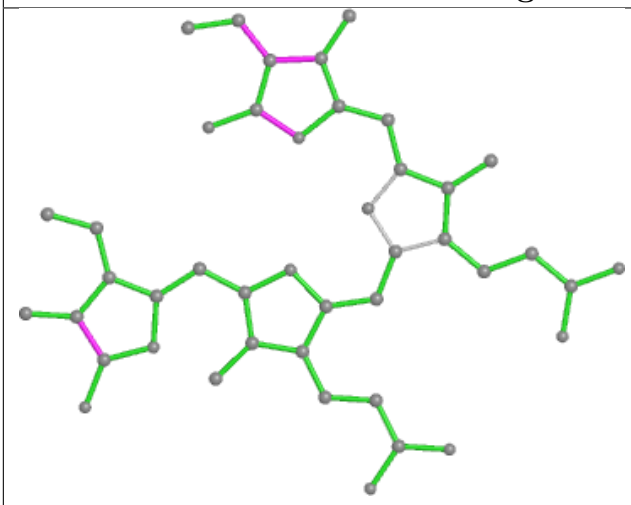


Rings

Ligand PEB E5 201



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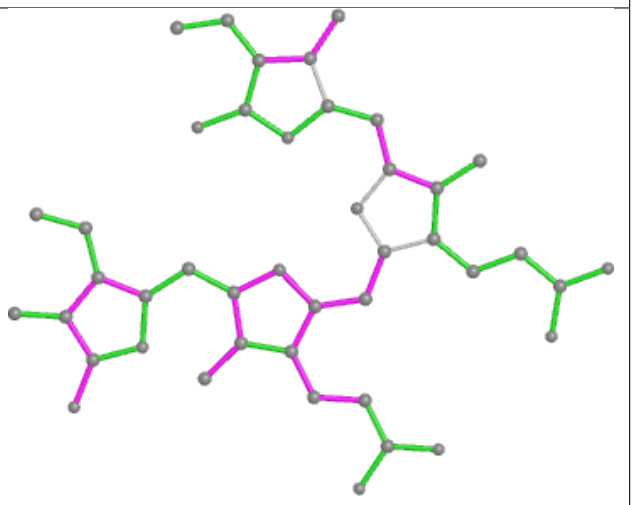
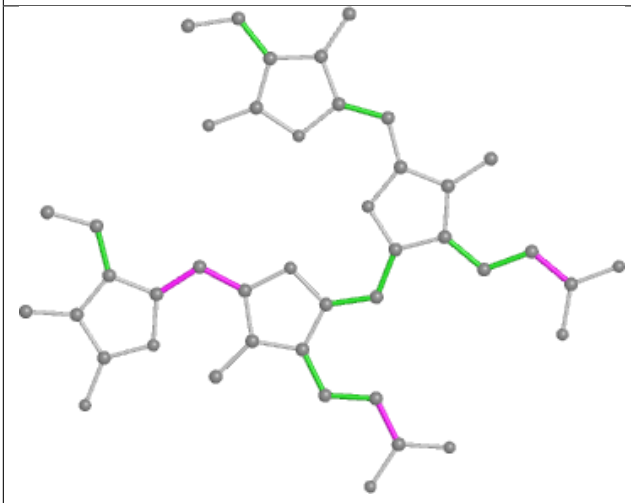


Bond angles



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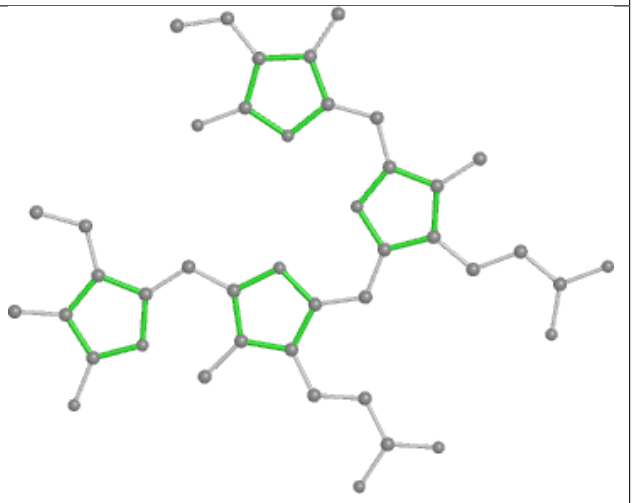

Rings

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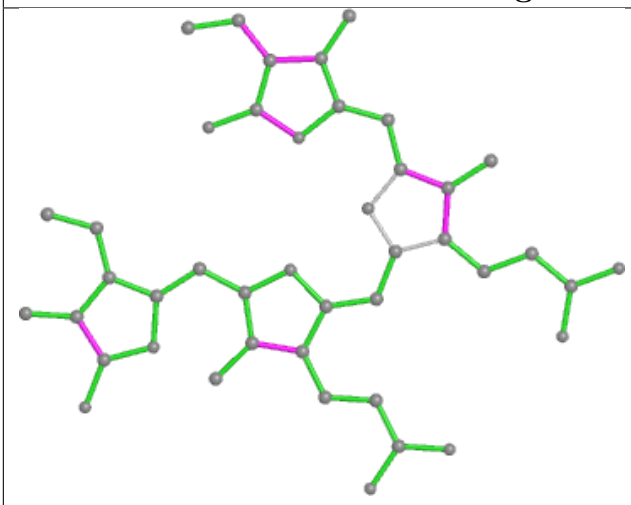

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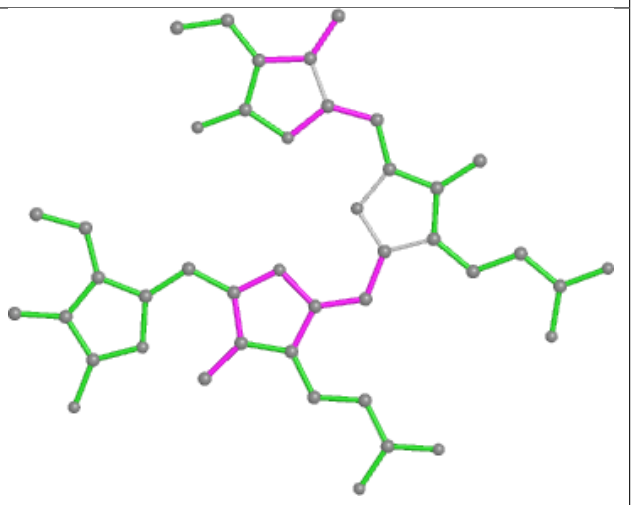

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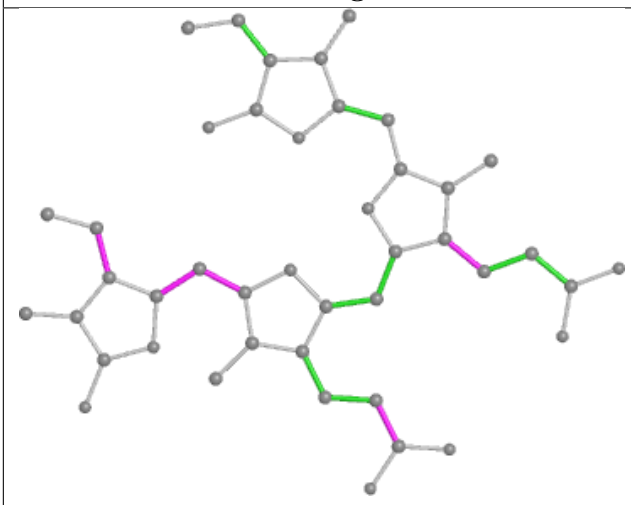

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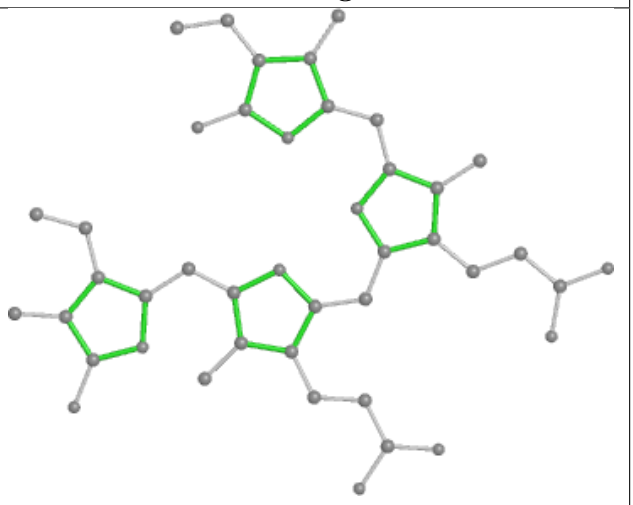
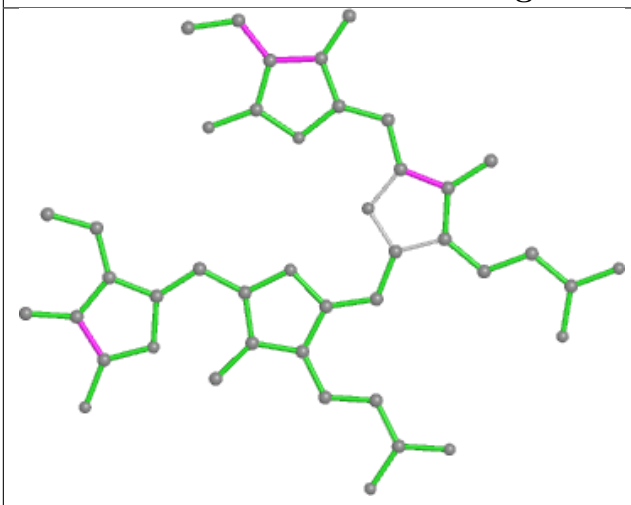


Rings

Ligand PEB A3 202



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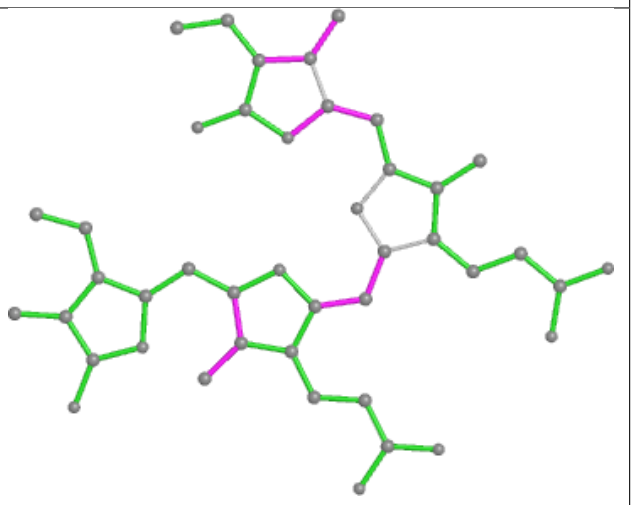

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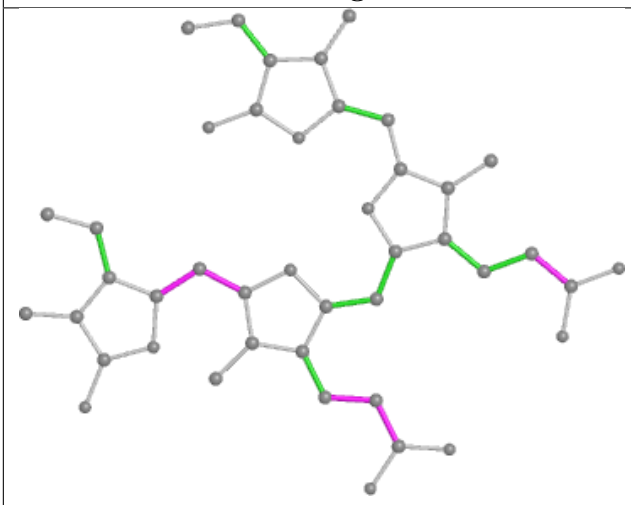

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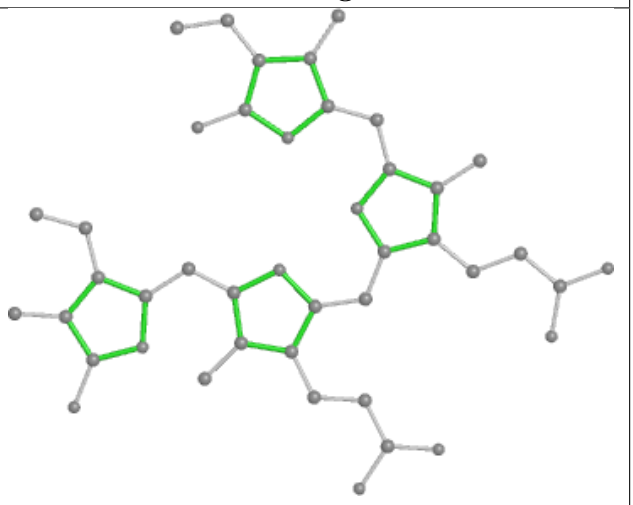
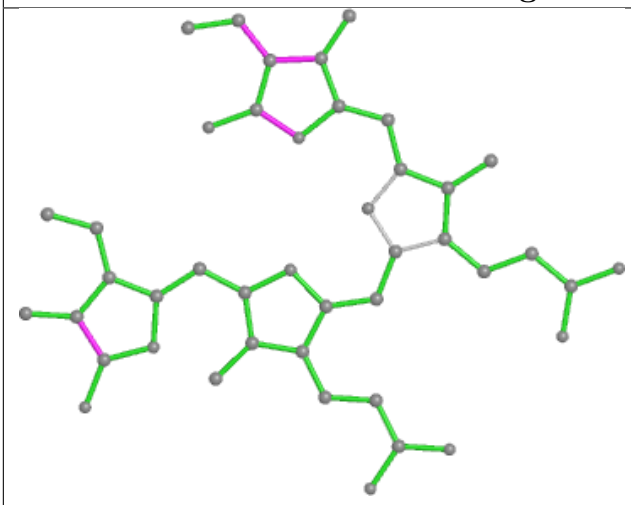


Rings

Ligand PEB v8 201



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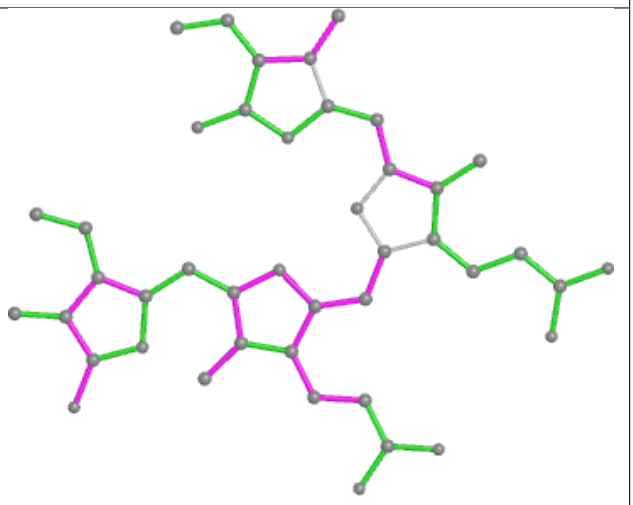

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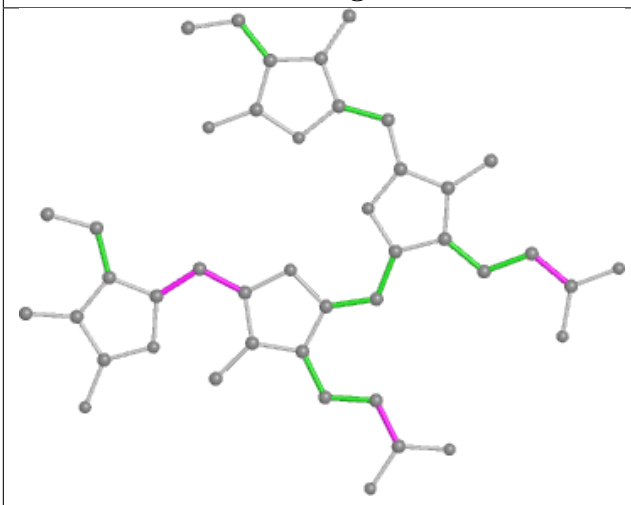

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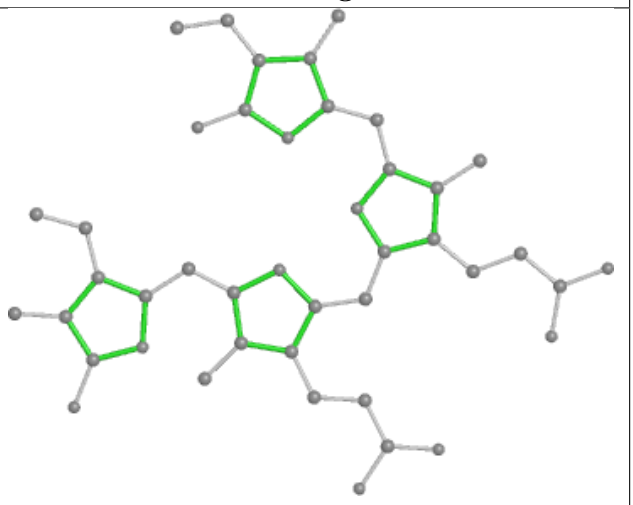

Rings

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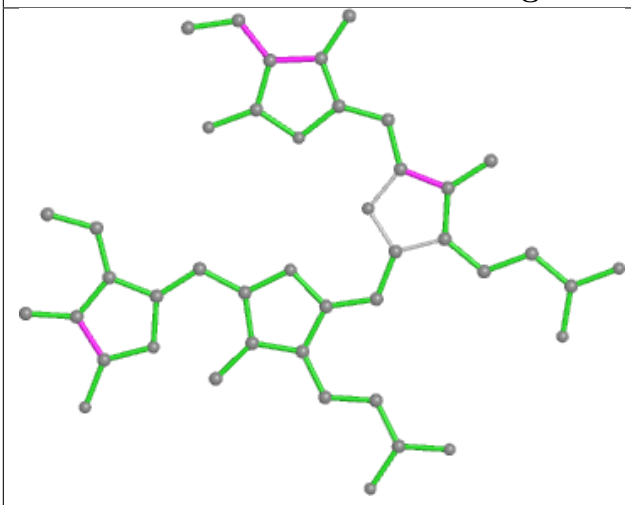

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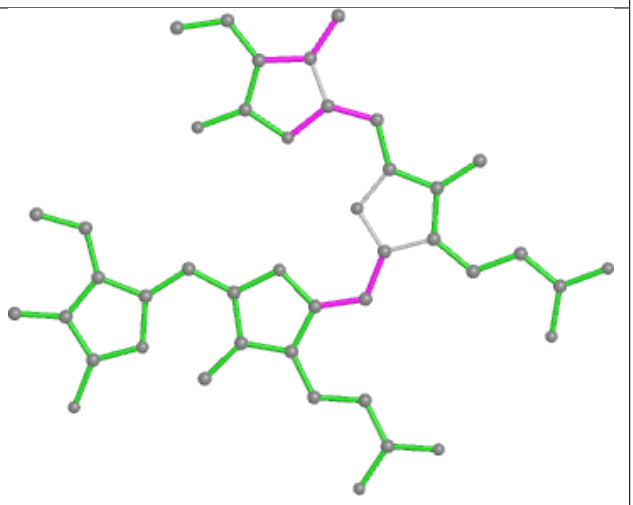

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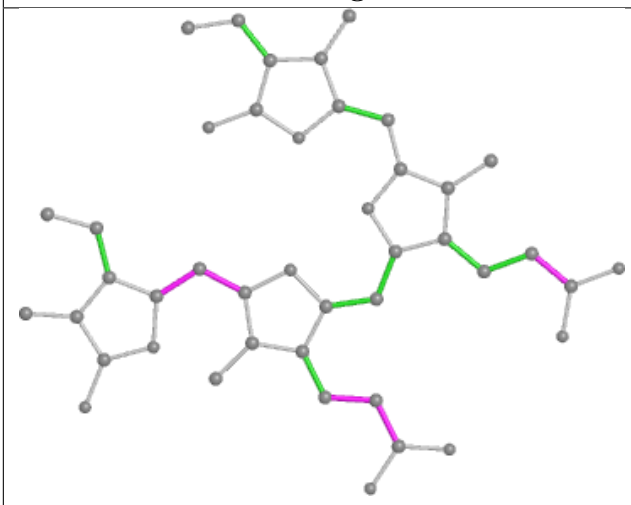

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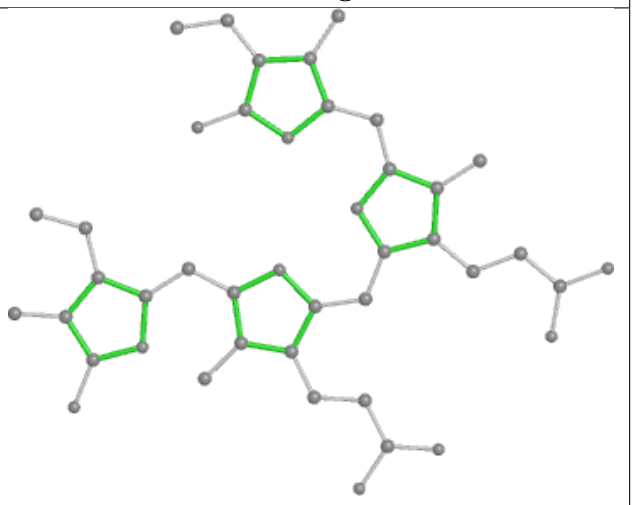

Rings

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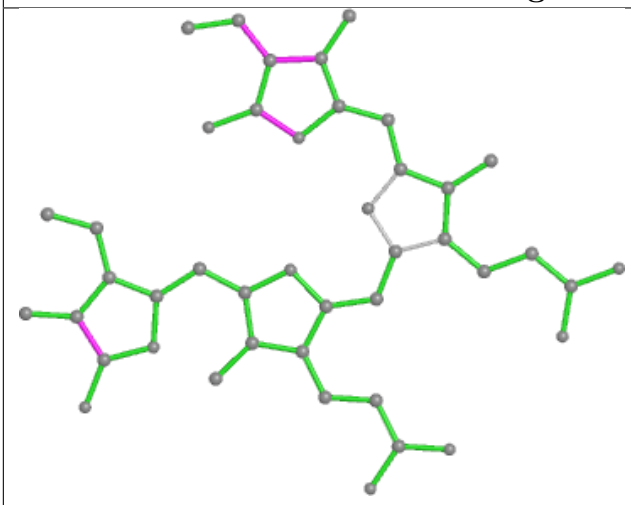

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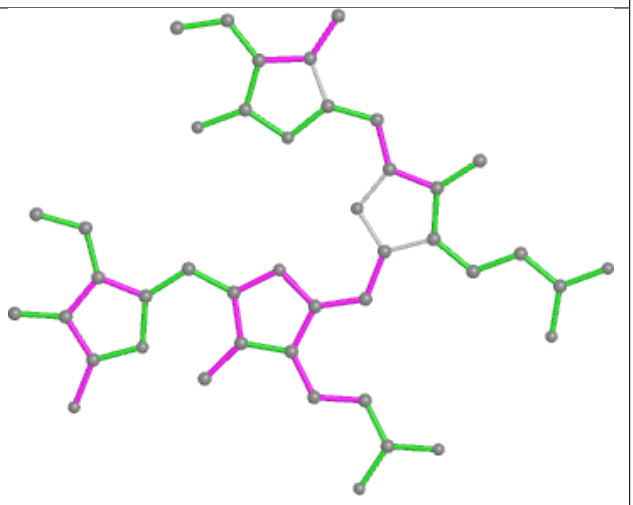

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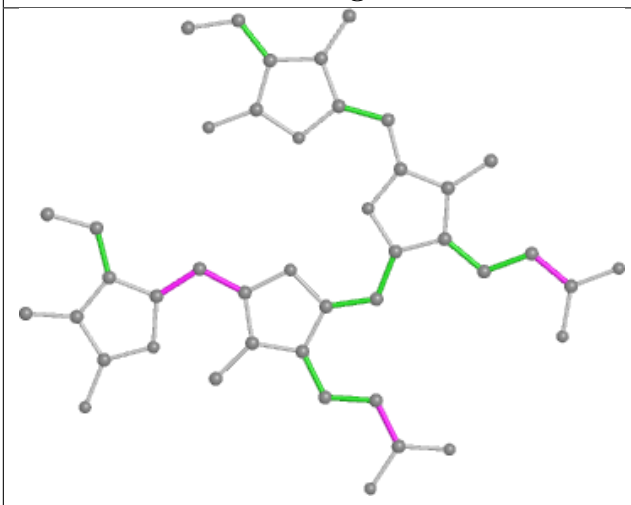
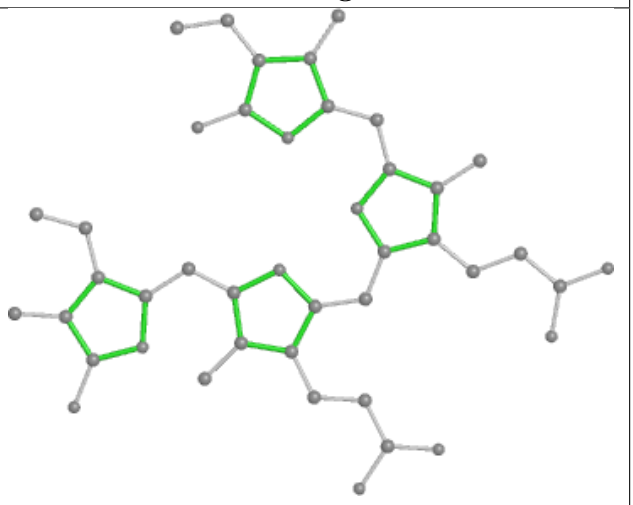
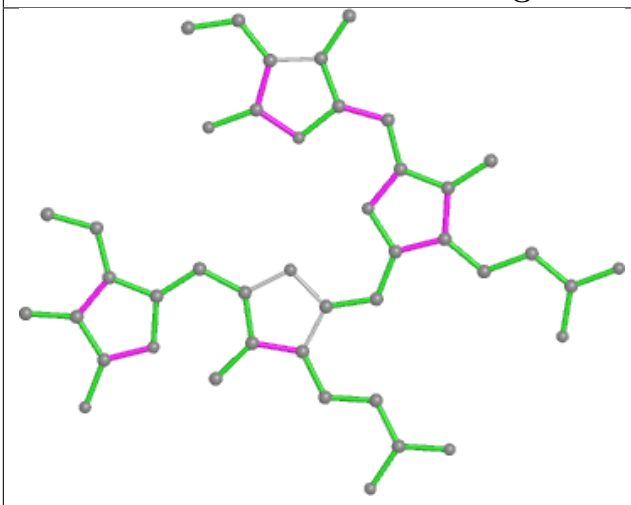


Torsions



Rings

Ligand PUB aY 405



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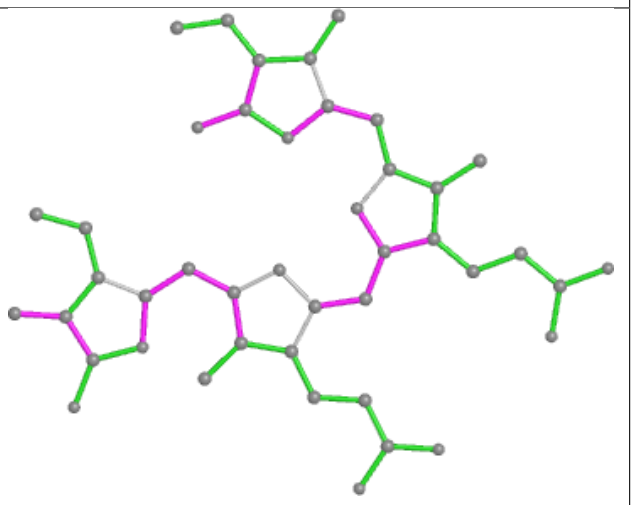
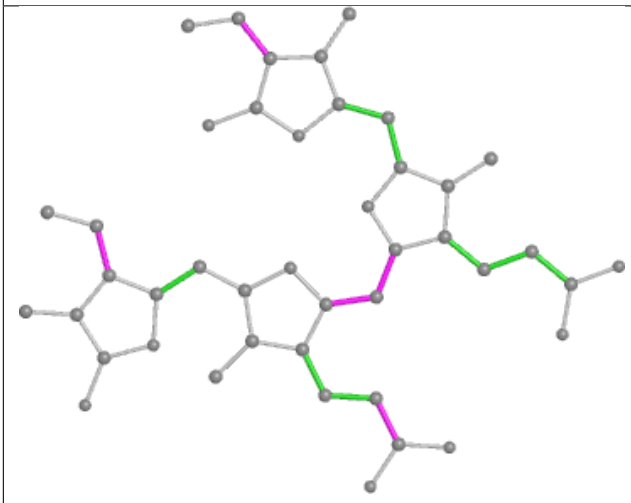


Bond angles



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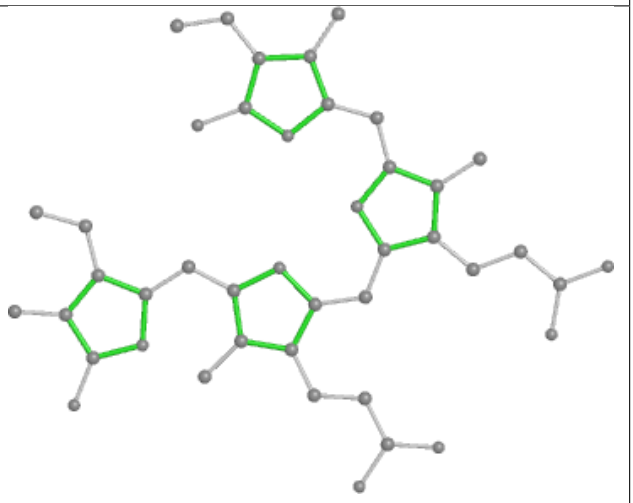
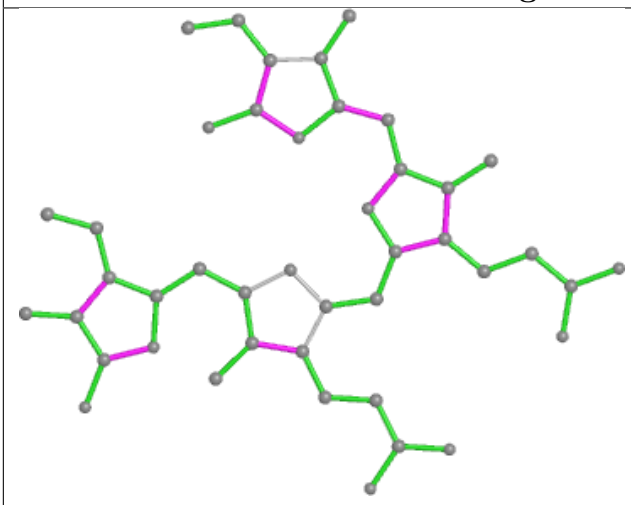


Rings

Ligand PUB r5 203



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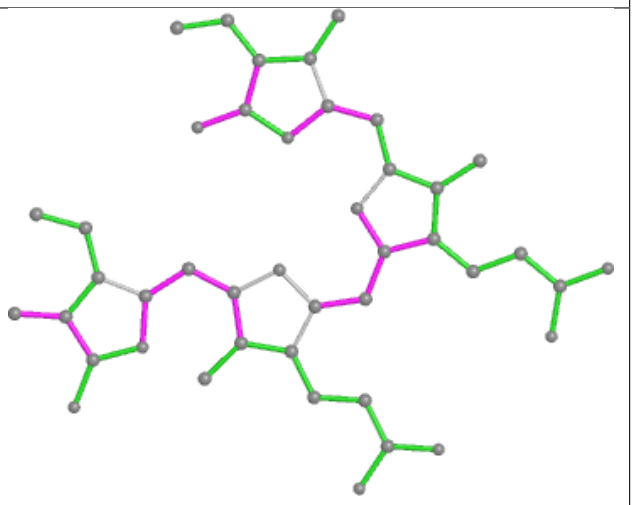

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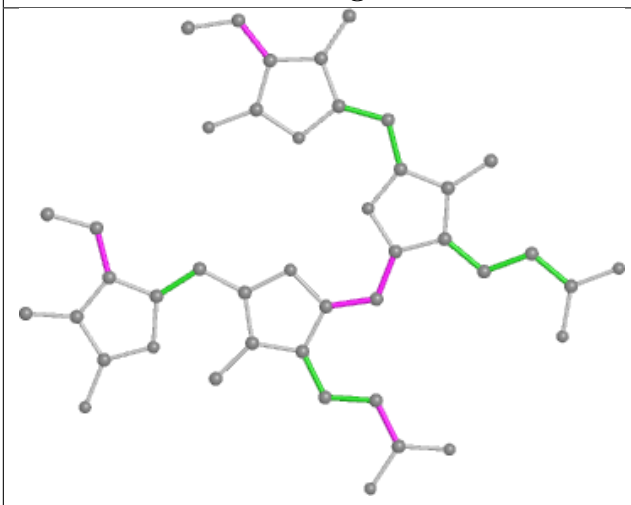

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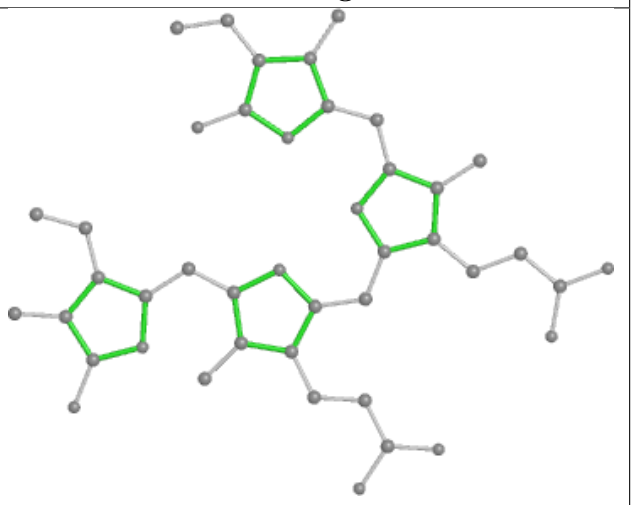
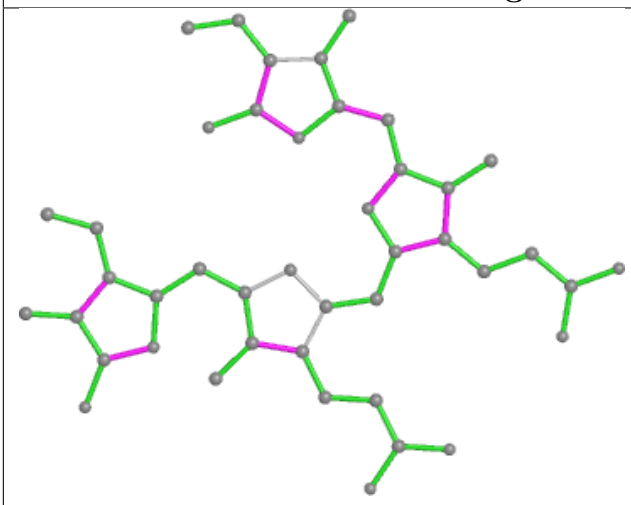


Rings

Ligand PUB kV 1003



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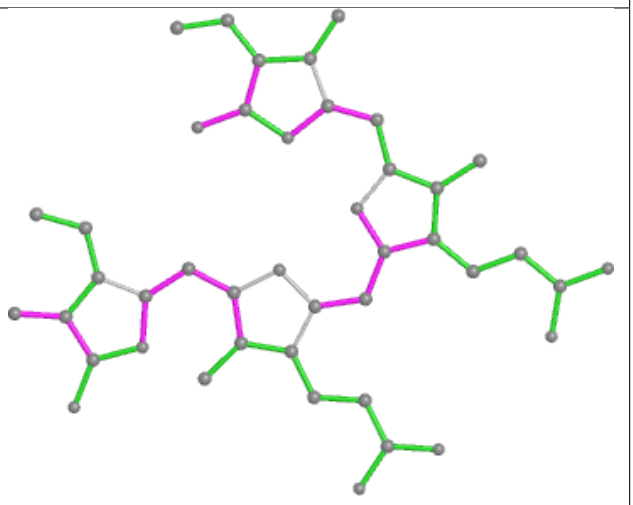

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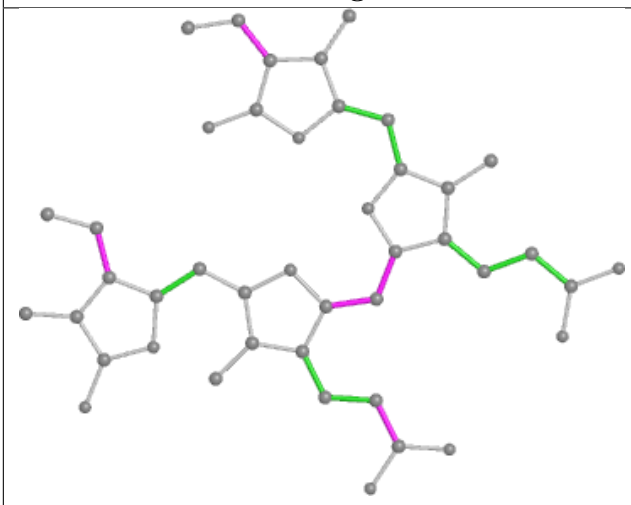

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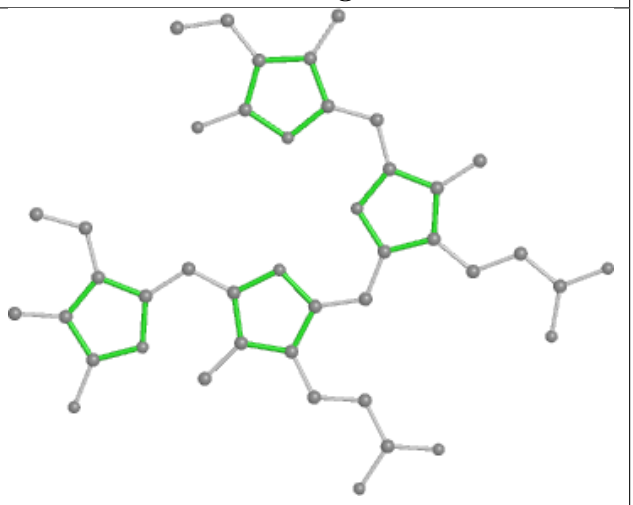
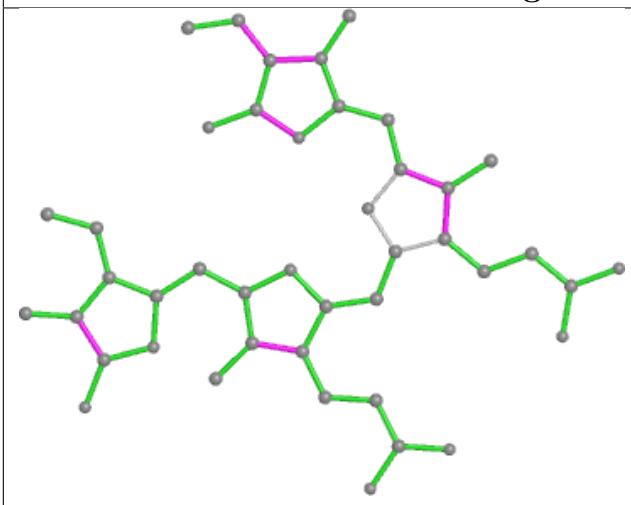


Rings

Ligand PEB j4 202



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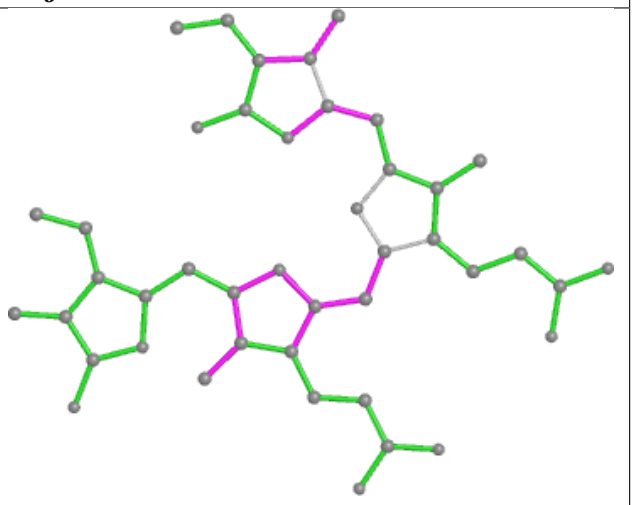

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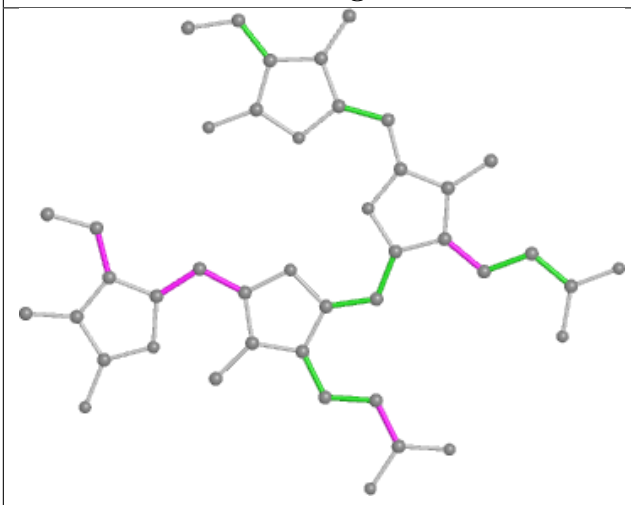

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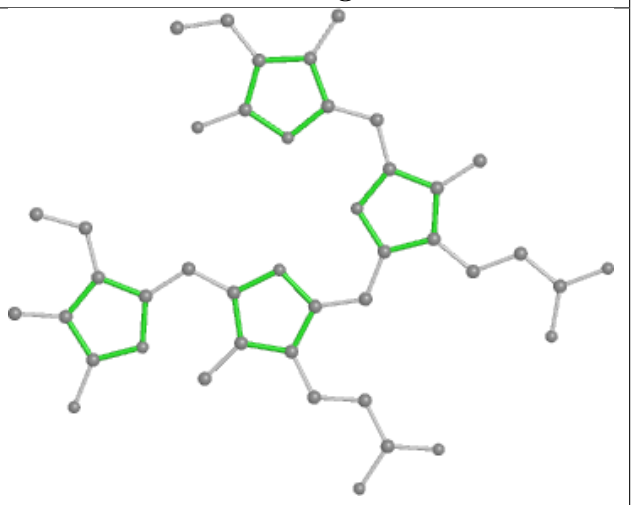

Rings

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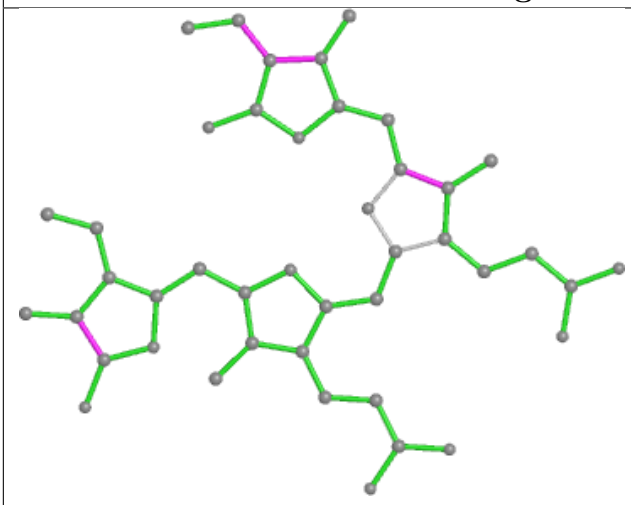

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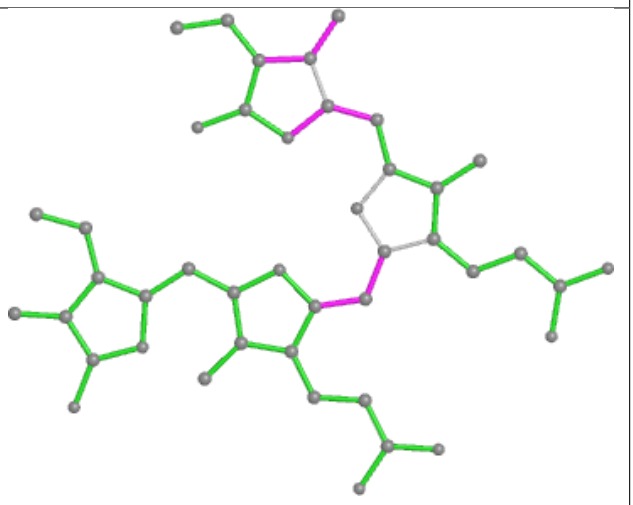

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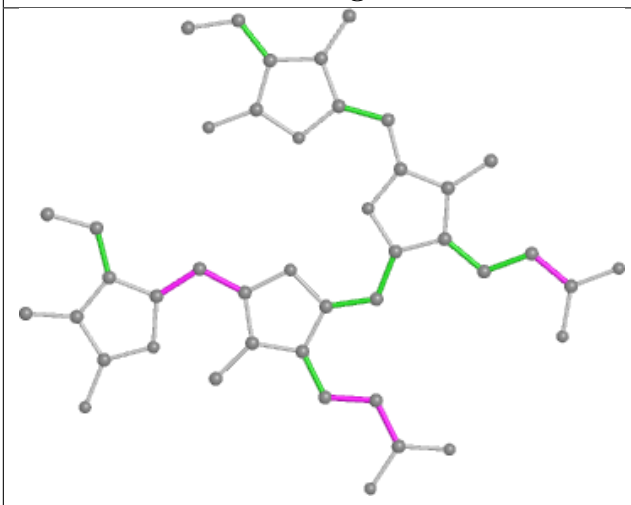

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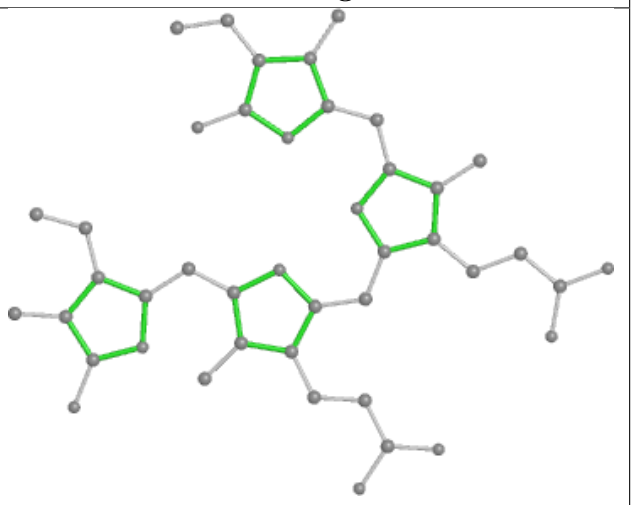

Rings

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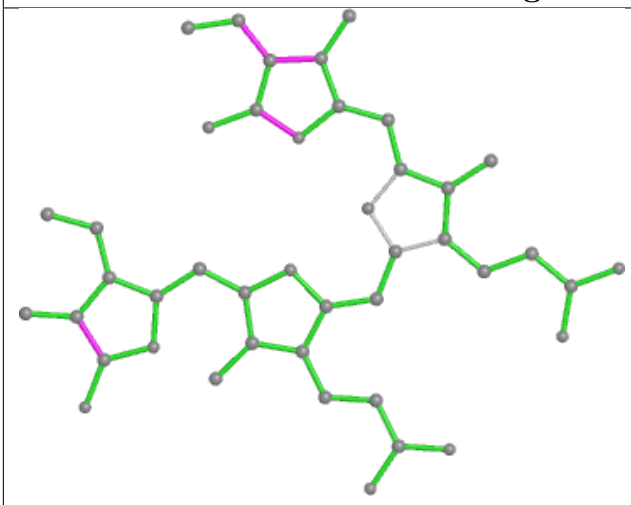

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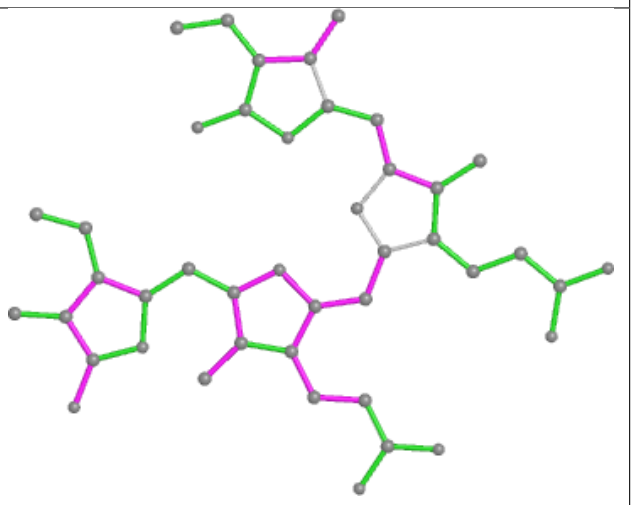

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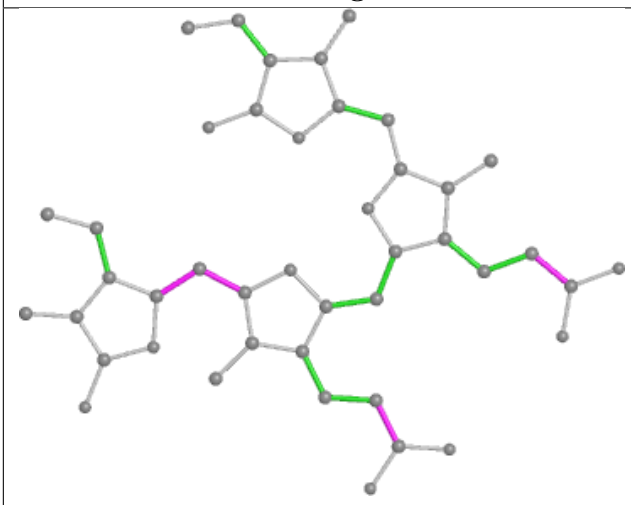

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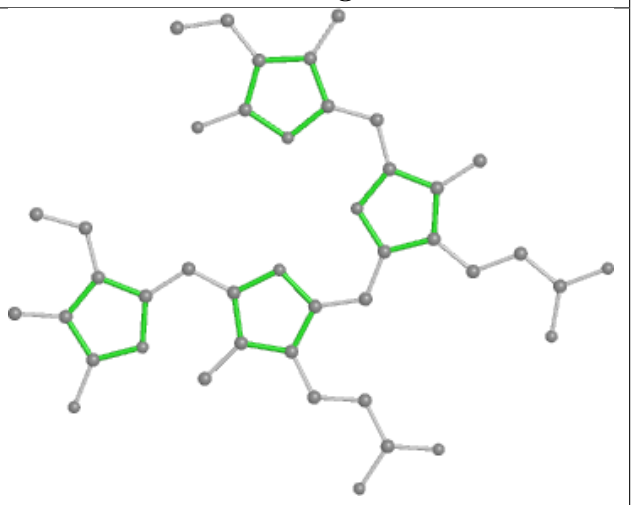
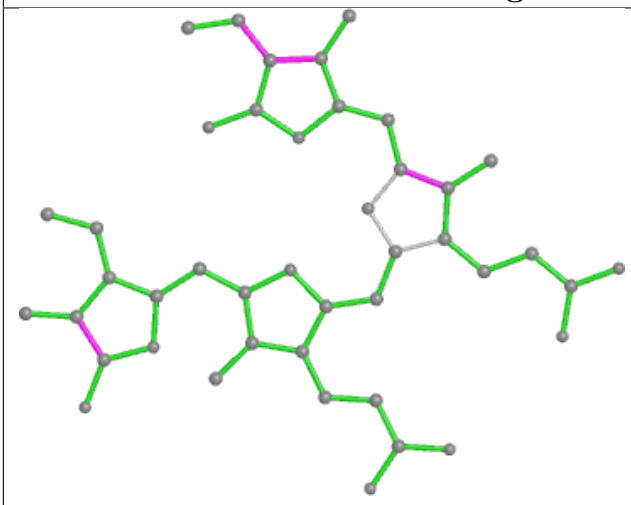


Rings

Ligand PEB O3 1002



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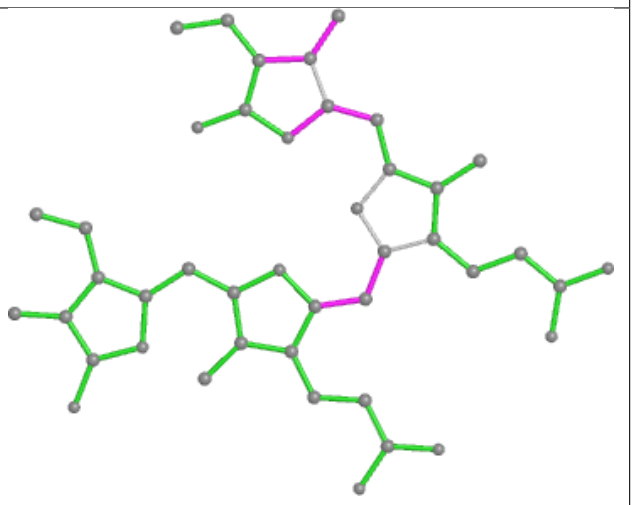

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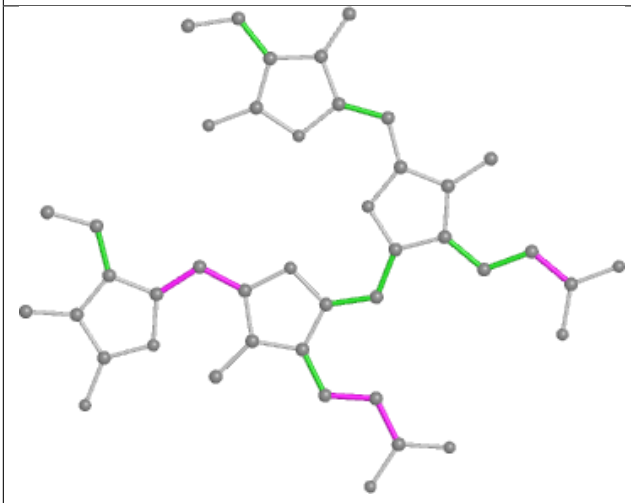

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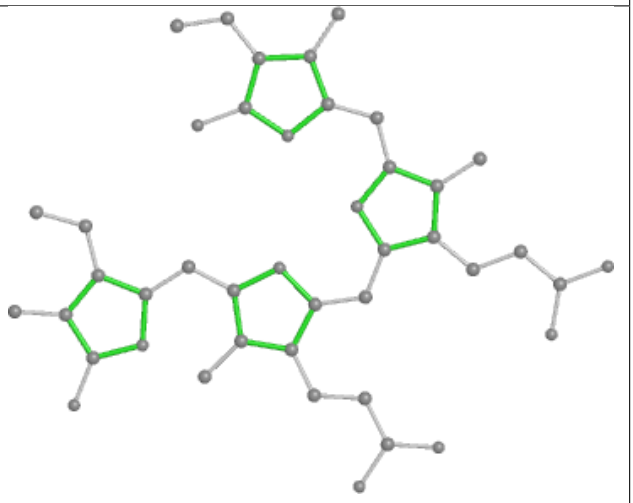
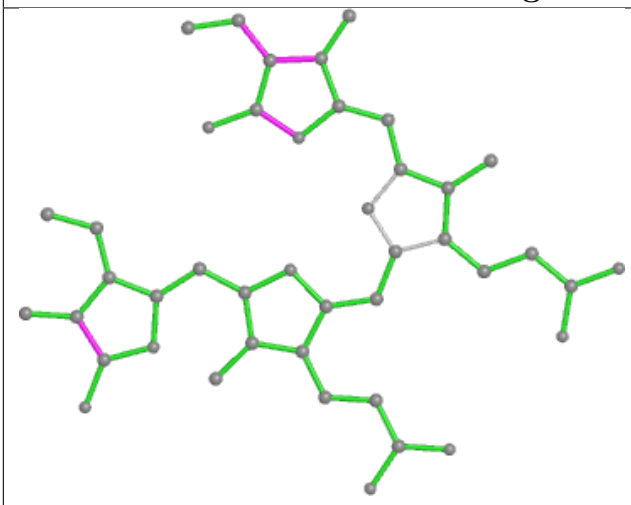


Rings

Ligand PEB ln 201



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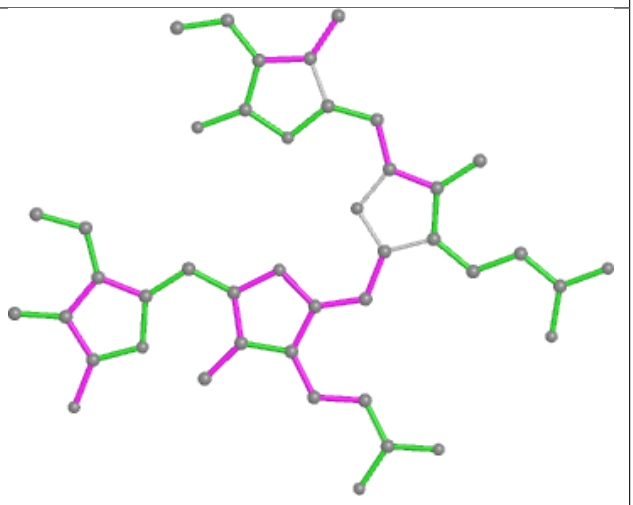

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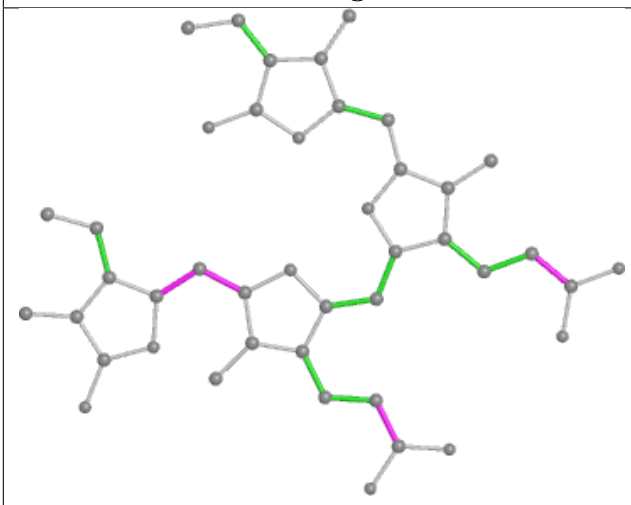

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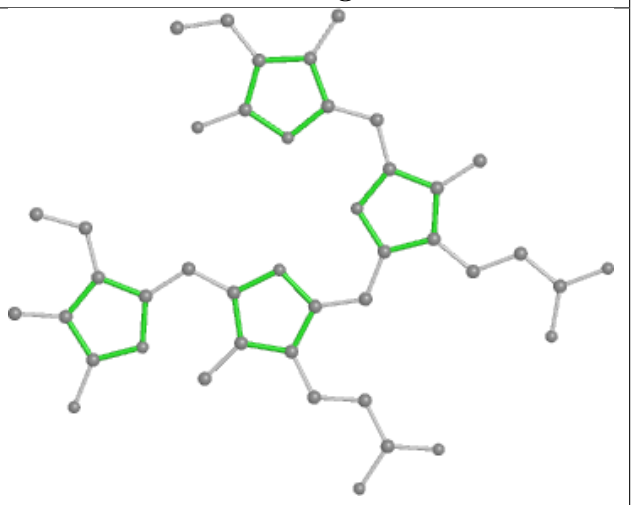
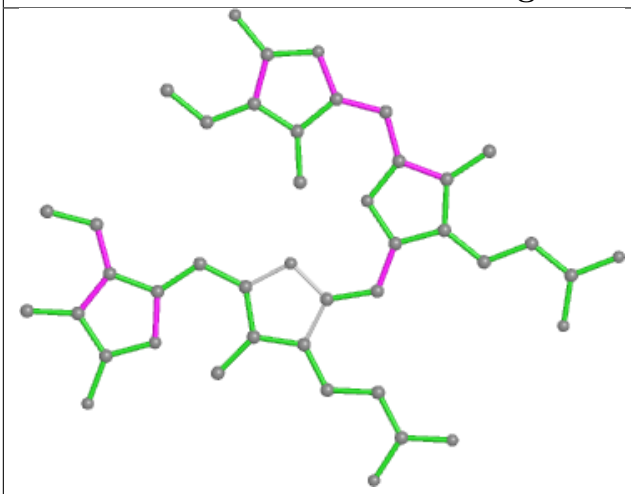


Rings

Ligand PVN e9 304



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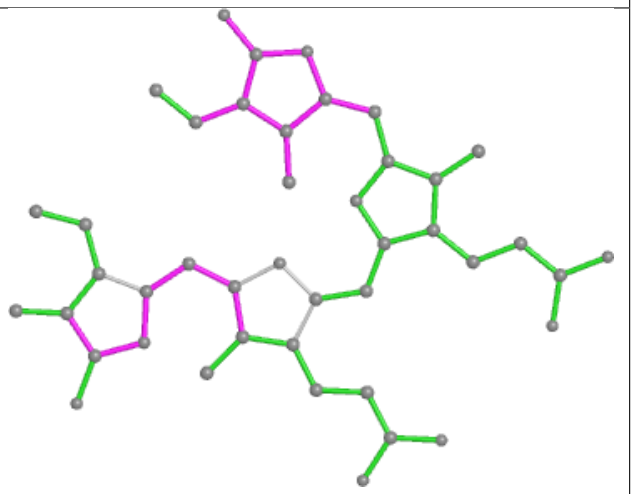

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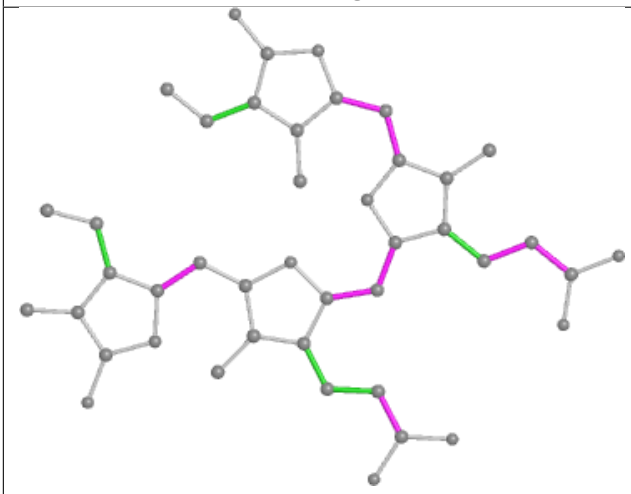

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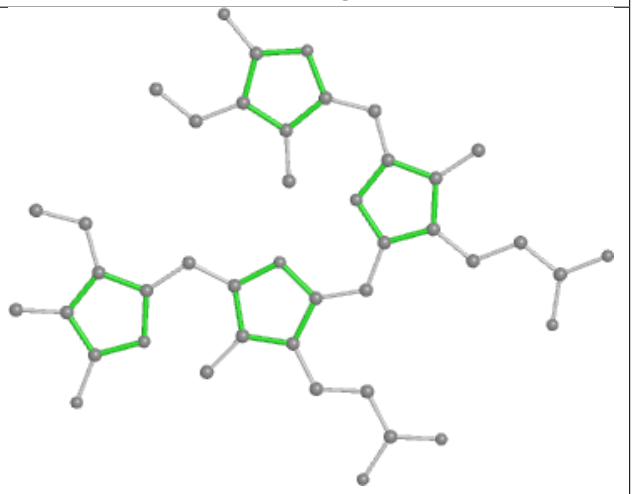
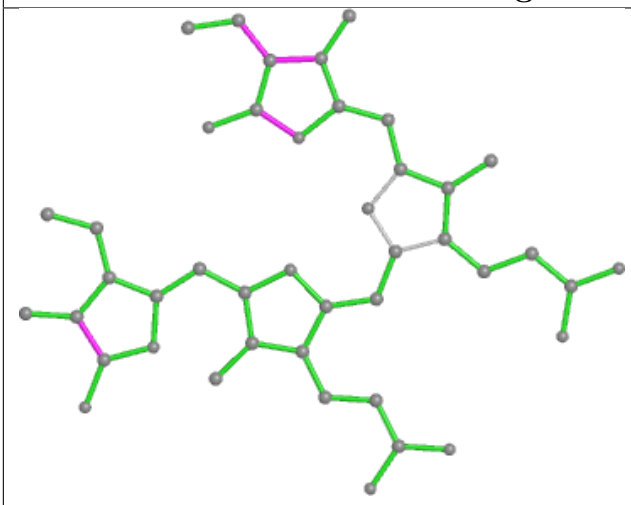


Rings

Ligand PEB X2 201



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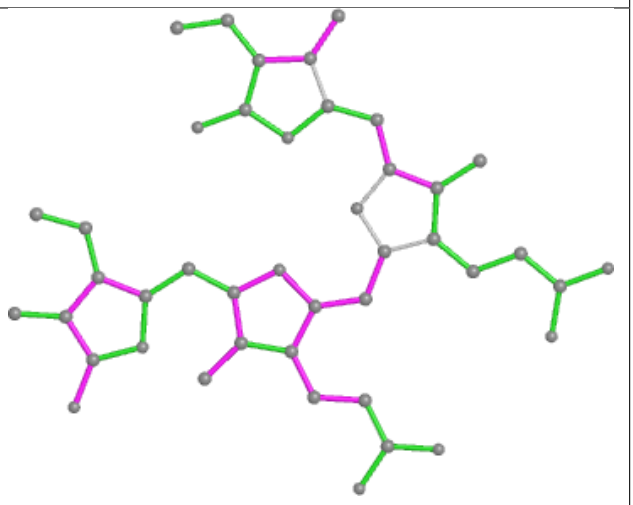

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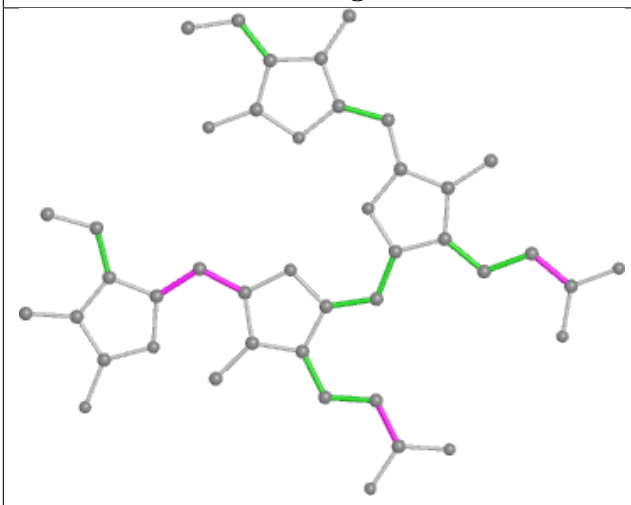

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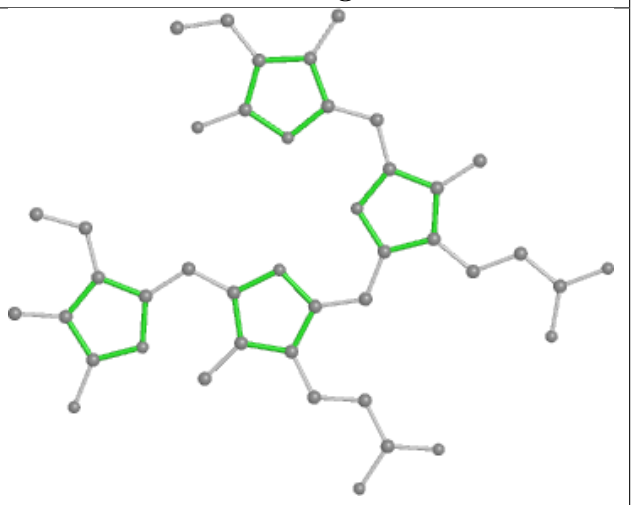
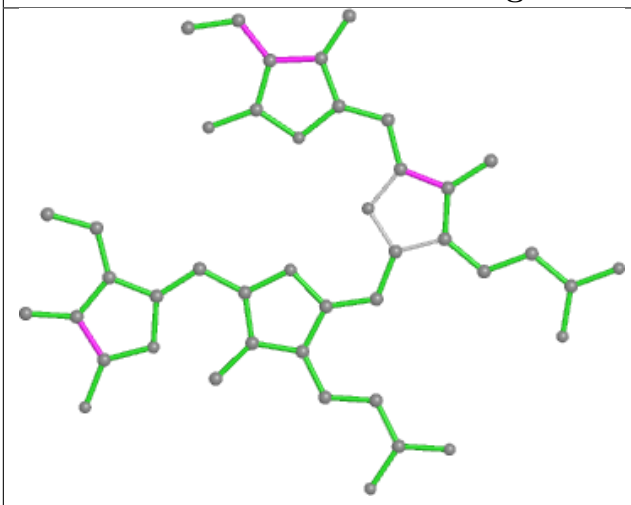


Rings

Ligand PEB Y7 1002



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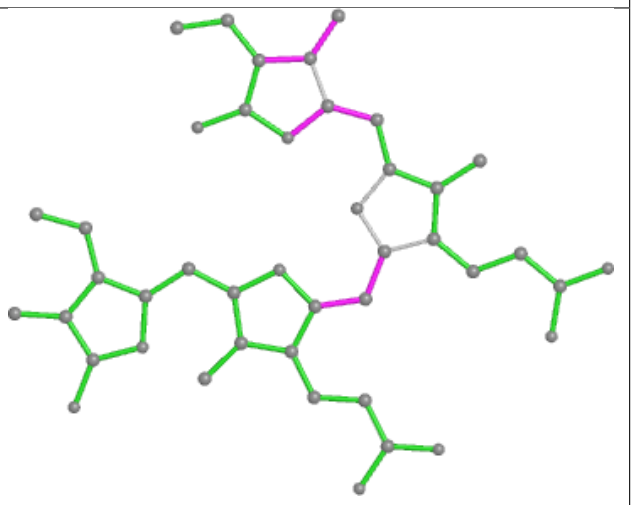

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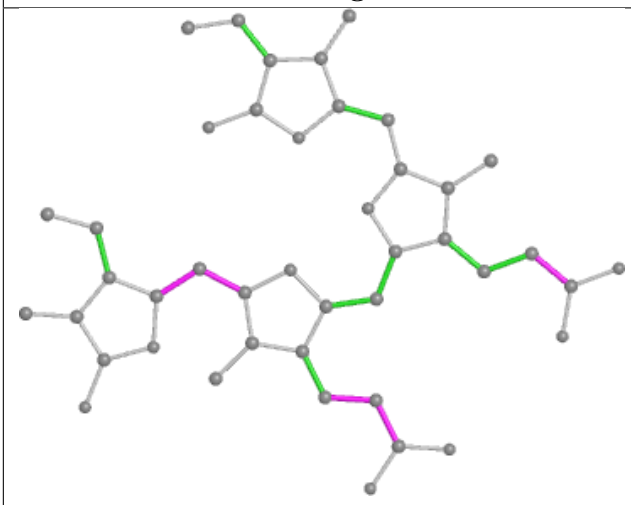

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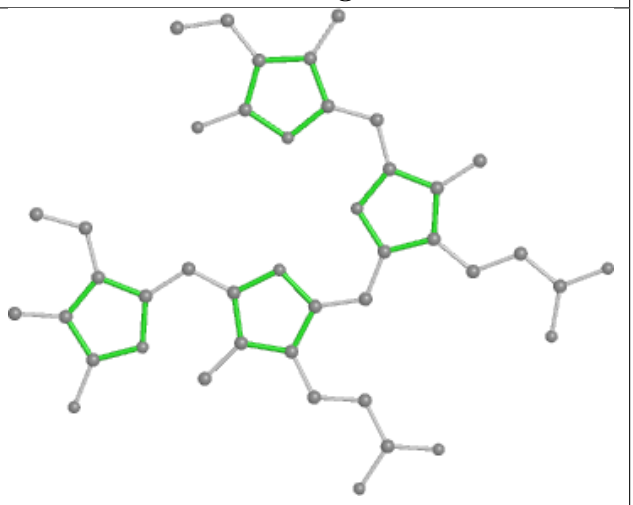
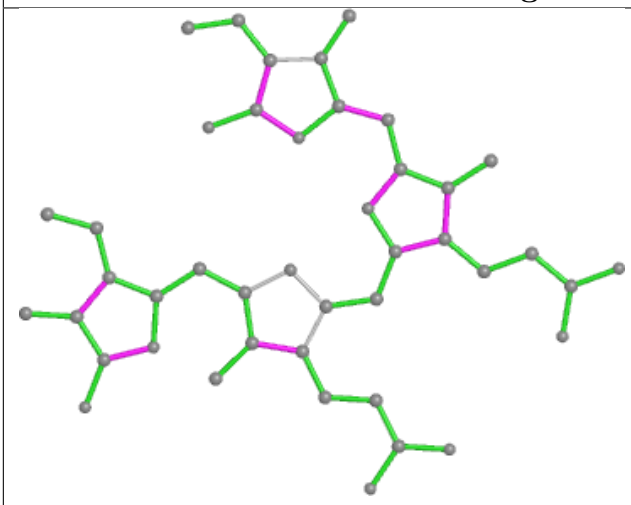


Rings

Ligand PUB dl 203



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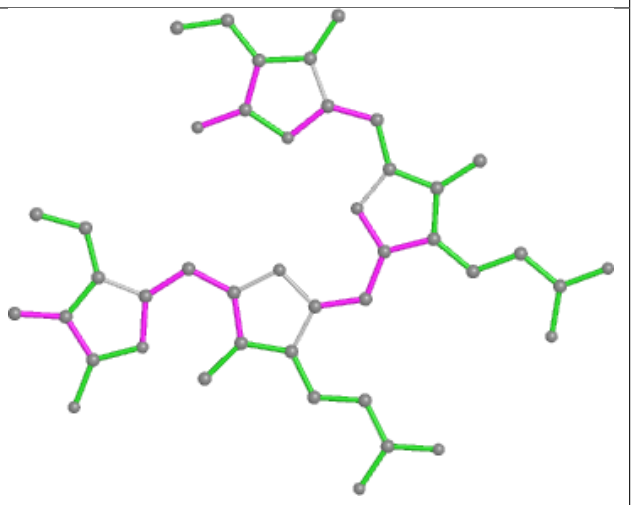

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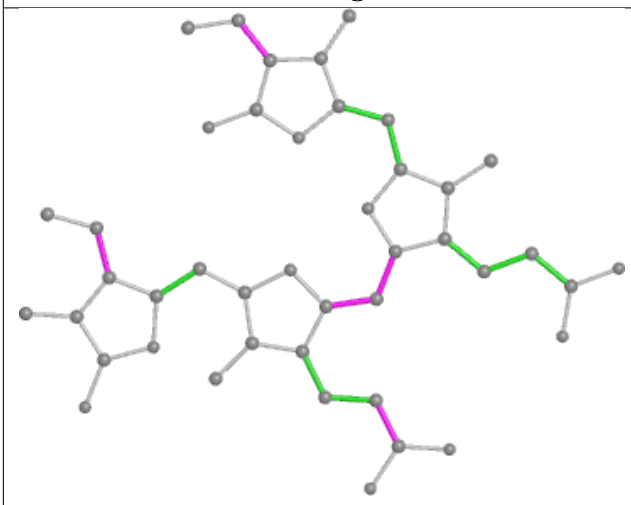

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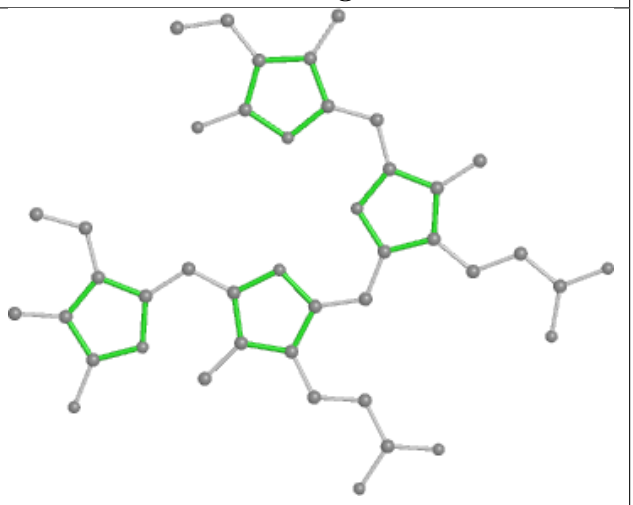
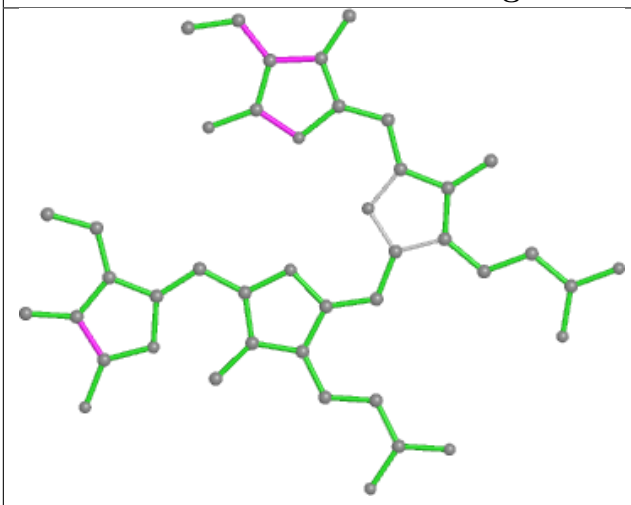


Rings

Ligand PEB M7 1001



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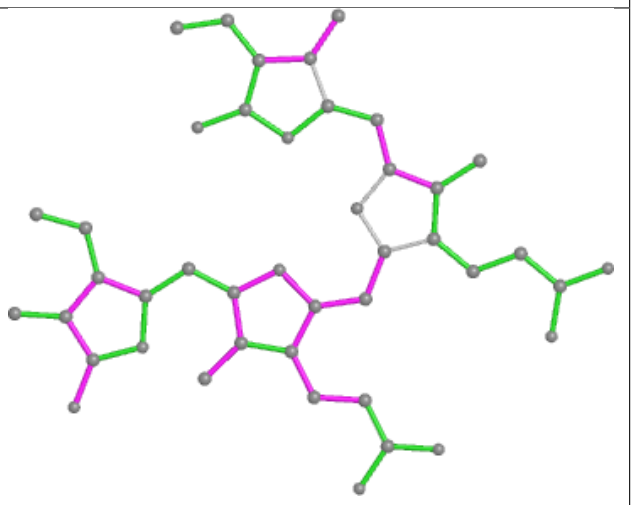
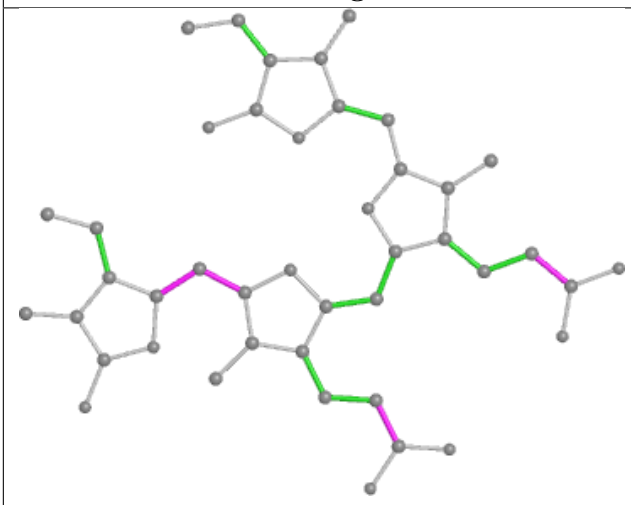


Bond angles



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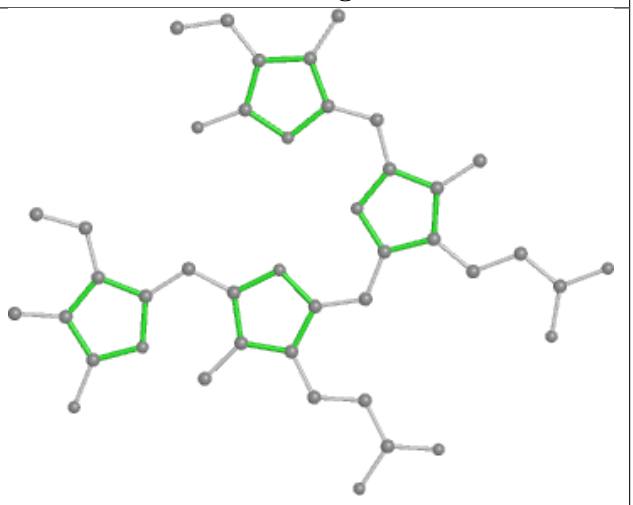
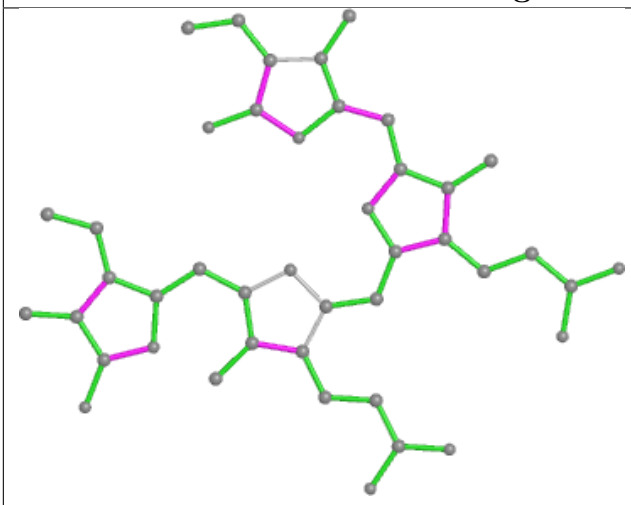
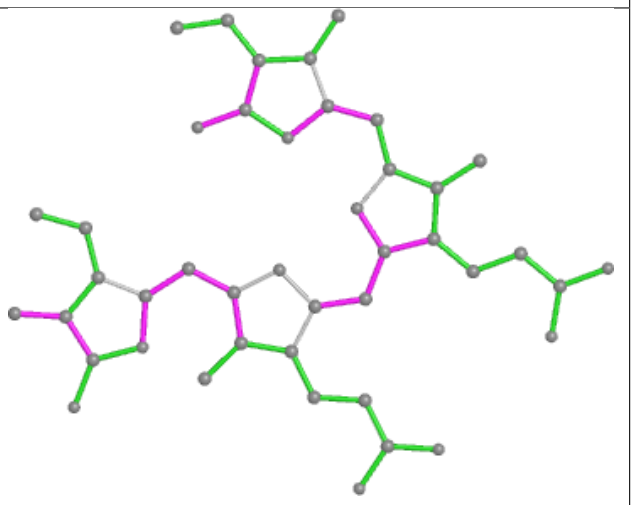


Rings

Ligand PUB V2 203



Bond lengths



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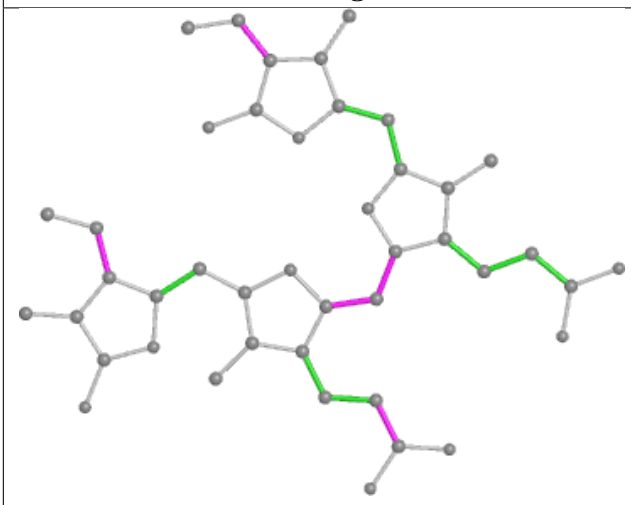
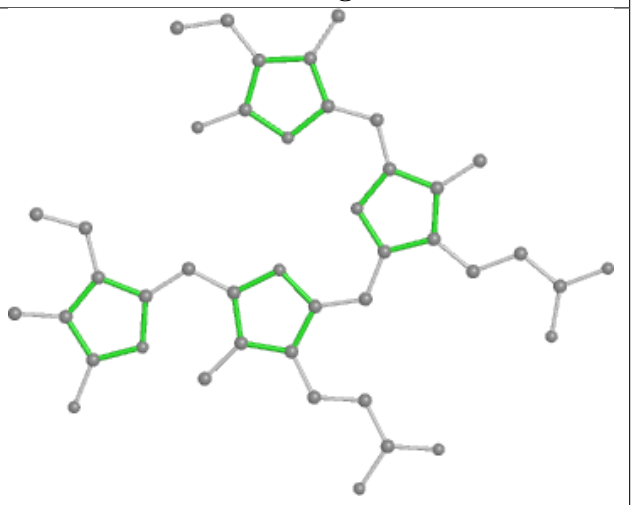
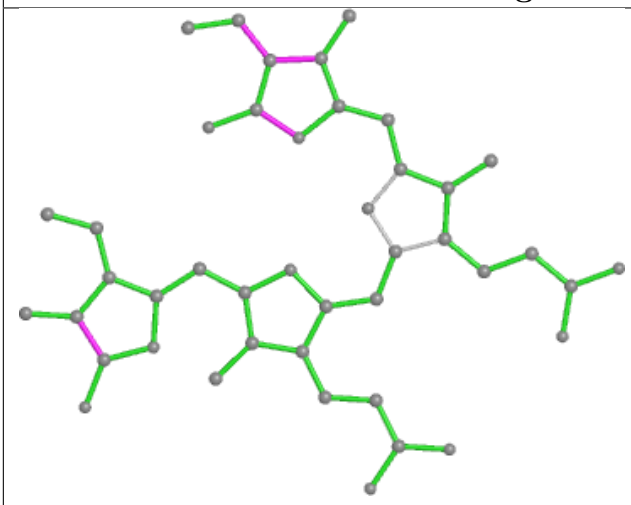


Torsions



Rings

Ligand PEB X3 201



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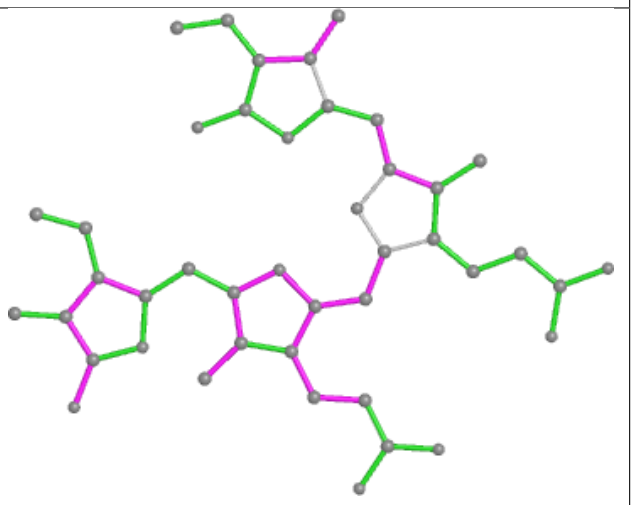

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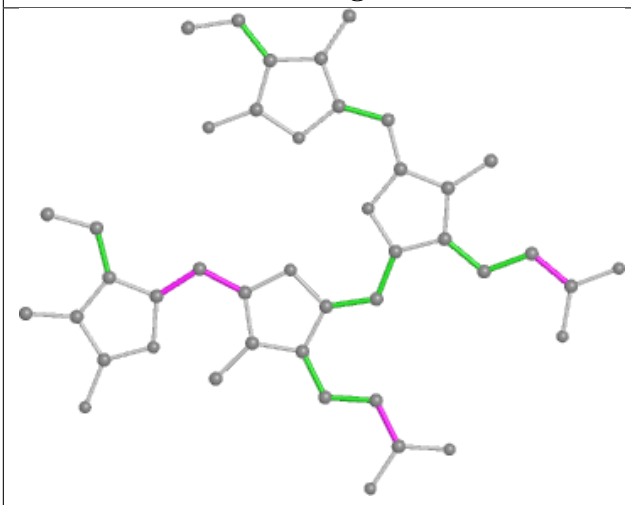

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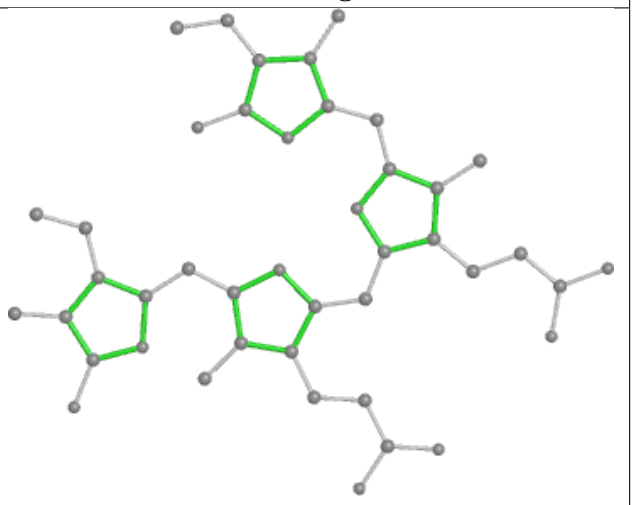
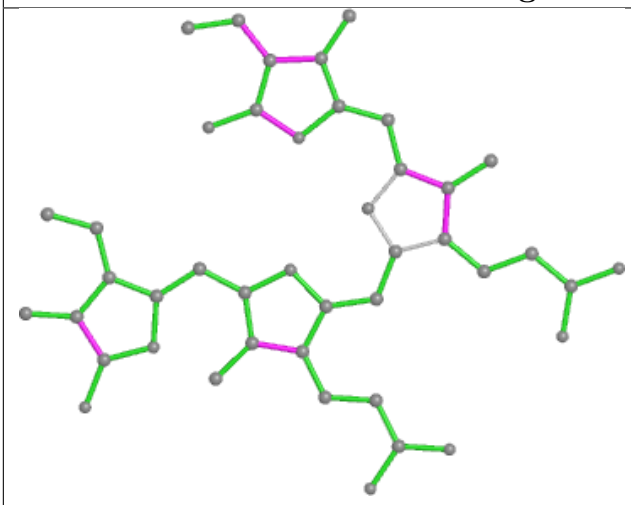


Rings

Ligand PEB gn 202



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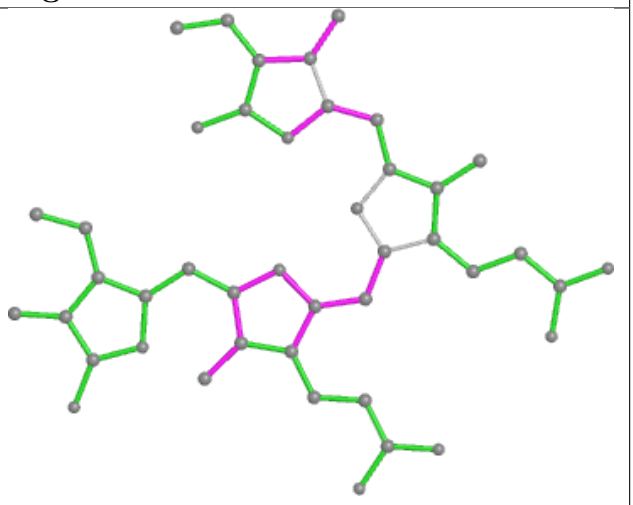

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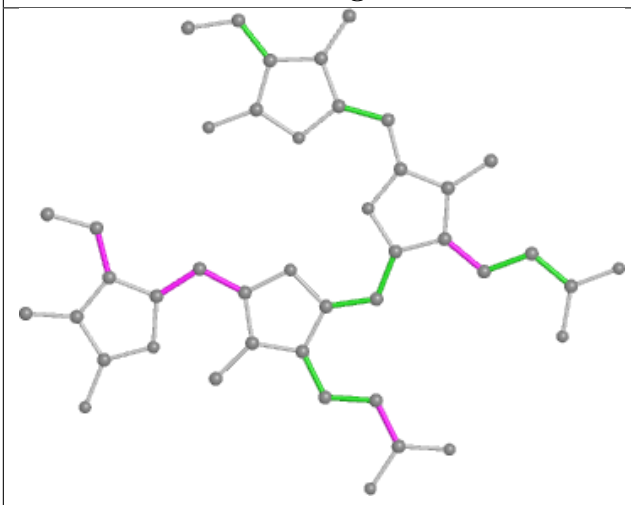

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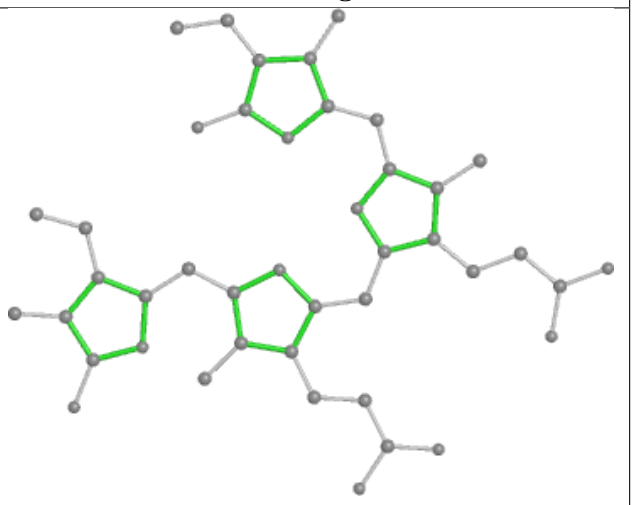

Rings

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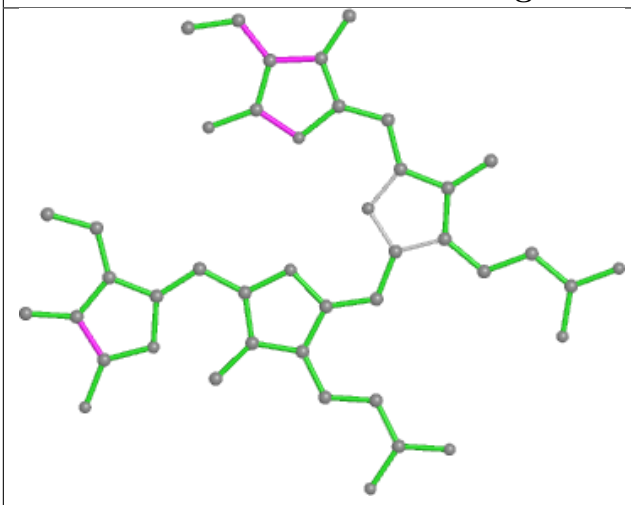

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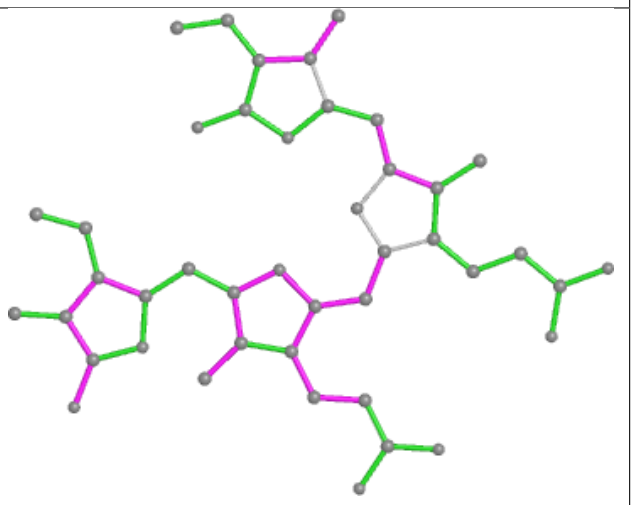

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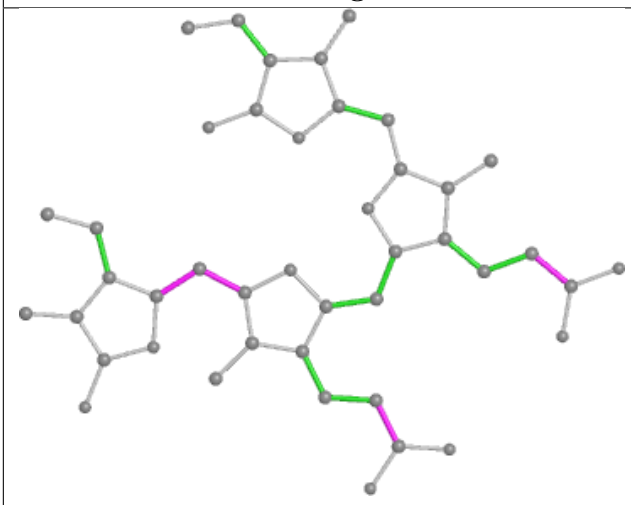

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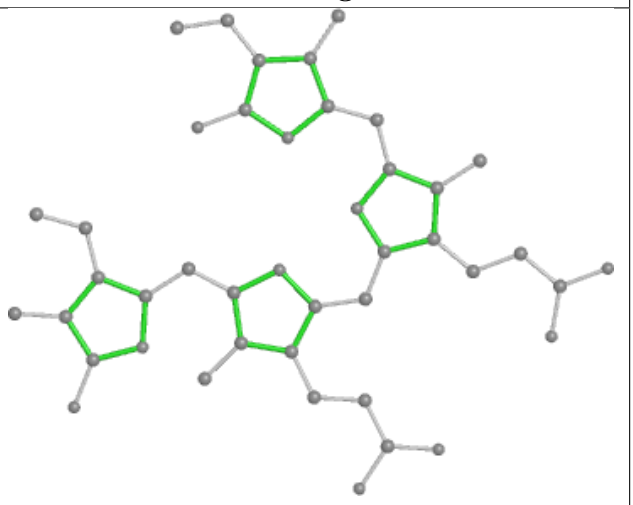
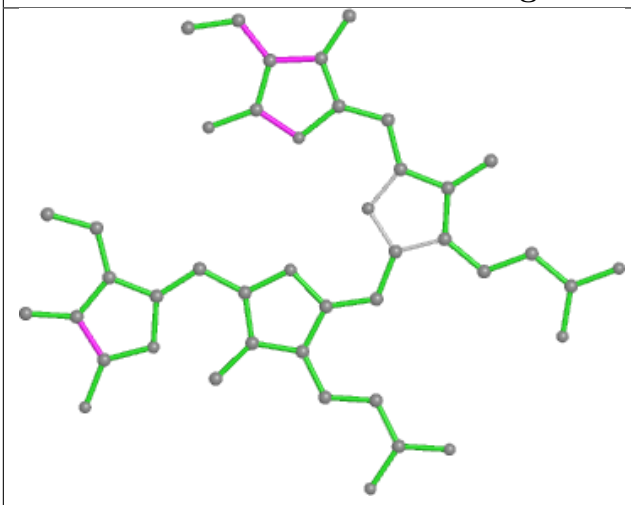


Rings

Ligand PEB de 201



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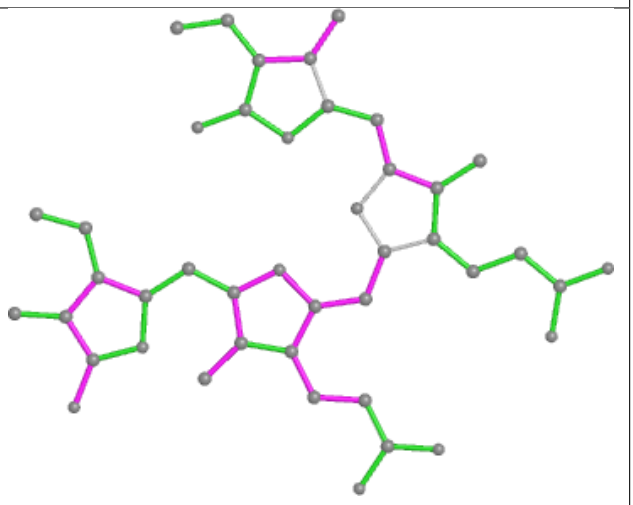

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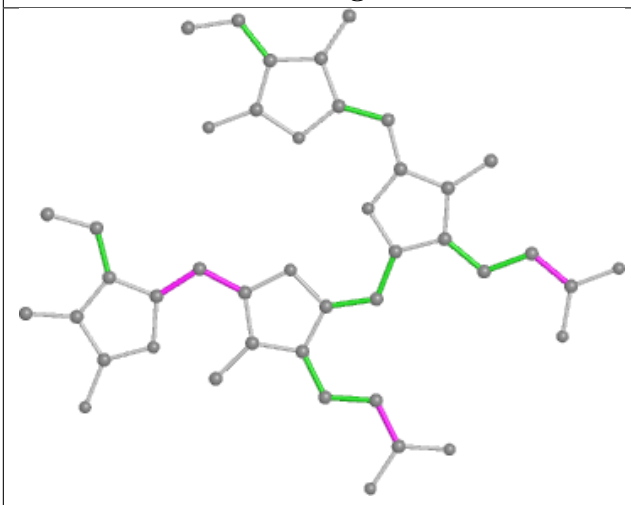

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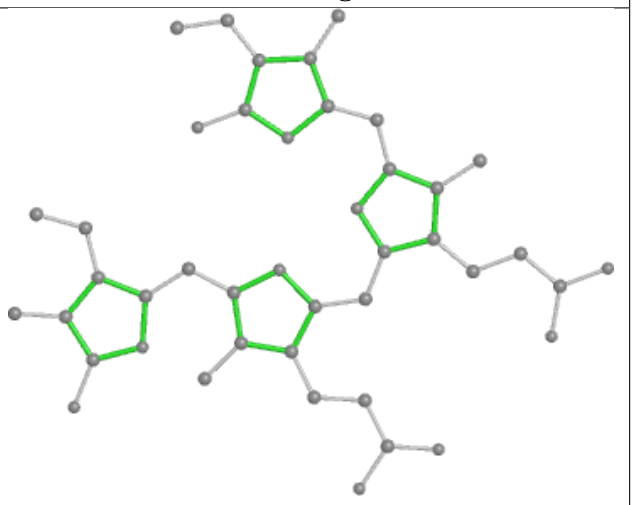
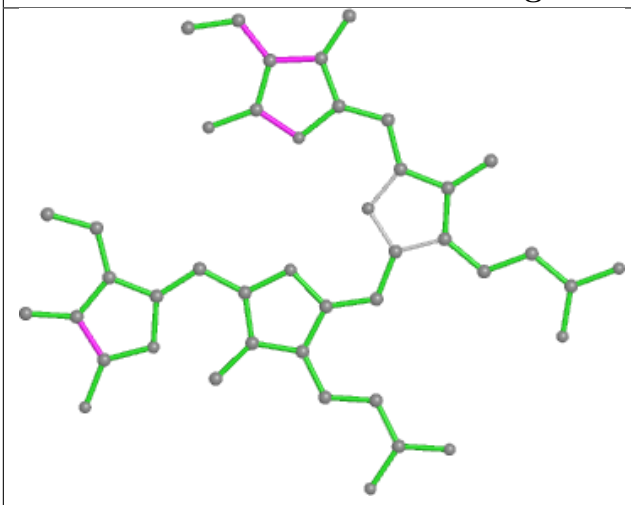


Rings

Ligand PEB lz 402



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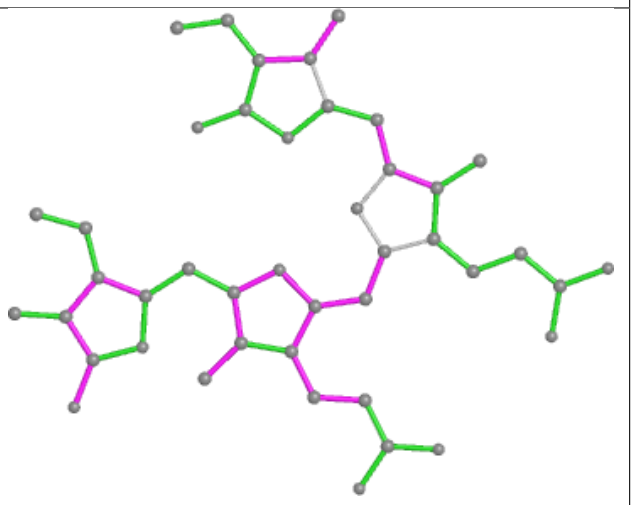

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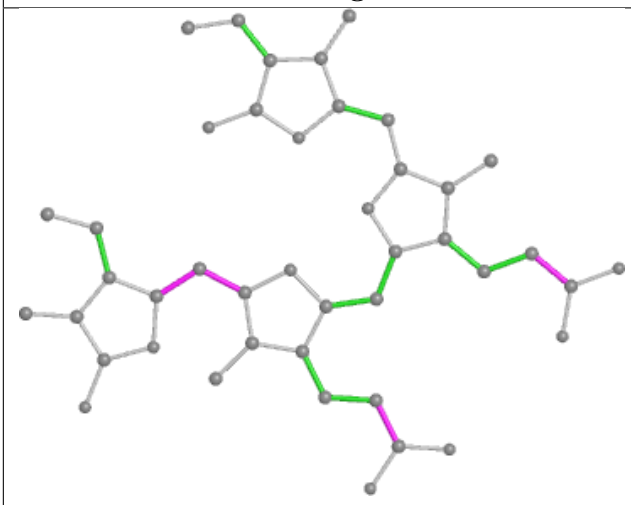

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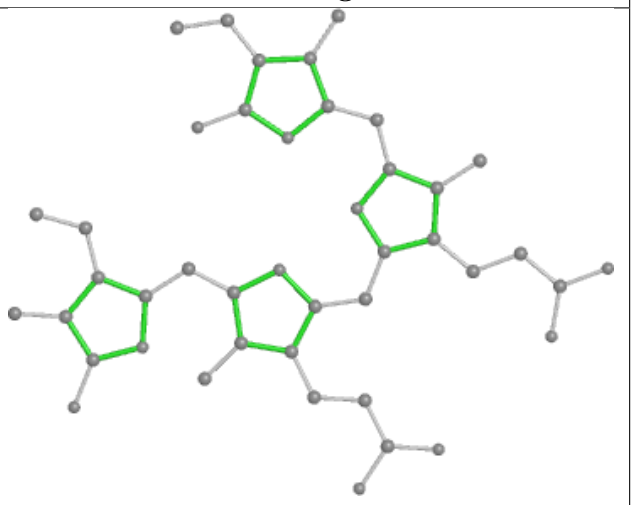

Rings

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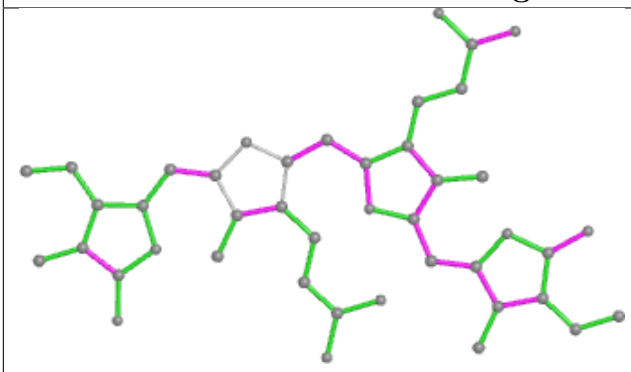

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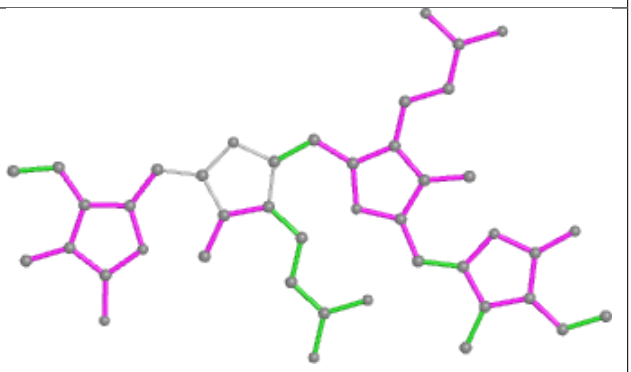

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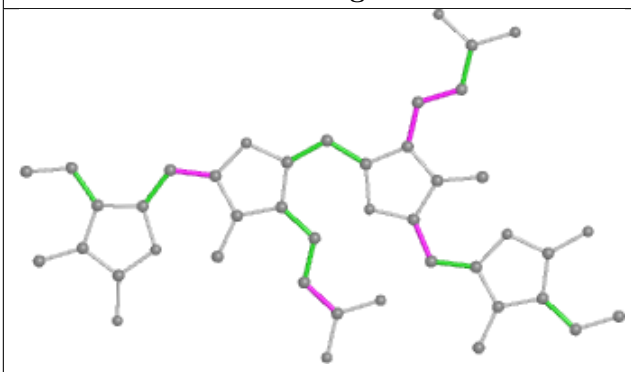

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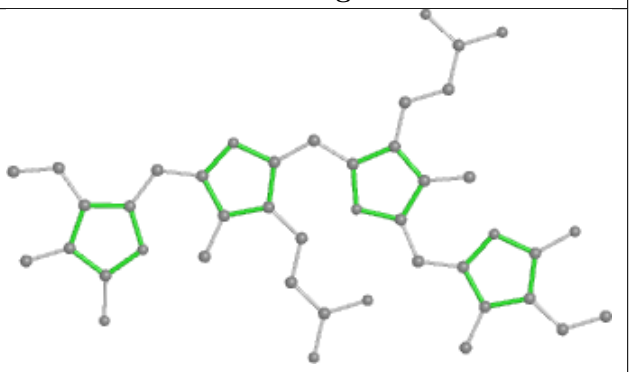
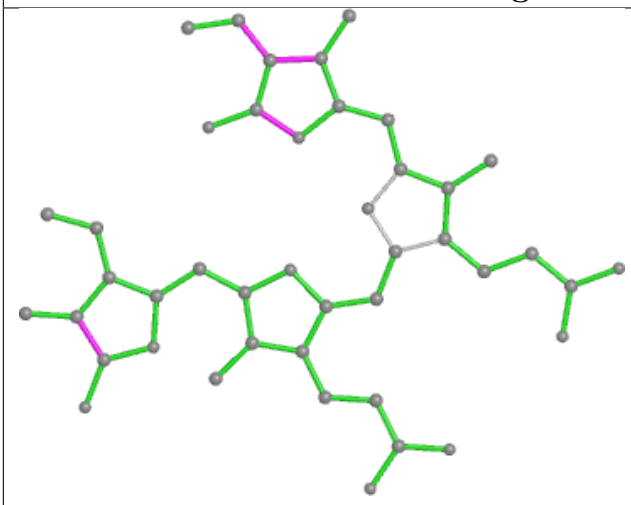


Rings

Ligand PEB M3 201



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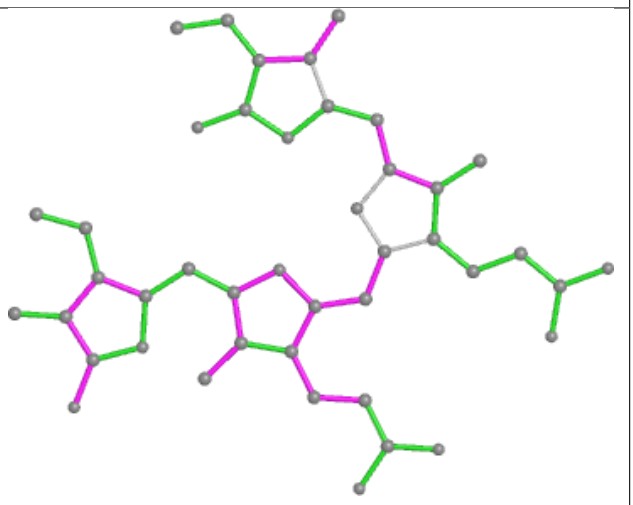

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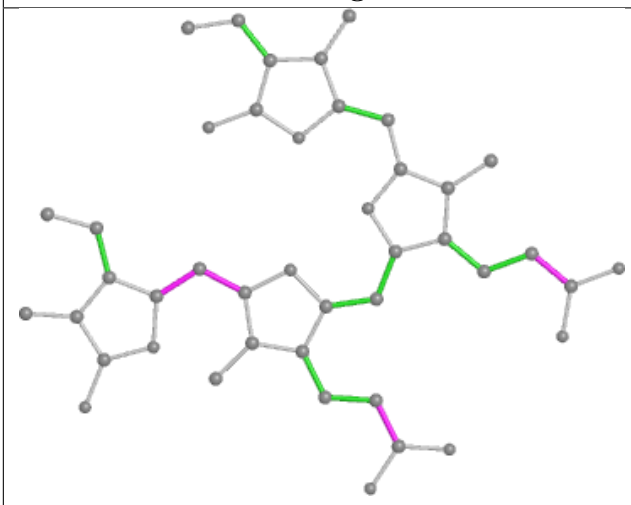

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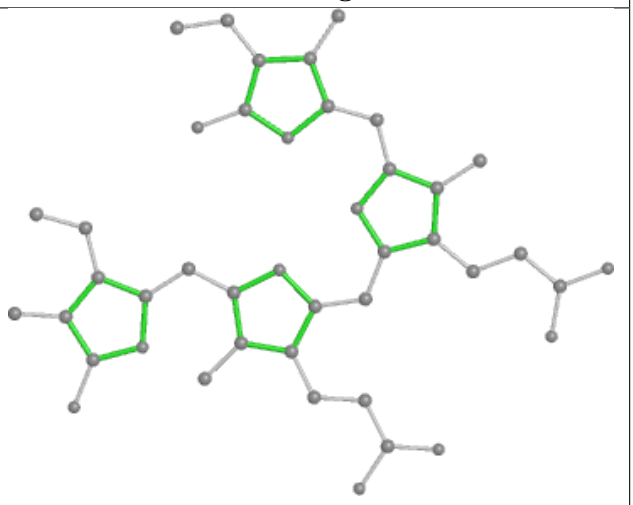
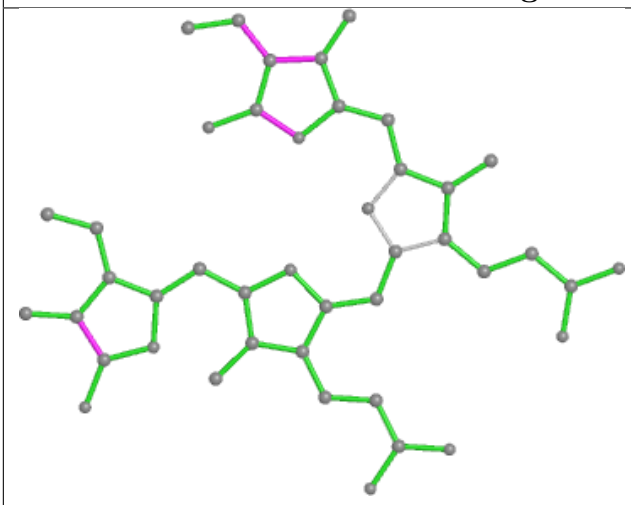


Rings

Ligand PEB z4 201



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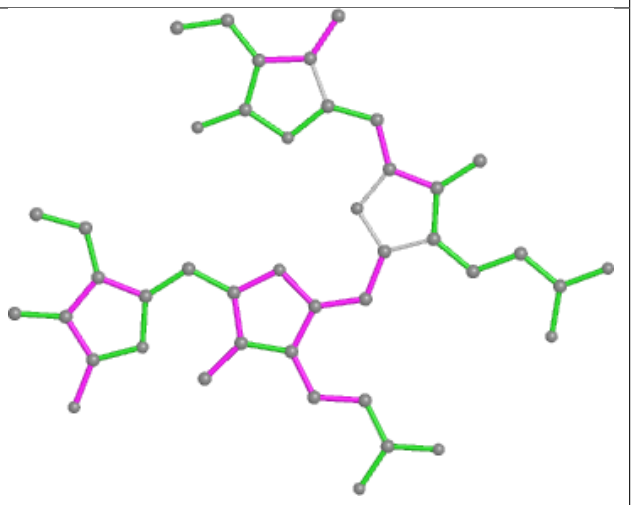

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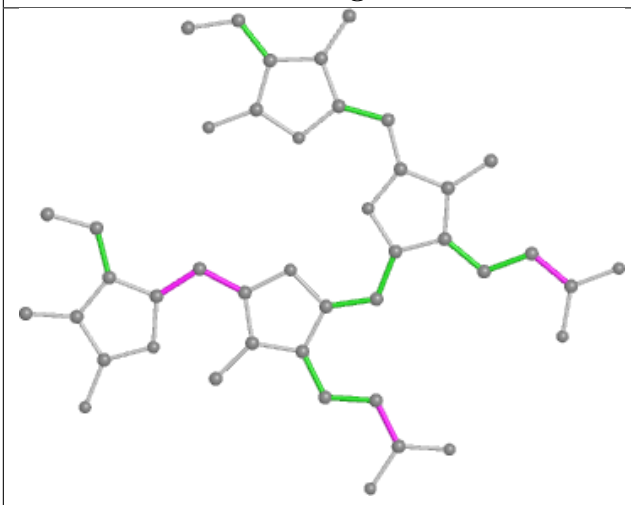

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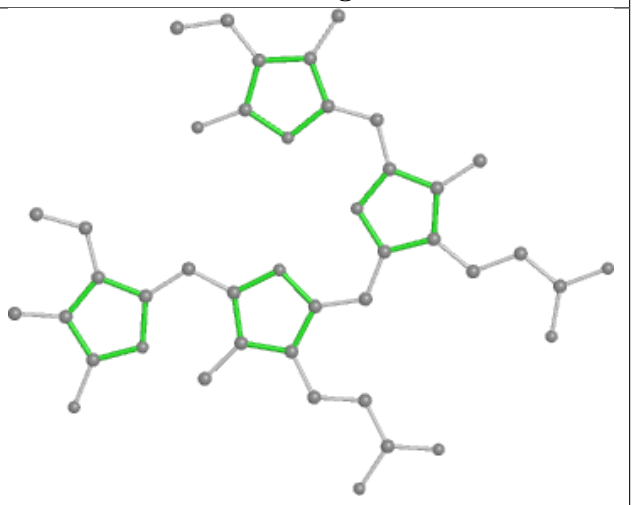

Rings

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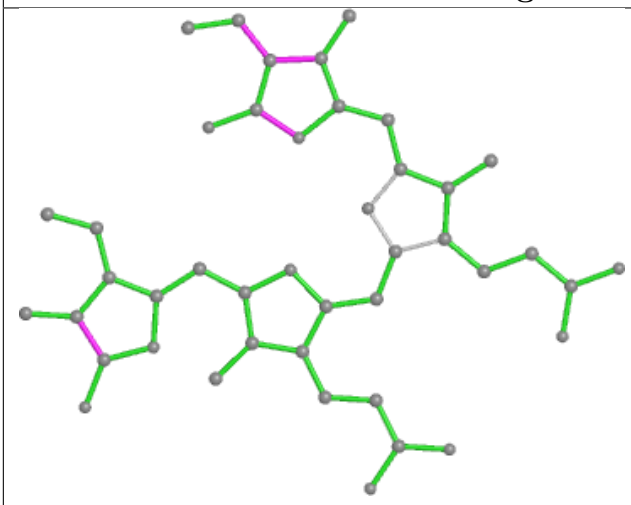

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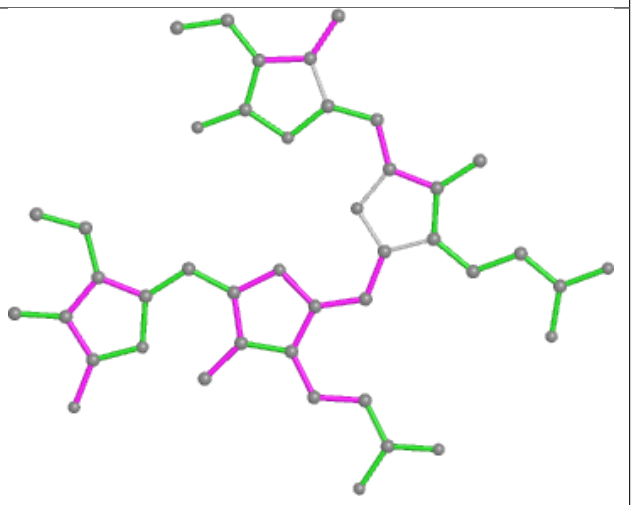

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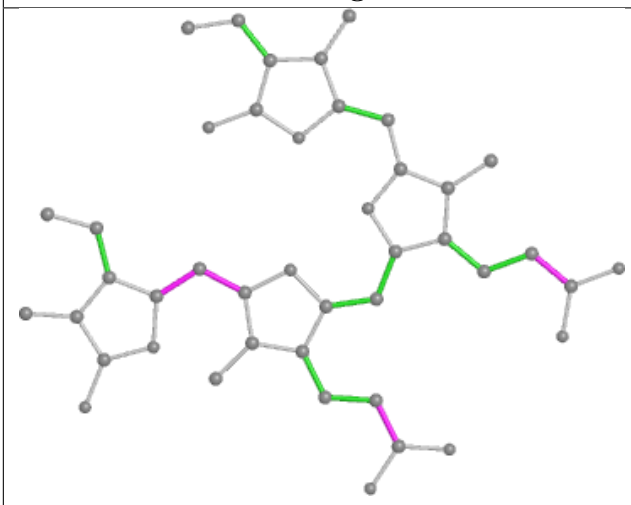

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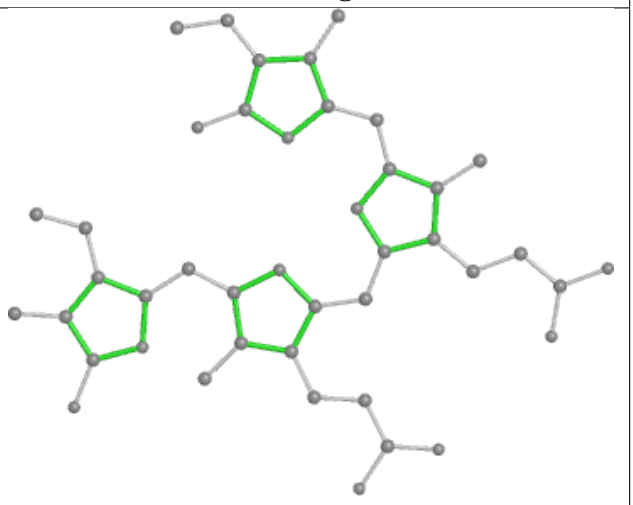
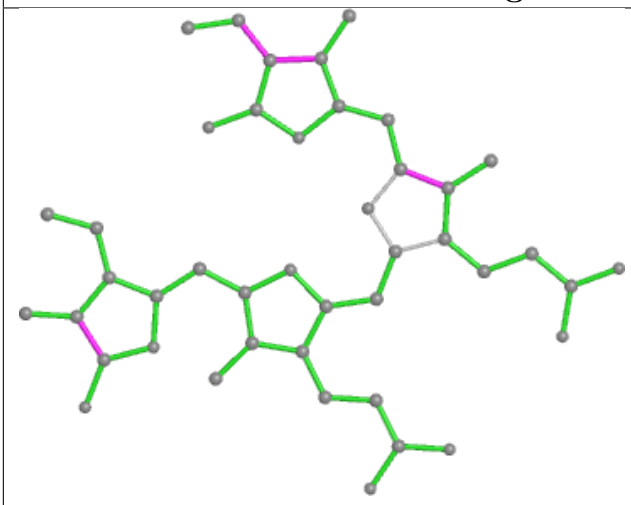


Rings

Ligand PEB K5 1002



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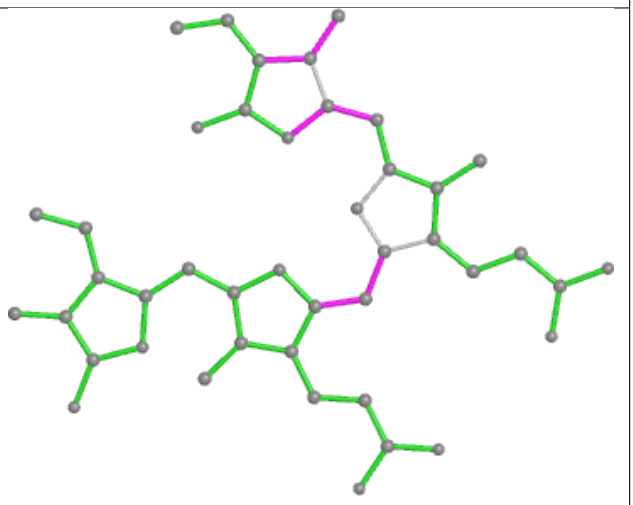

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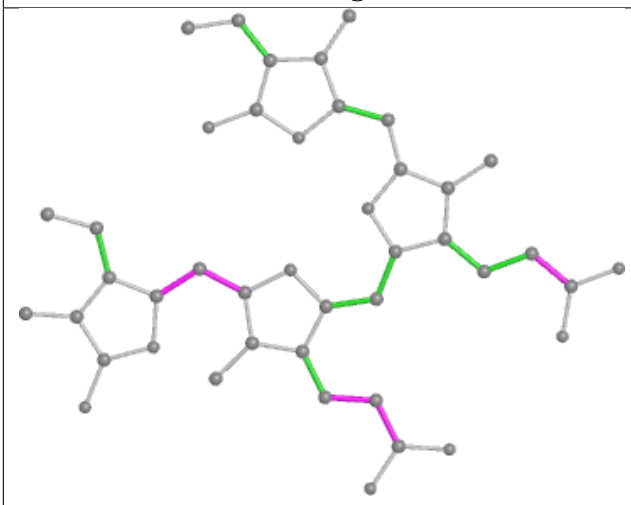

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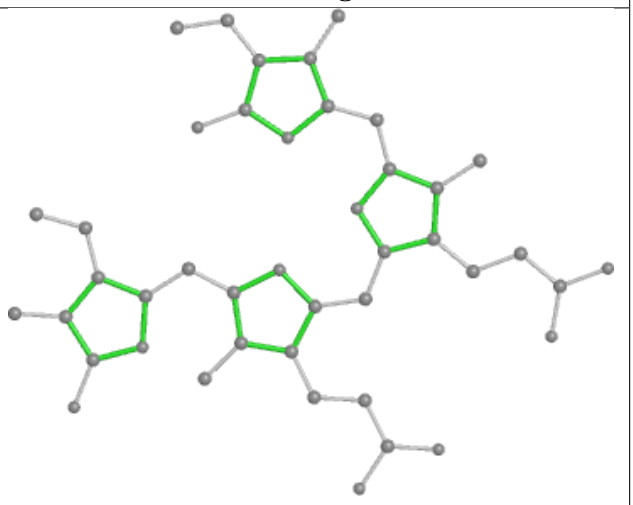
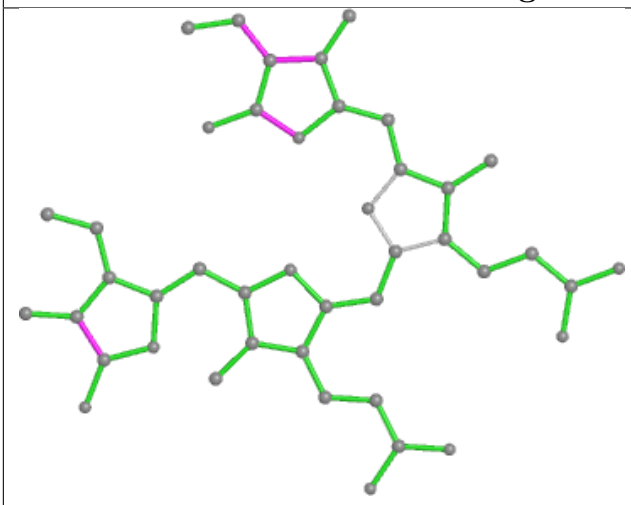


Rings

Ligand PEB S4 201



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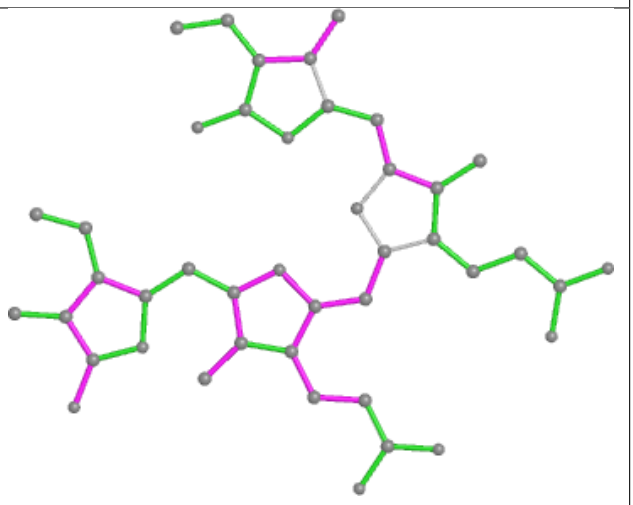

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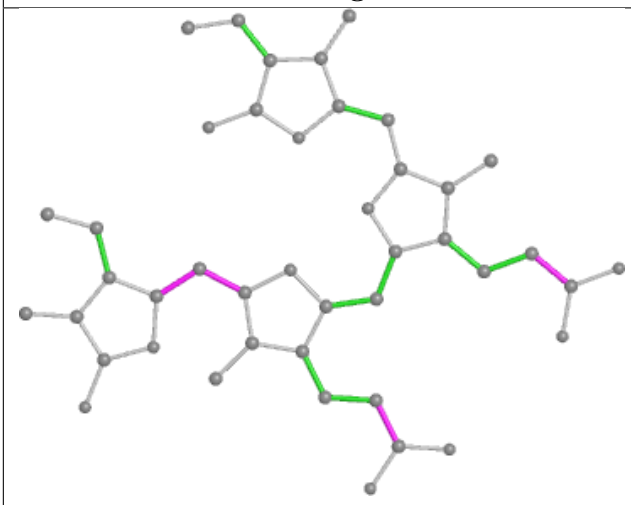

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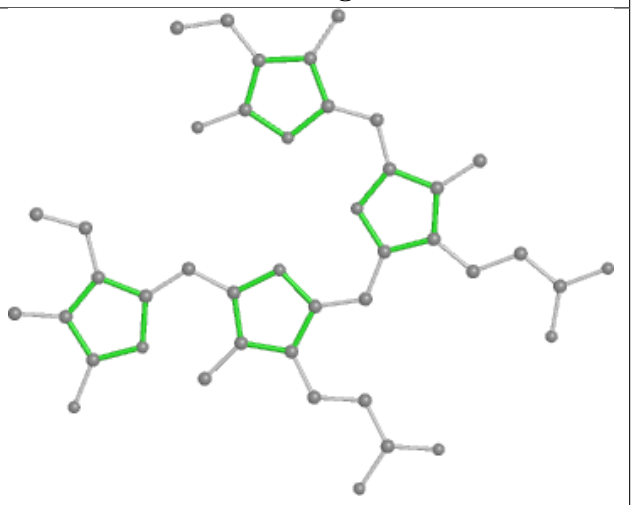
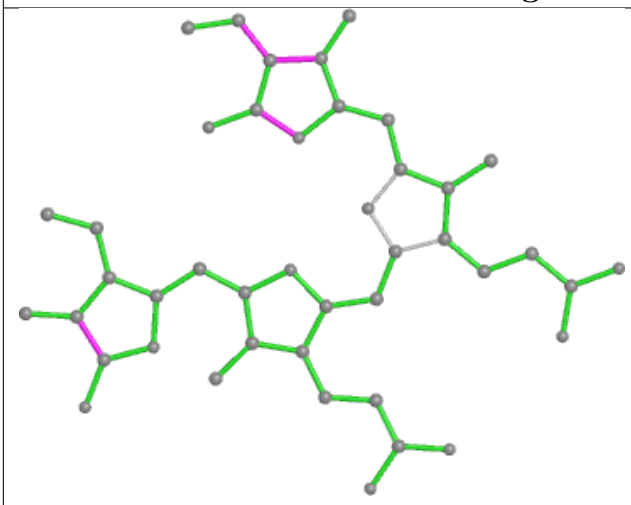


Rings

Ligand PEB t6 202



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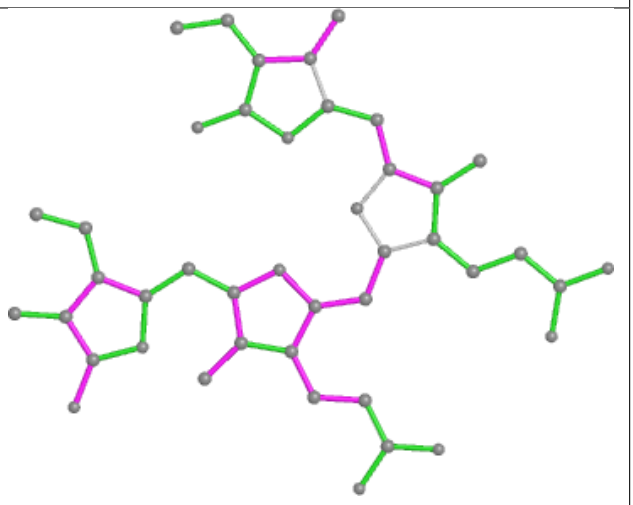

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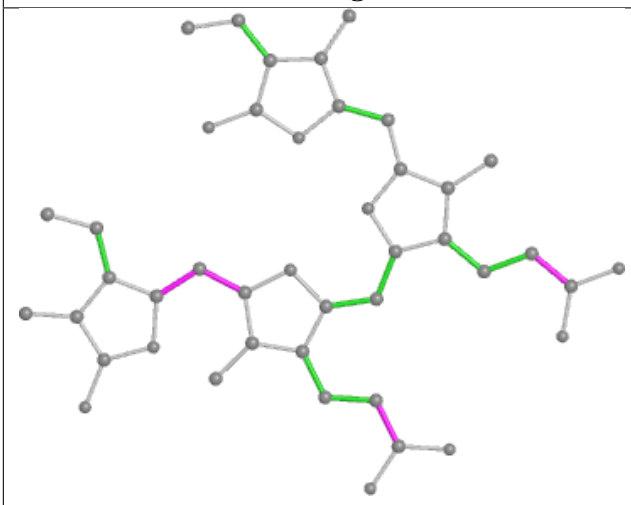

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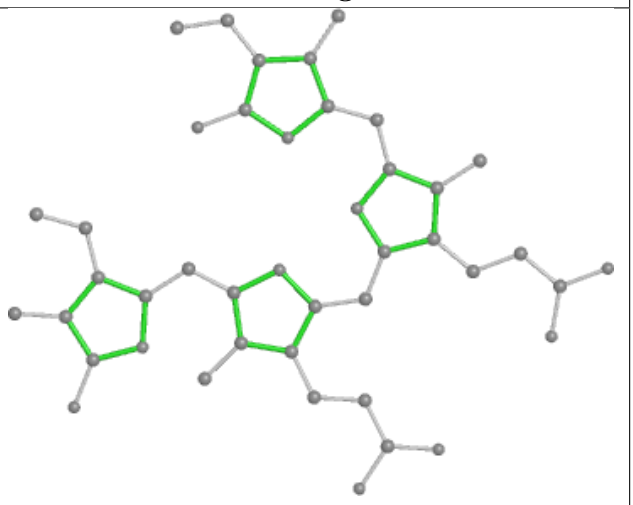
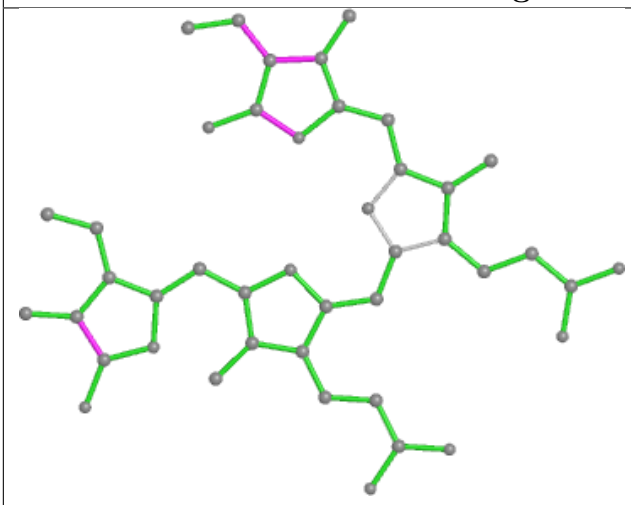


Rings

Ligand PEB ez 1002



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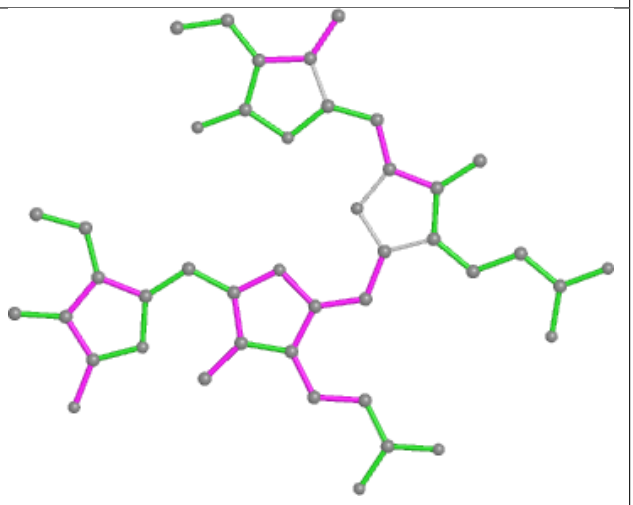
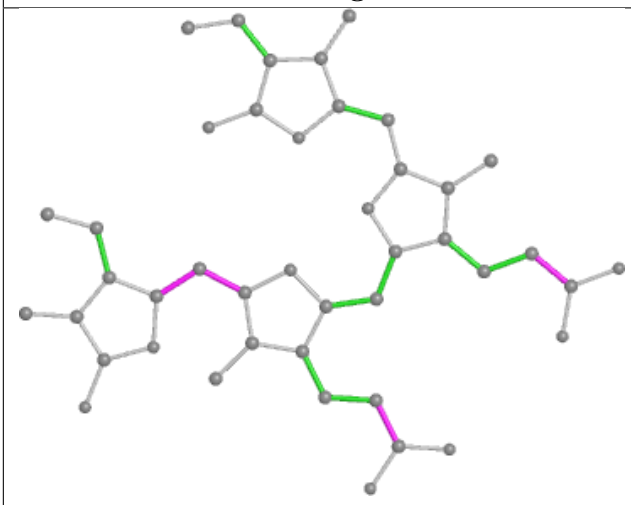
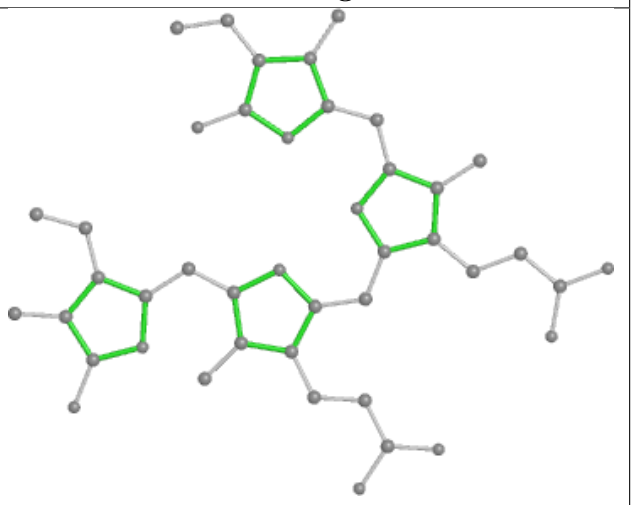


Bond angles

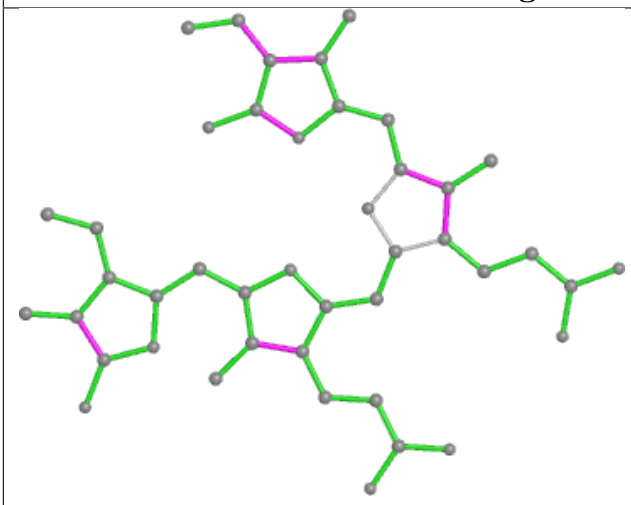


Torsions



Rings

Ligand PEB h2 202



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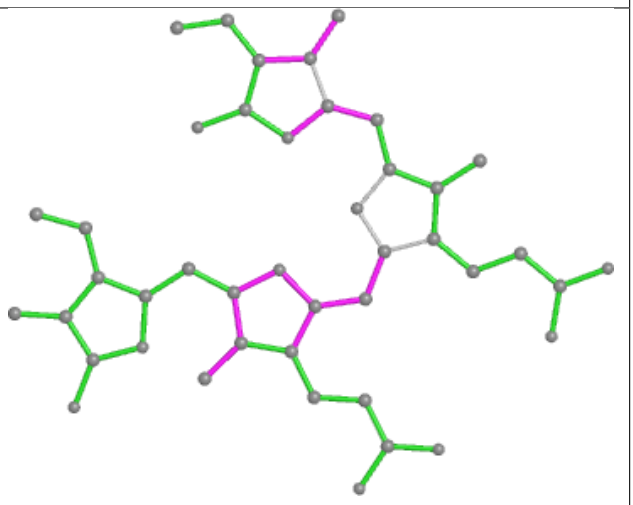

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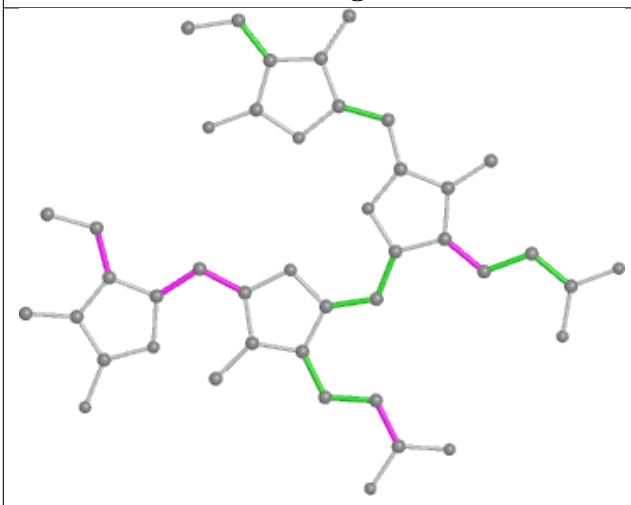

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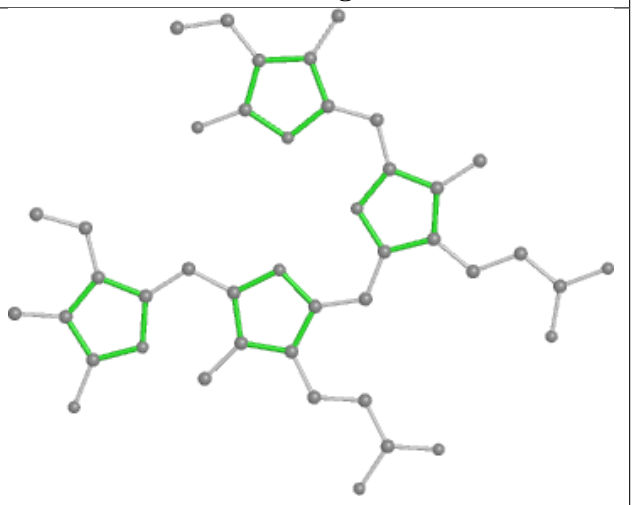
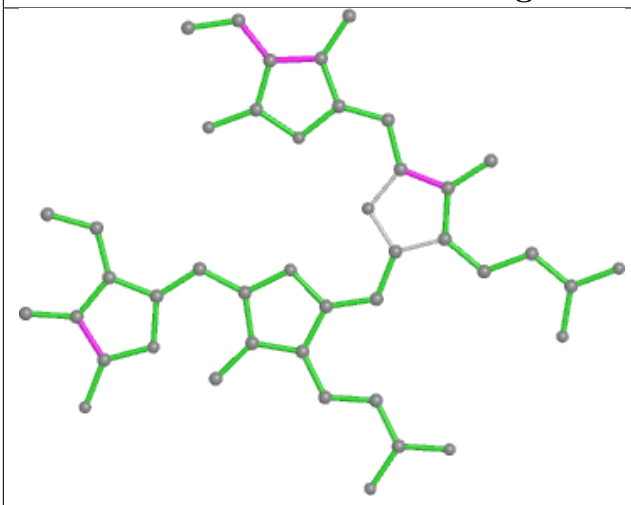


Rings

Ligand PEB O9 202



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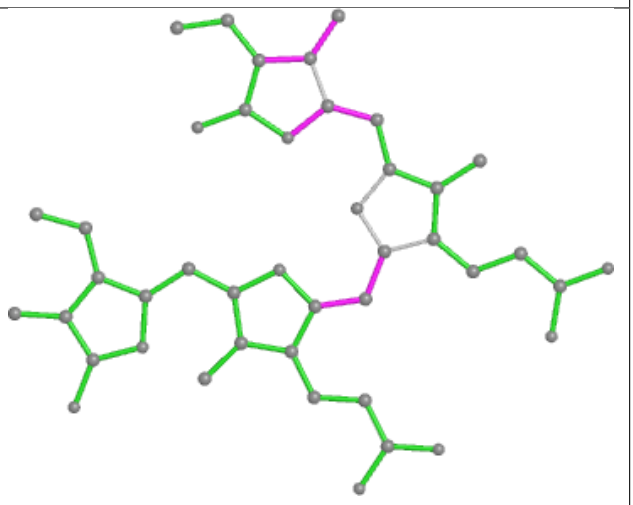

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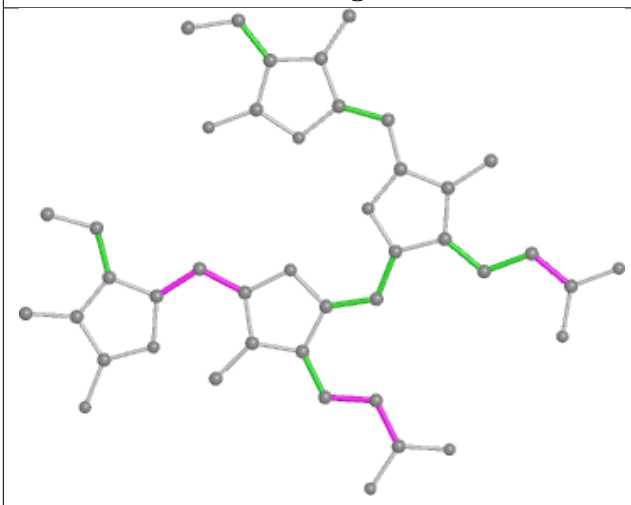

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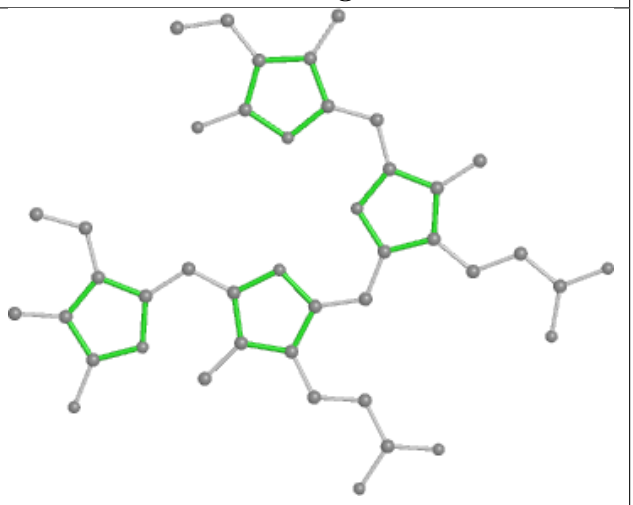
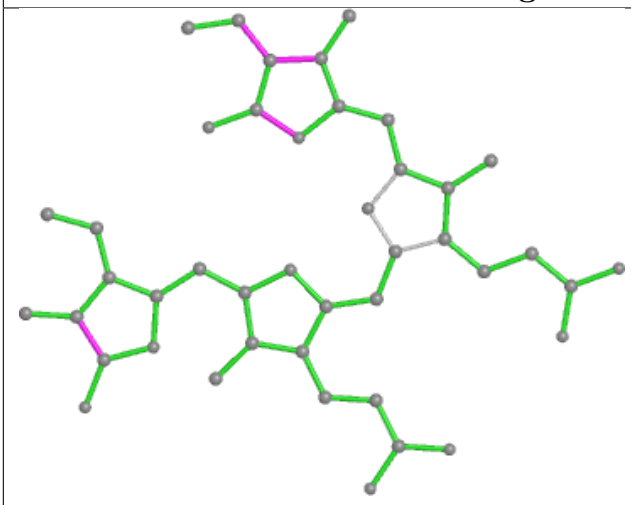


Rings

Ligand PEB p4 201



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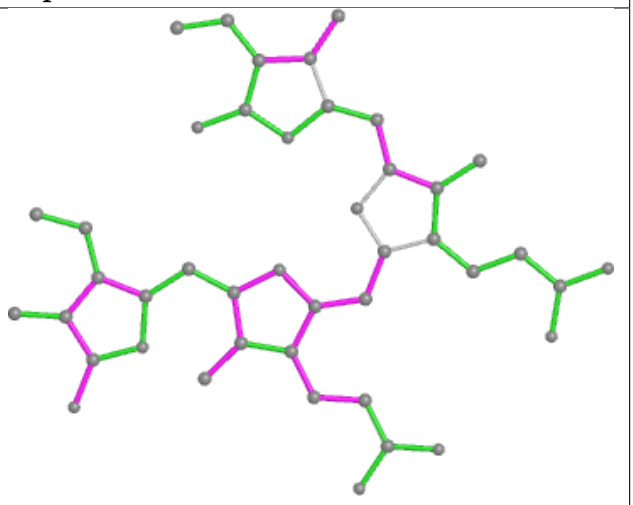
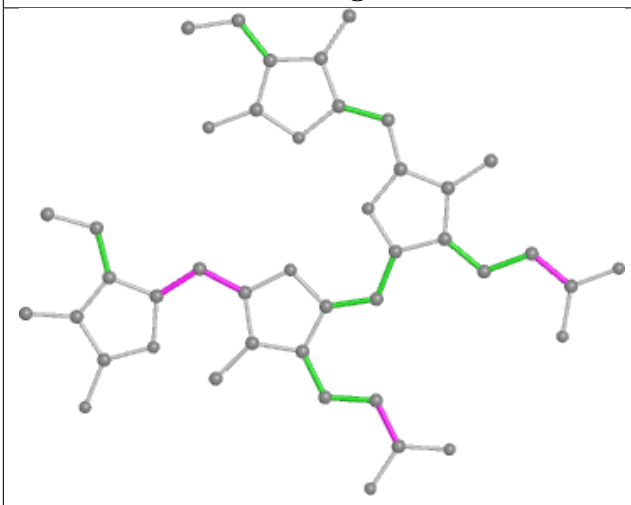


Bond angles



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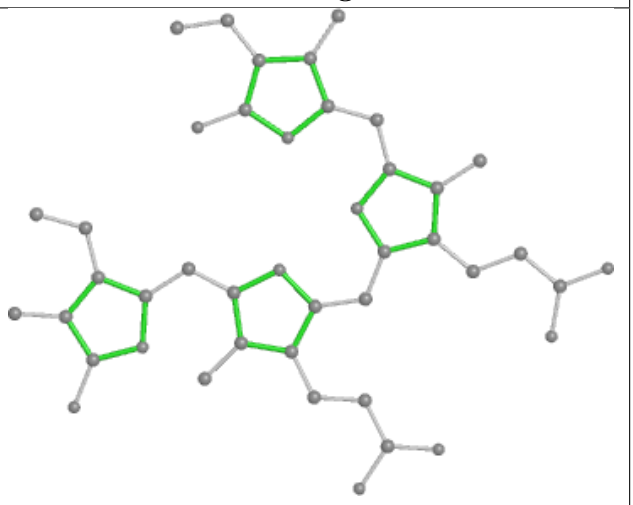
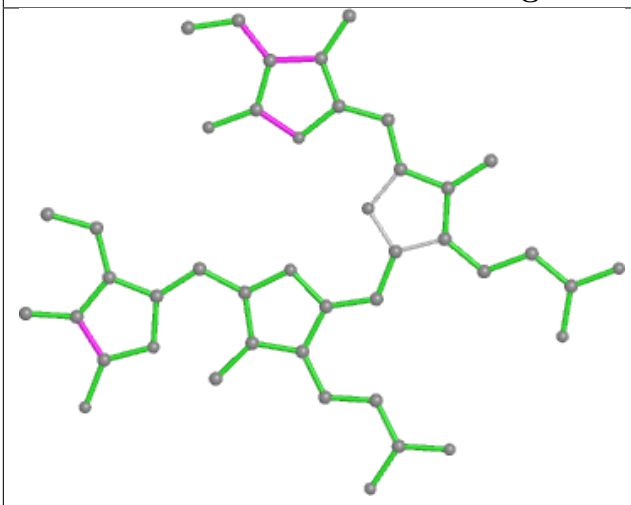


Rings

Ligand PEB t7 201



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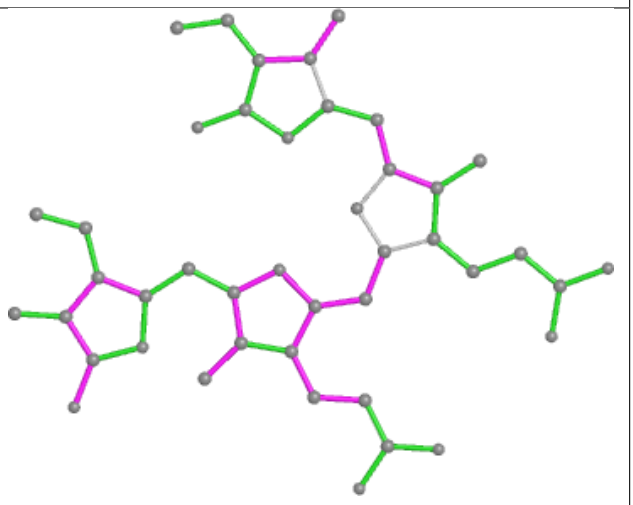

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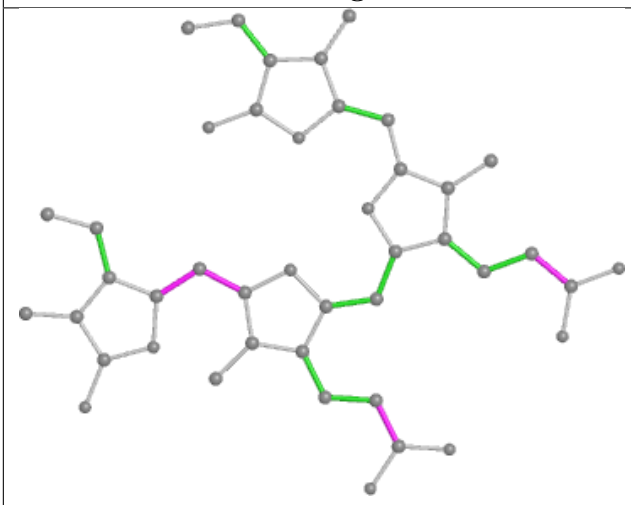

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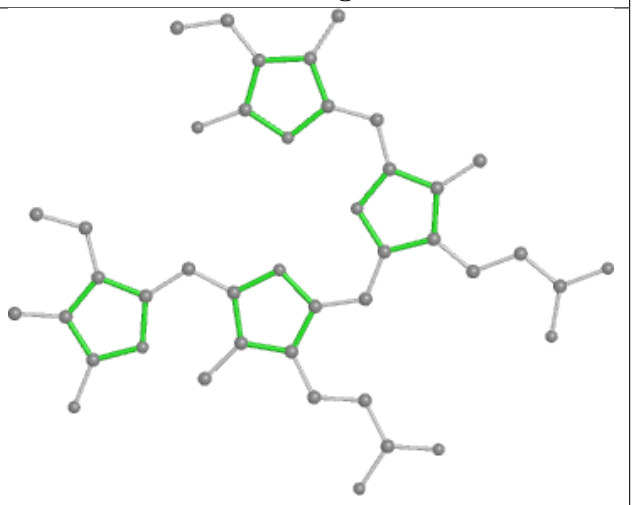
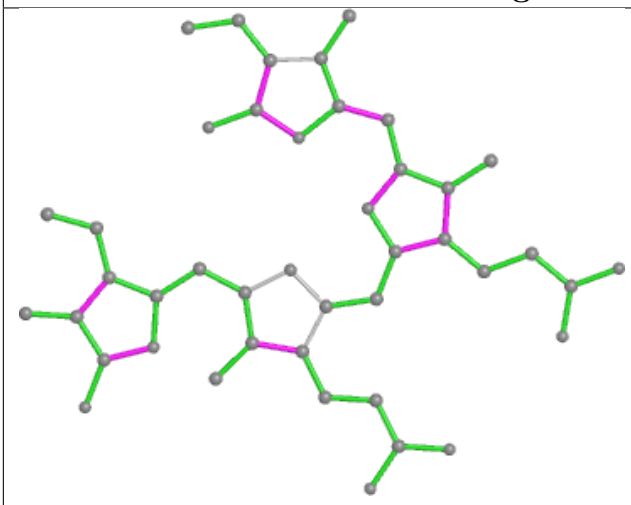


Rings

Ligand PUB G8 203



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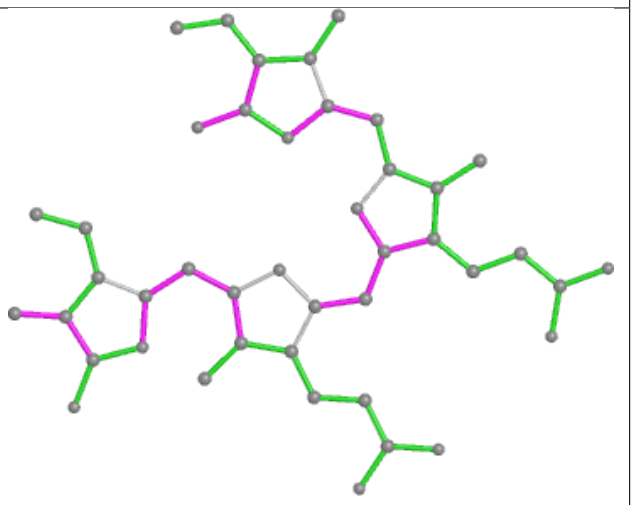

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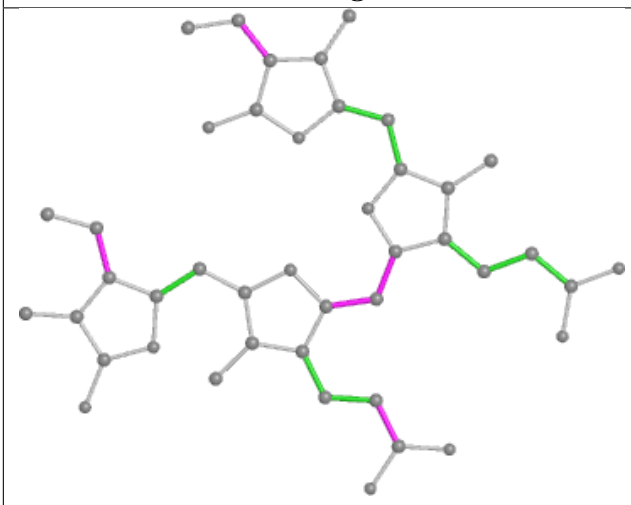

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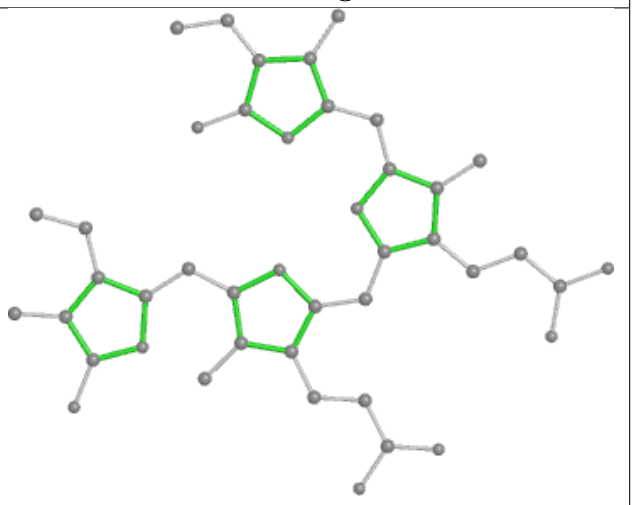
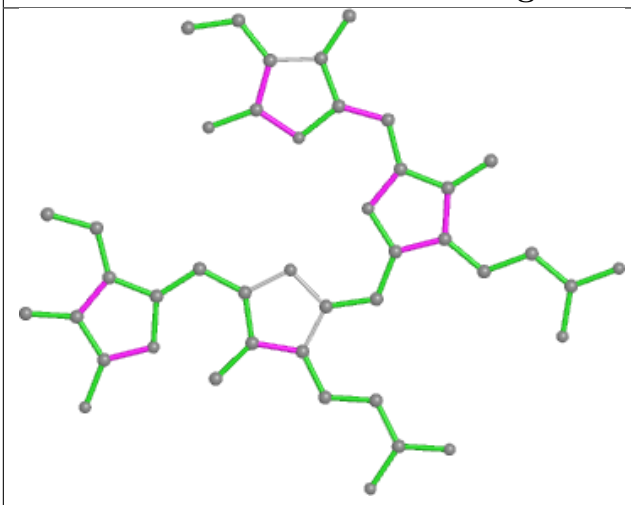


Rings

Ligand PUB y8 203



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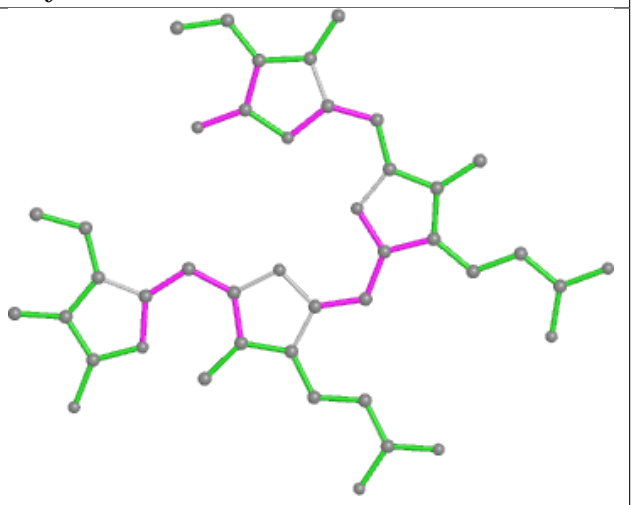

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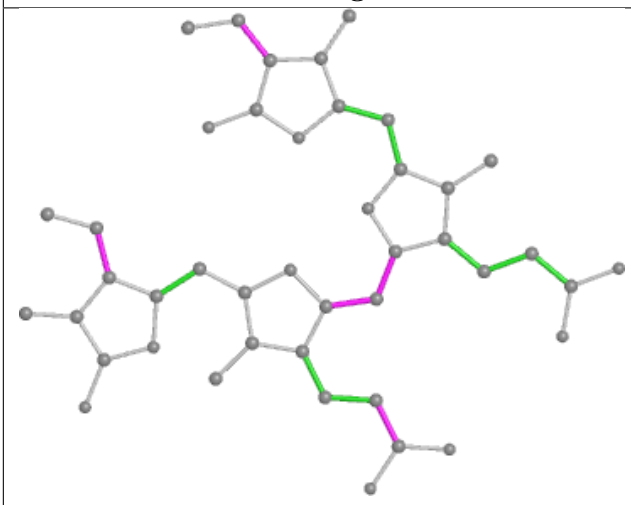

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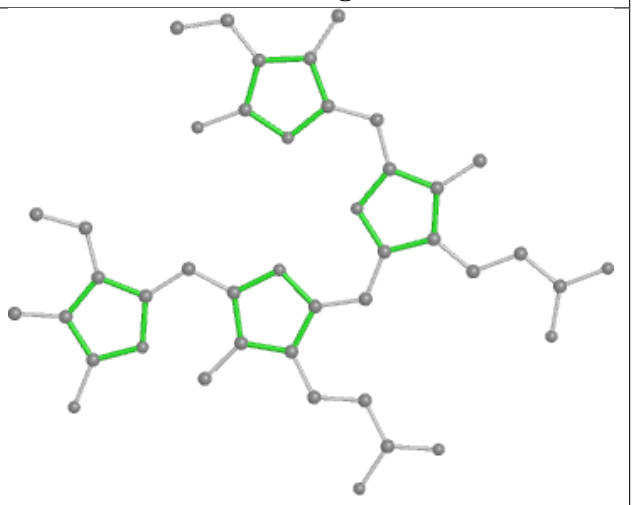
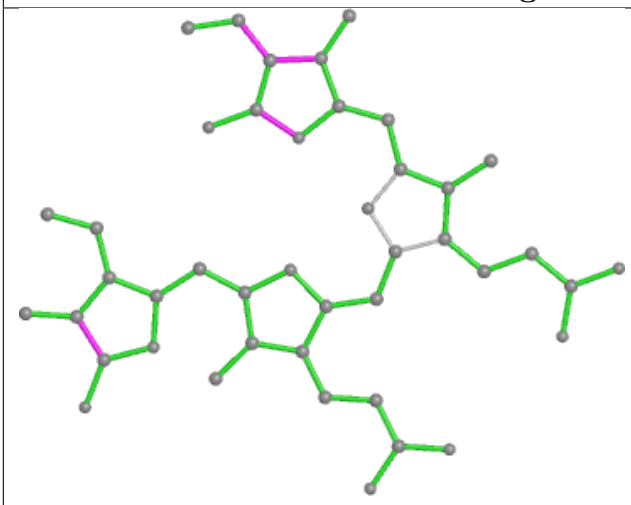


Rings

Ligand PEB fw 201



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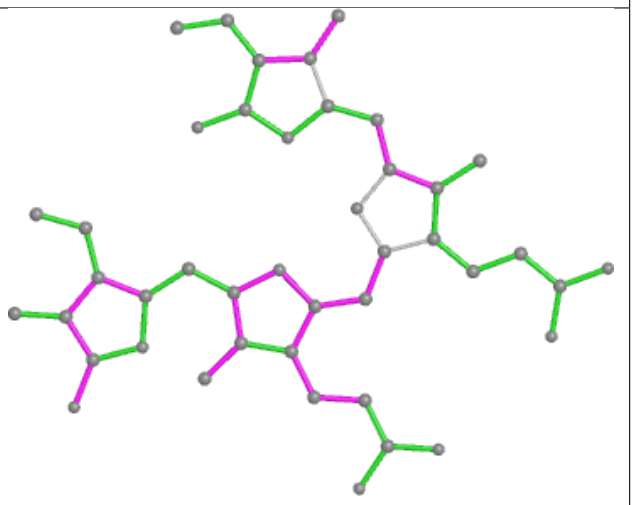

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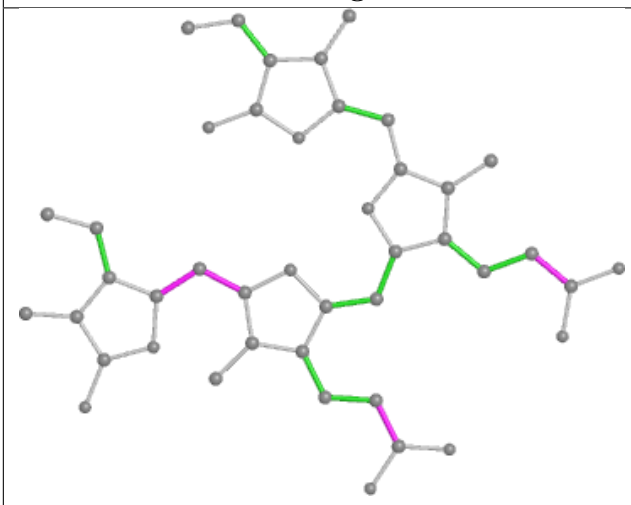

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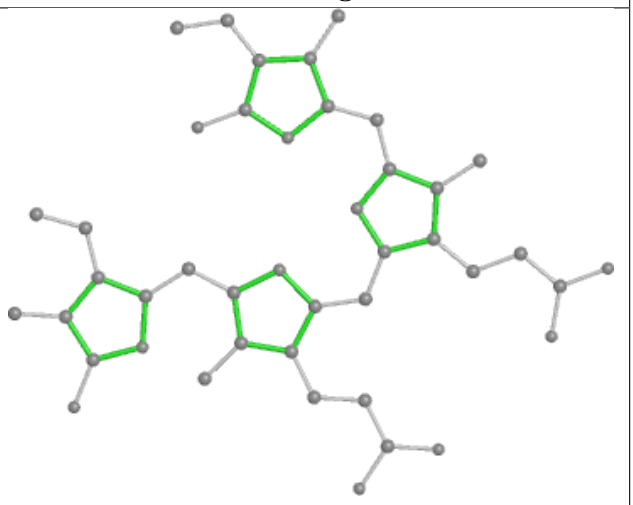
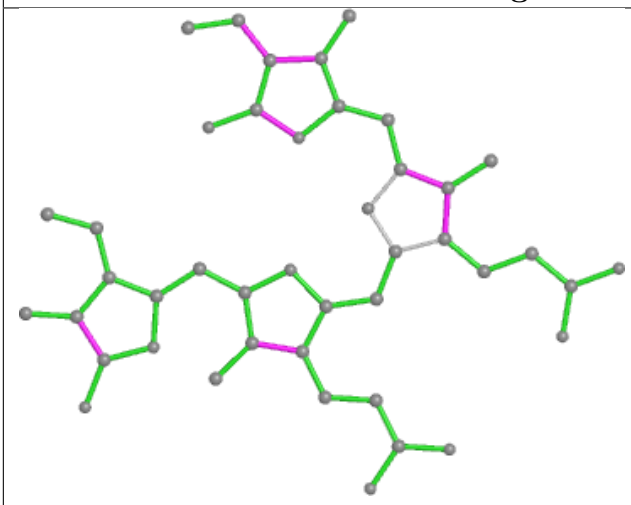


Rings

Ligand PEB 34 1002



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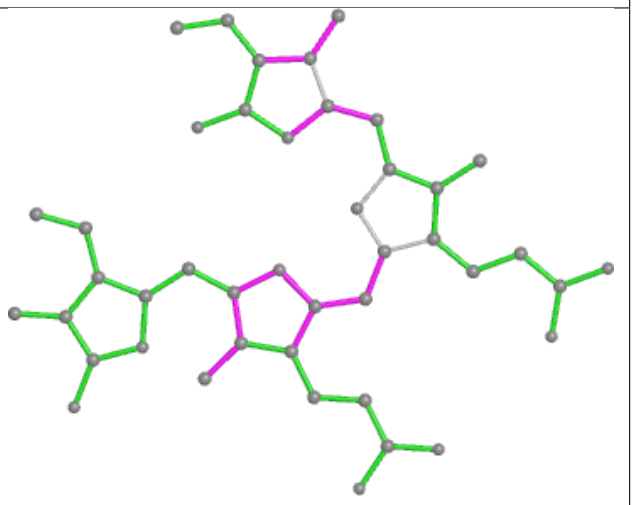

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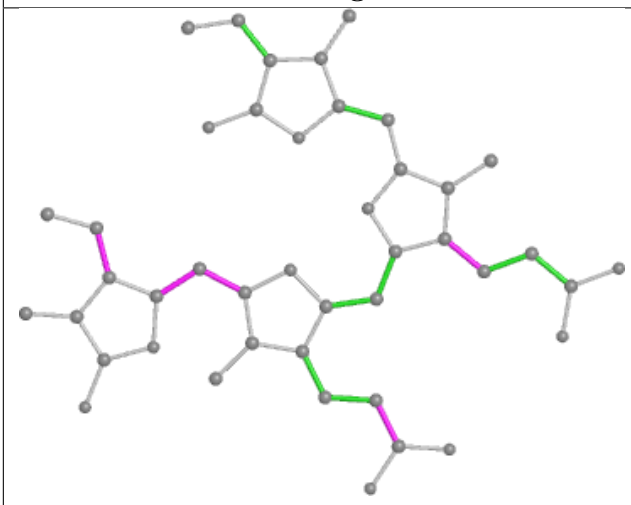

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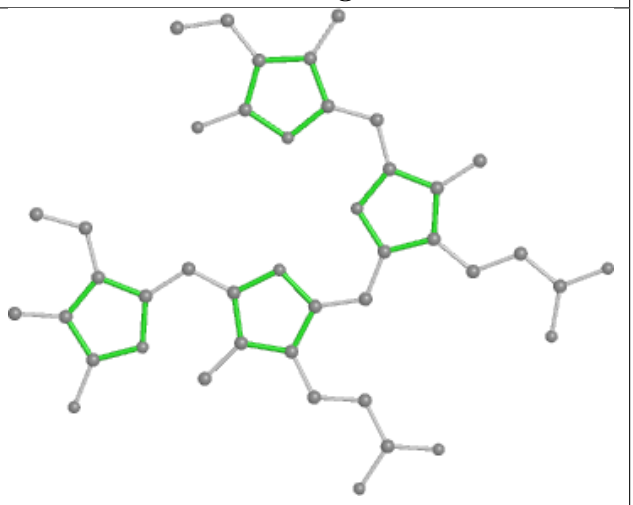
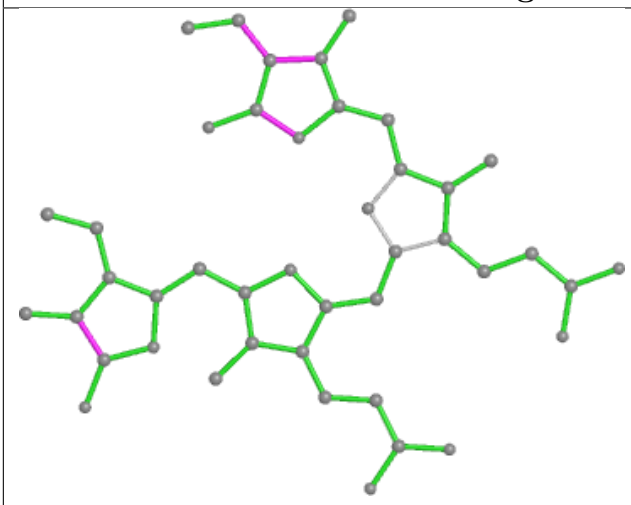


Rings

Ligand PEB E6 201



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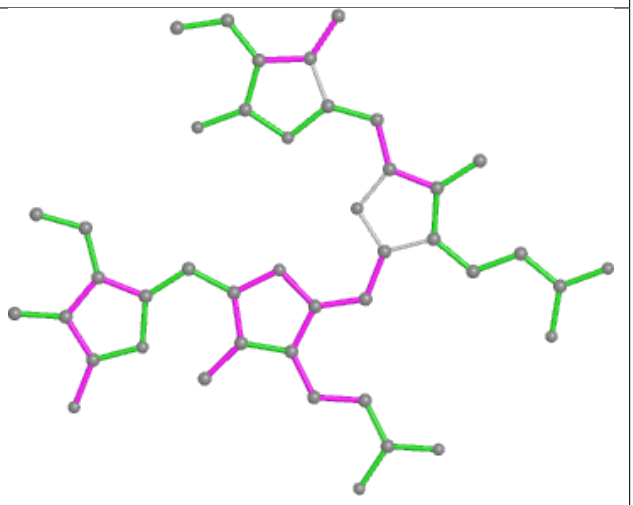

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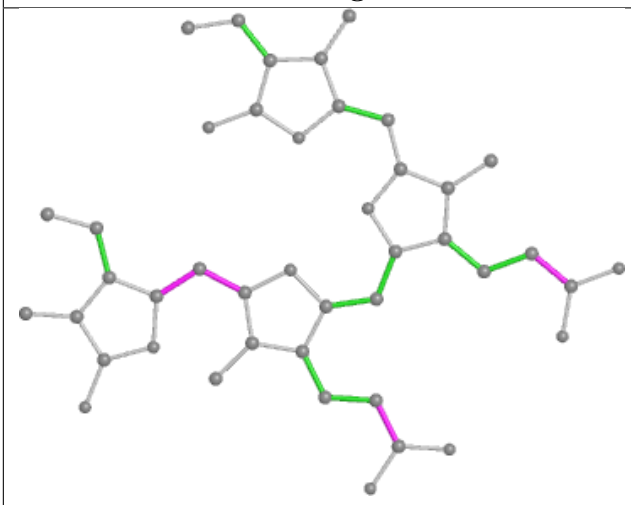

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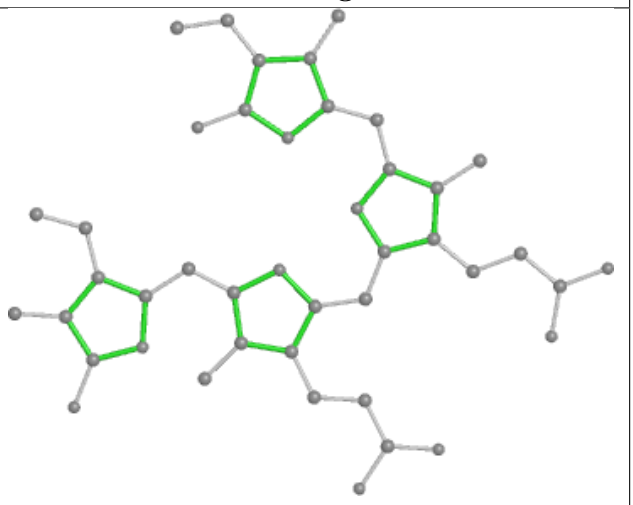
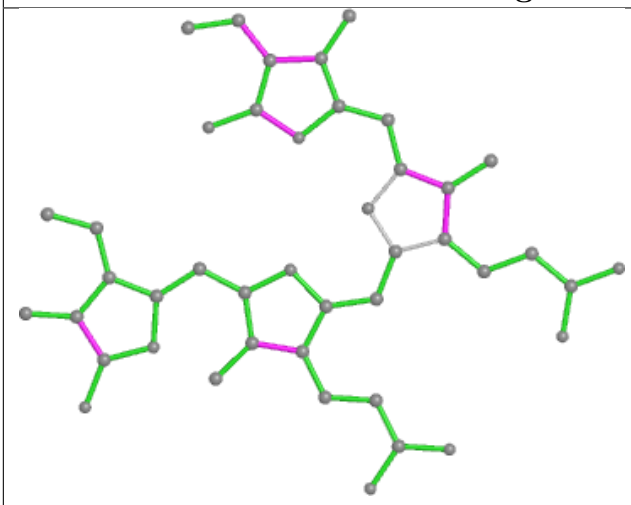


Rings

Ligand PEB aD 202



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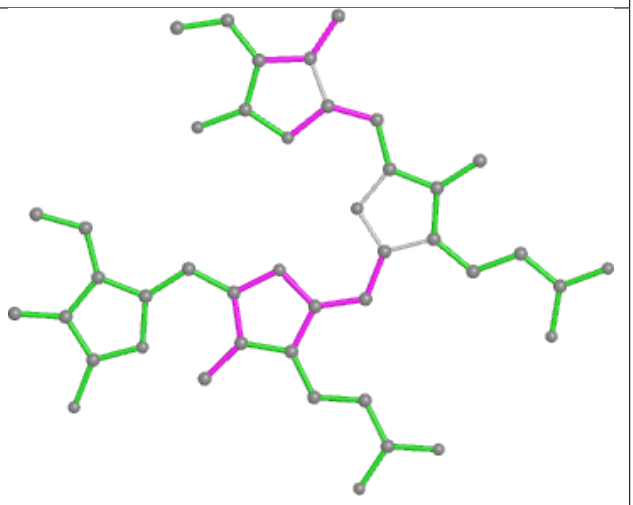

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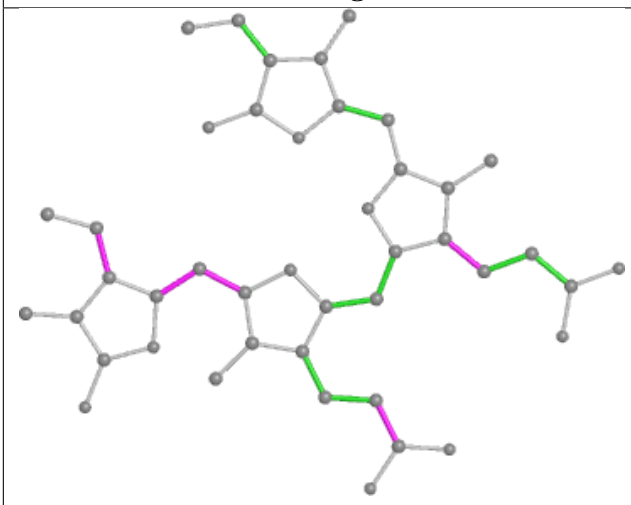

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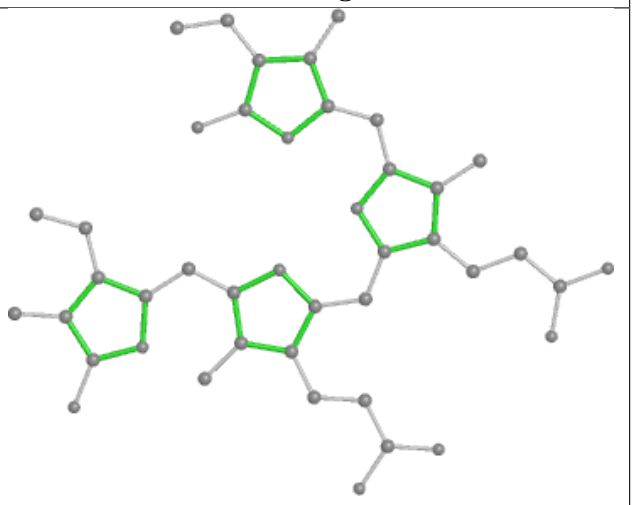
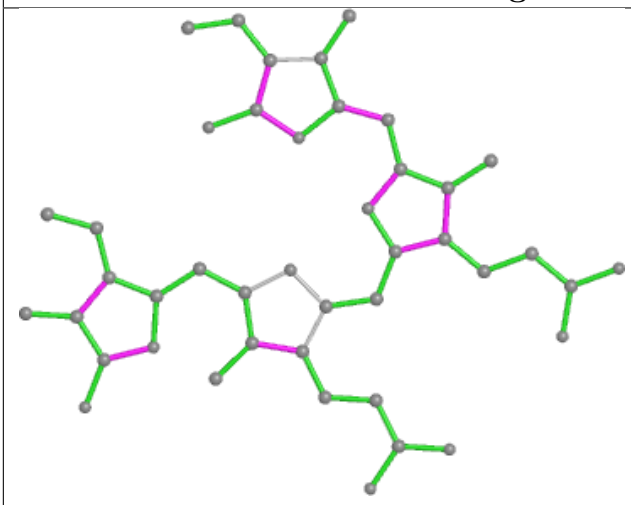


Rings

Ligand PUB jP 1003



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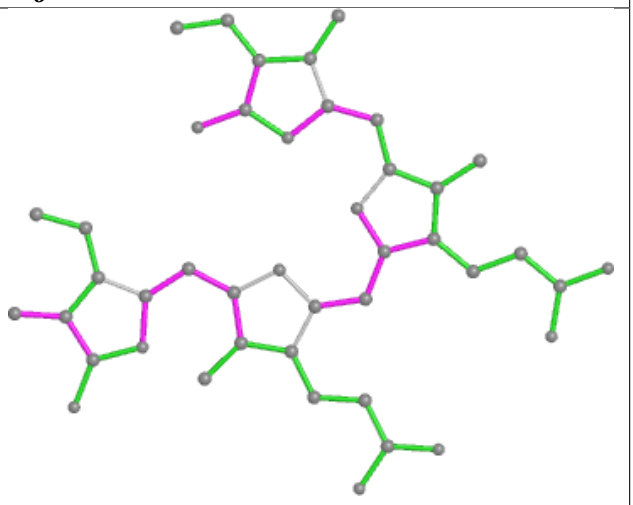

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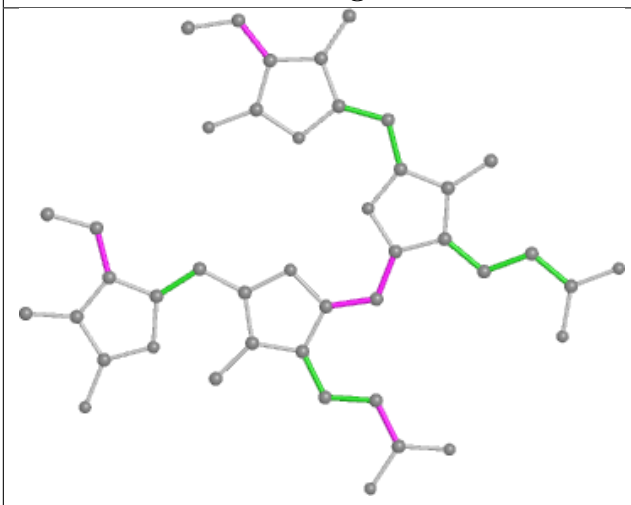

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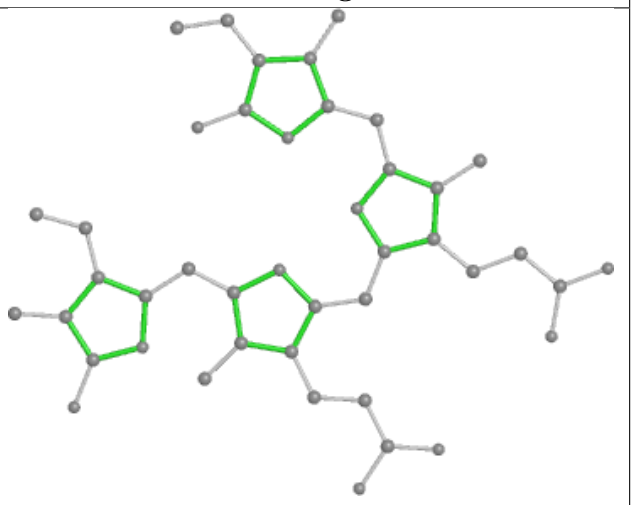
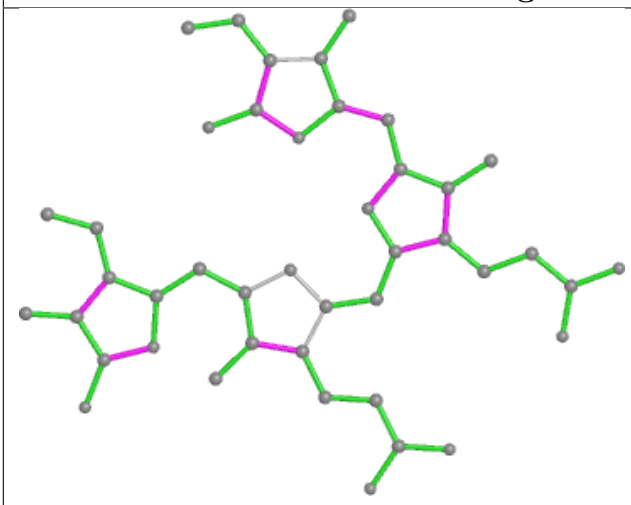


Rings

Ligand PUB J5 203



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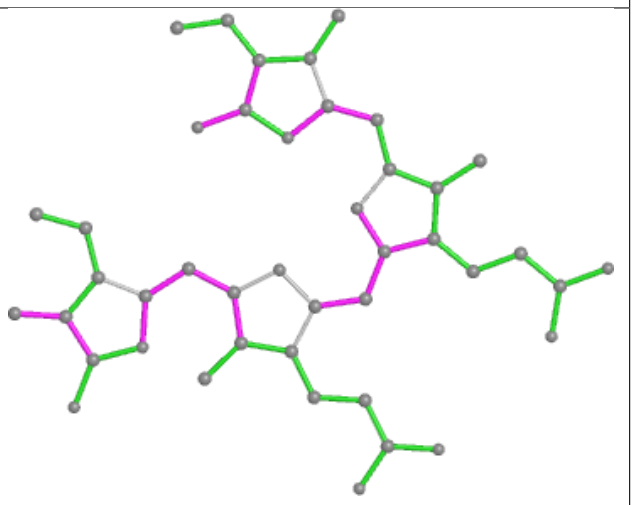

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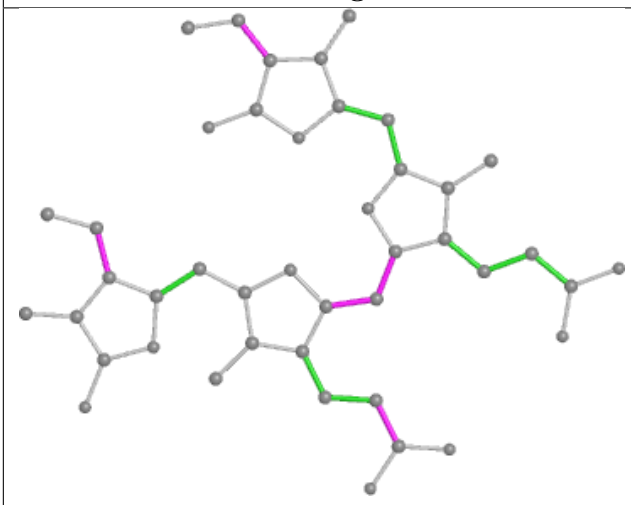

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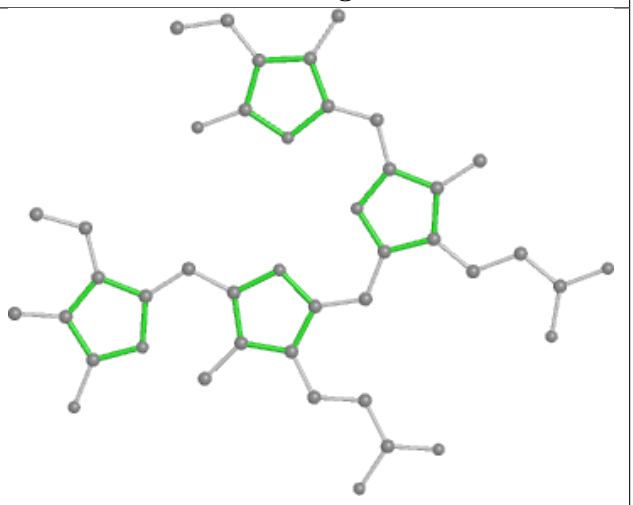
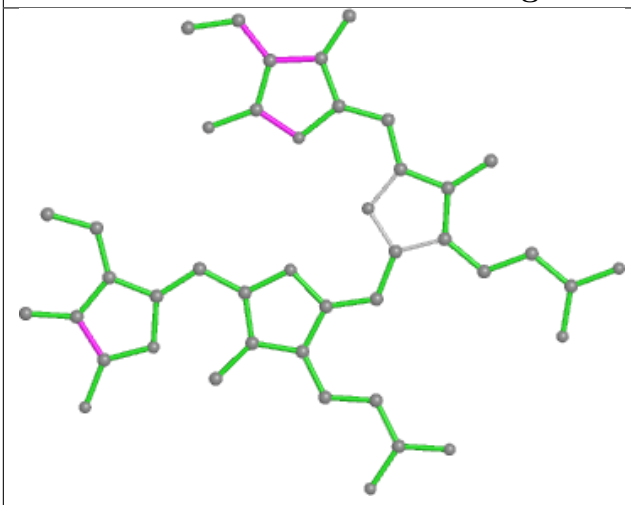


Rings

Ligand PEB r2 202



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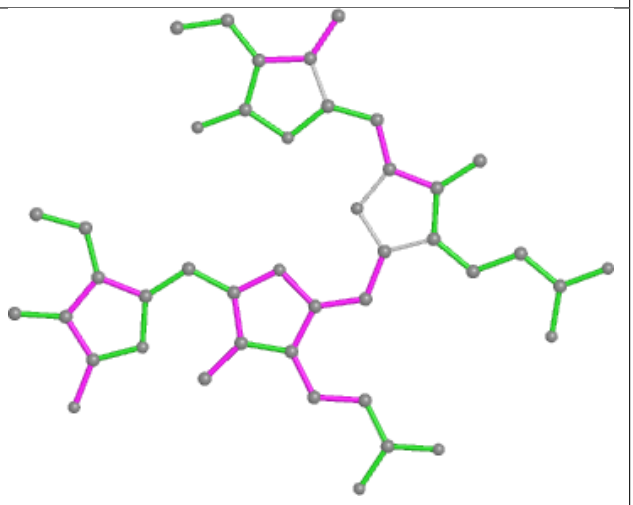
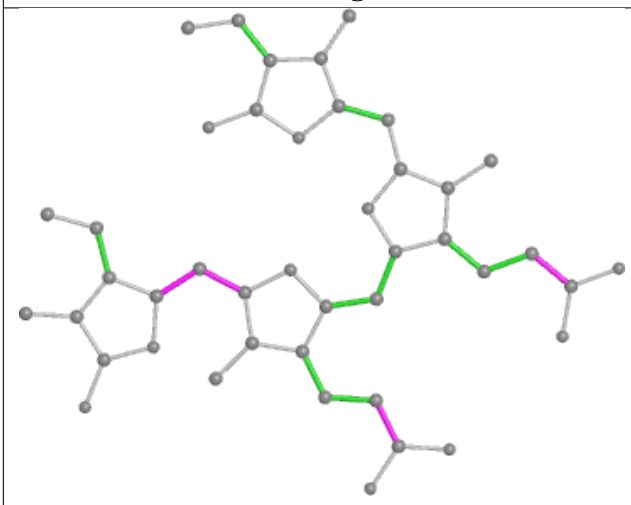
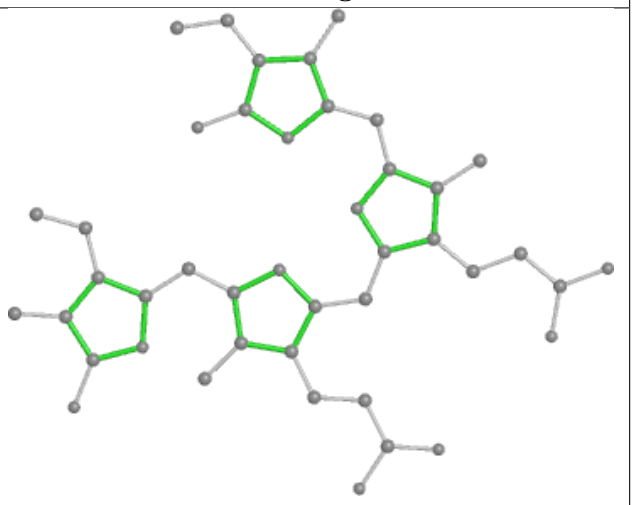


Bond angles

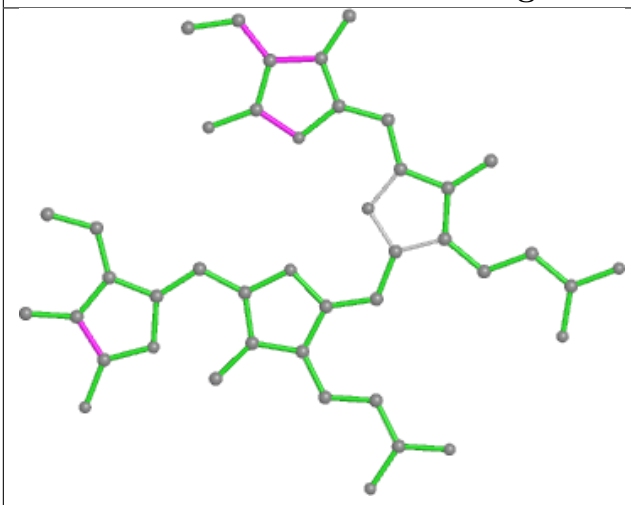


Torsions



Rings

Ligand PEB dh 201



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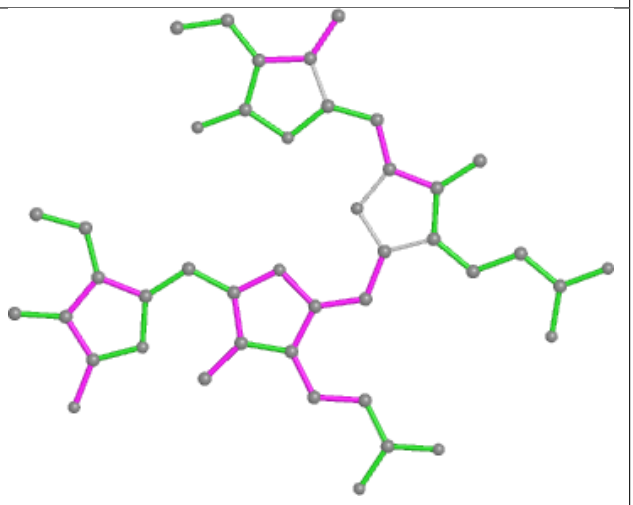

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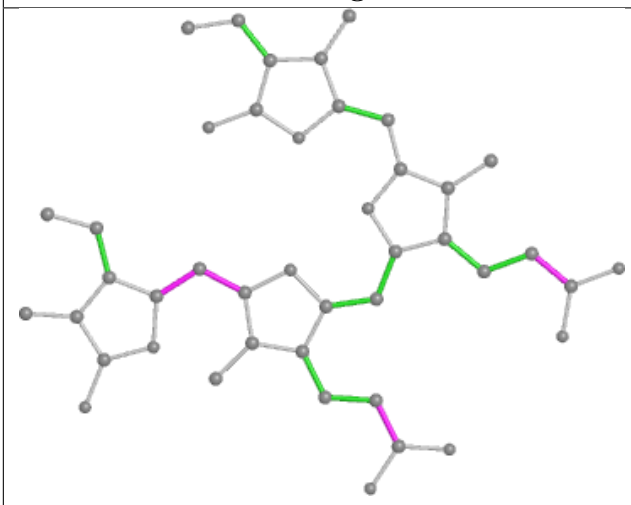

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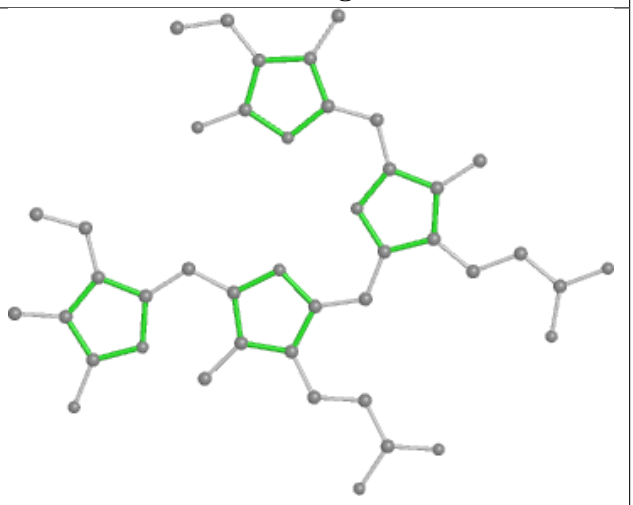
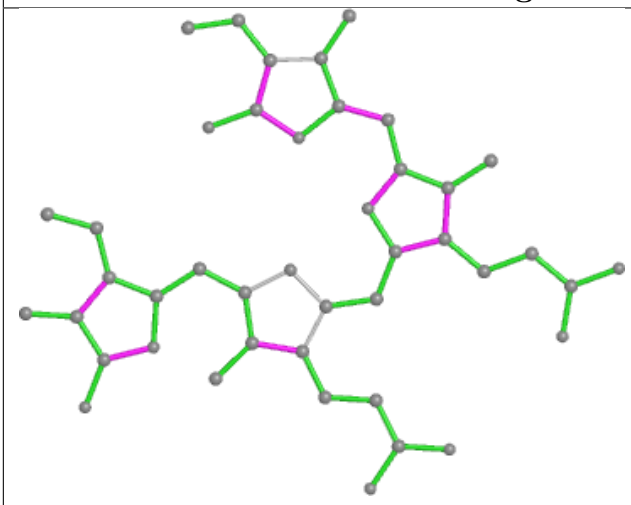


Rings

Ligand PUB F5 203



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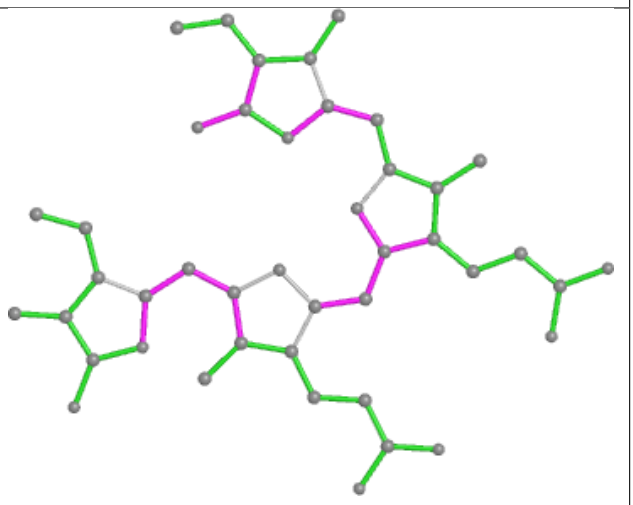

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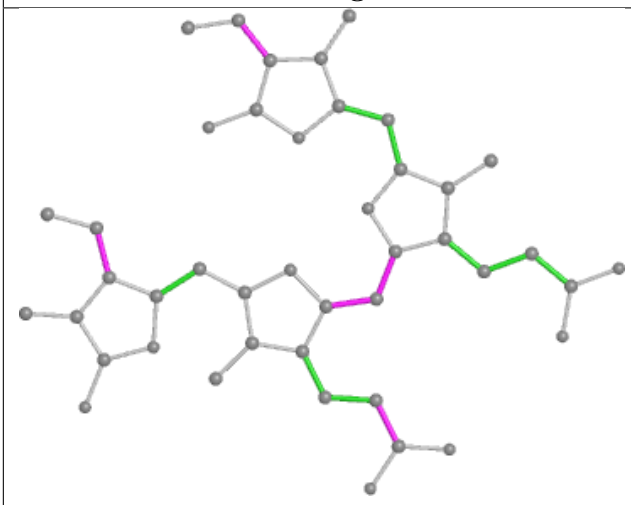

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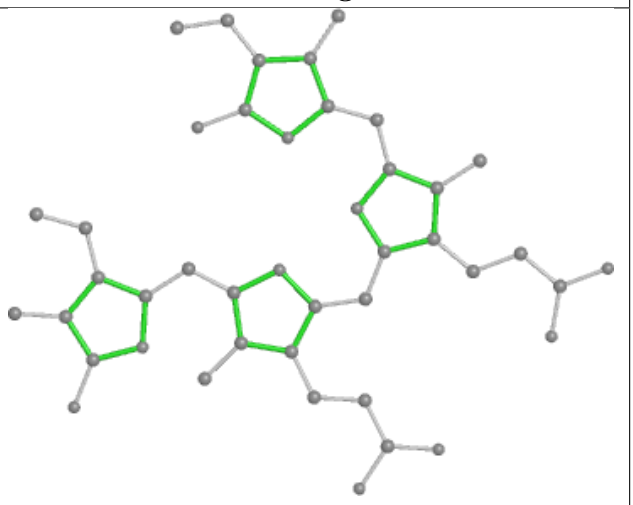
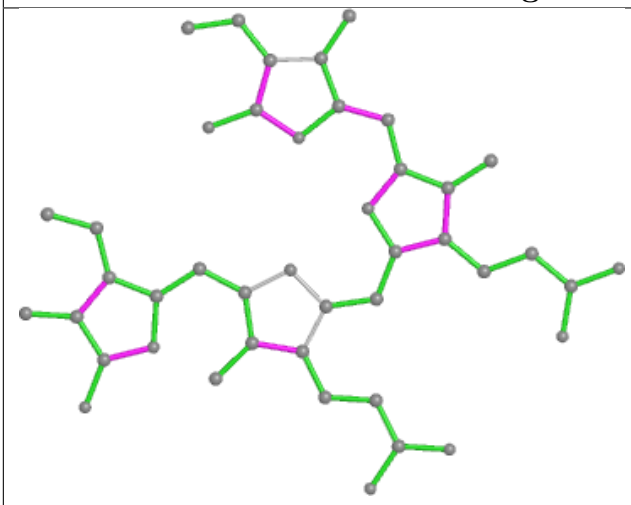


Rings

Ligand PUB l2 203



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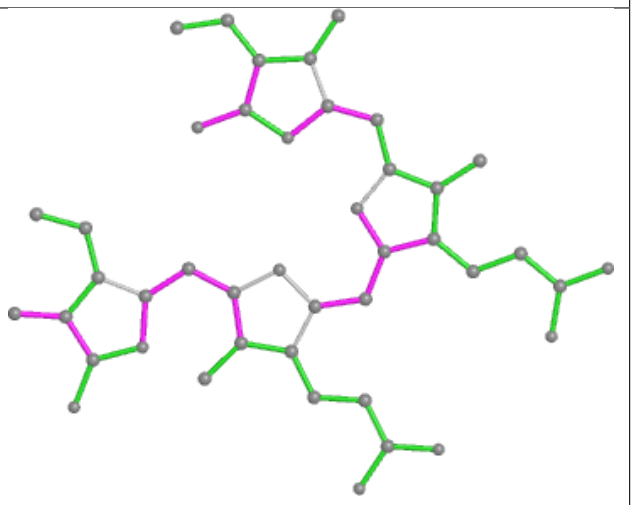

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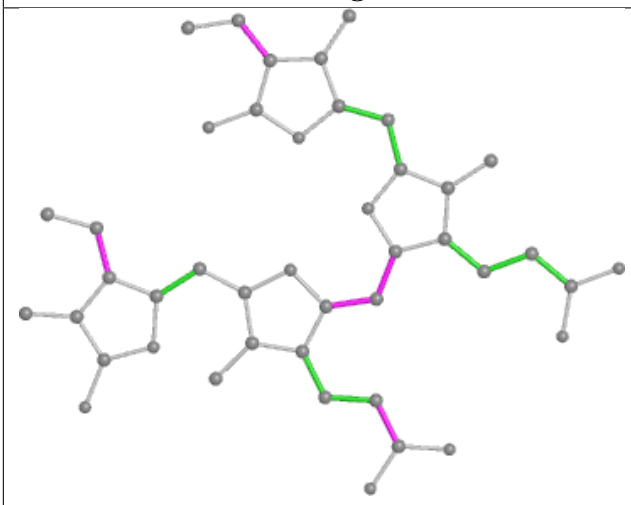

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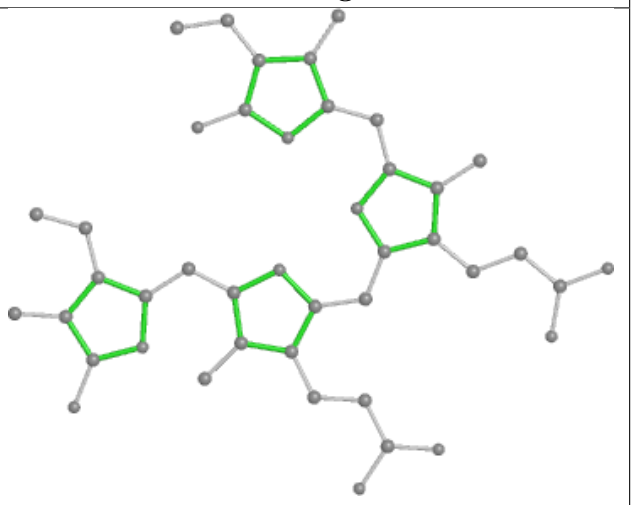
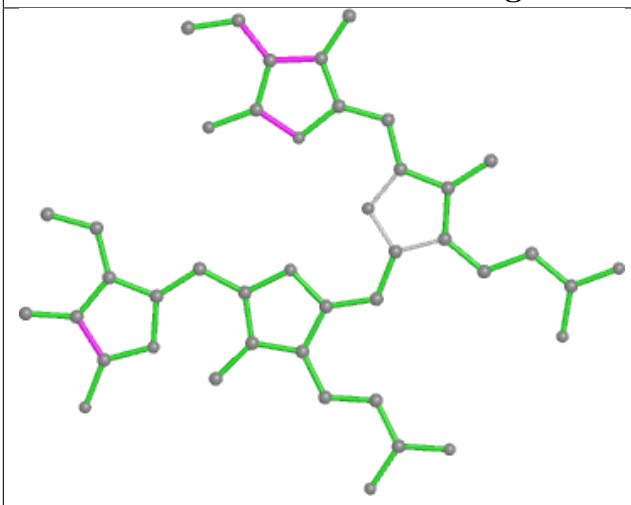


Rings

Ligand PEB bK 1001



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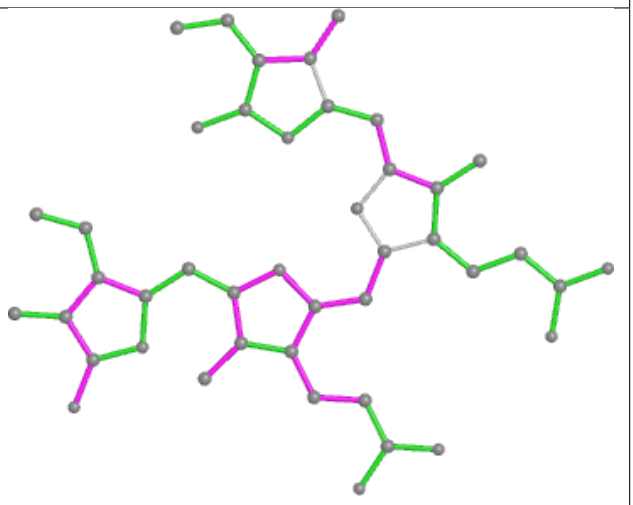
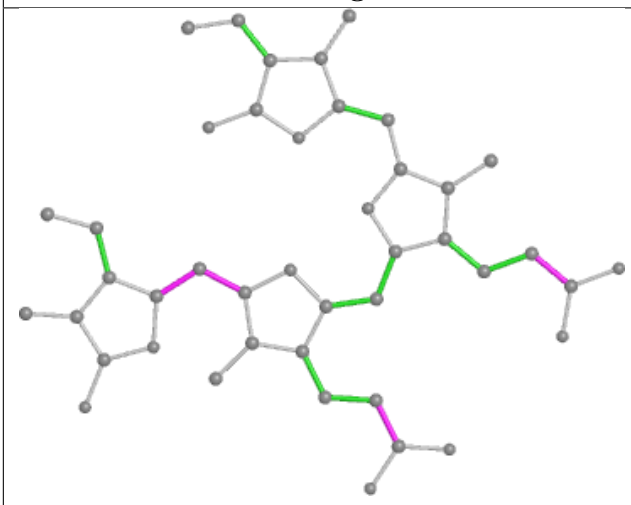


Bond angles



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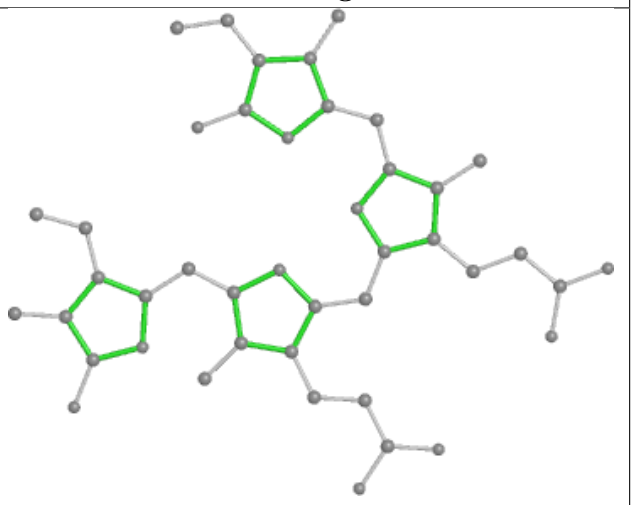
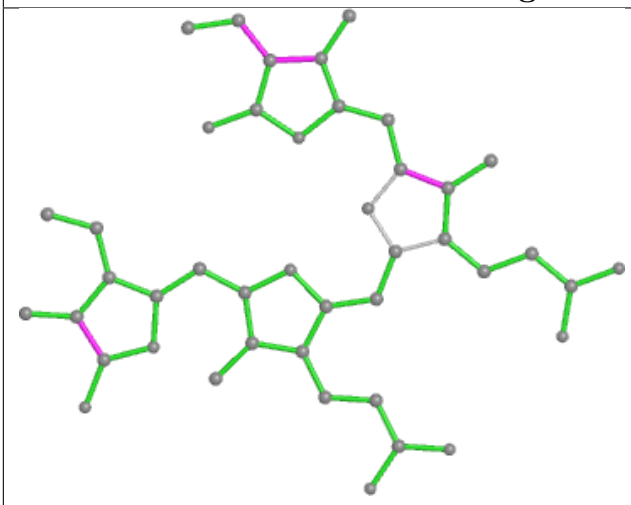


Rings

Ligand PEB S3 202



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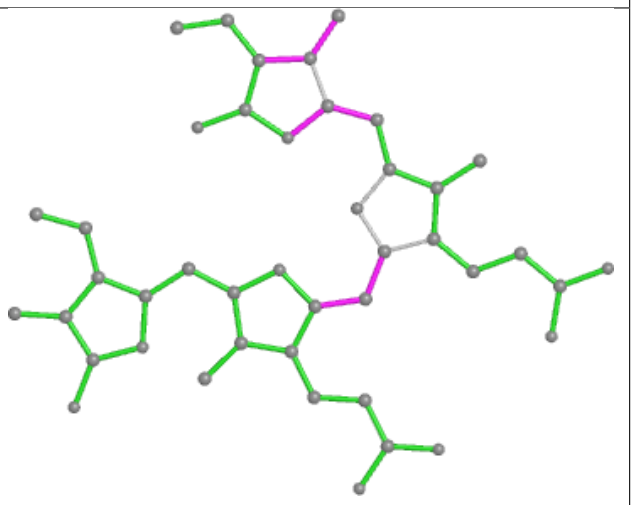

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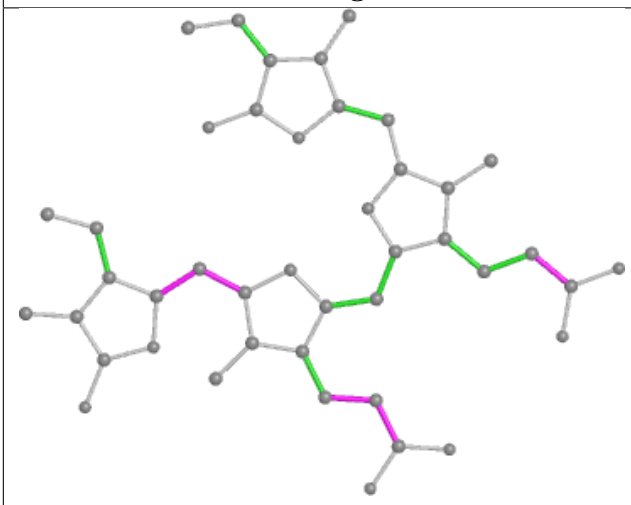

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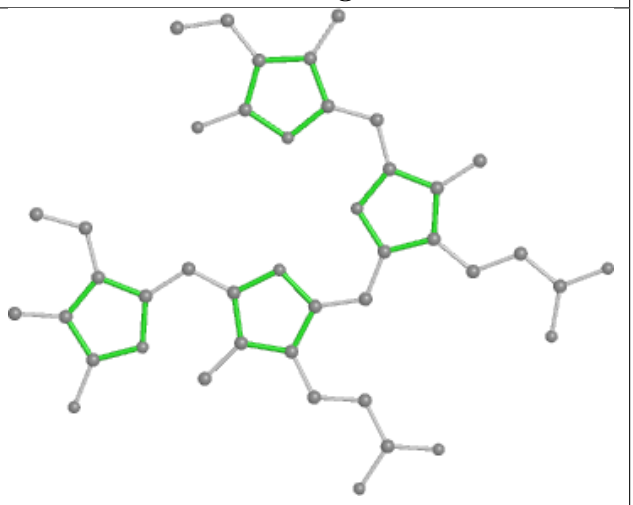
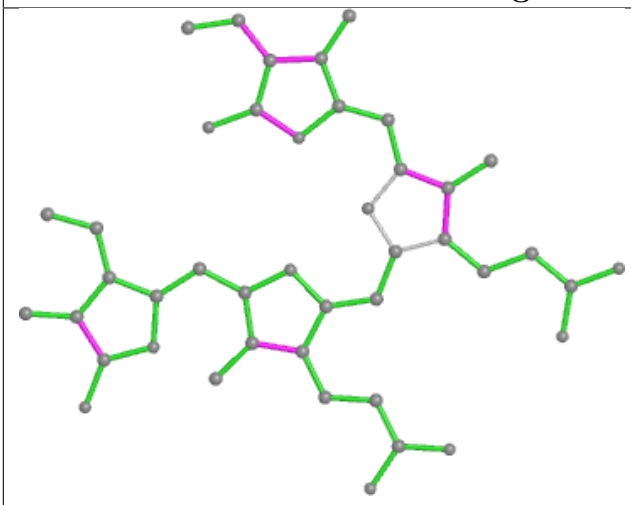


Rings

Ligand PEB jL 1002



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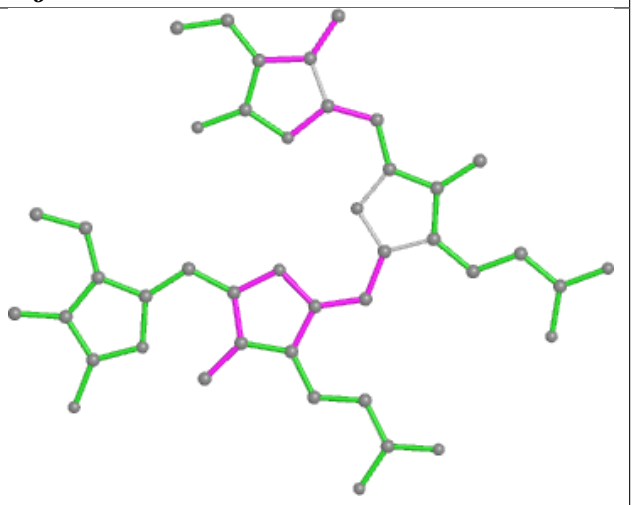

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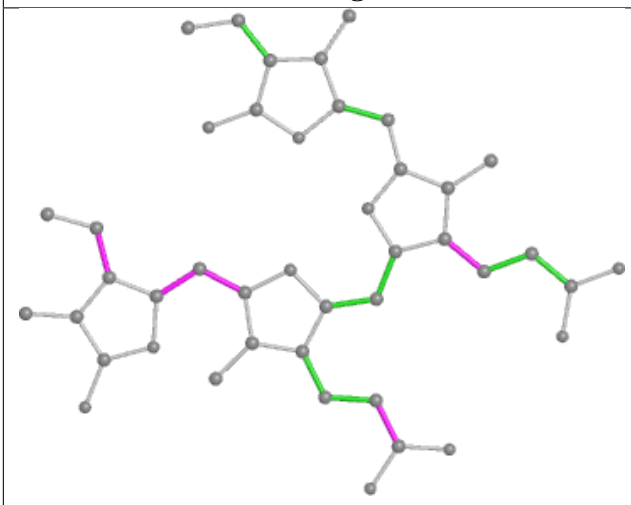

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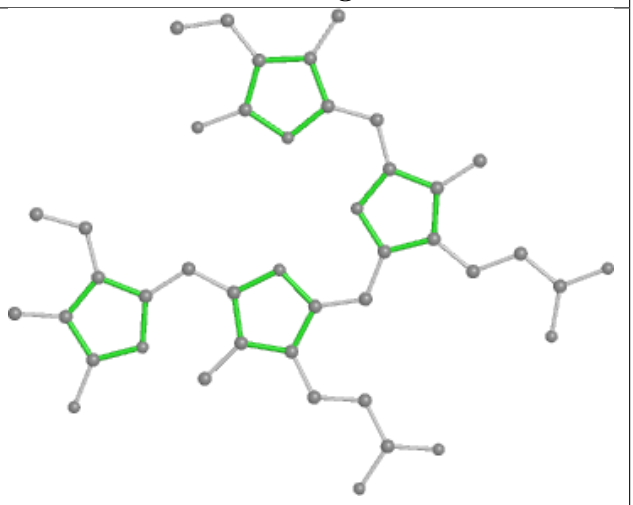

Rings

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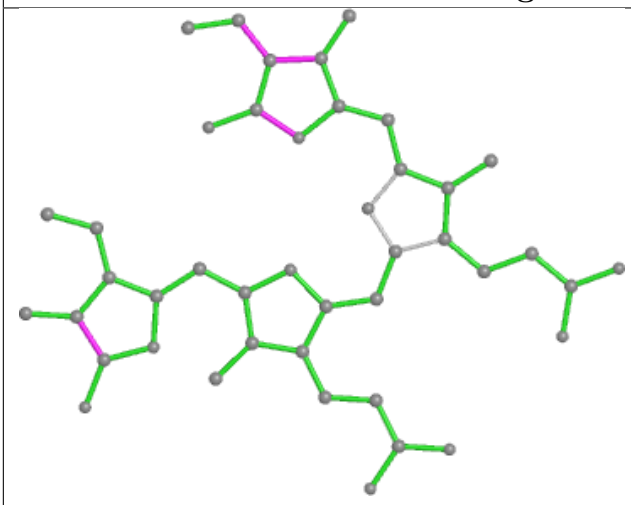

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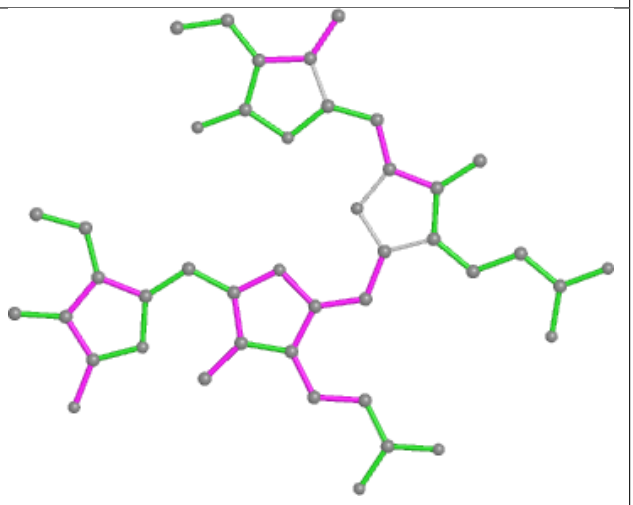

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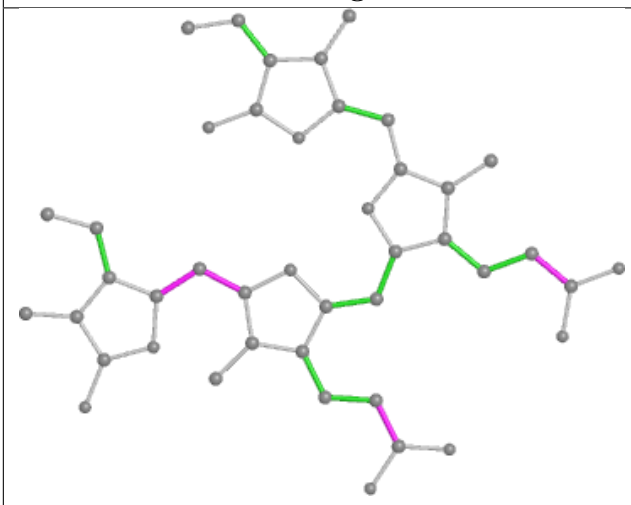

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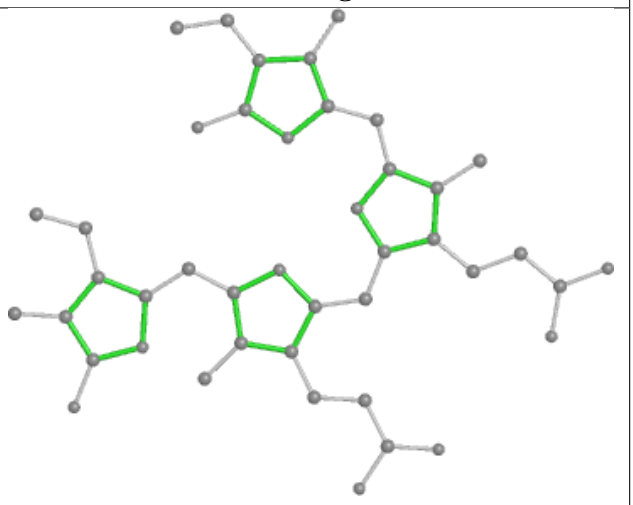
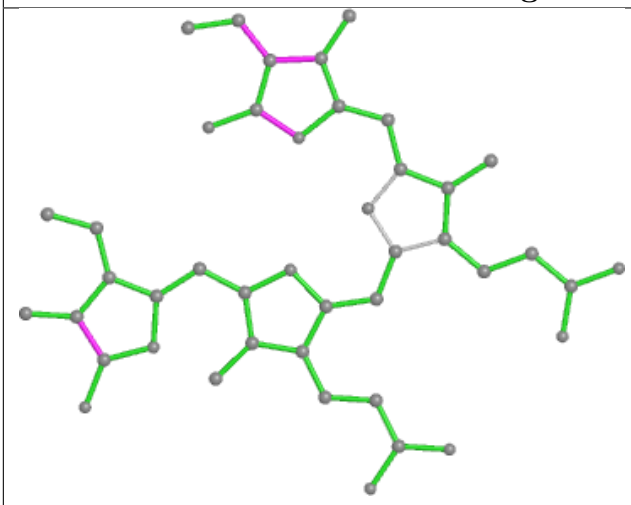


Rings

Ligand PEB z8 202



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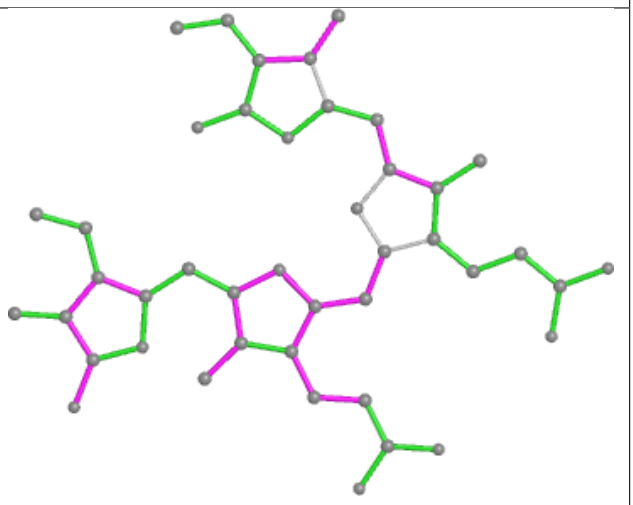
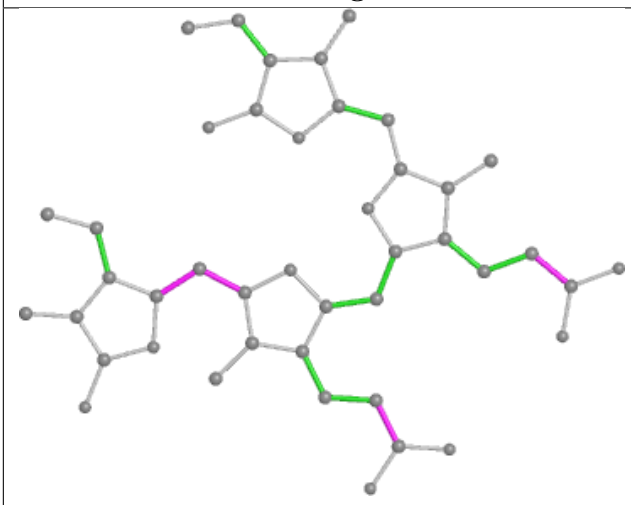


Bond angles



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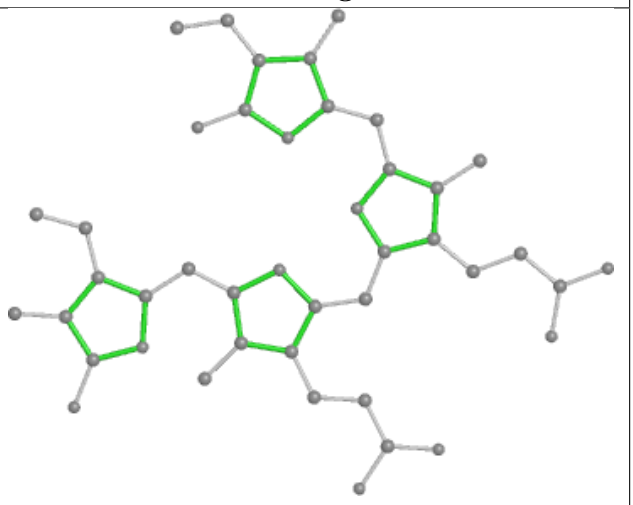
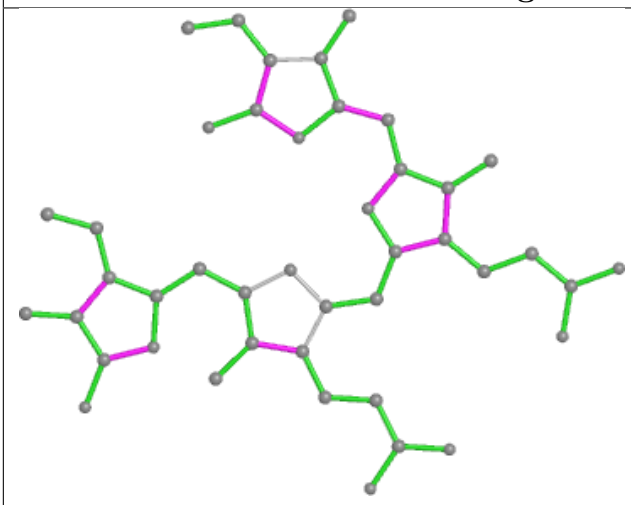


Rings

Ligand PUB gv 203



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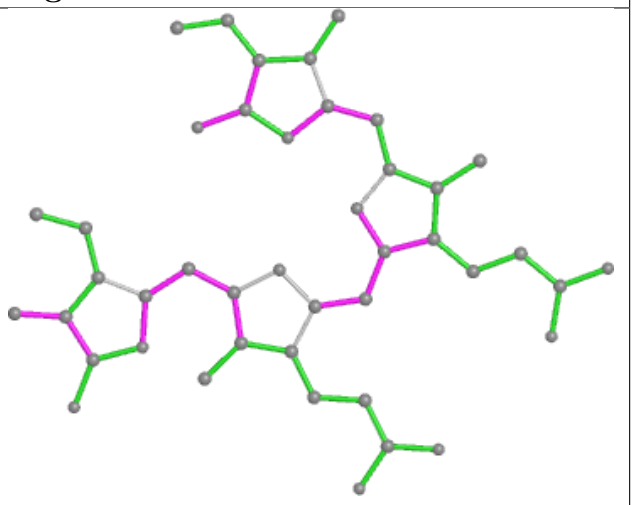

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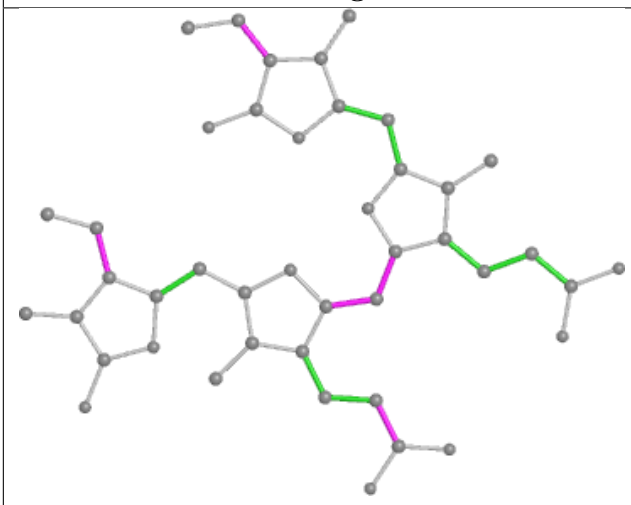

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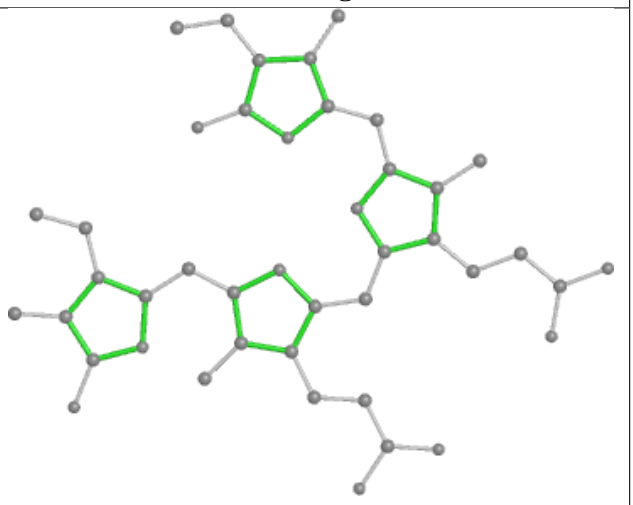
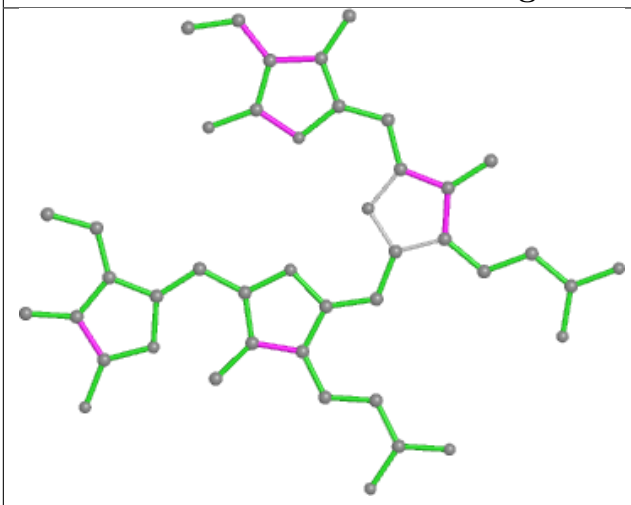


Rings

Ligand PEB p4 202



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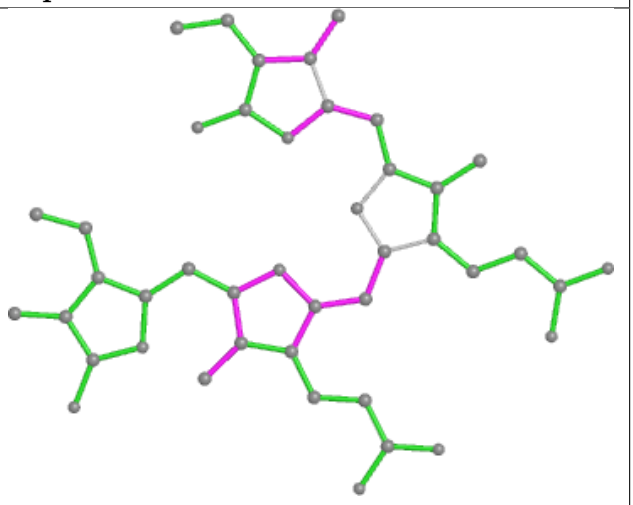

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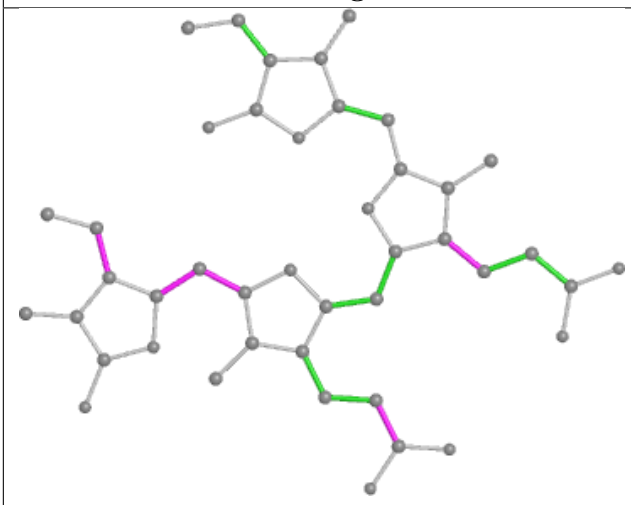

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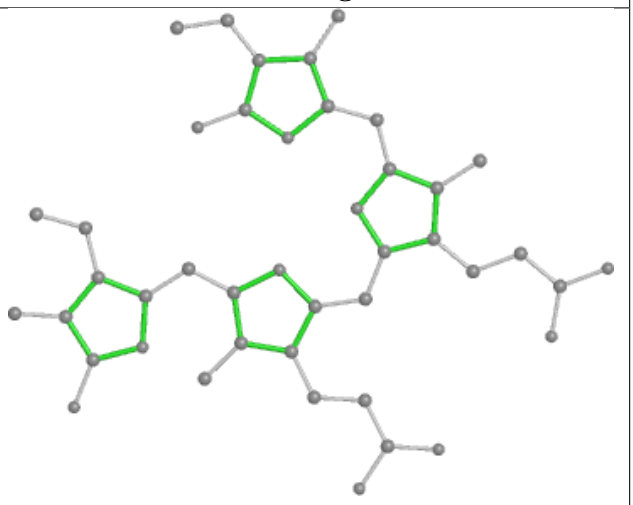
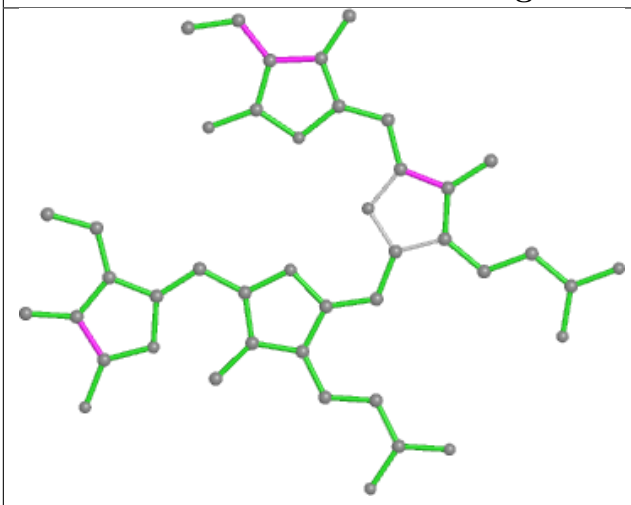


Rings

Ligand PEB A4 202



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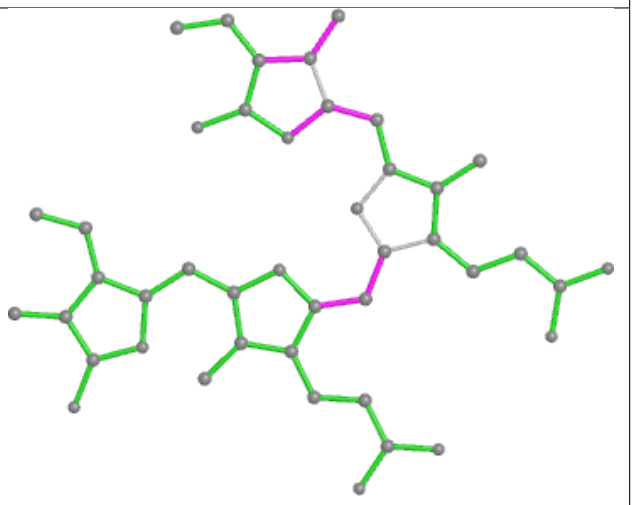

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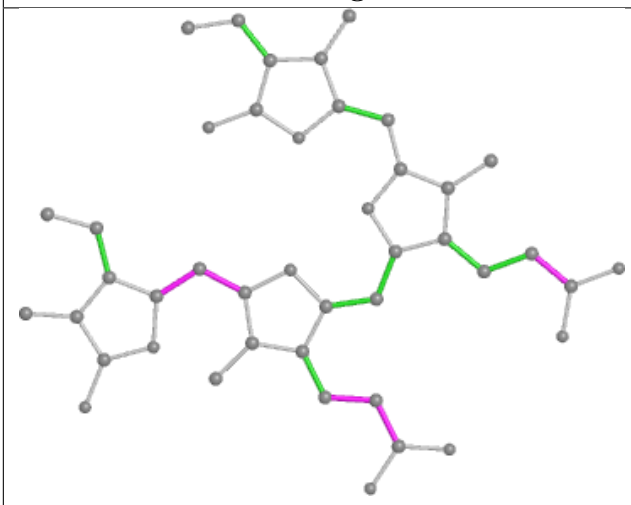

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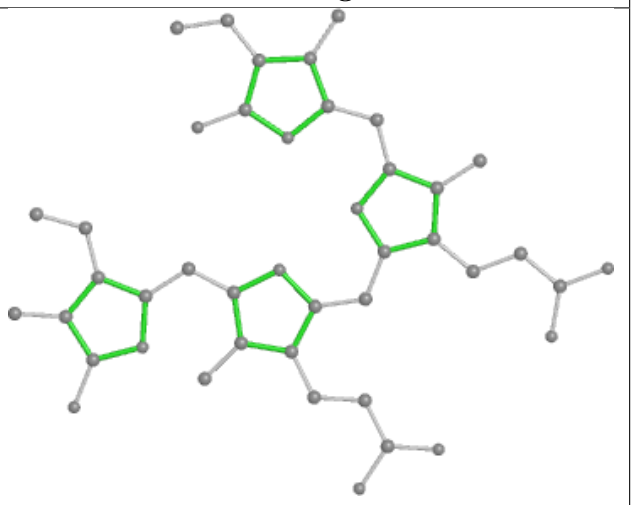
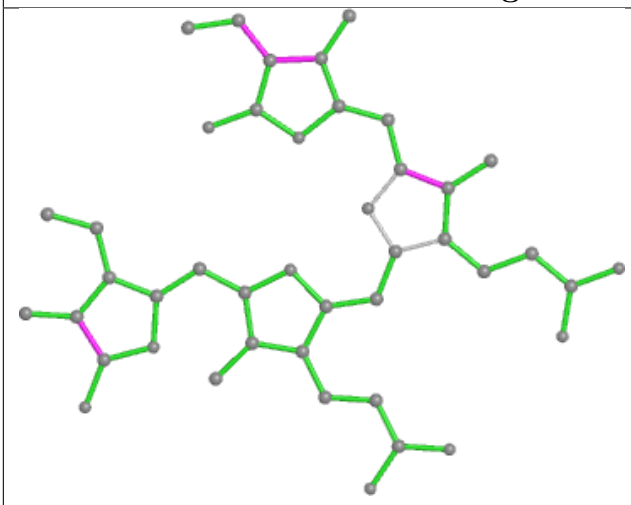


Rings

Ligand PEB hM 1002



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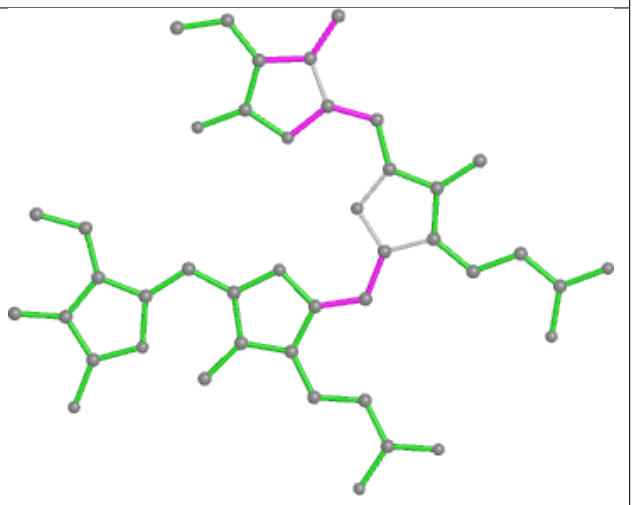

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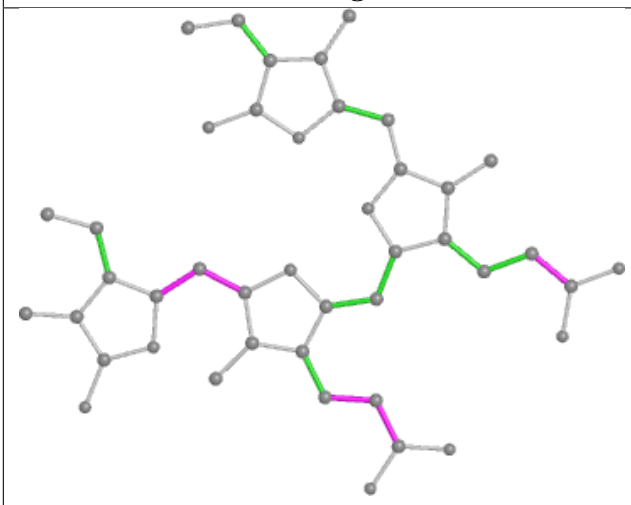

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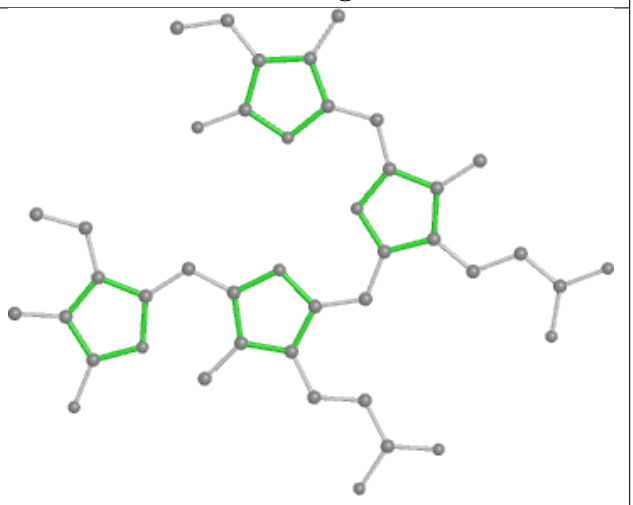
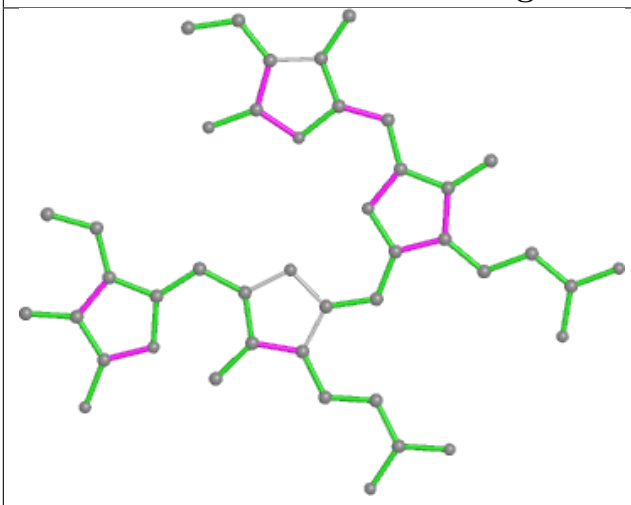


Rings

Ligand PUB d3 303



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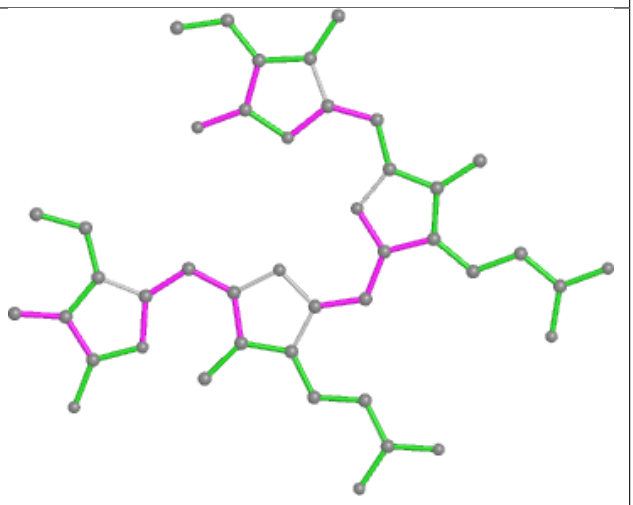
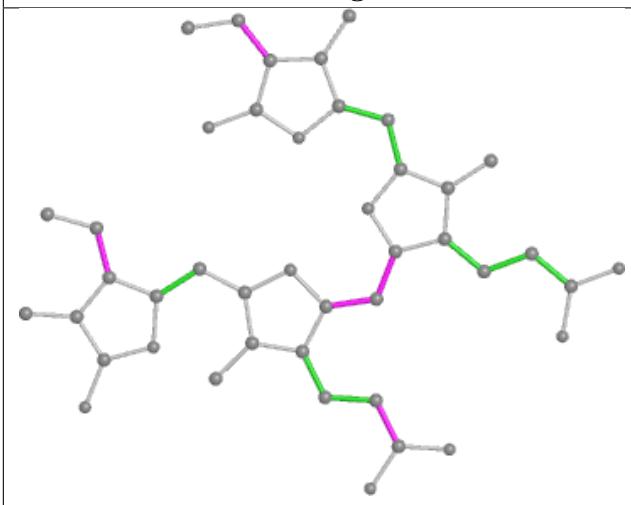


Bond angles



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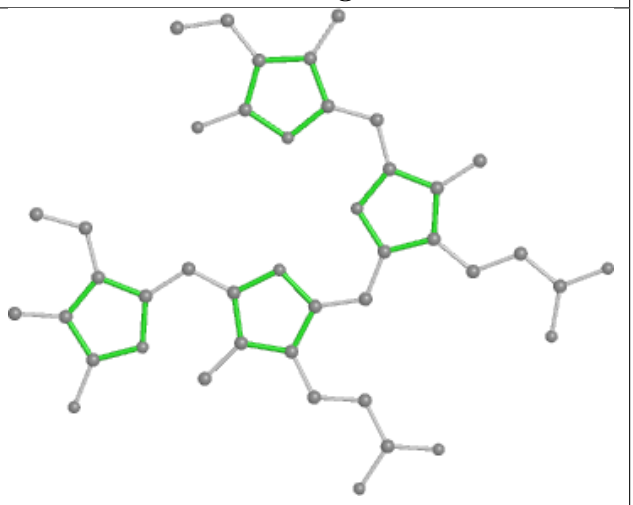
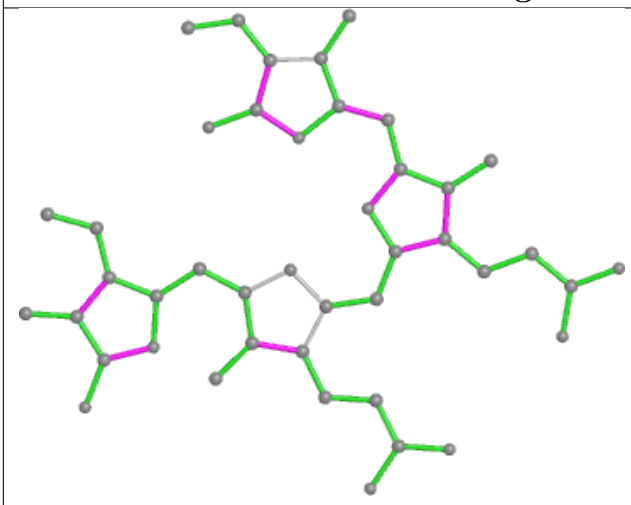


Rings

Ligand PUB hZ 405



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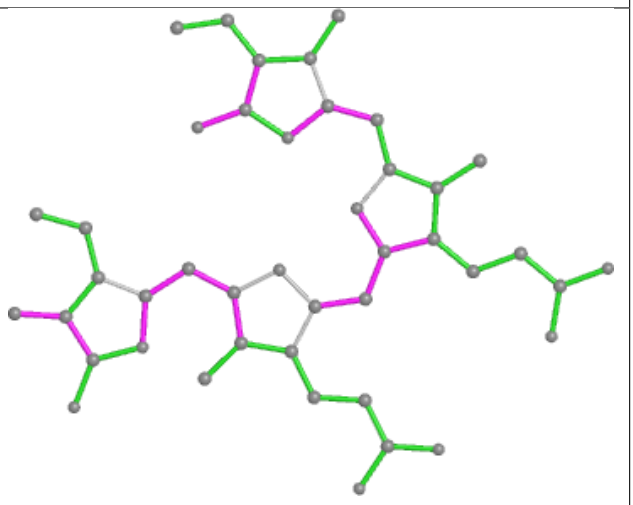

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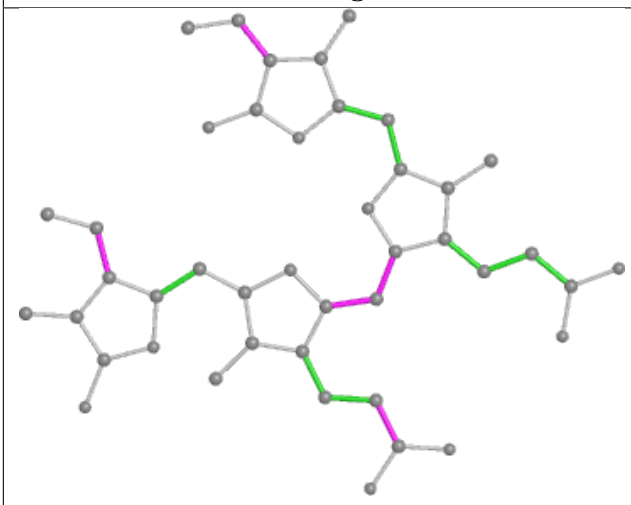
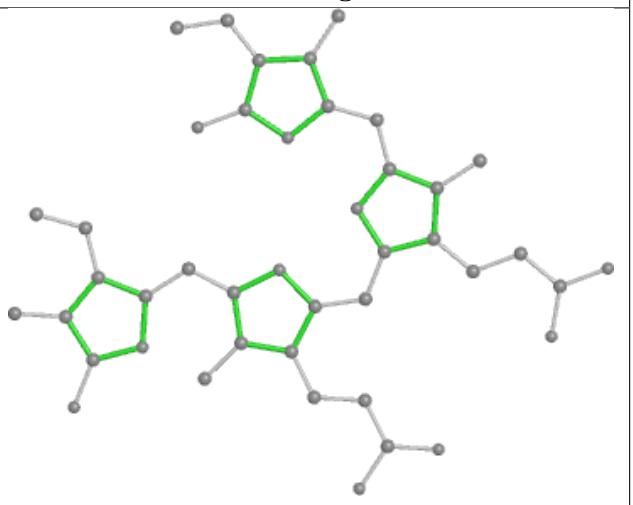
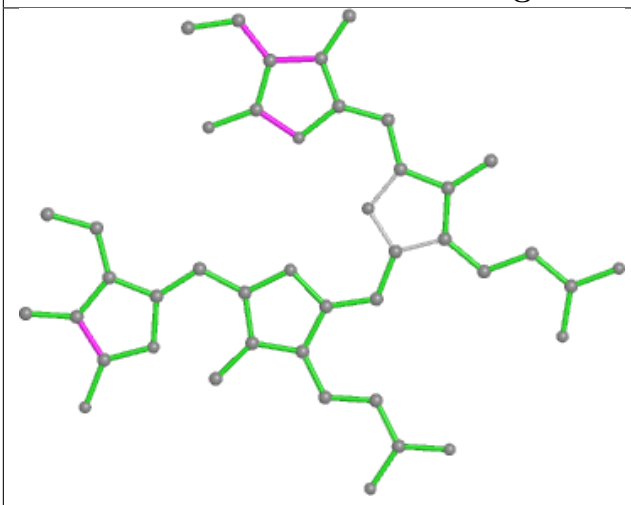


Torsions



Rings

Ligand PEB dH 202



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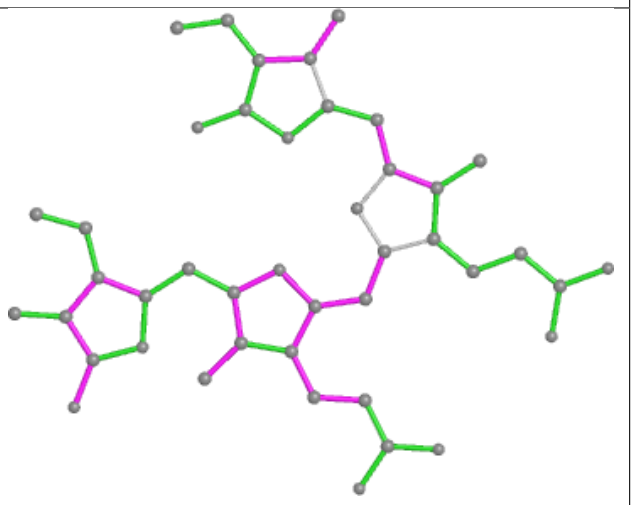

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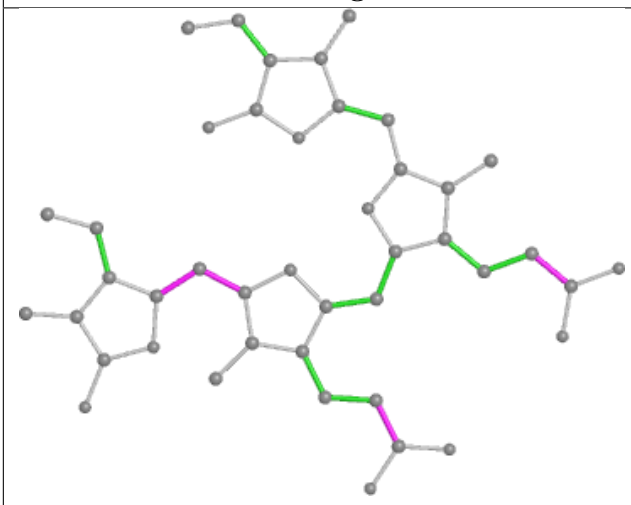

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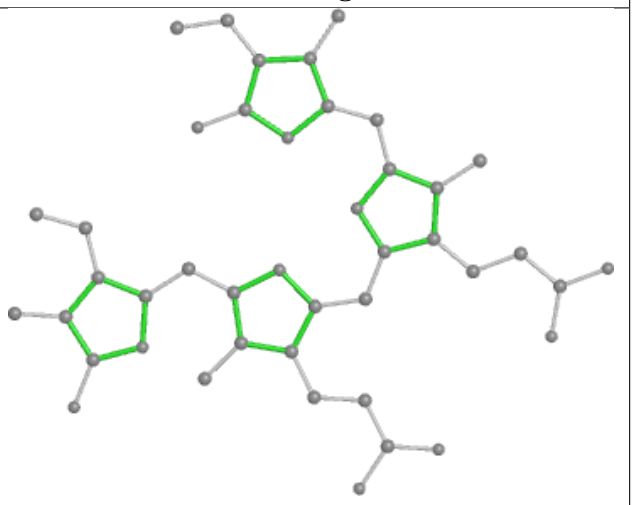
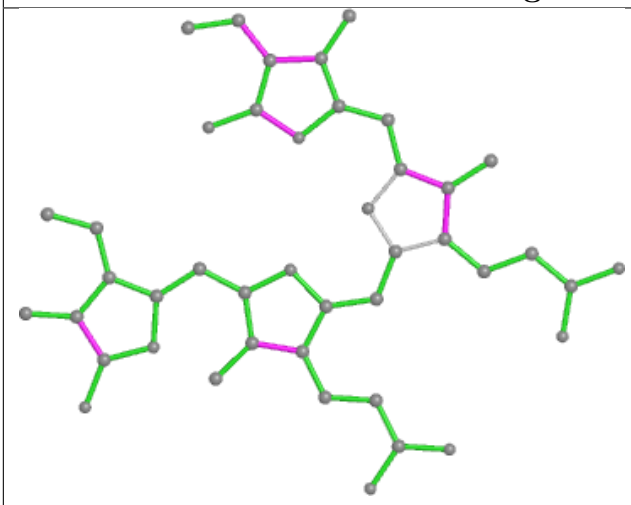


Rings

Ligand PEB gi 202



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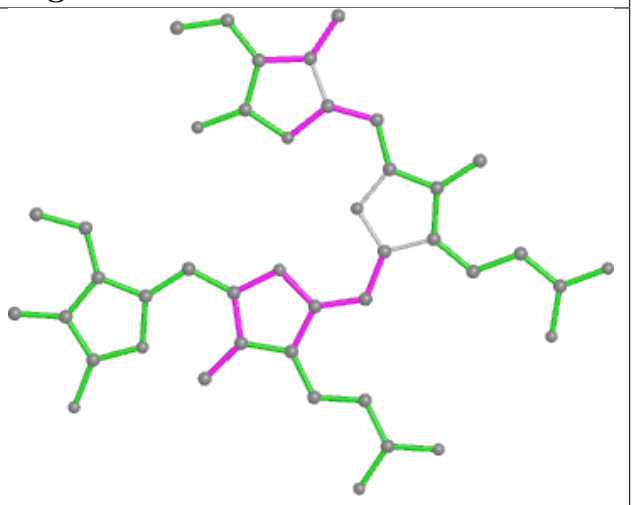

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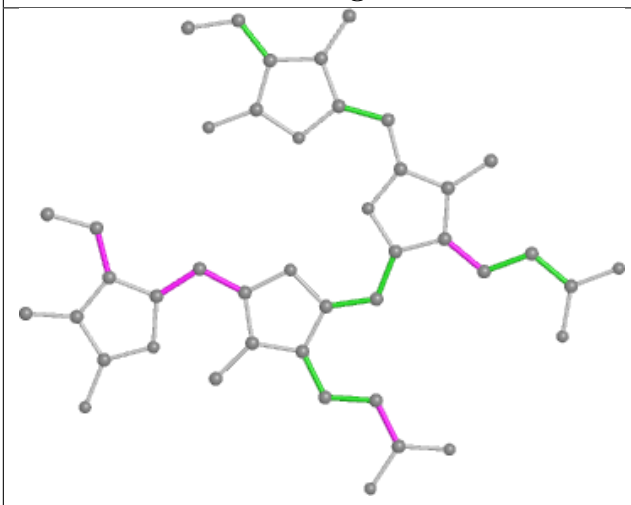

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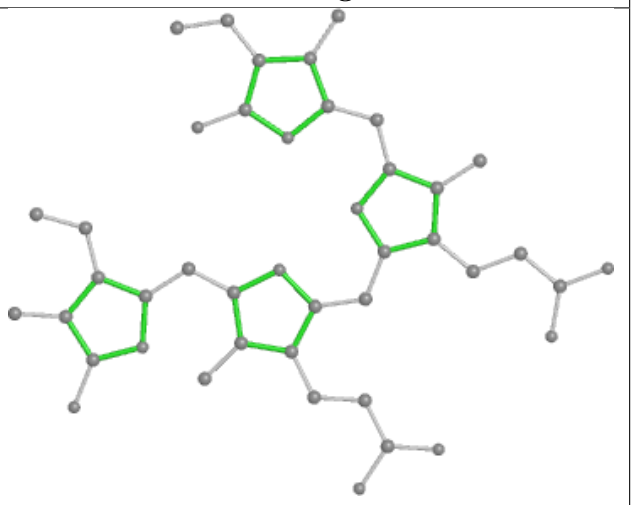

Rings

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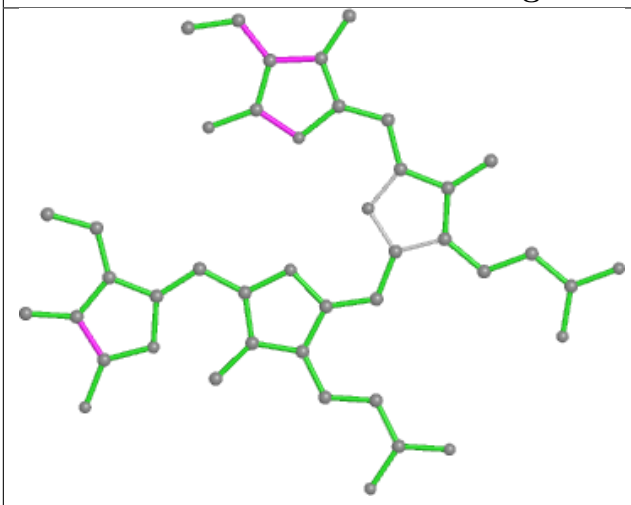

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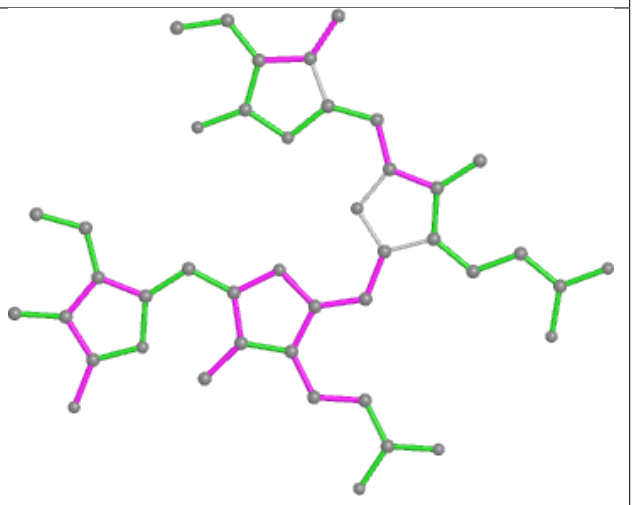

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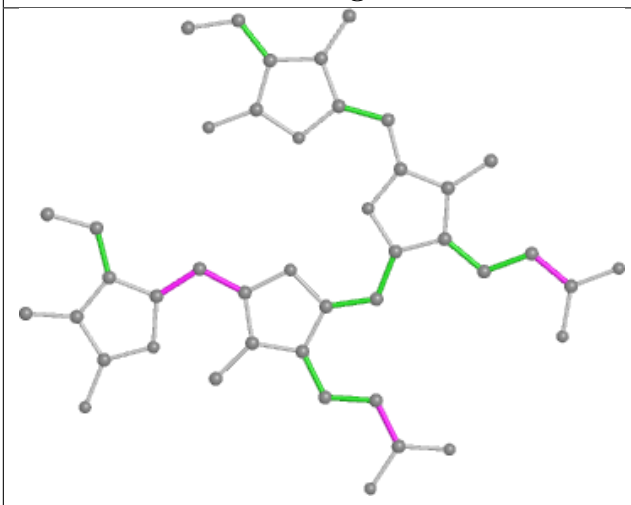

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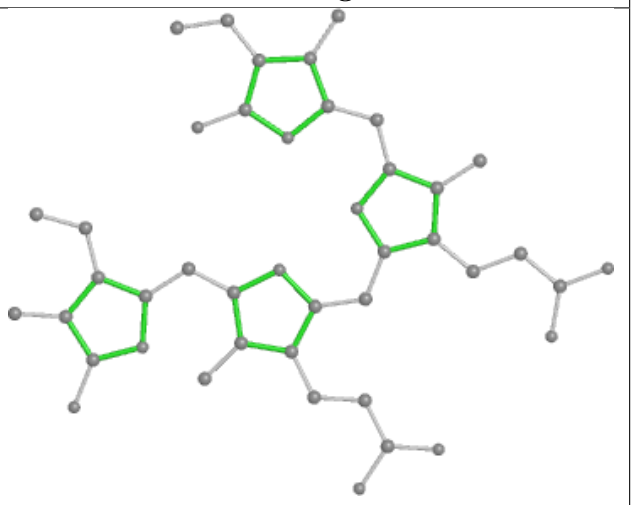

Rings

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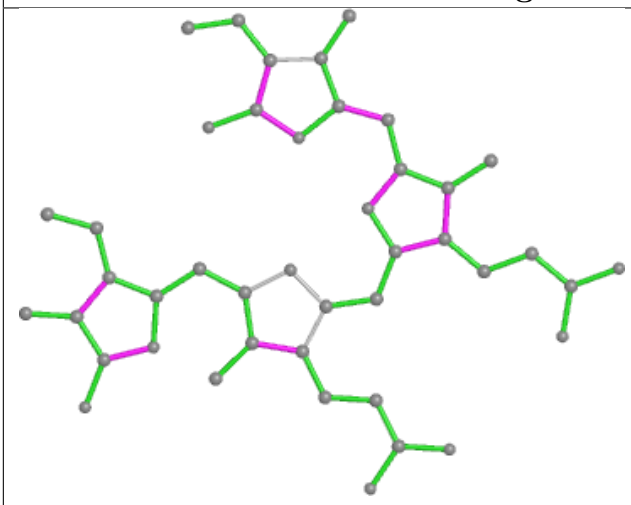

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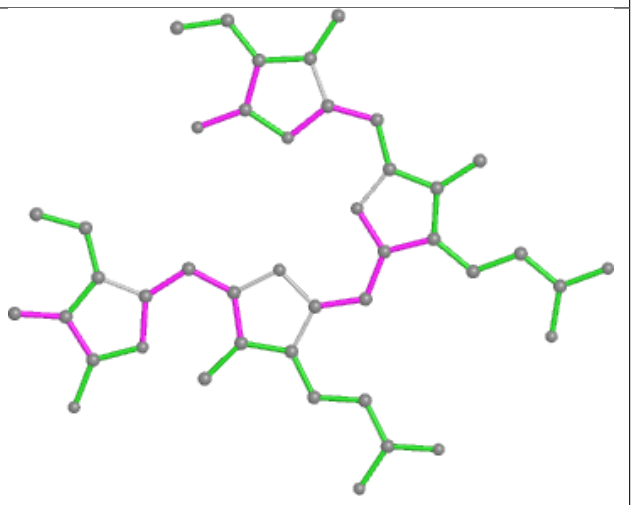

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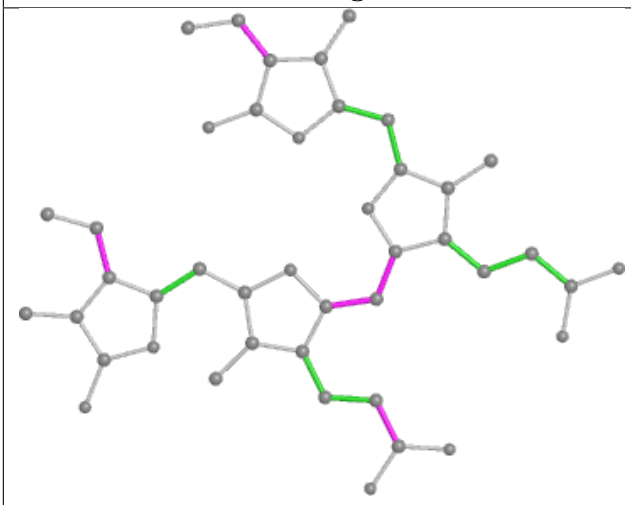

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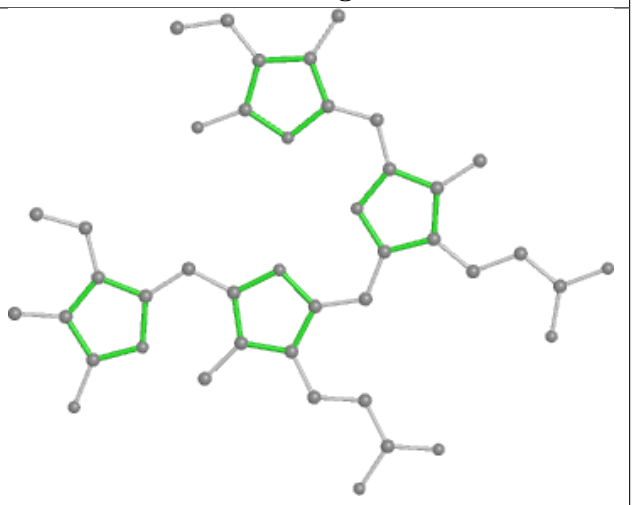

Rings

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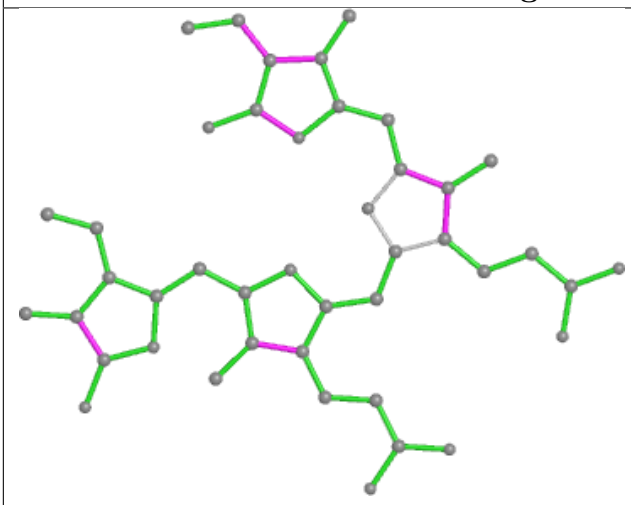

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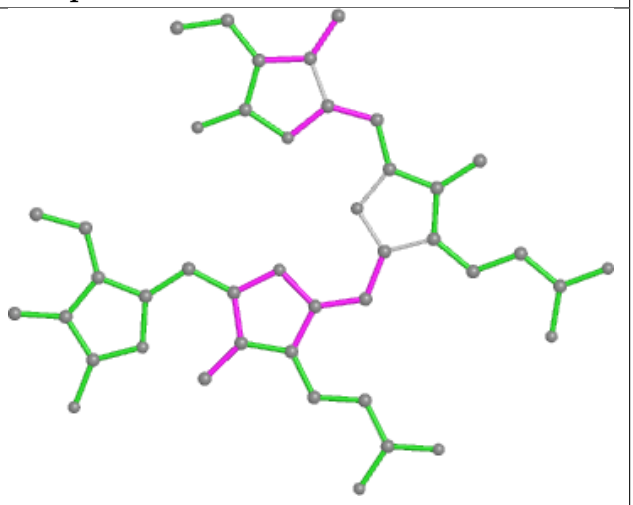

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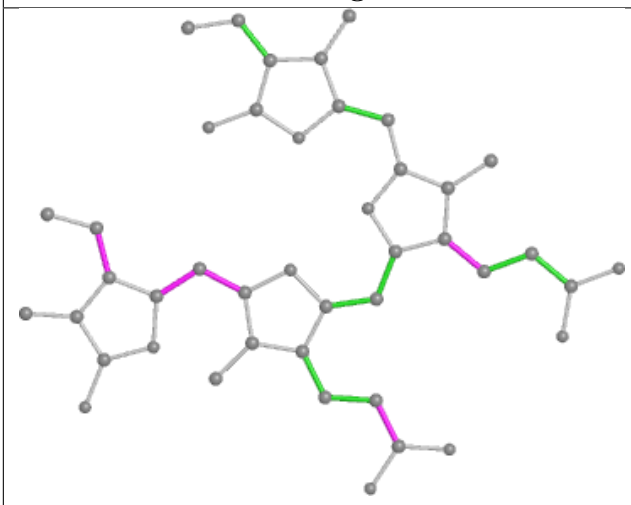

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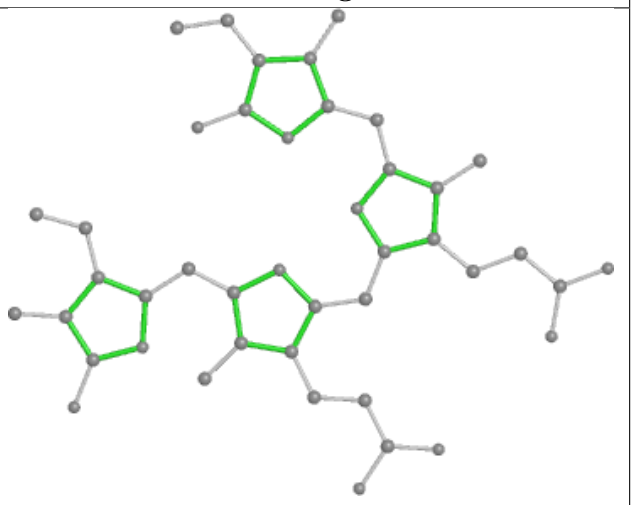

Rings

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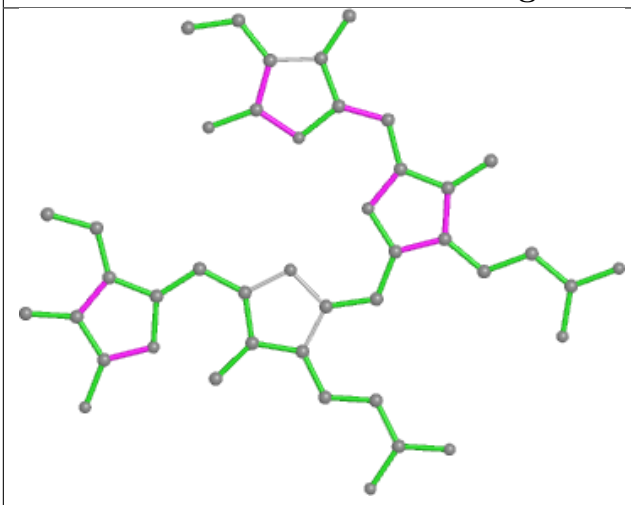

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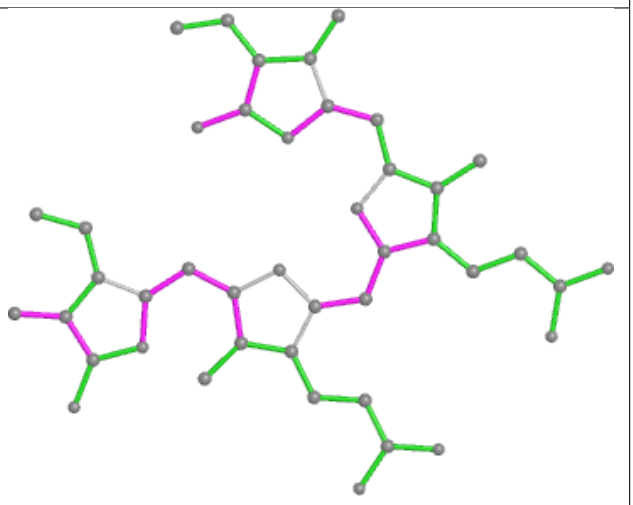

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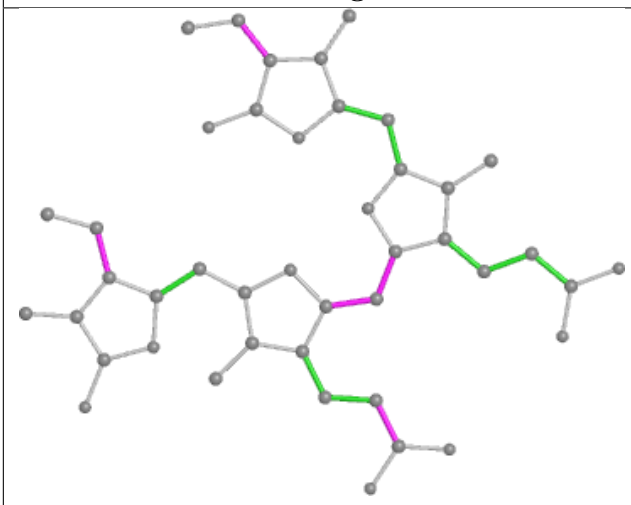

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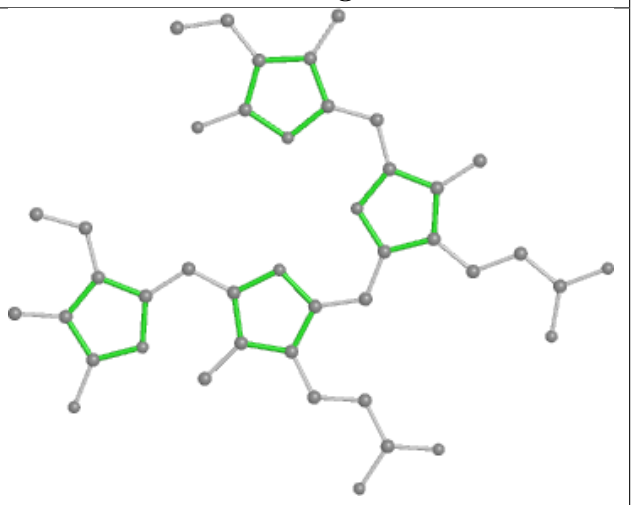

Rings

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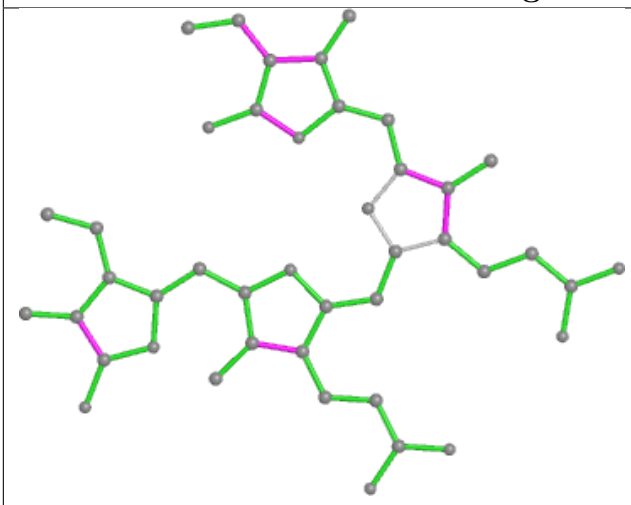

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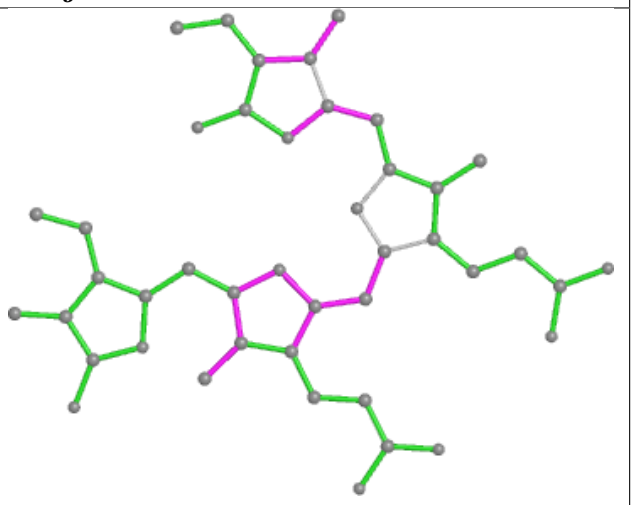

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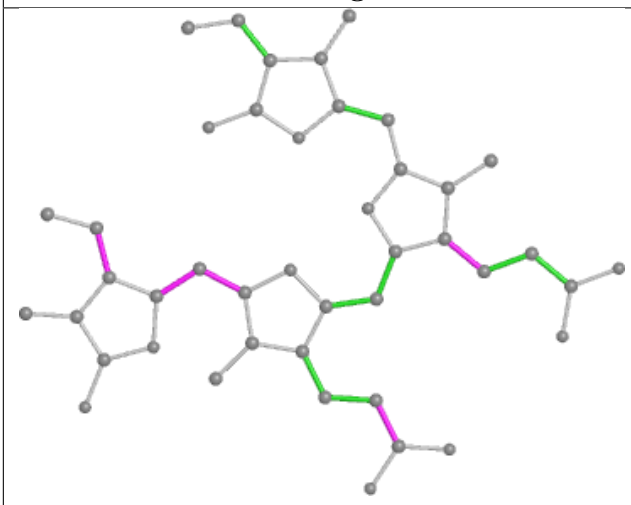

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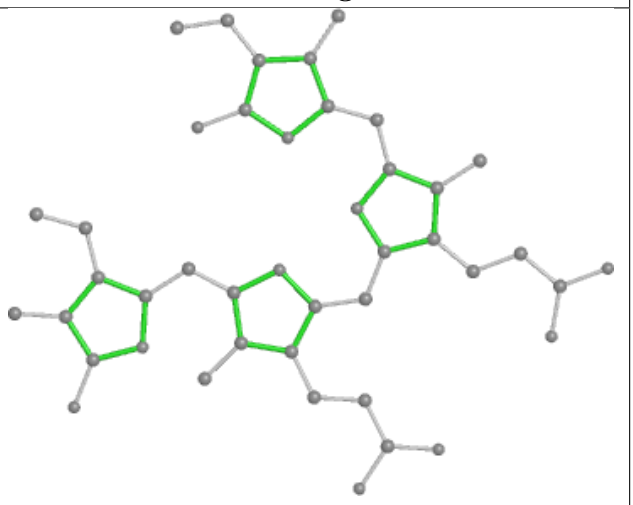

Rings

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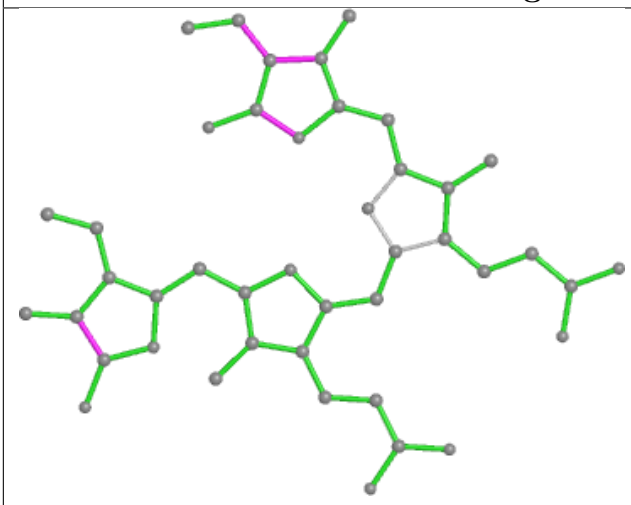

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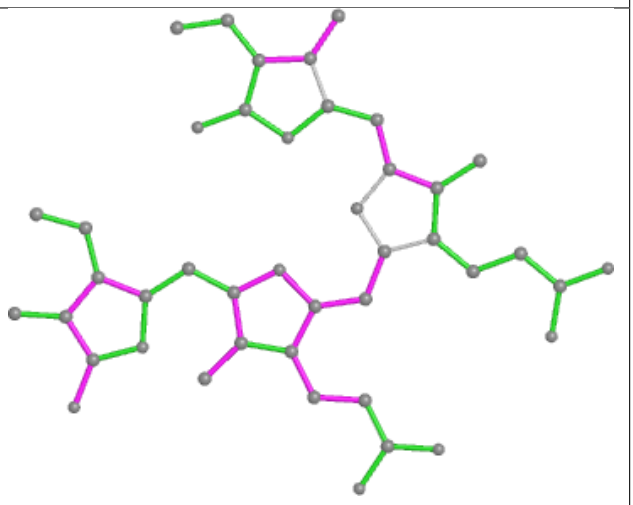

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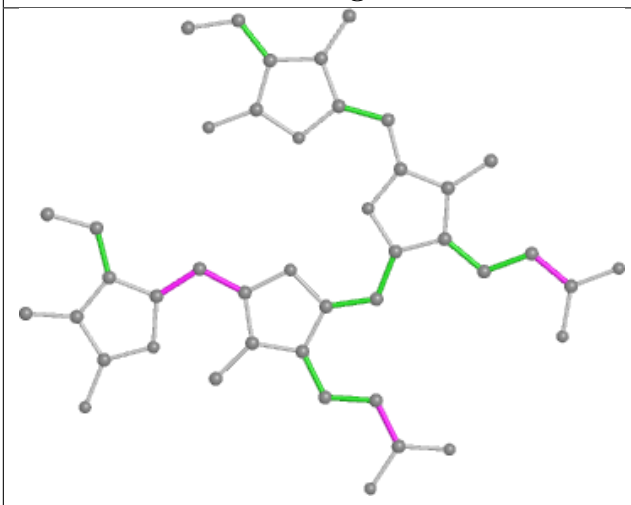

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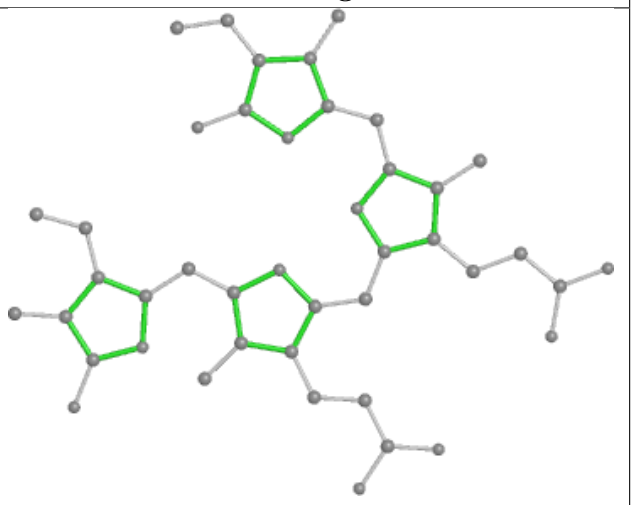

Rings

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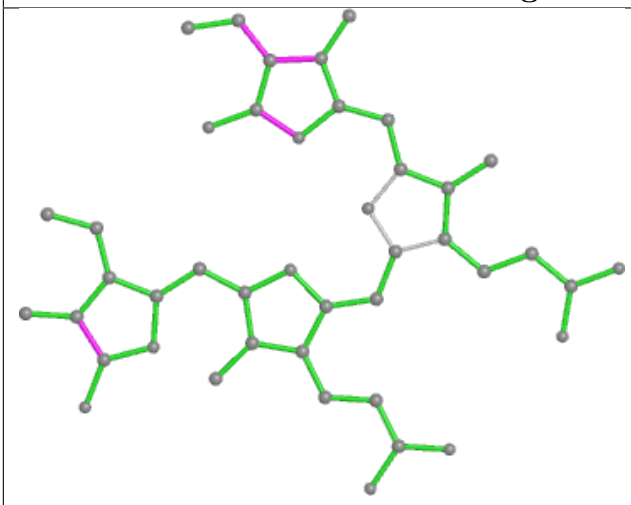

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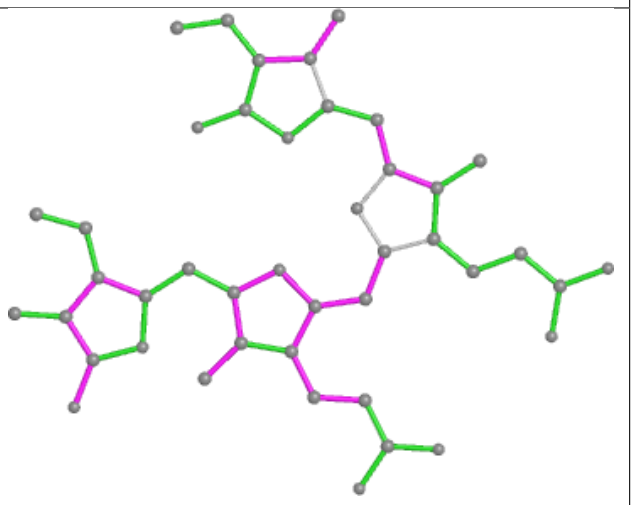

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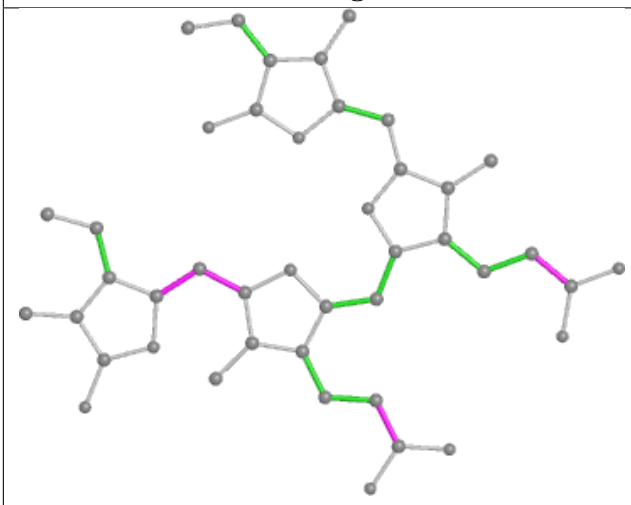

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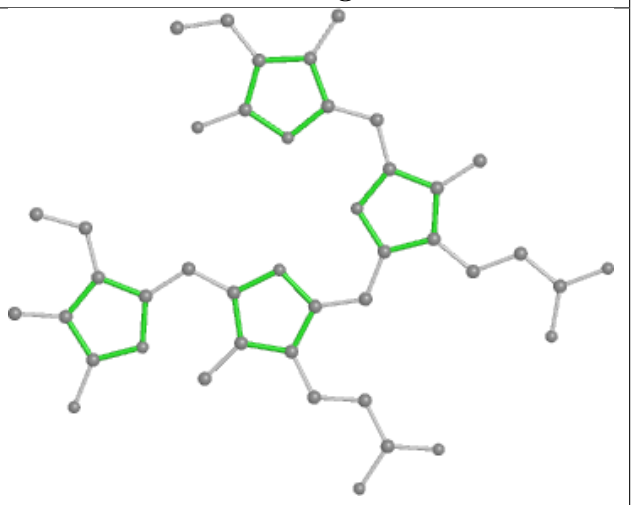

Rings

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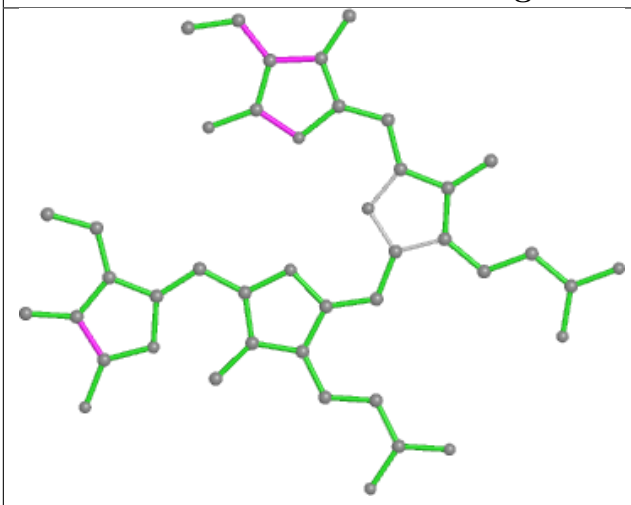

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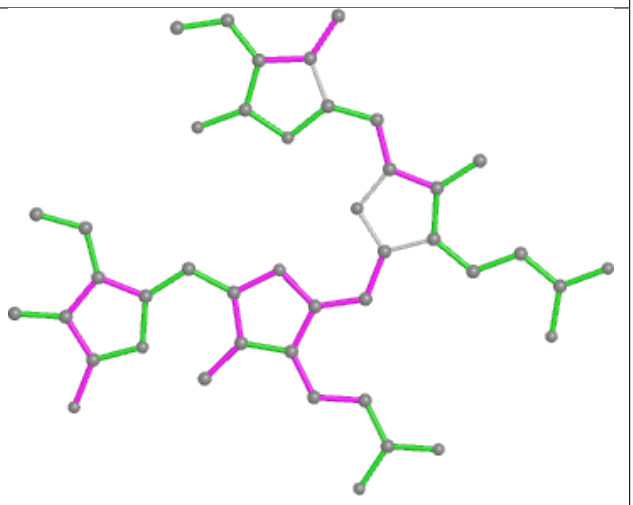

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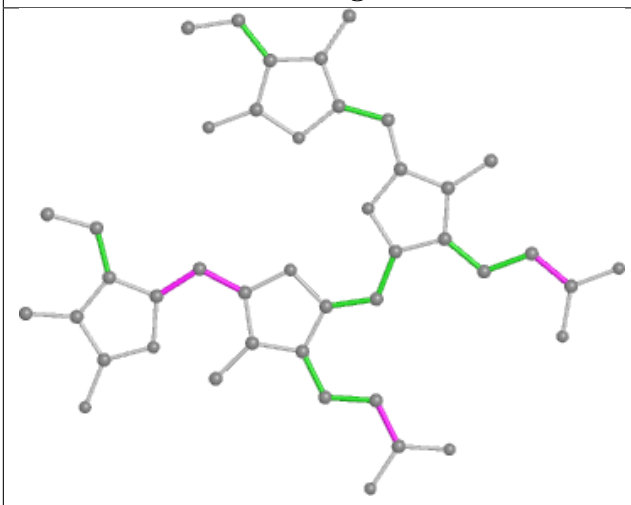

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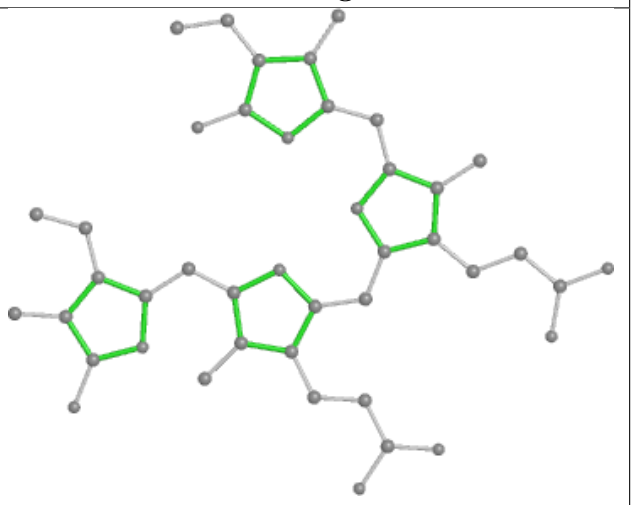

Rings

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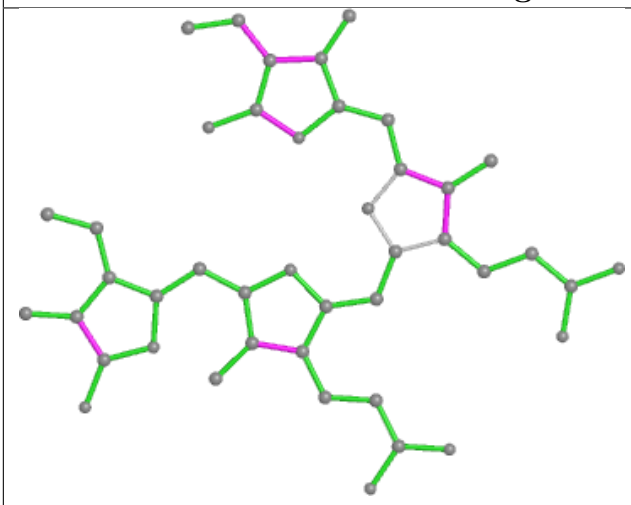

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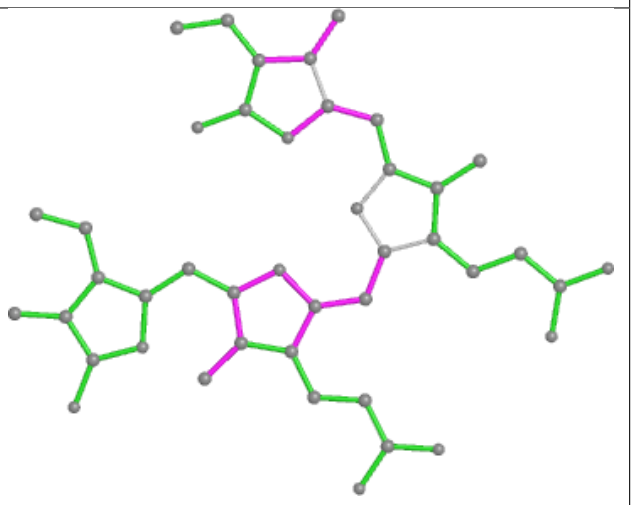

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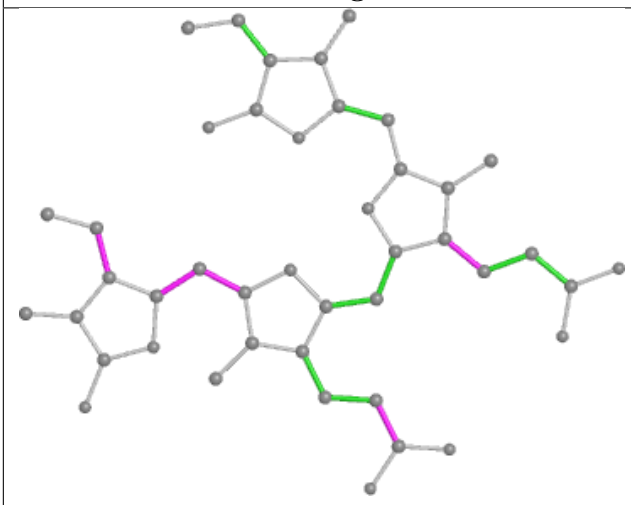

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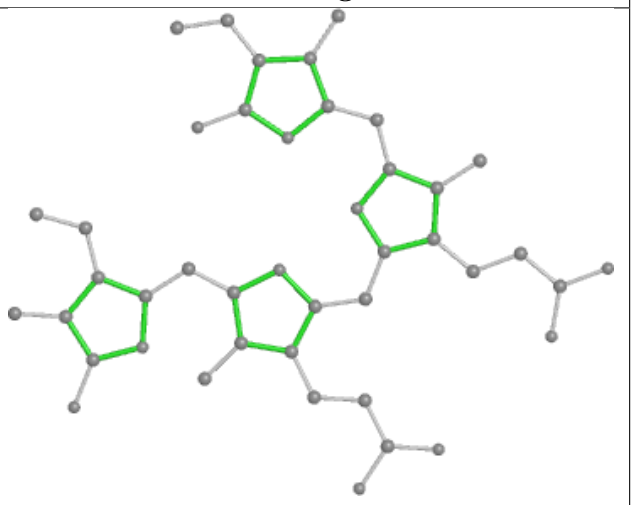

Rings

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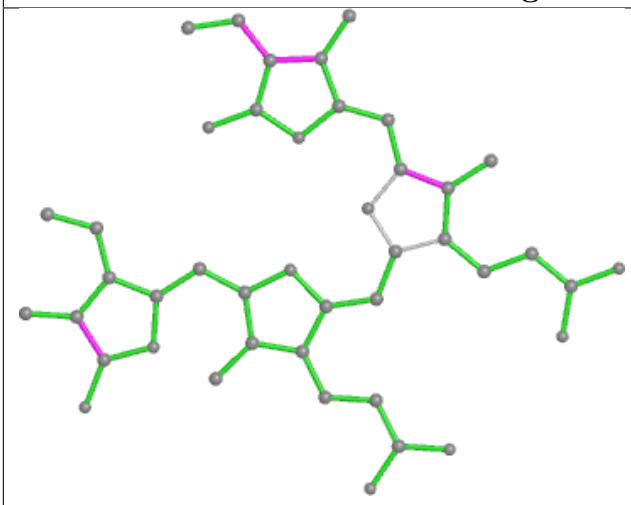

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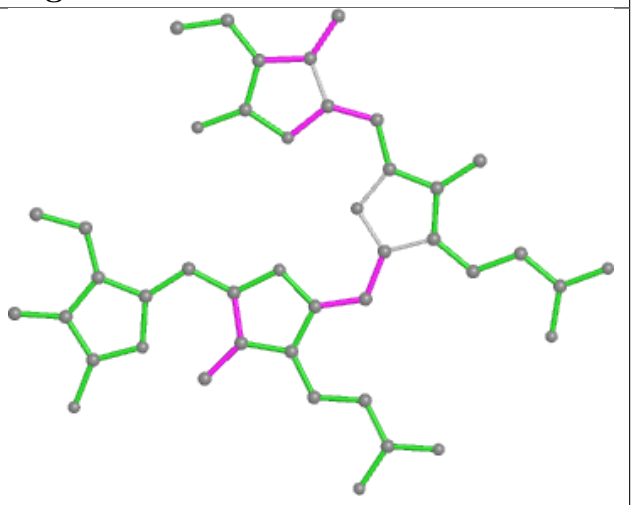

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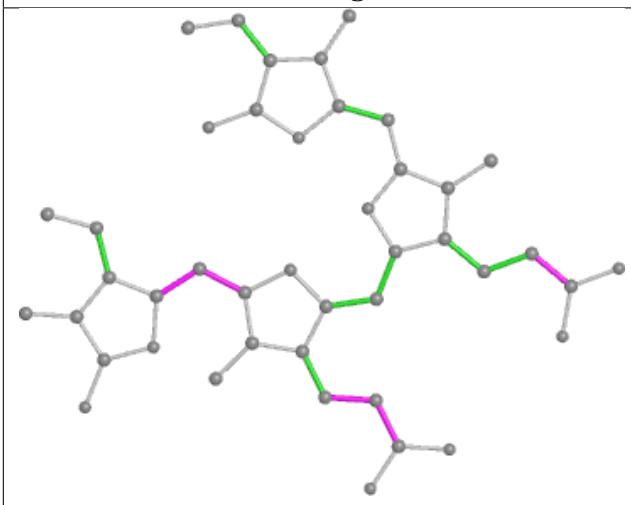

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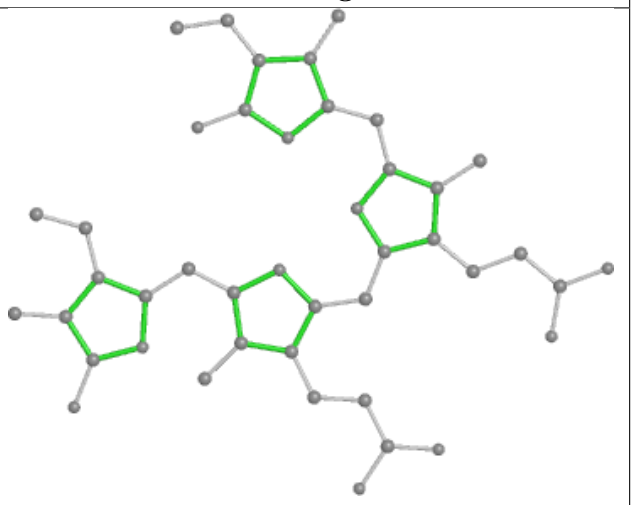
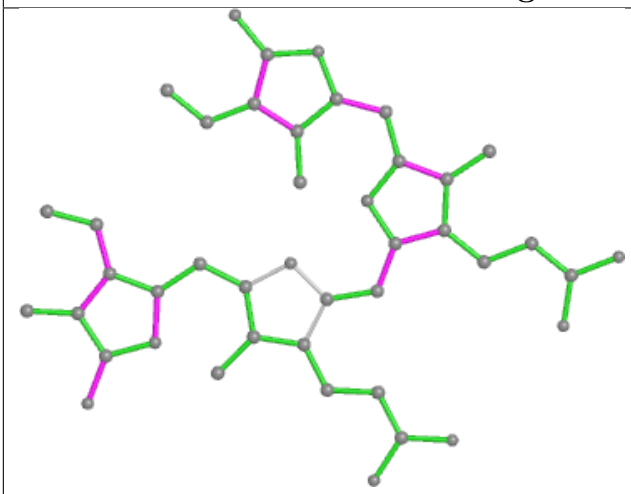


Rings

Ligand PVN c3 303



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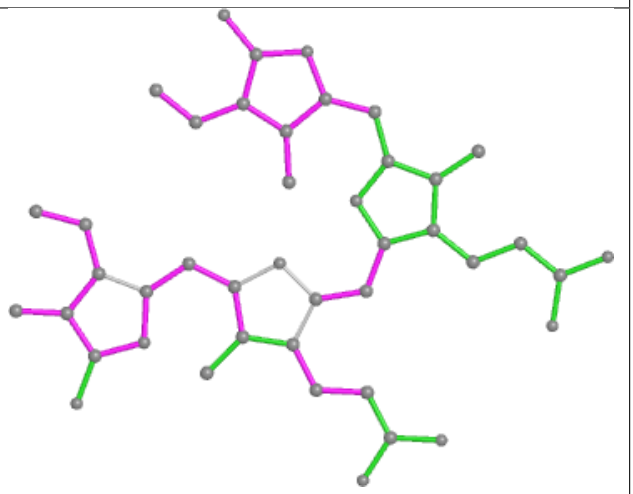
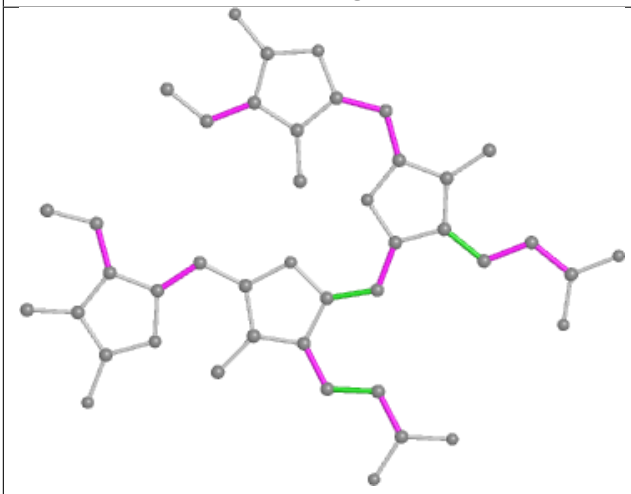
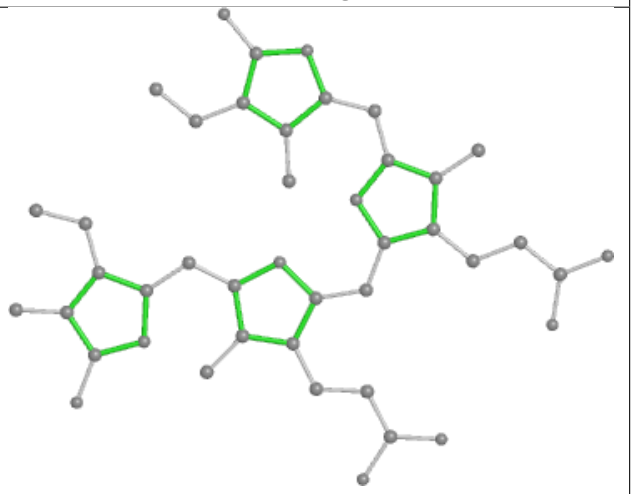


Bond angles

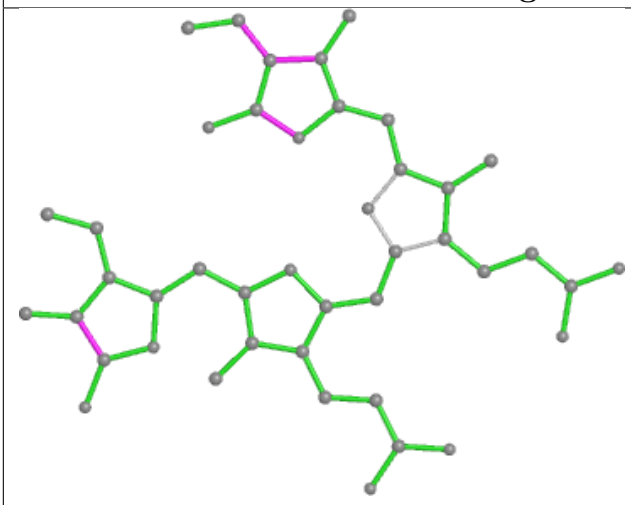


Torsions



Rings

Ligand PEB v4 201



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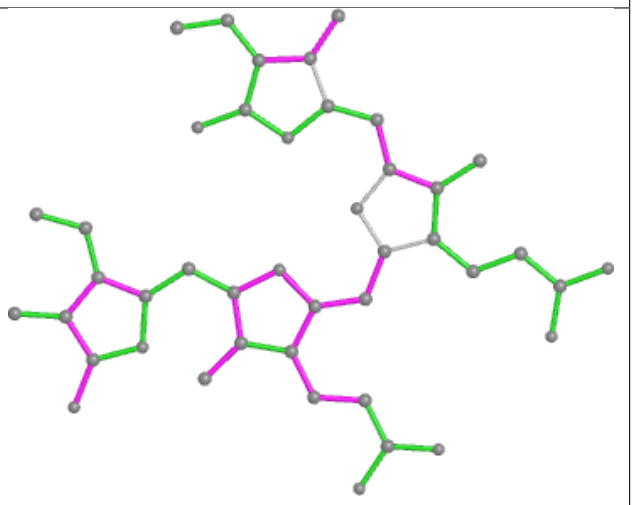

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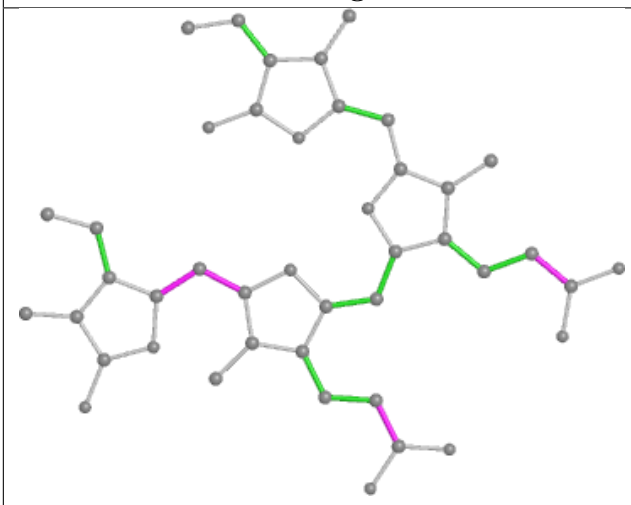

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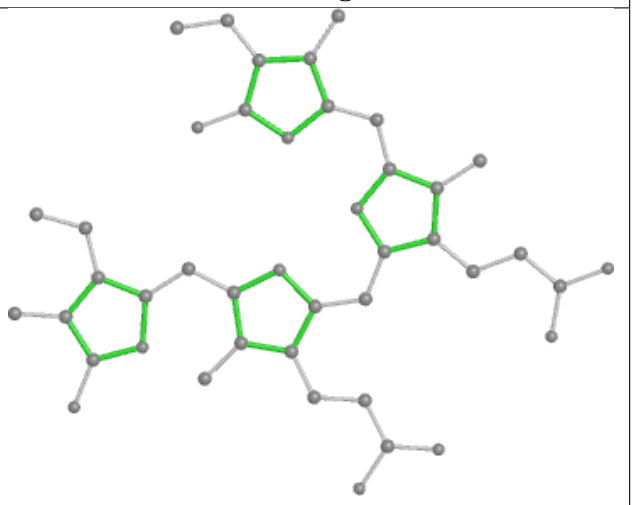
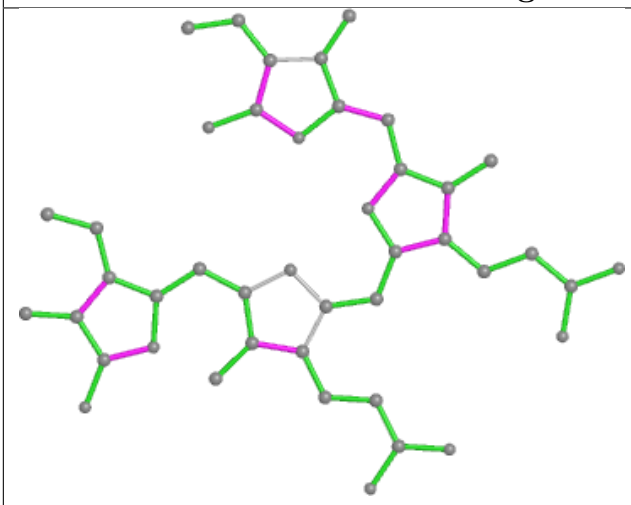


Rings

Ligand PUB bz 203



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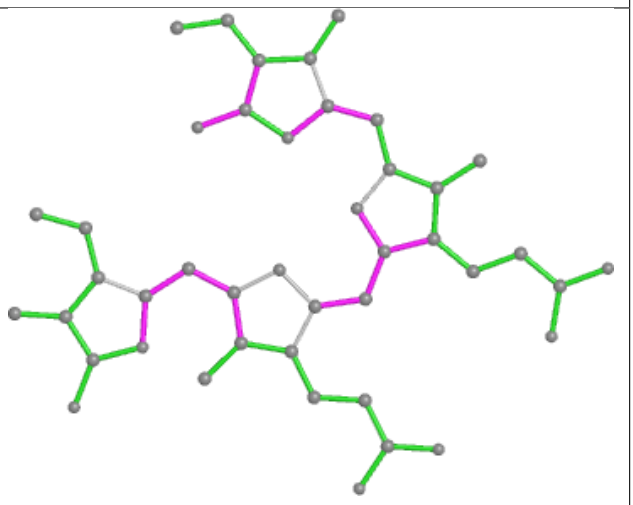

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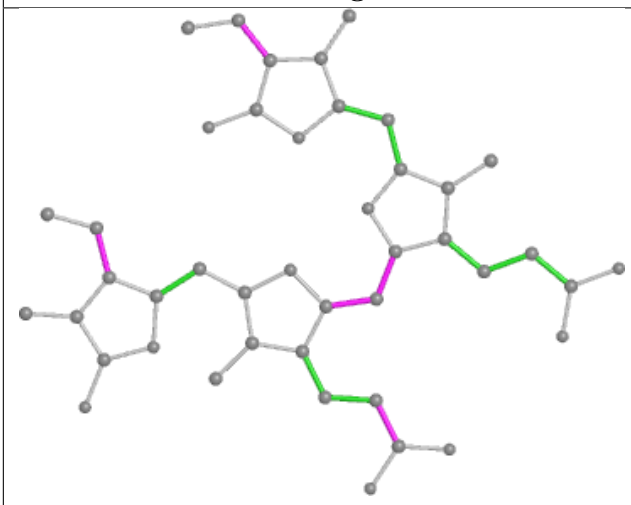

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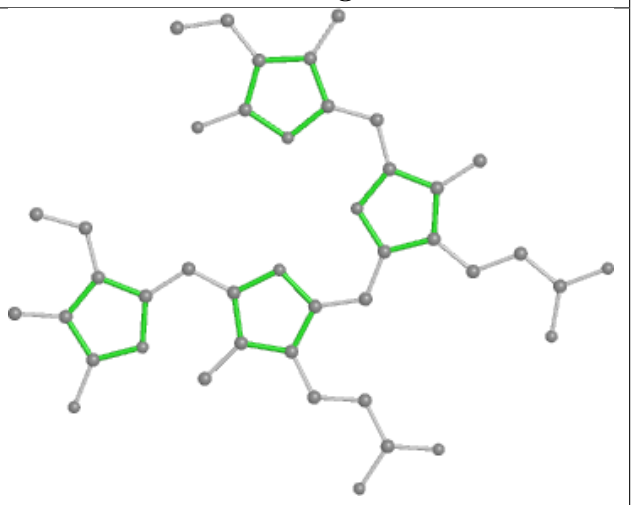
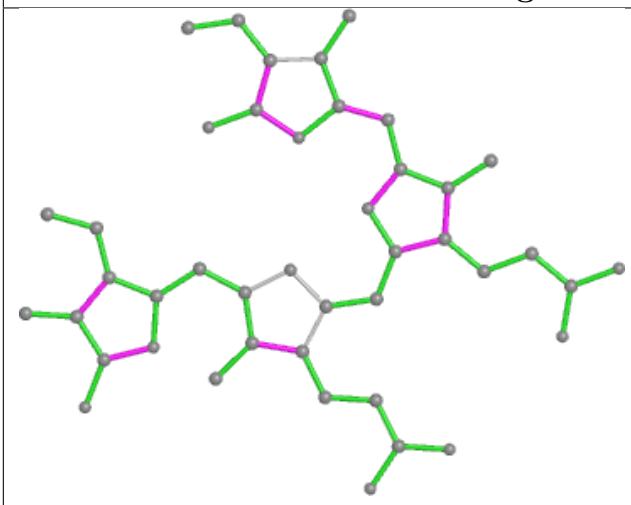


Rings

Ligand PUB gp 203



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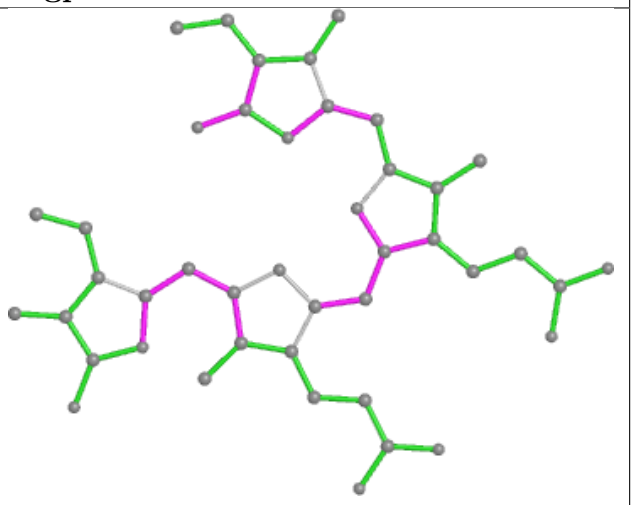

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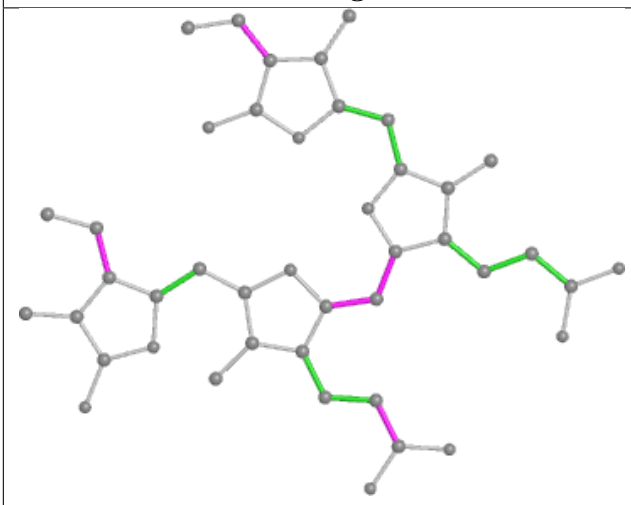

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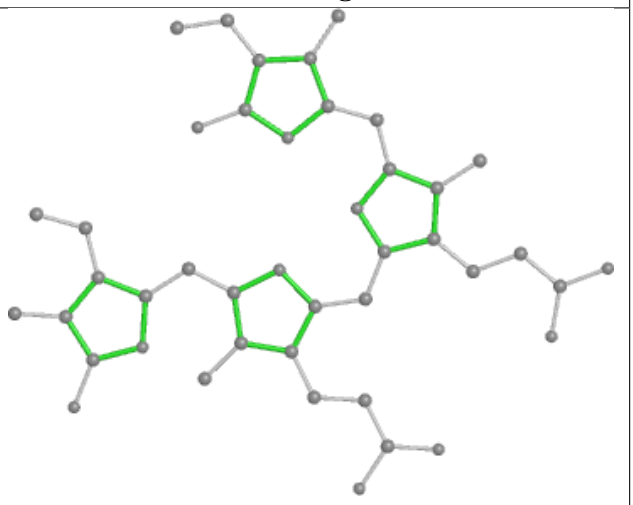
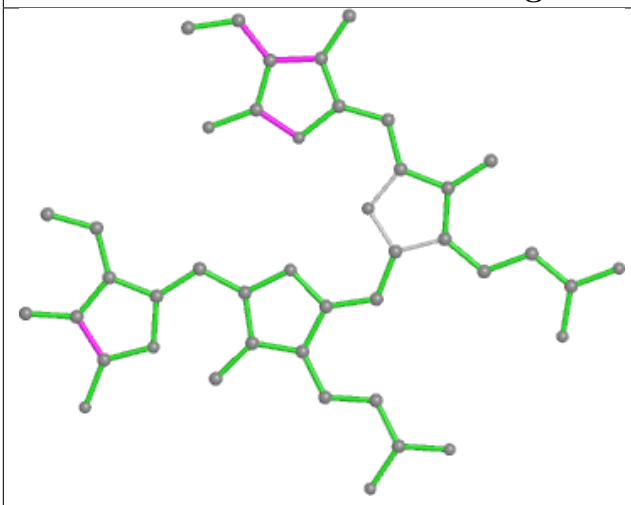


Rings

Ligand PEB fr 201



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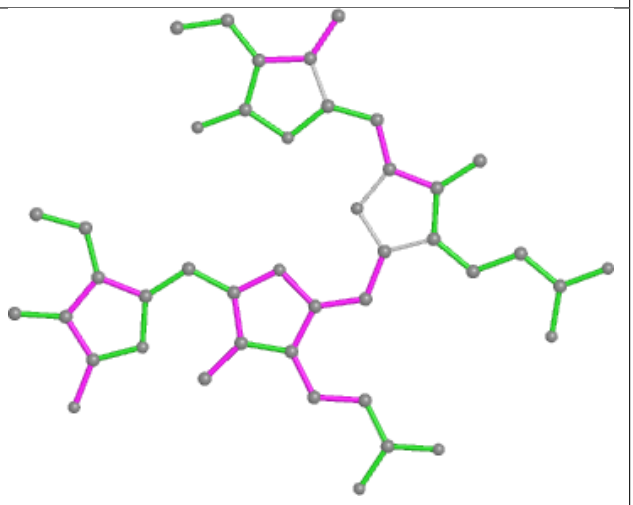

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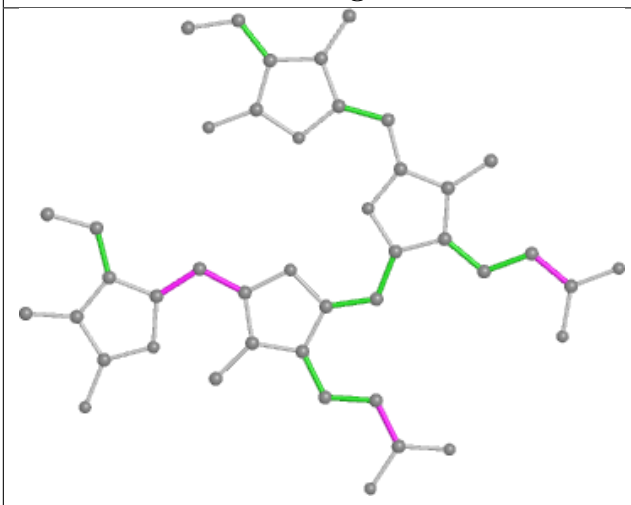

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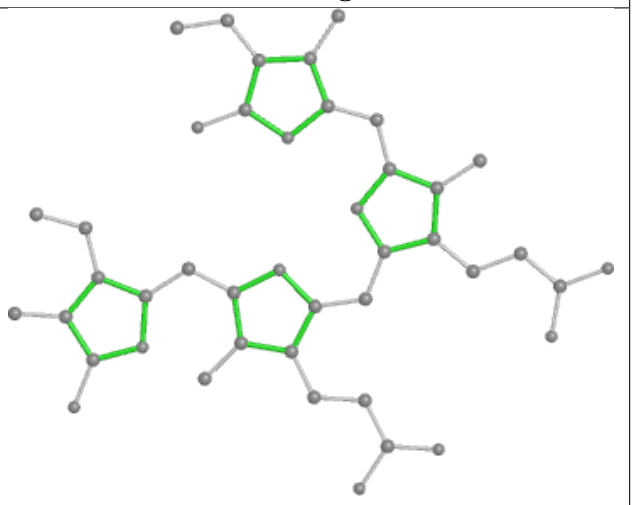
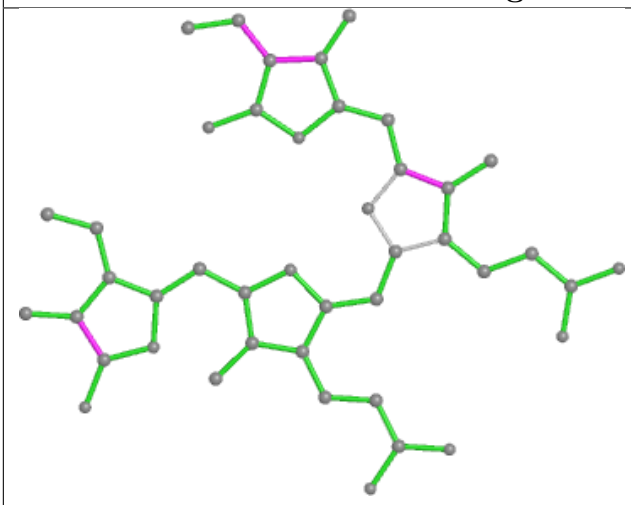


Rings

Ligand PEB A2 1001



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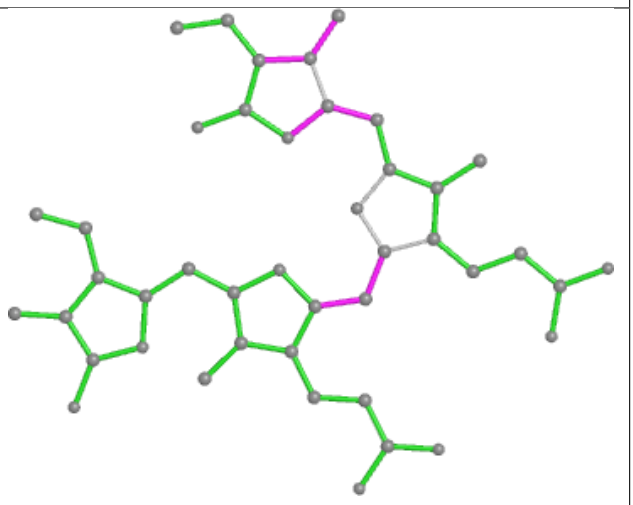

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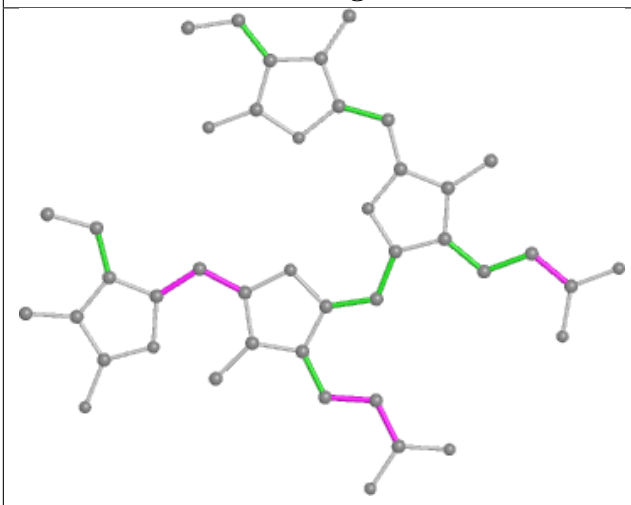

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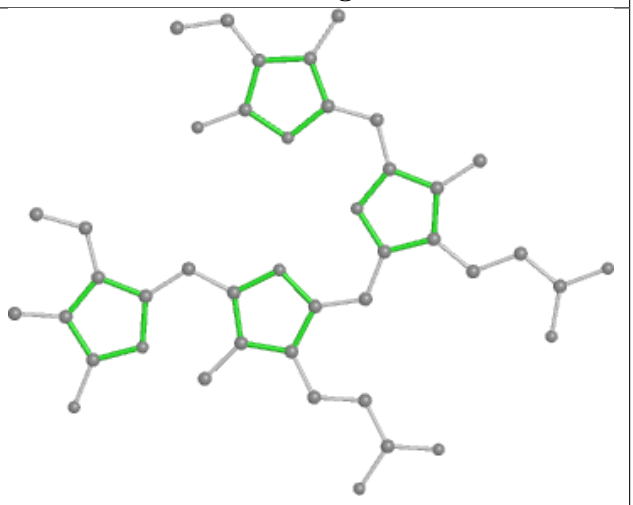

Rings

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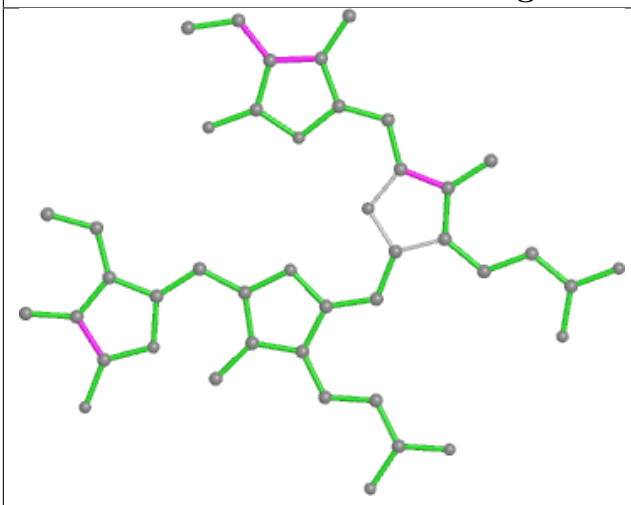

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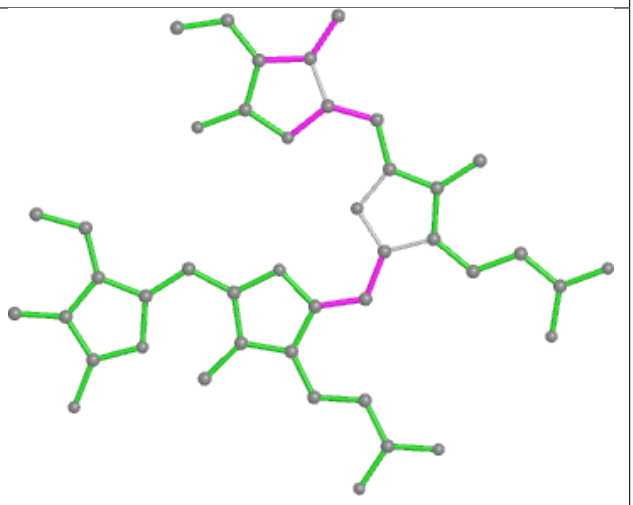

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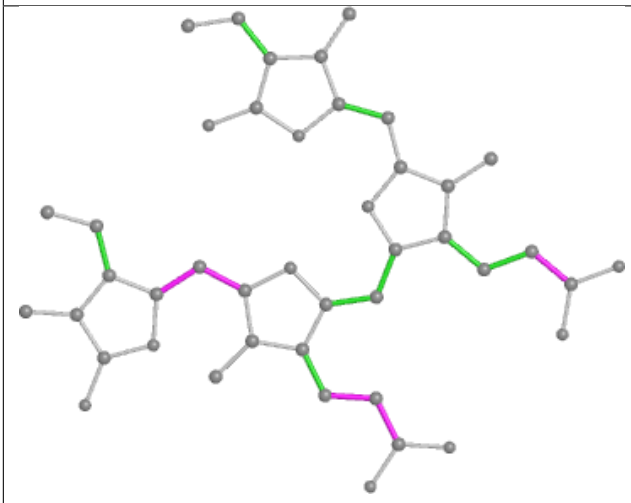

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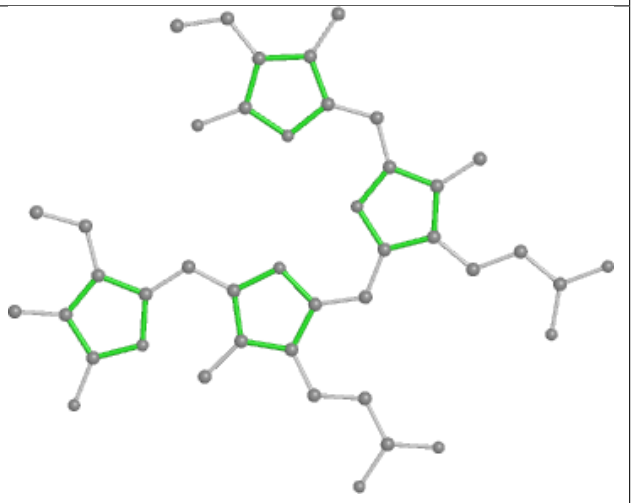

Rings

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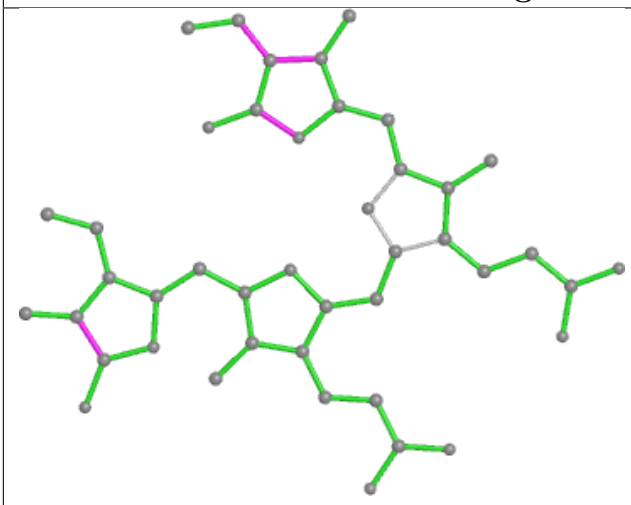

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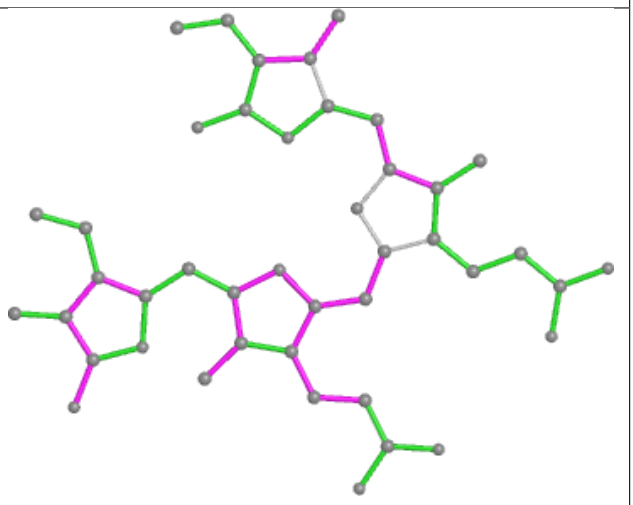

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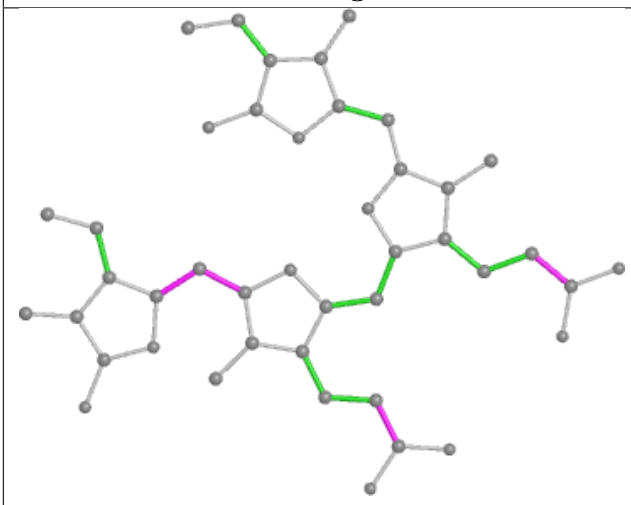

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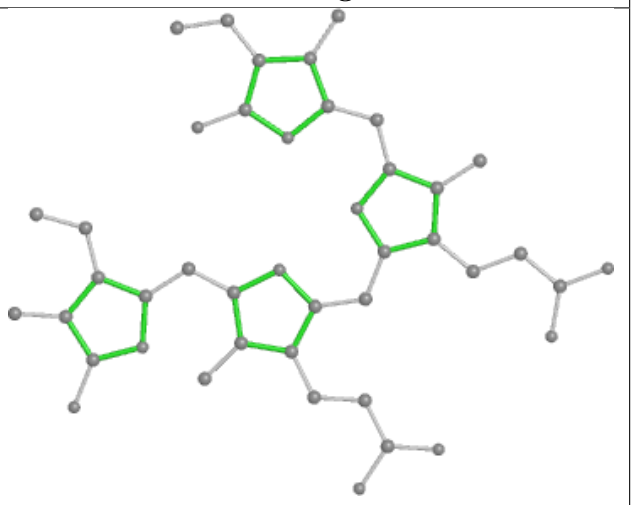
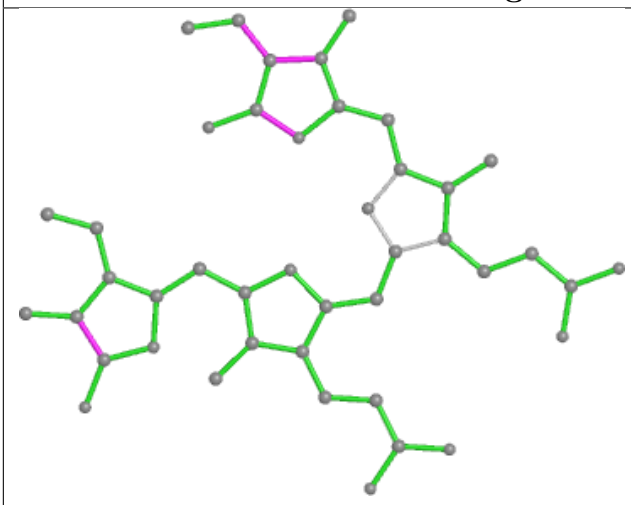


Rings

Ligand PEB kU 1001



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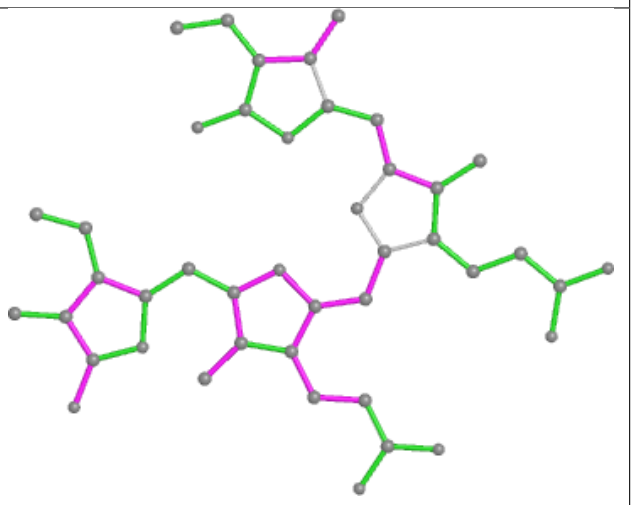

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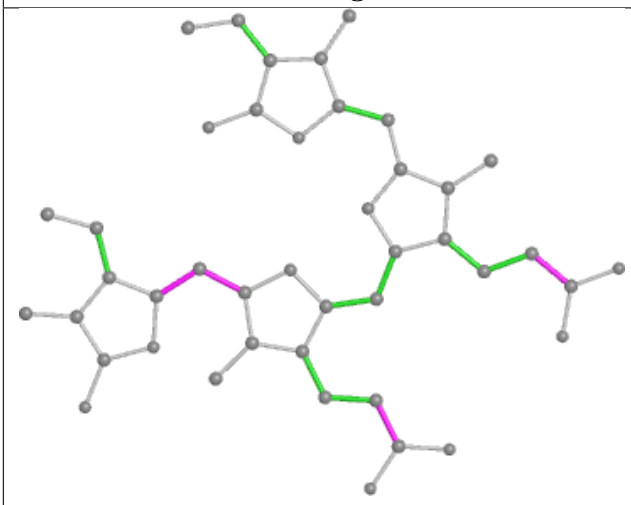

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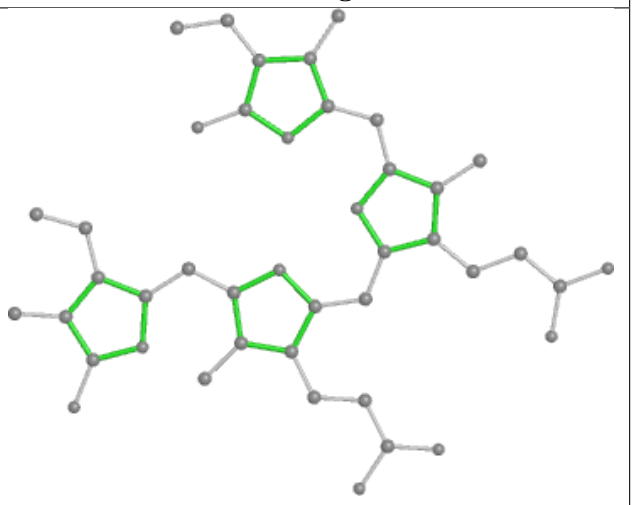
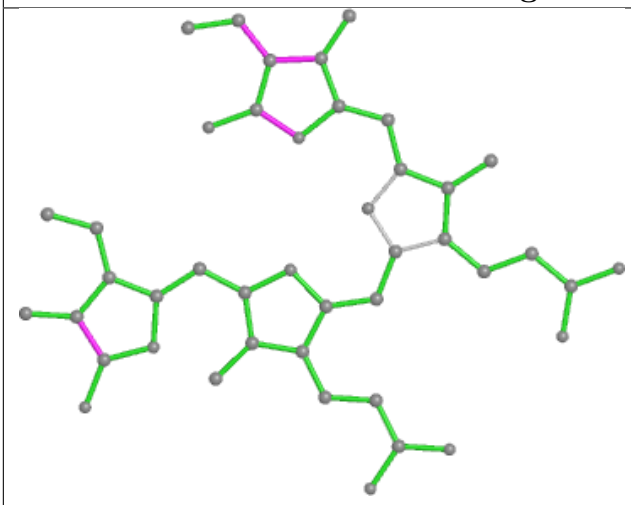


Rings

Ligand PEB a9 601



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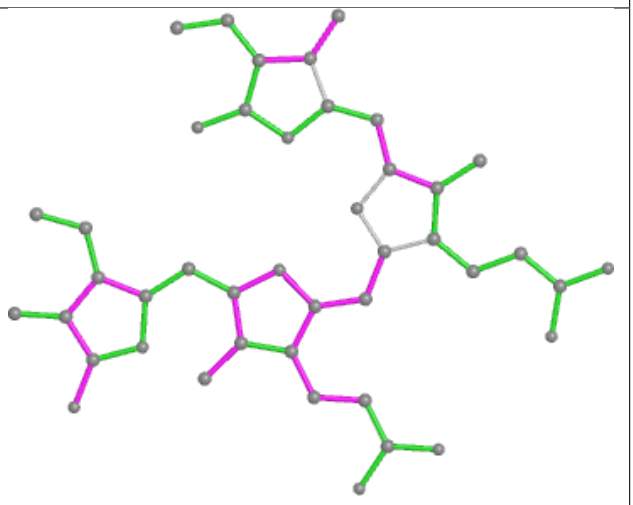

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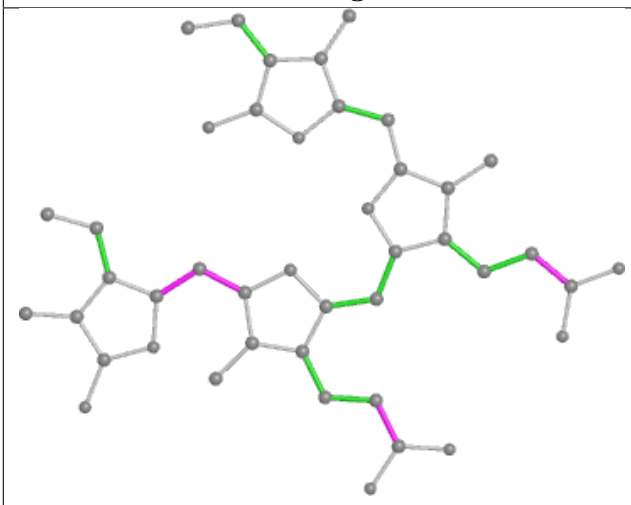

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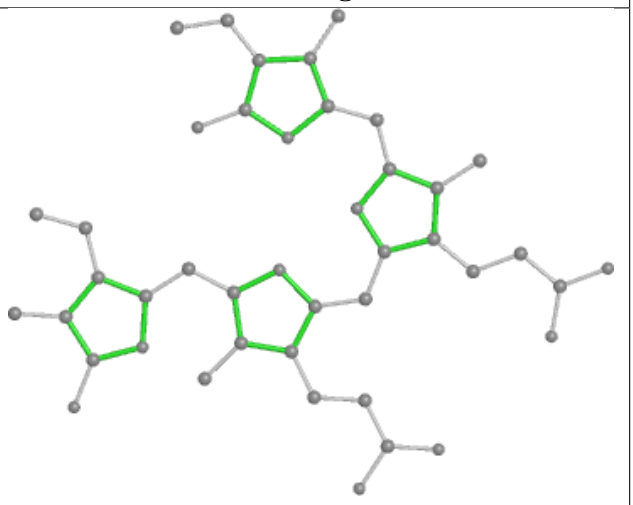
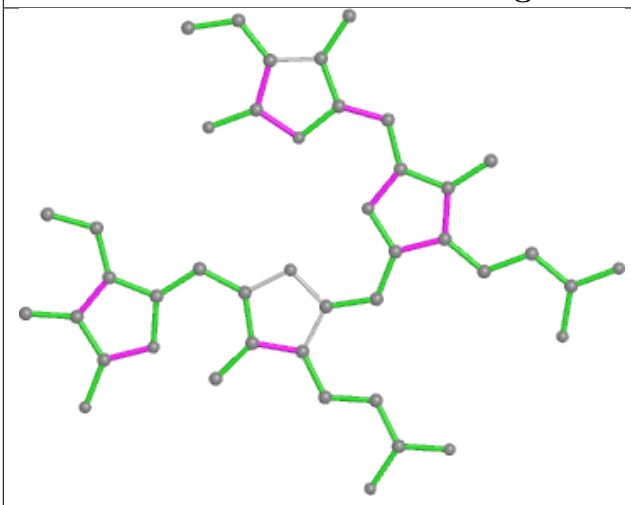


Rings

Ligand PUB cO 203



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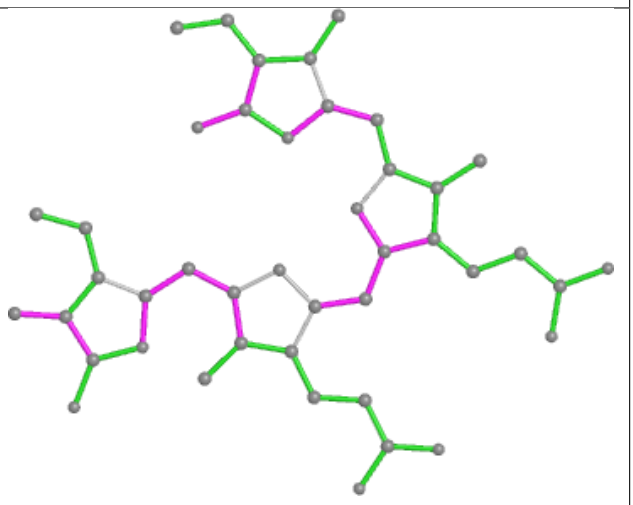

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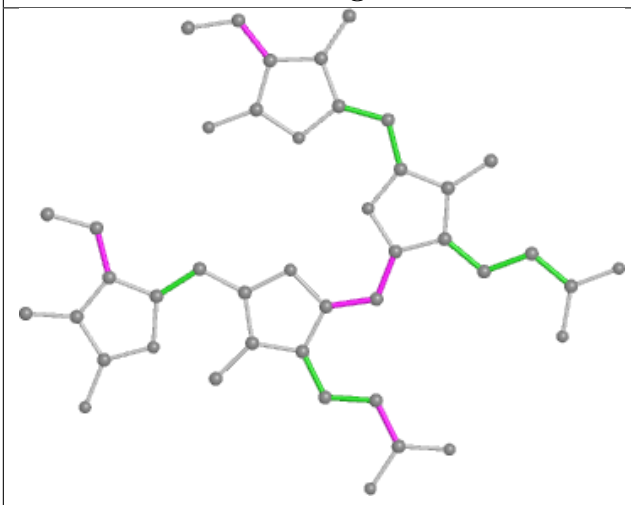

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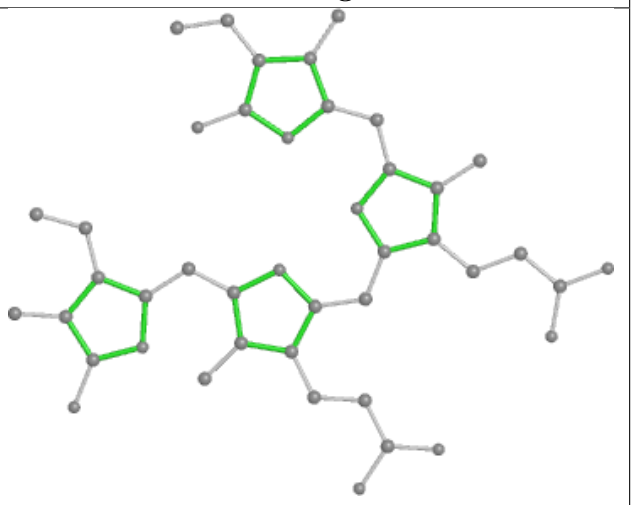

Rings

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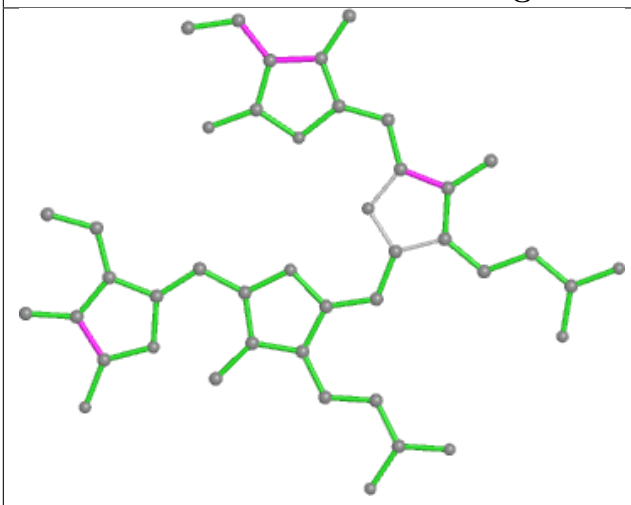

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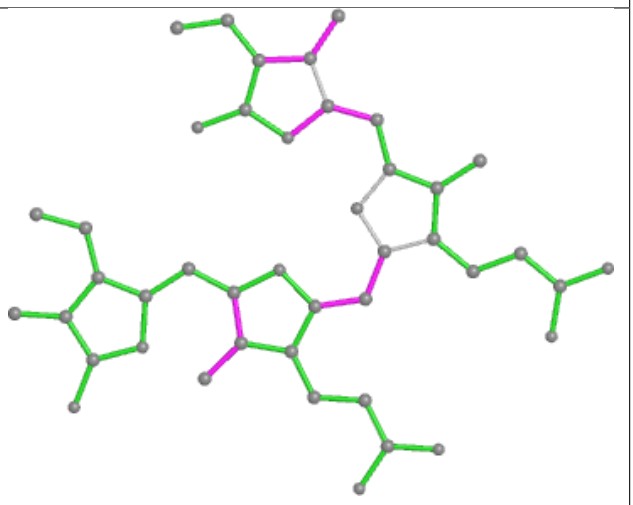

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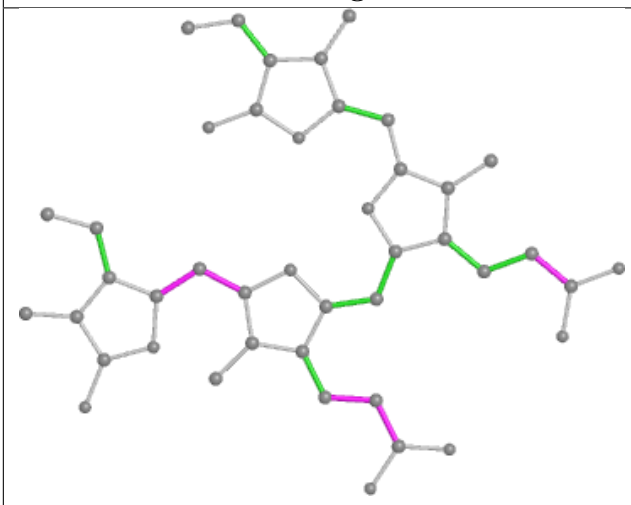

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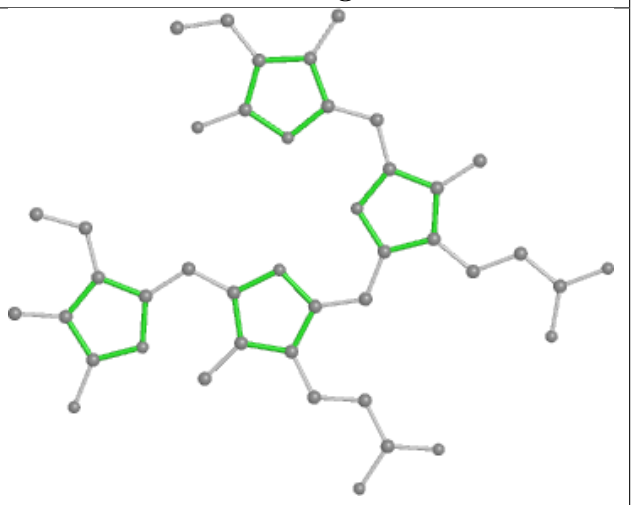
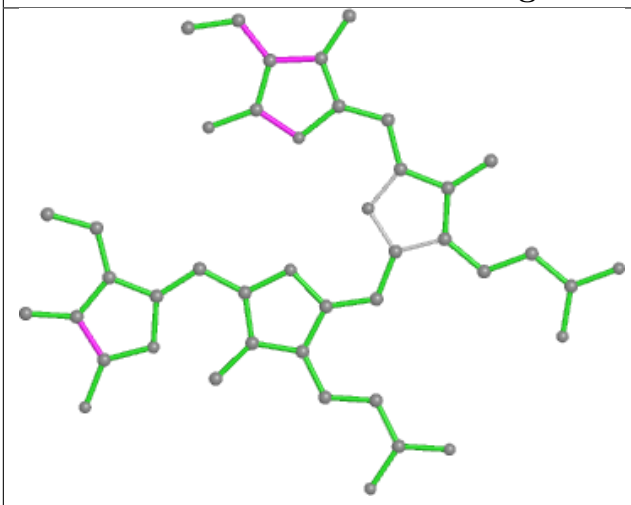


Rings

Ligand PEB S6 202



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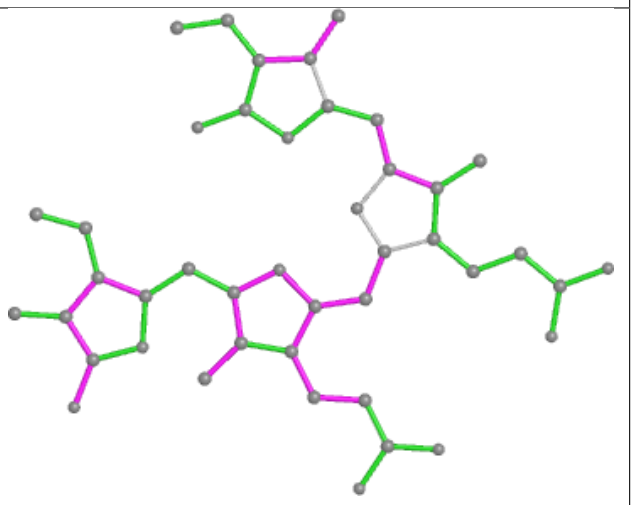

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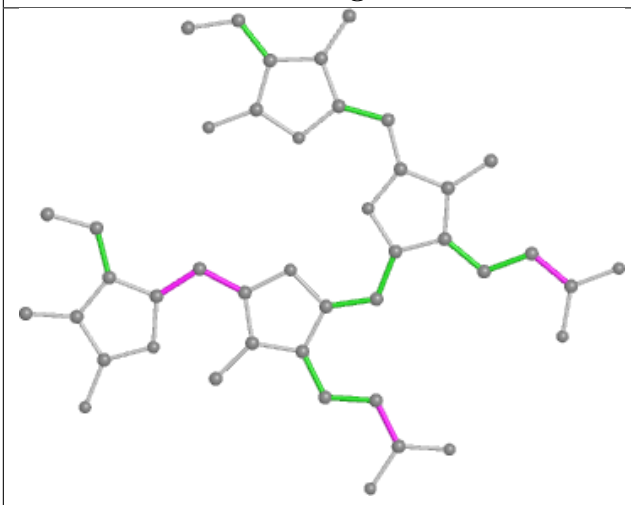

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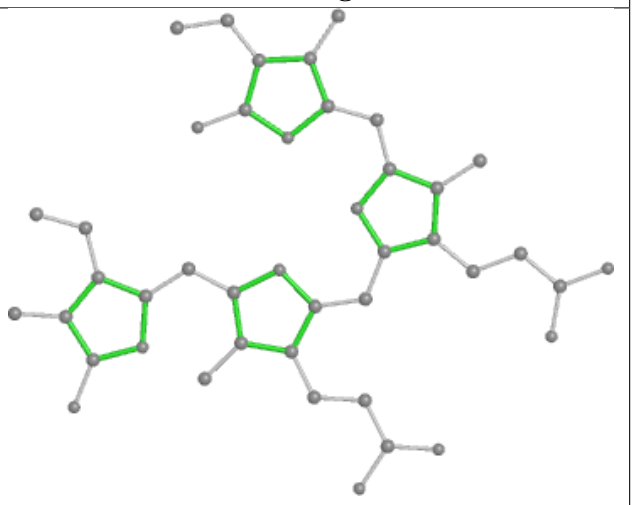
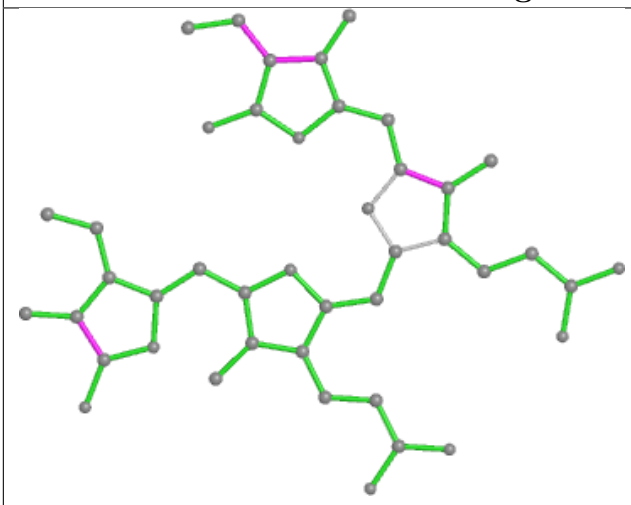


Rings

Ligand PEB N2 201



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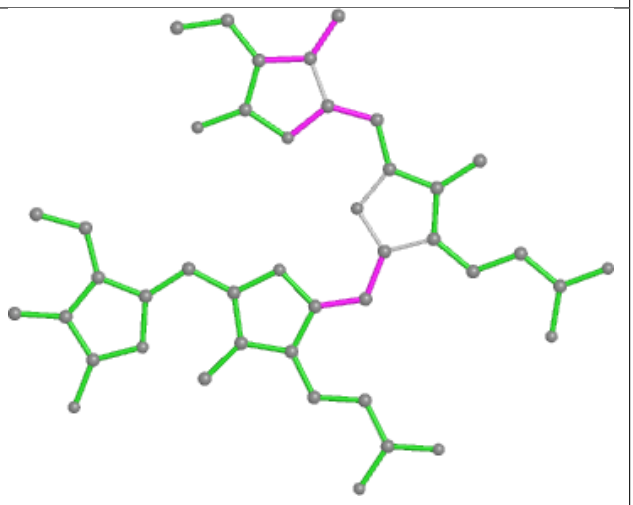
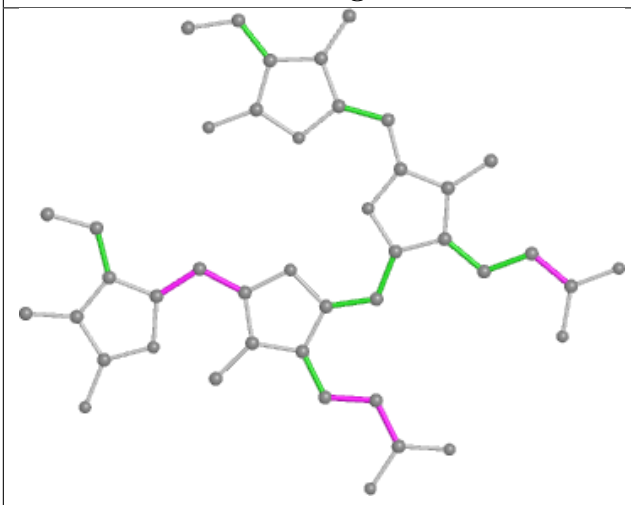
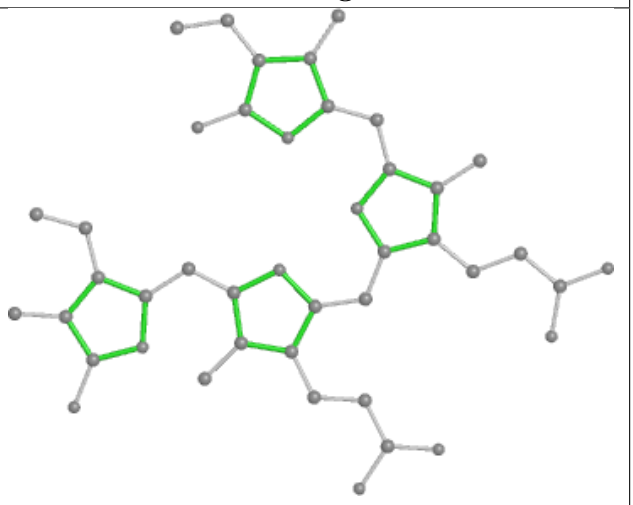


Bond angles

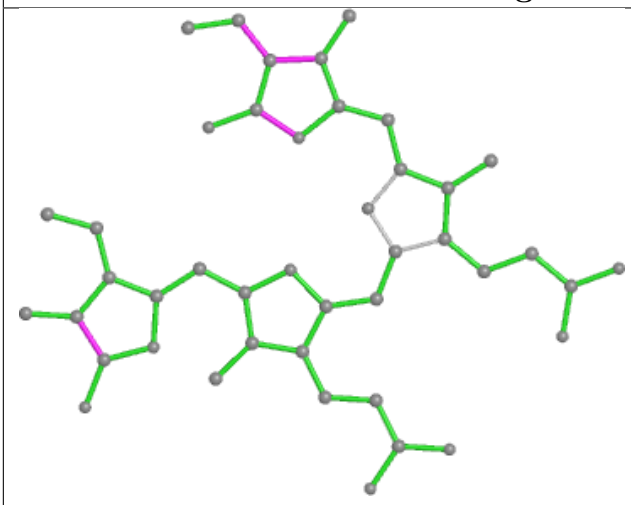


Torsions



Rings

Ligand PEB eG 201



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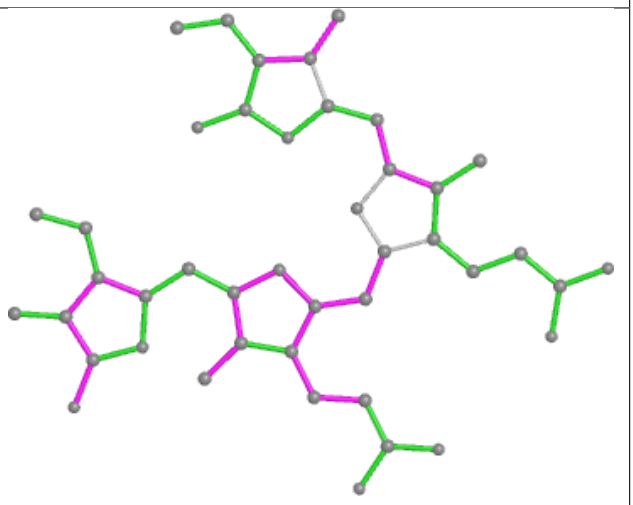
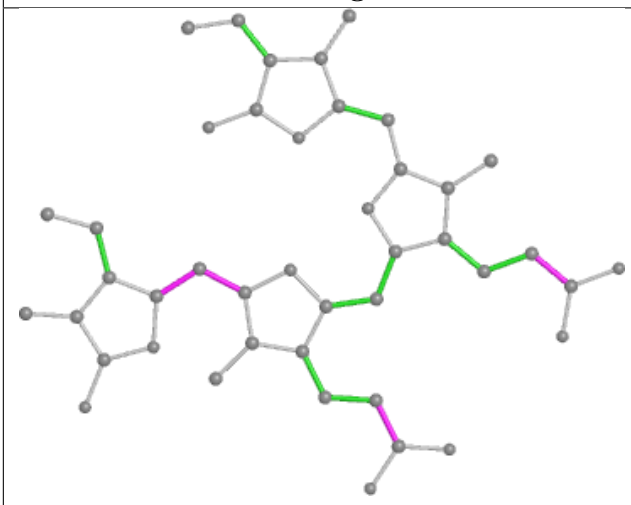


Bond angles



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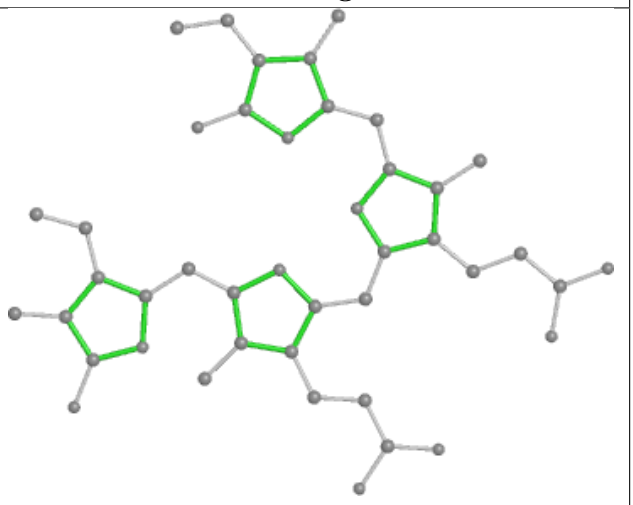
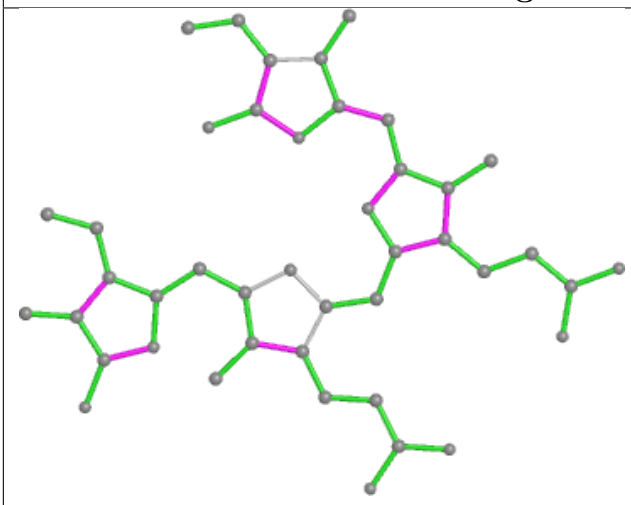


Rings

Ligand PUB L3 203



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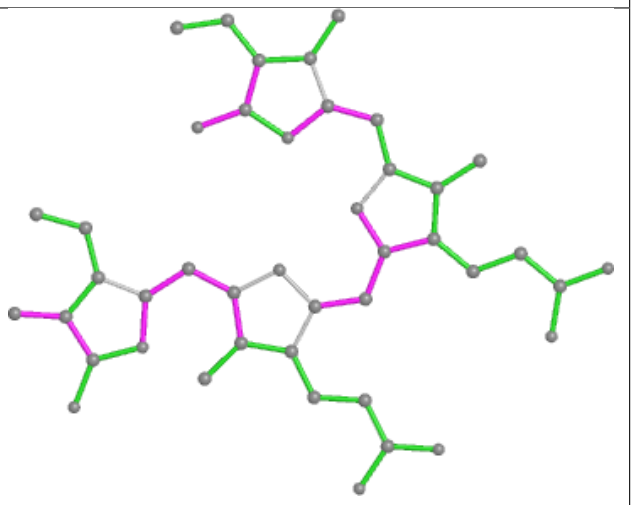

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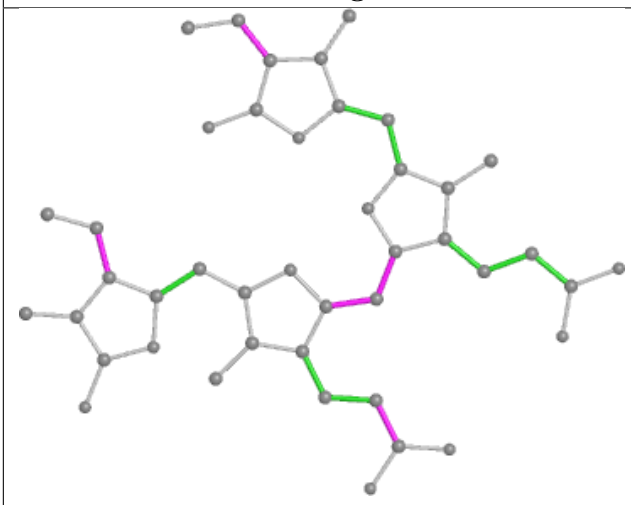

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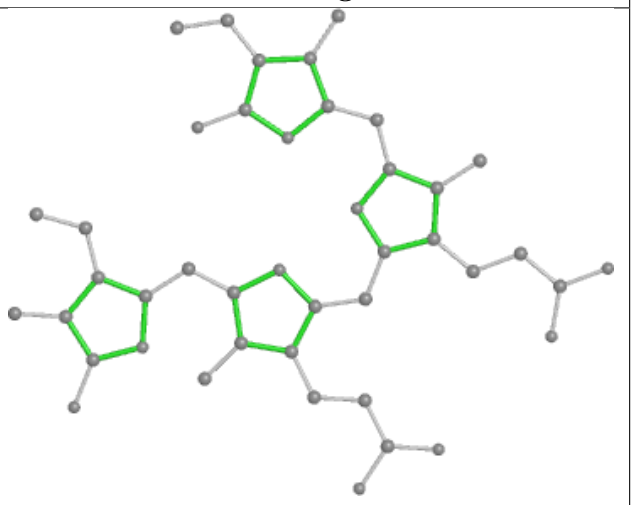
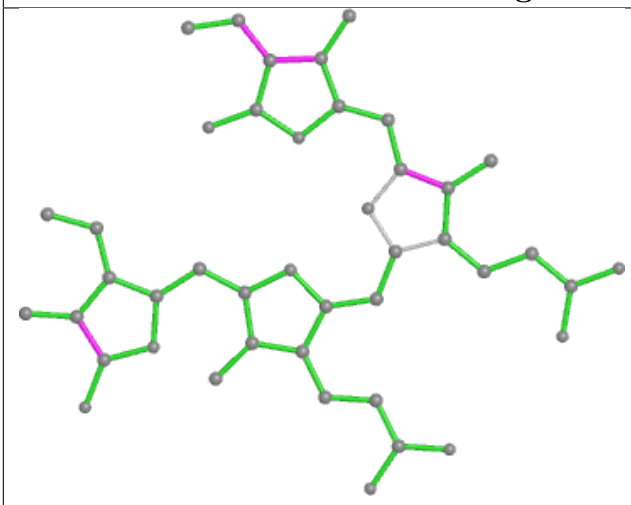


Rings

Ligand PEB U6 202



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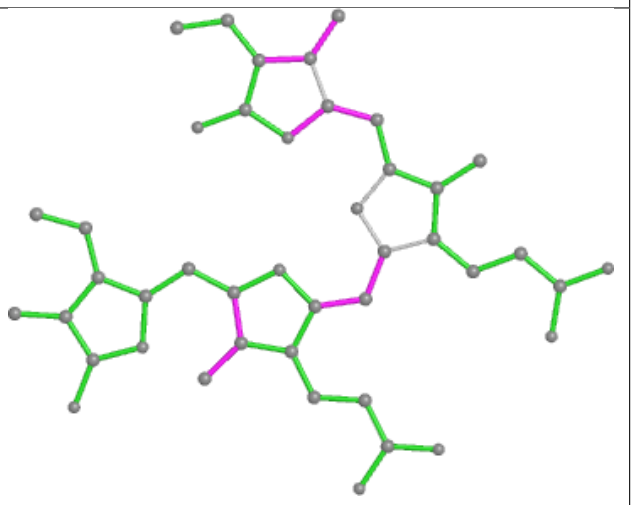

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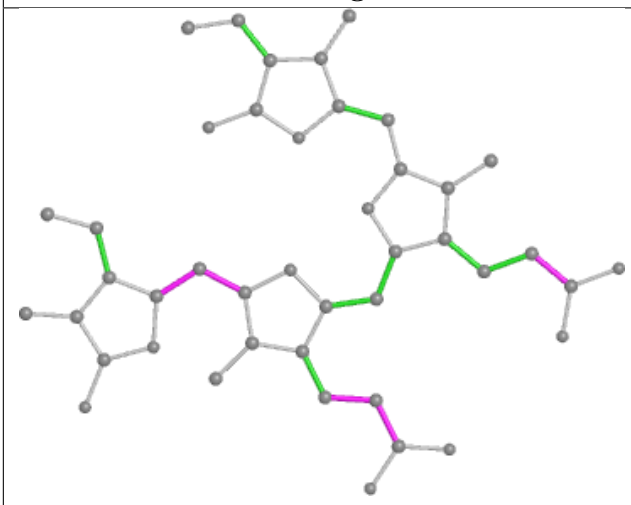

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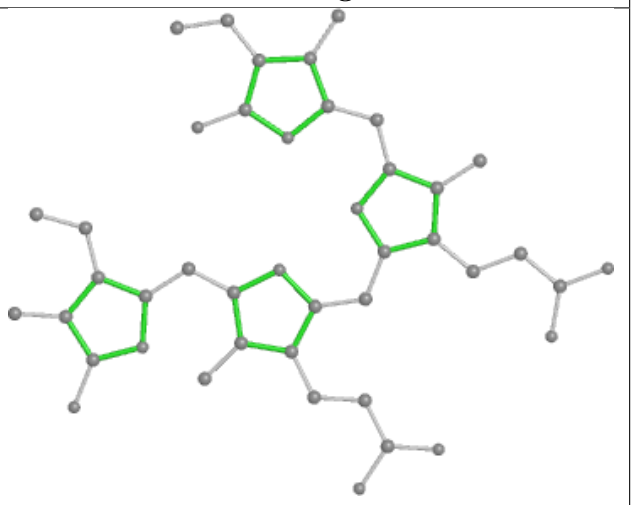
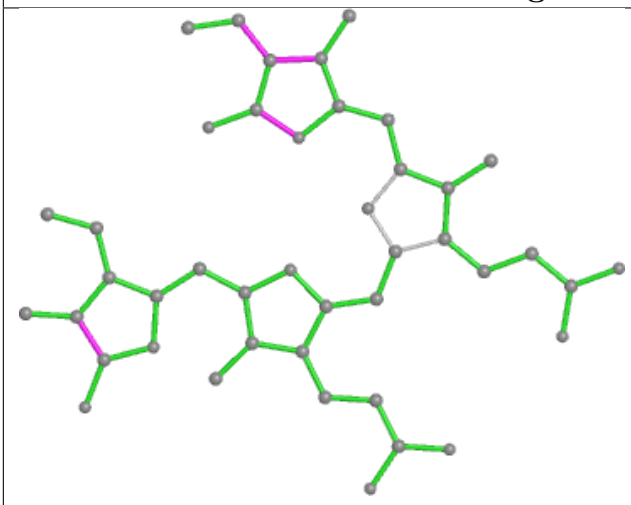


Rings

Ligand PEB fi 201



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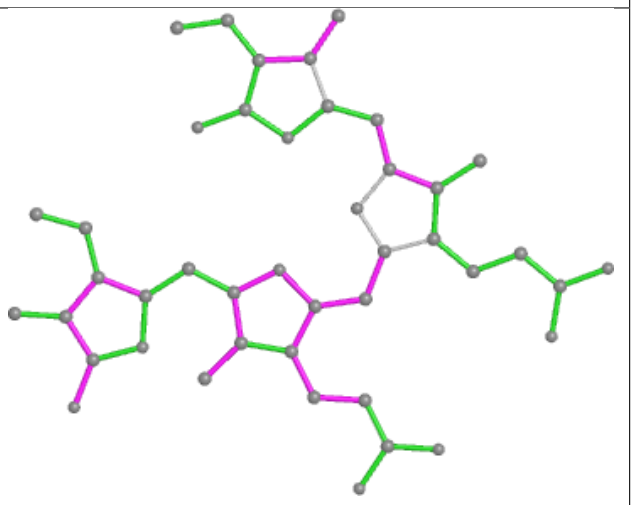

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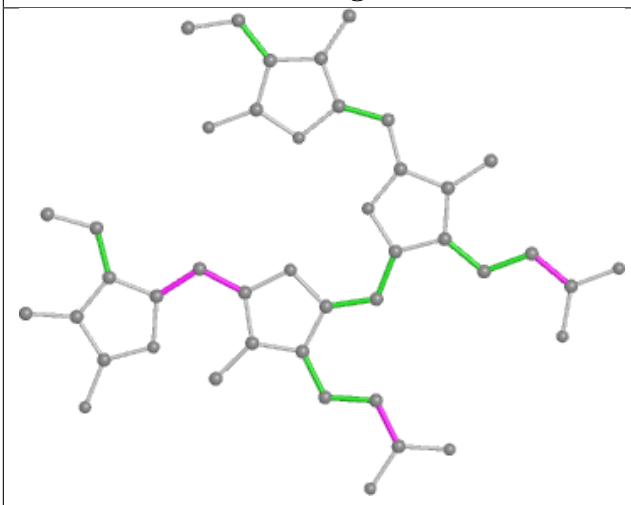

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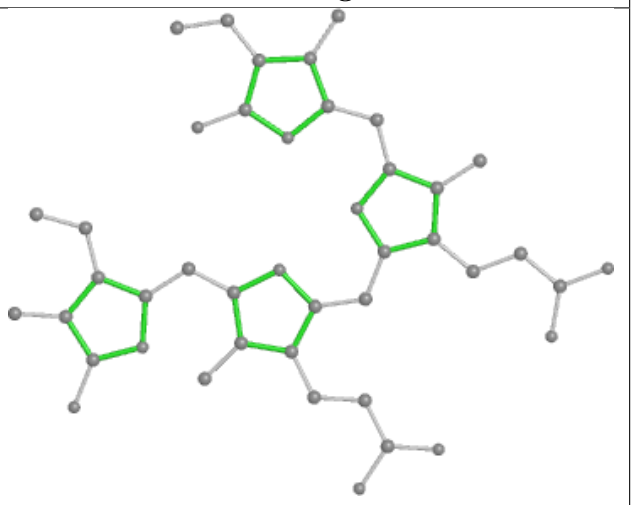
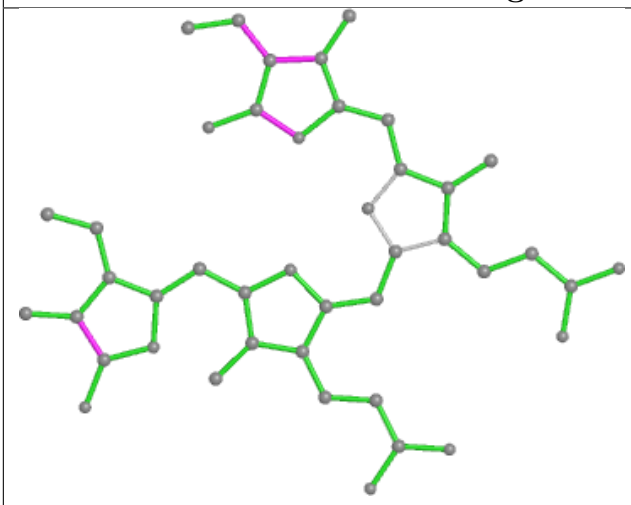


Rings

Ligand PEB hE 1001



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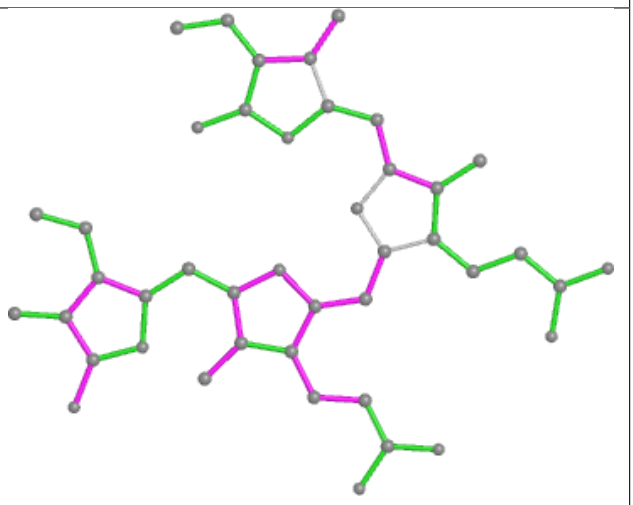

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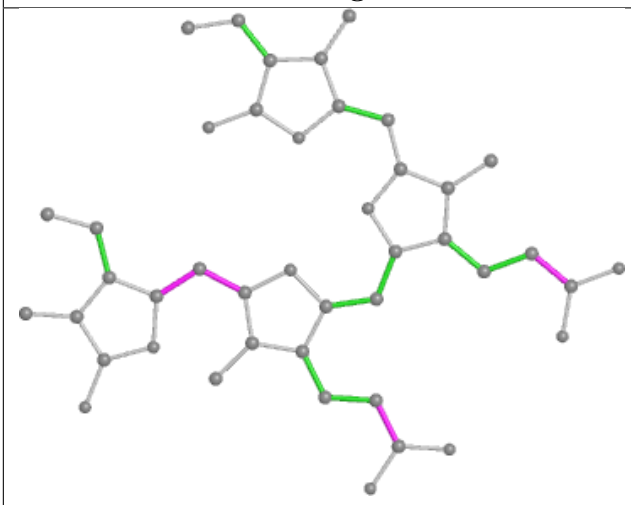

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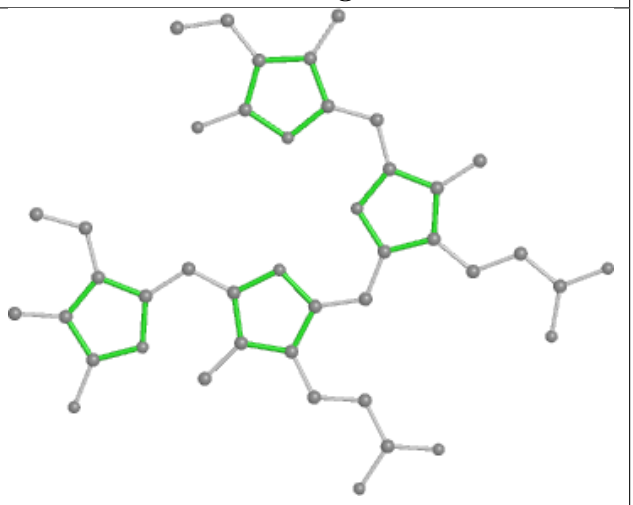
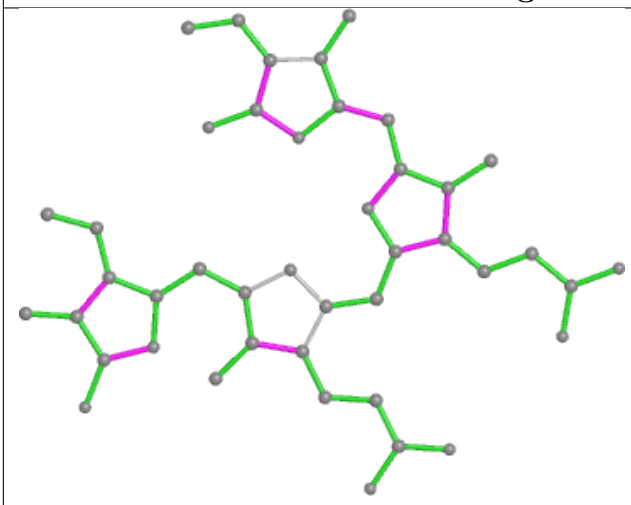


Rings

Ligand PUB y6 204



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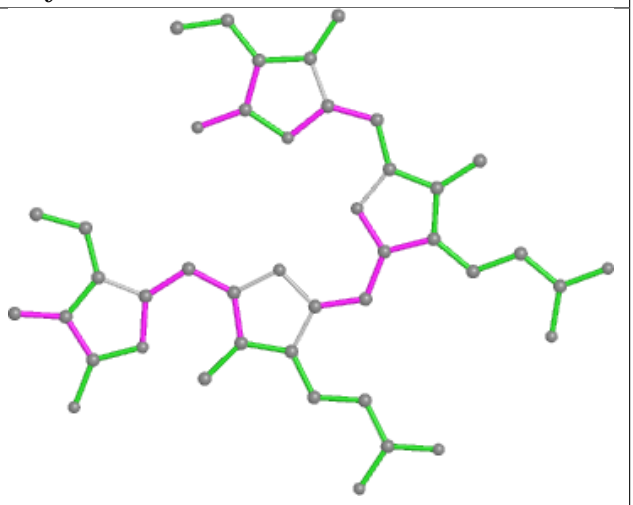

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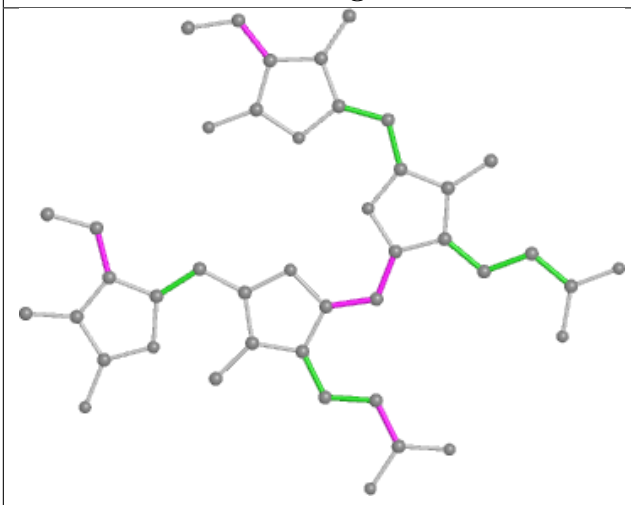

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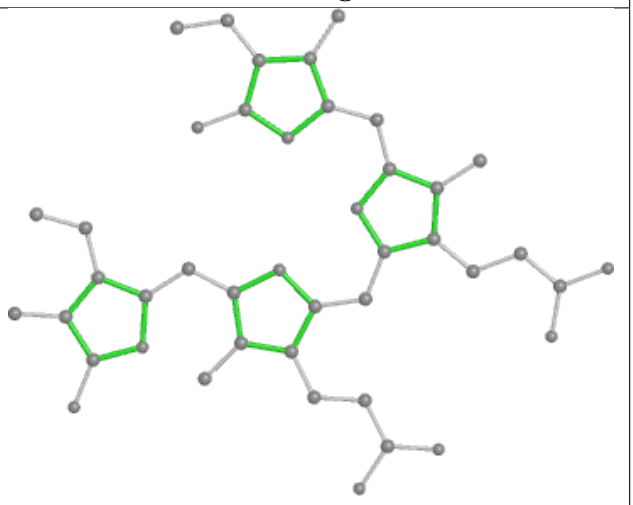

Rings

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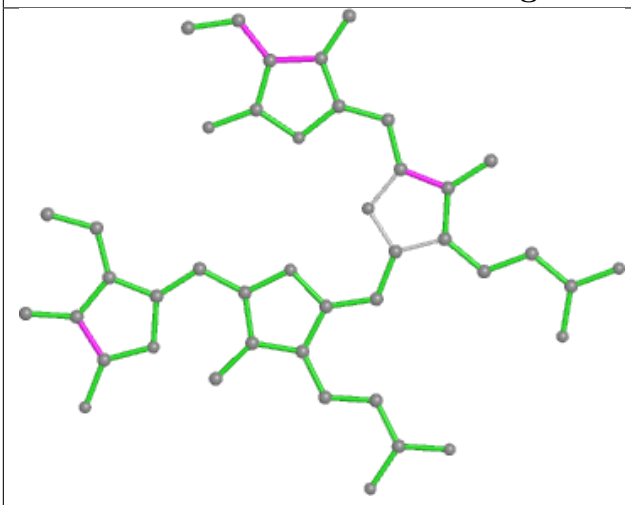

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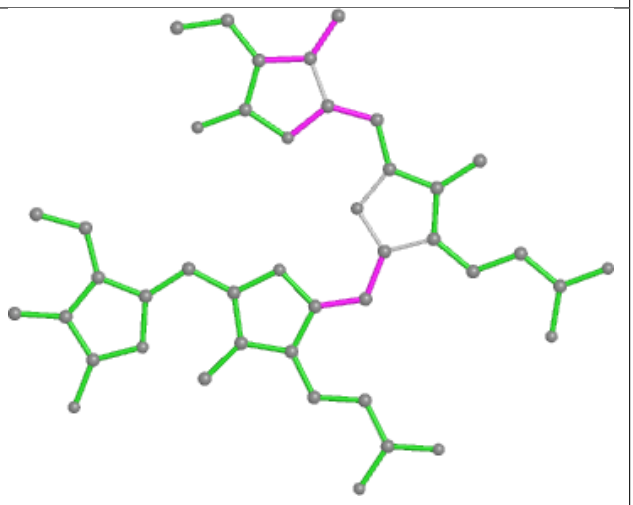

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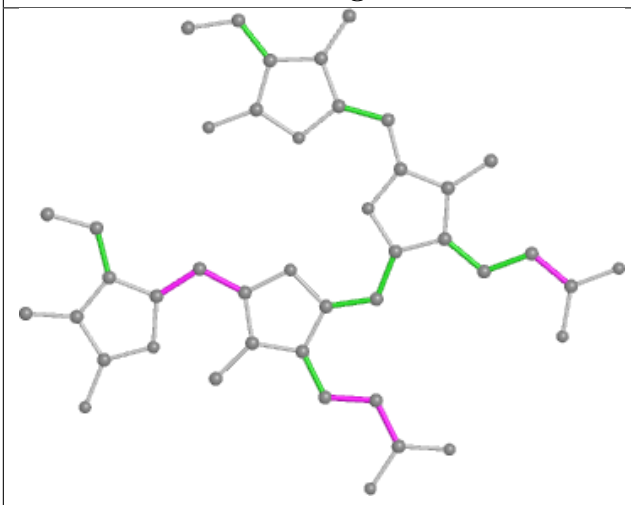

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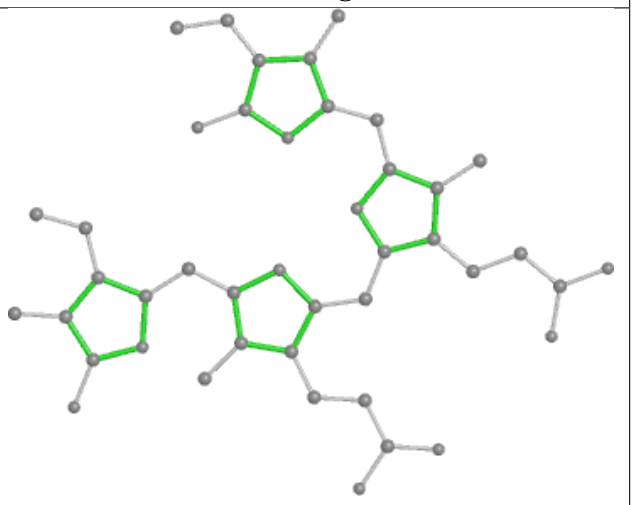
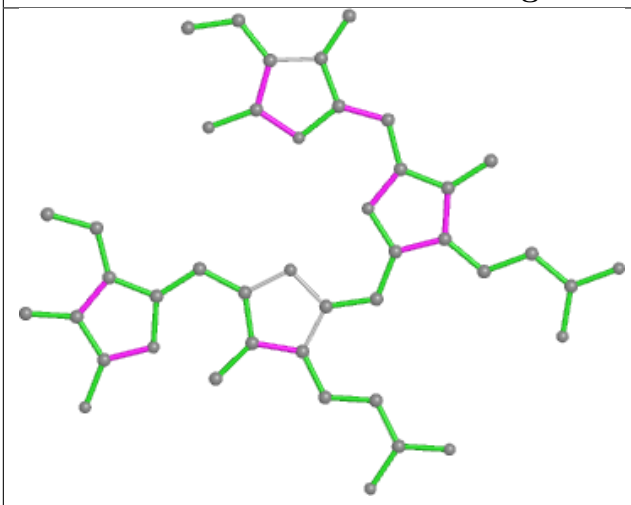


Rings

Ligand PUB f3 203



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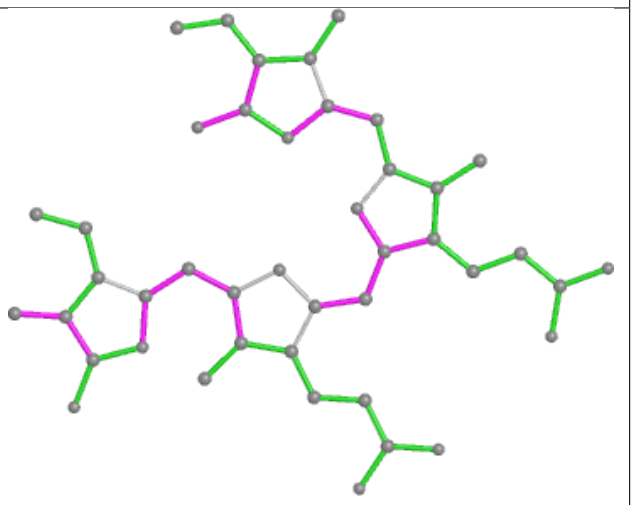

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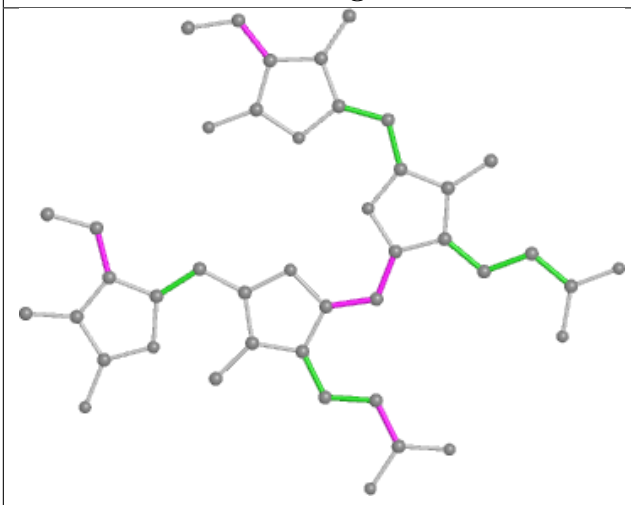

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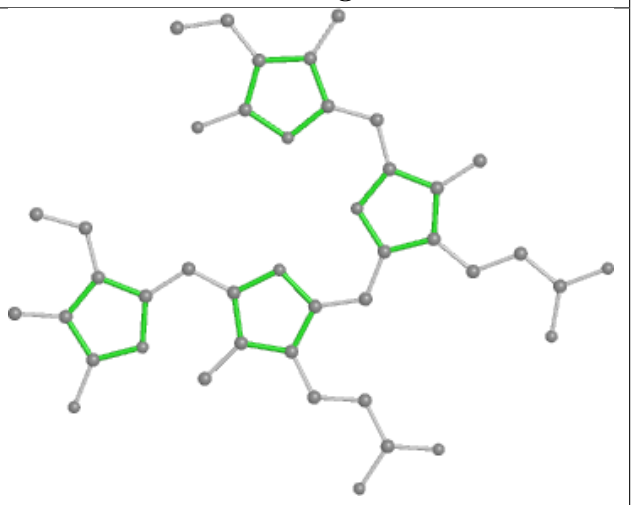

Rings

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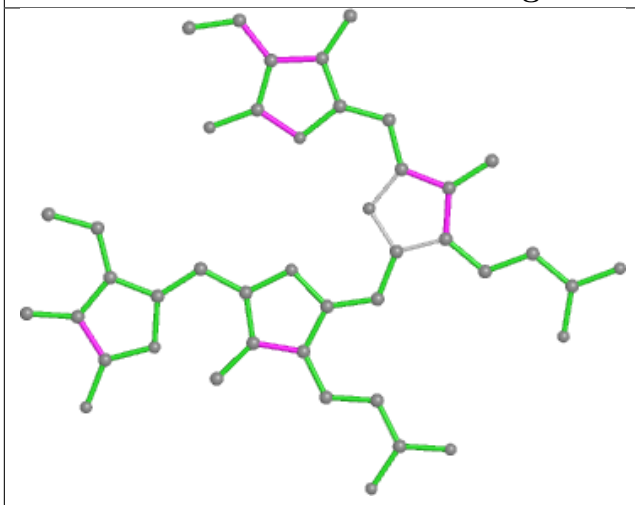

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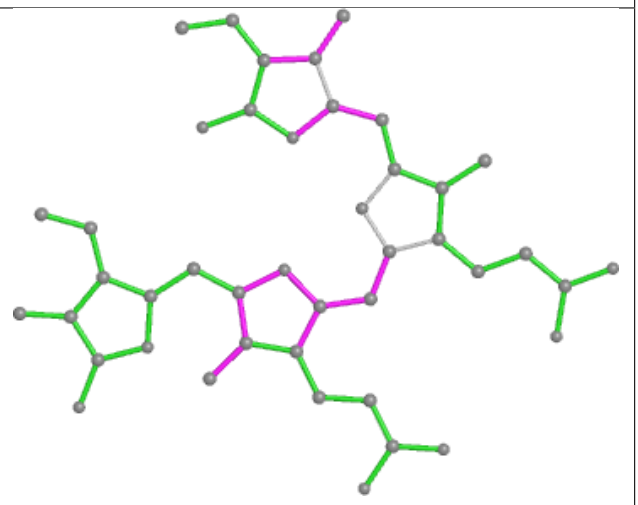

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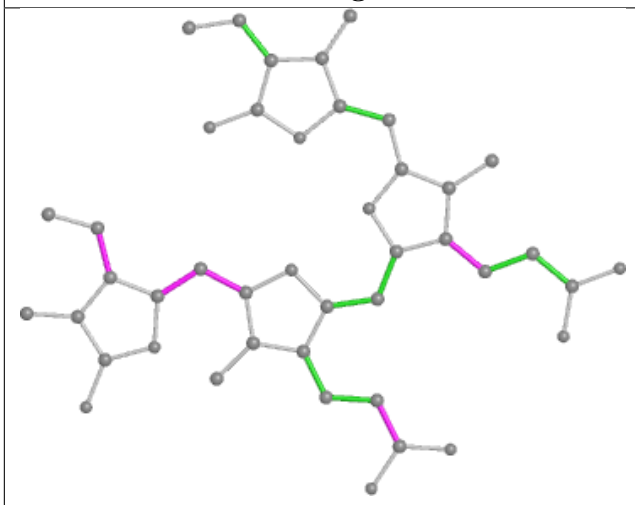

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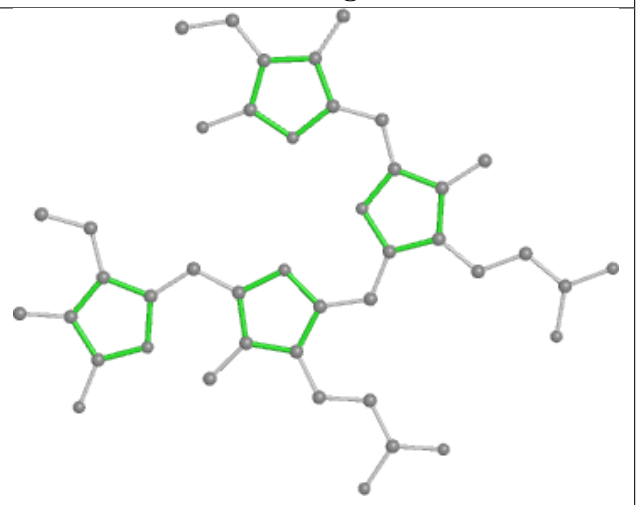
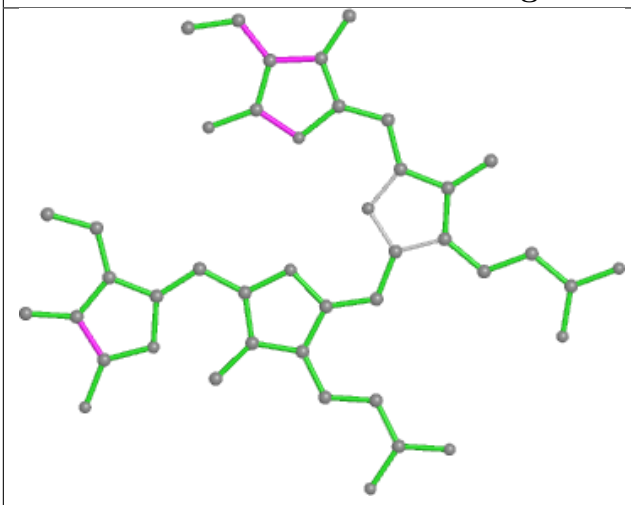


Rings

Ligand PEB c3 302



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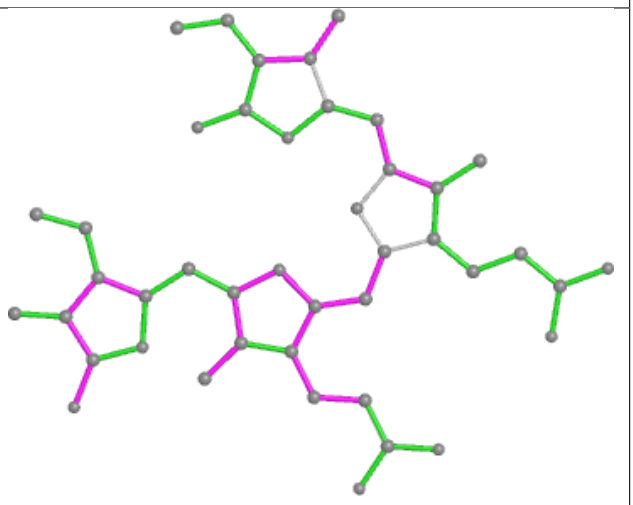

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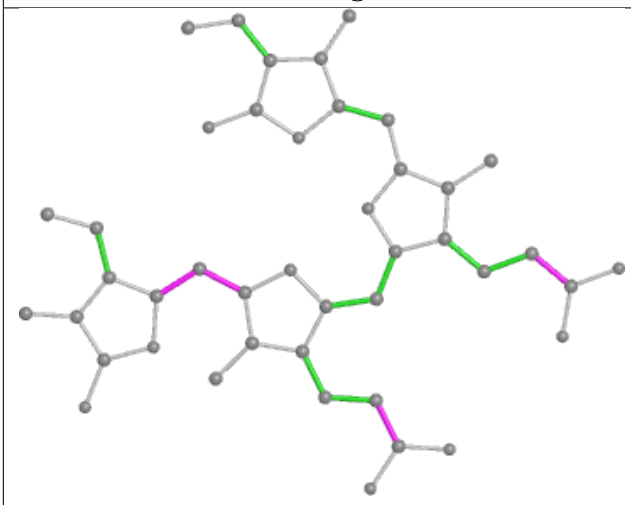

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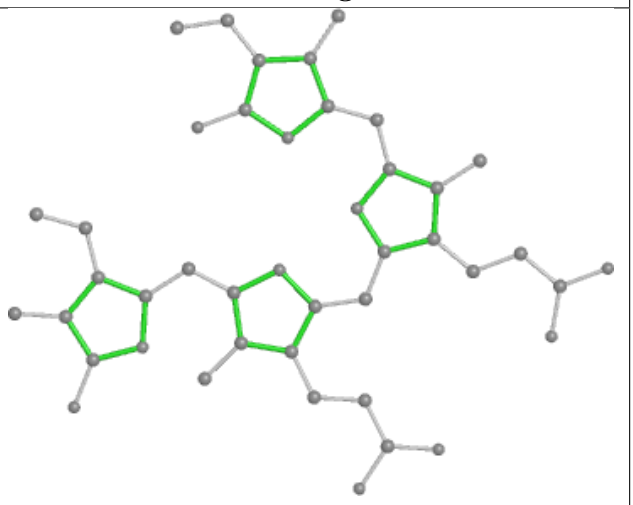
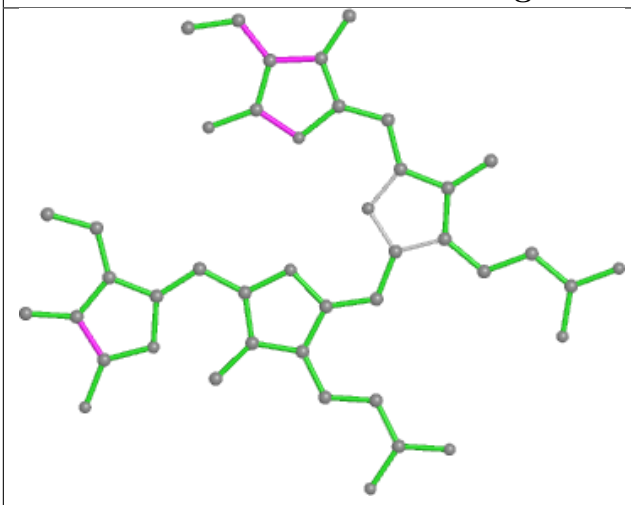


Rings

Ligand PEB dX 201



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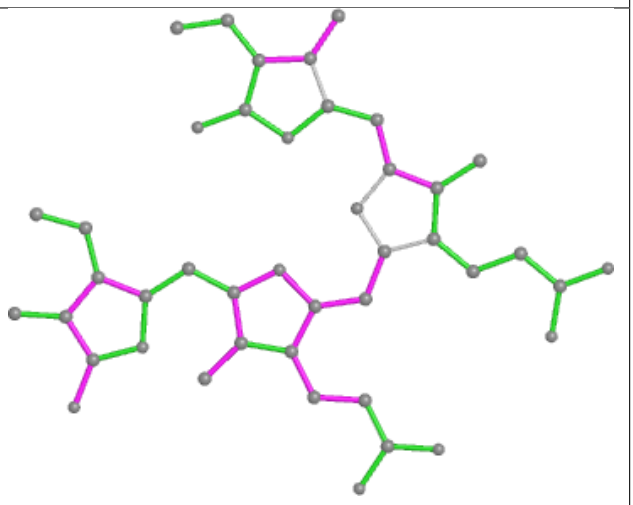

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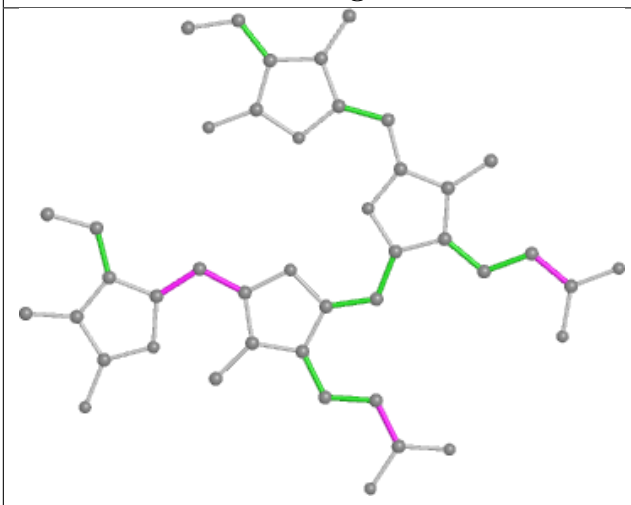

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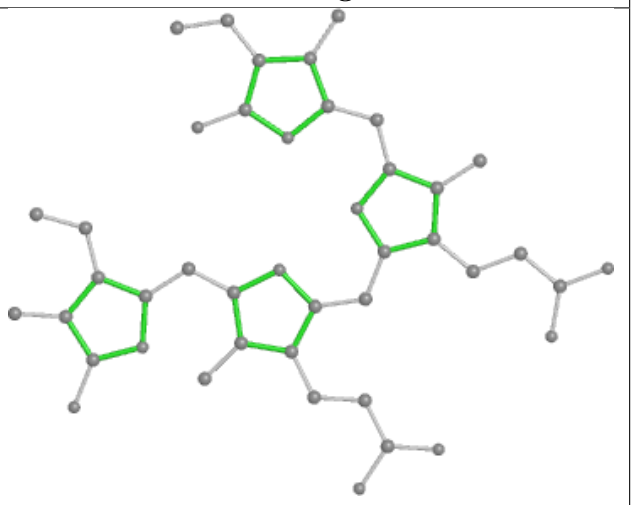
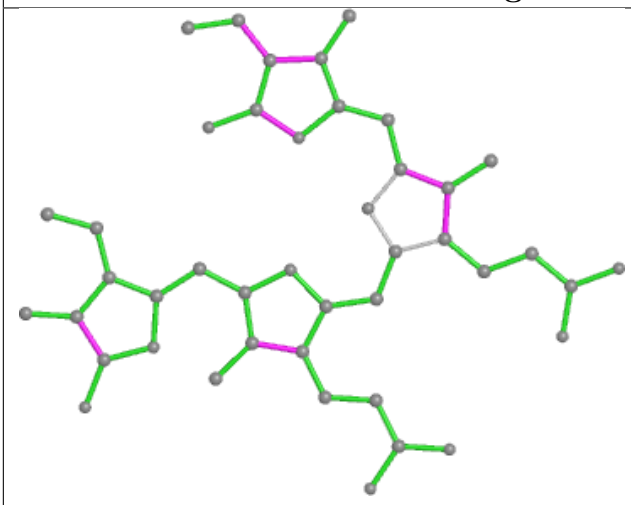


Rings

Ligand PEB m5 1003



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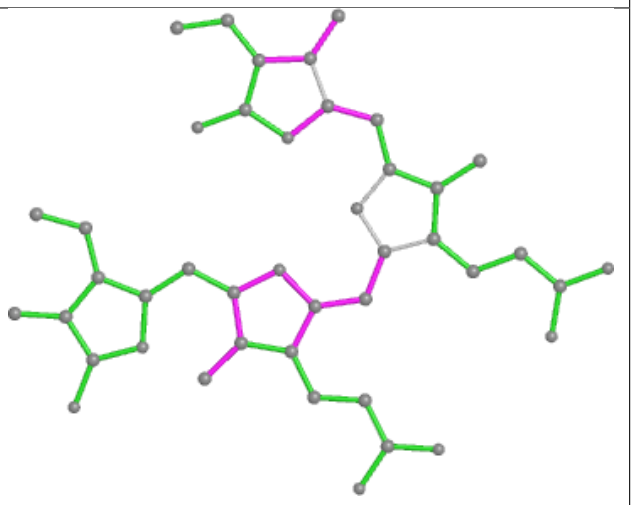
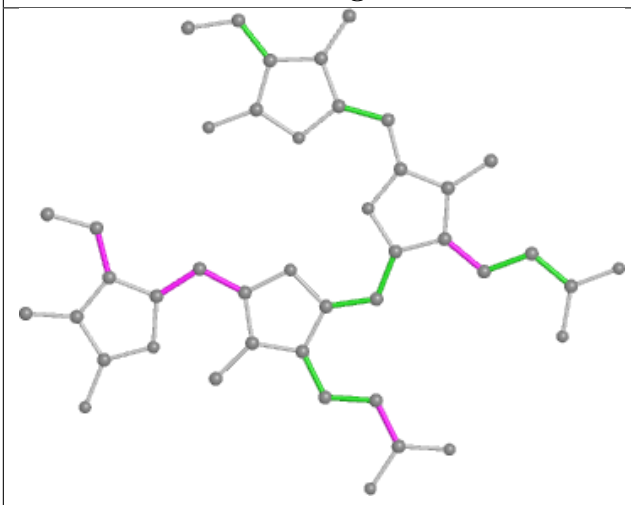


Bond angles



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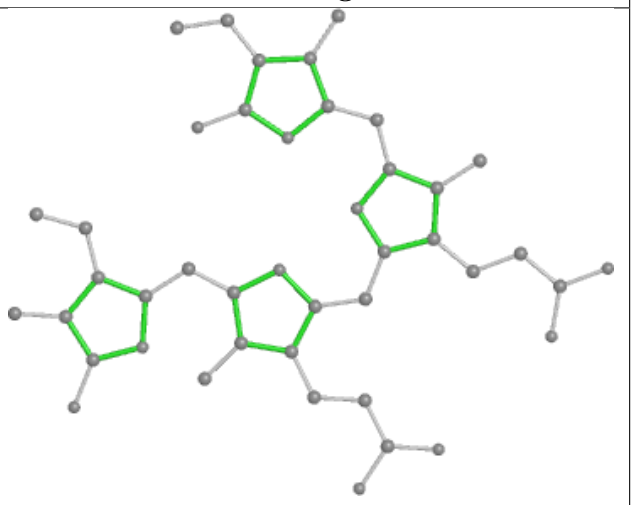
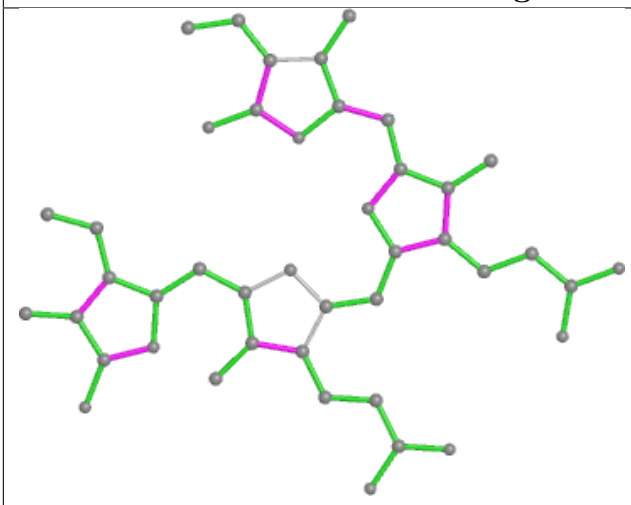


Rings

Ligand PUB V4 203



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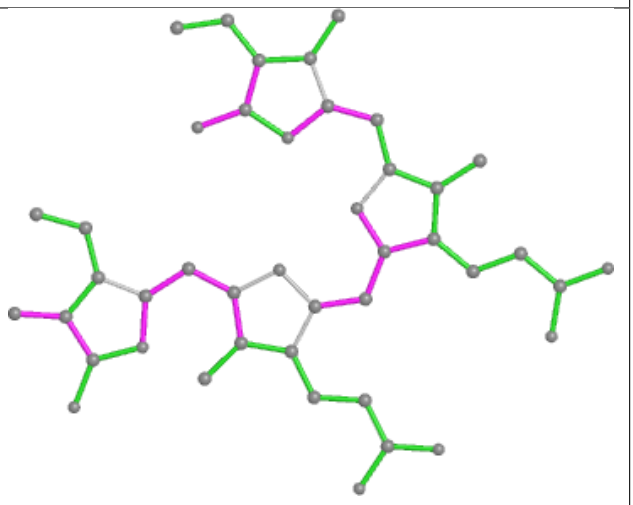
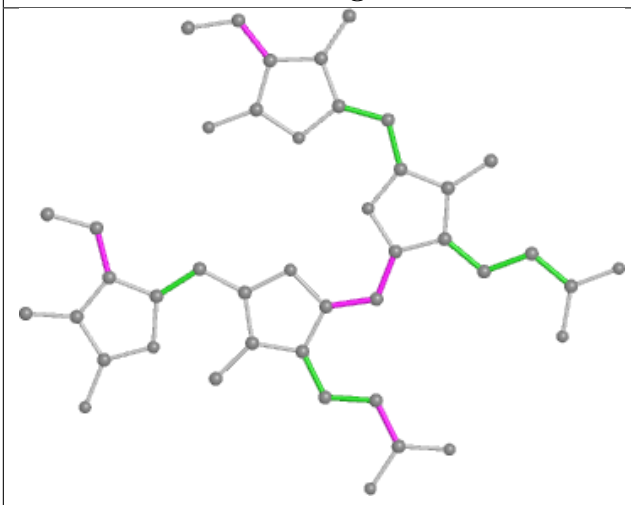


Bond angles



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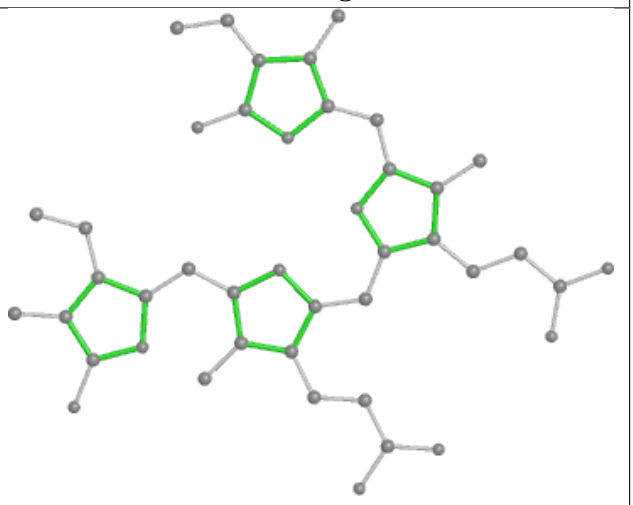
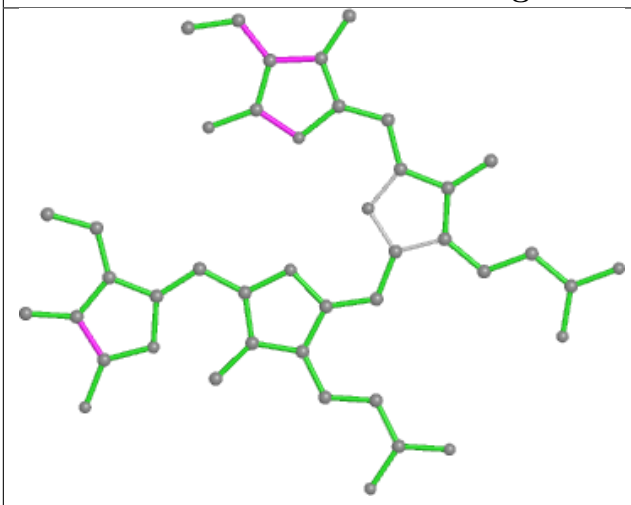


Rings

Ligand PEB iE 1001



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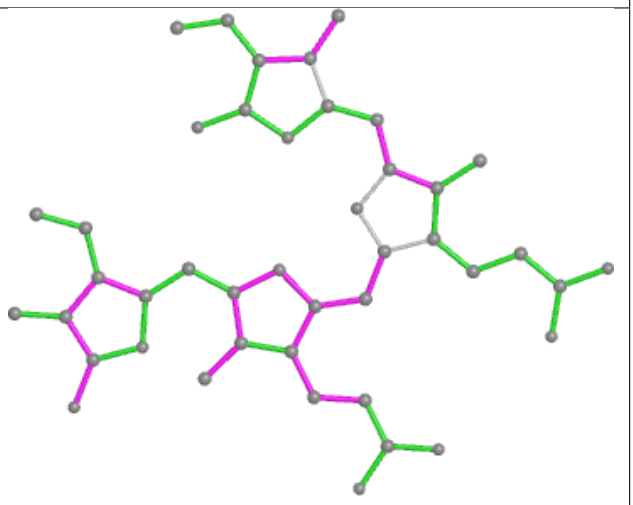

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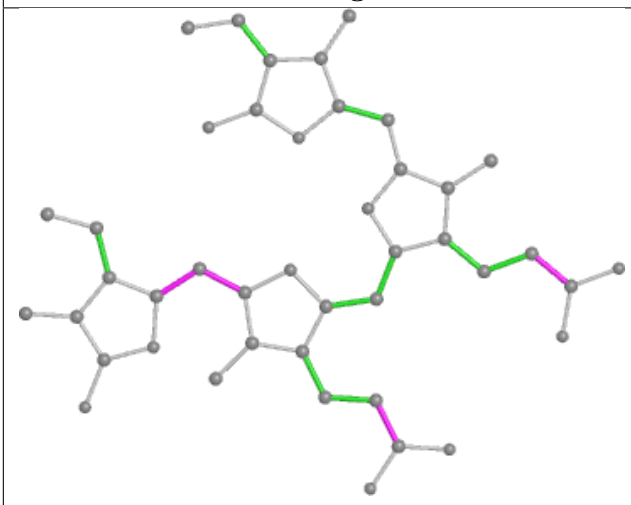
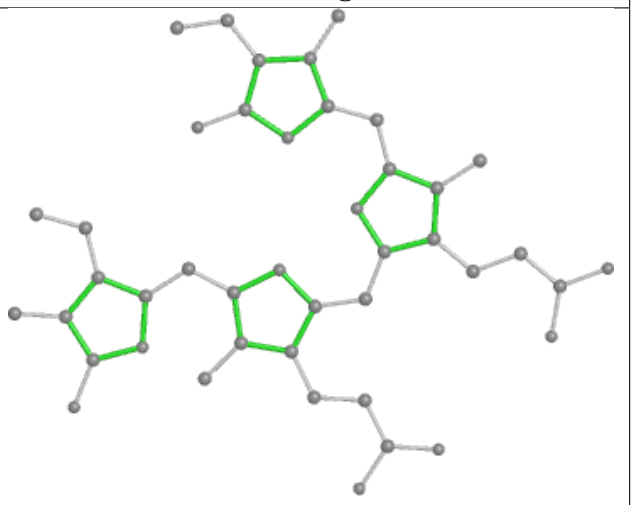
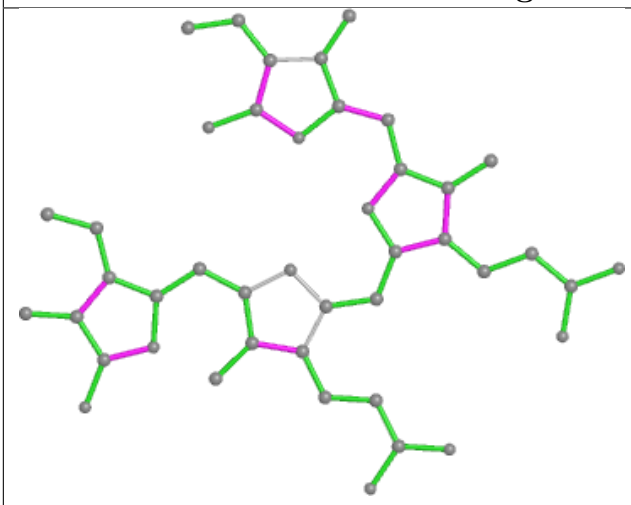


Torsions



Rings

Ligand PUB L9 203



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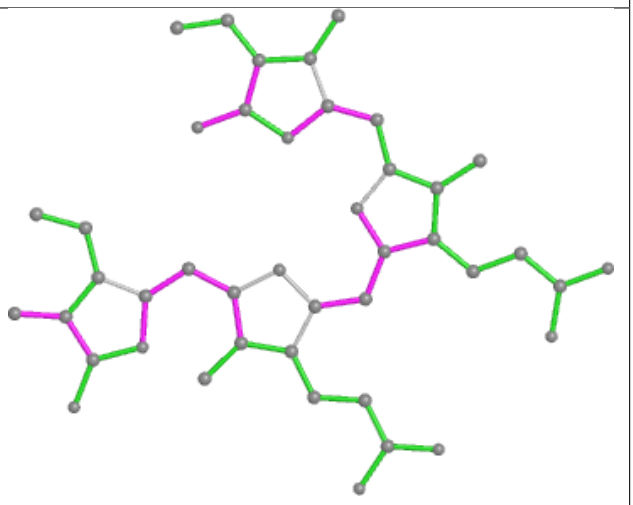

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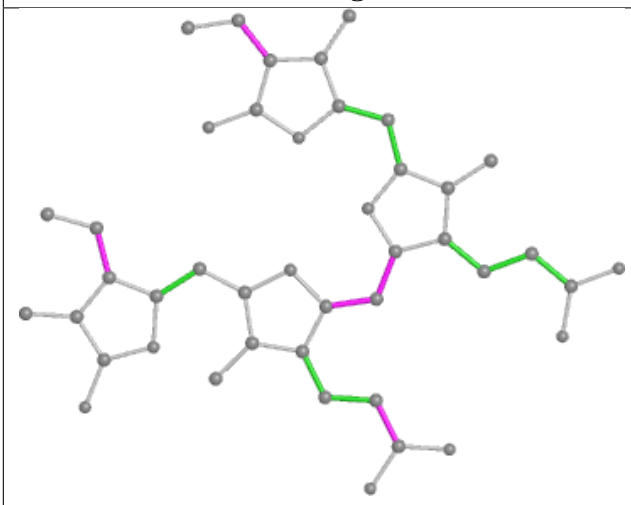

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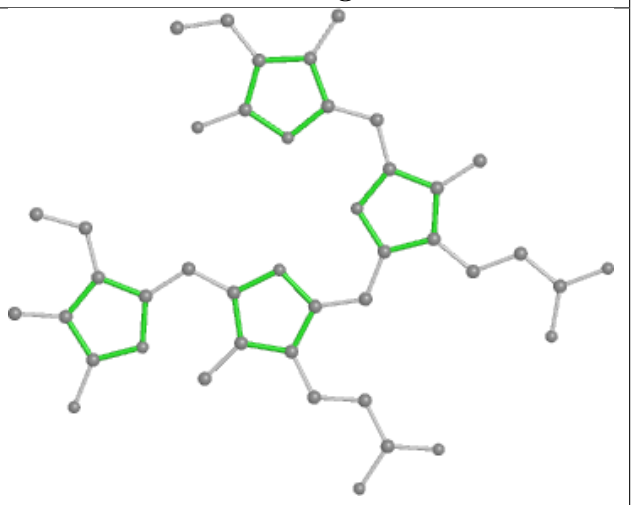
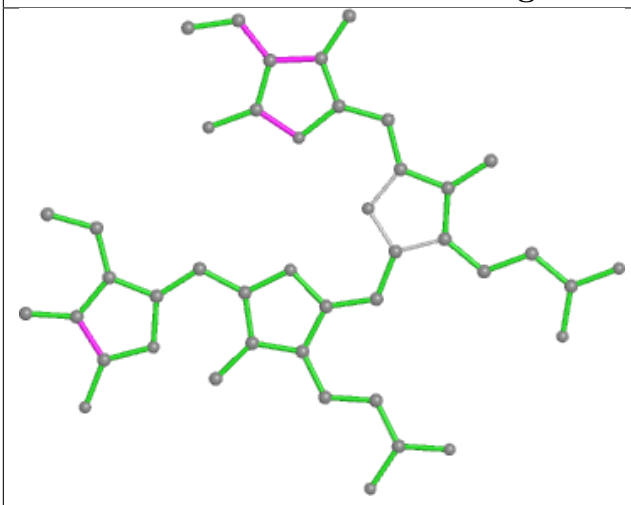


Rings

Ligand PEB bS 201



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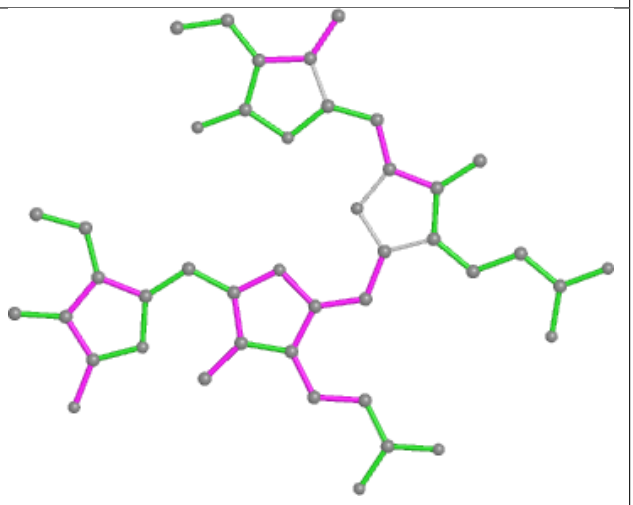

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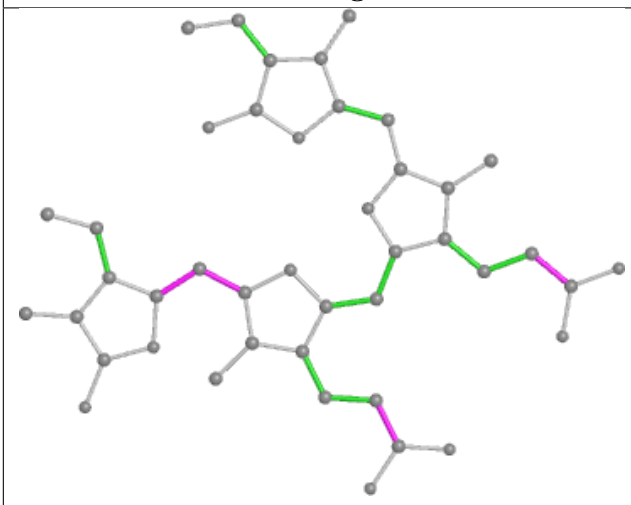

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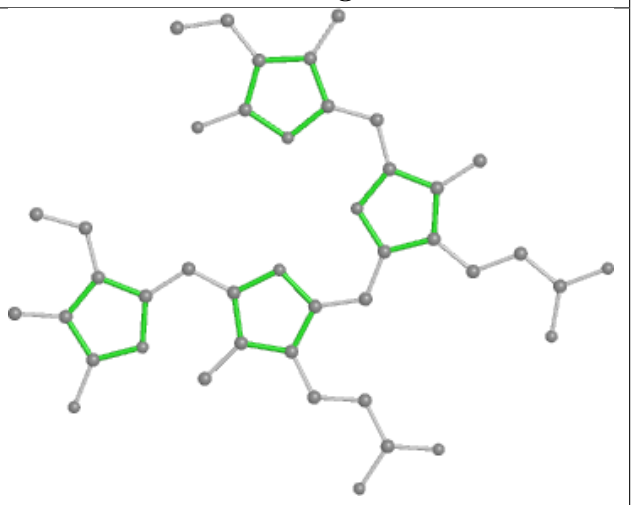

Rings

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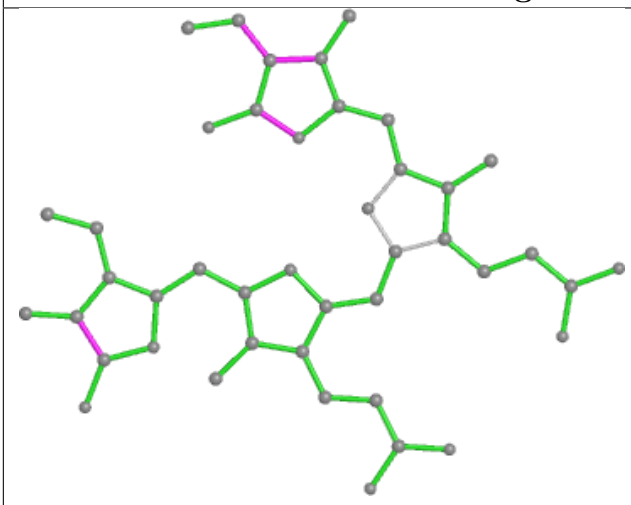

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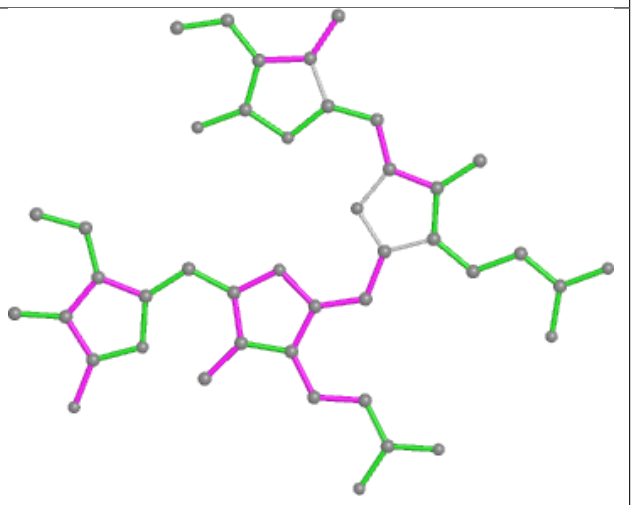

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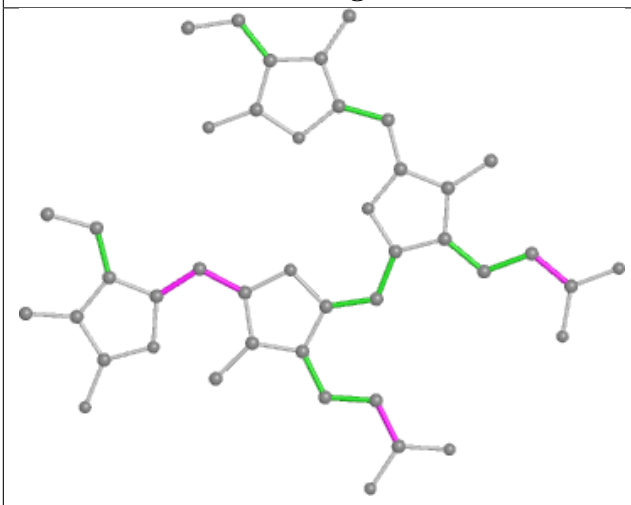

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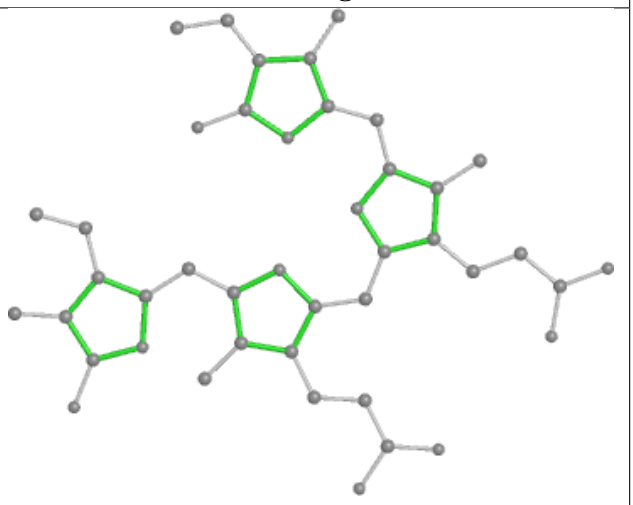
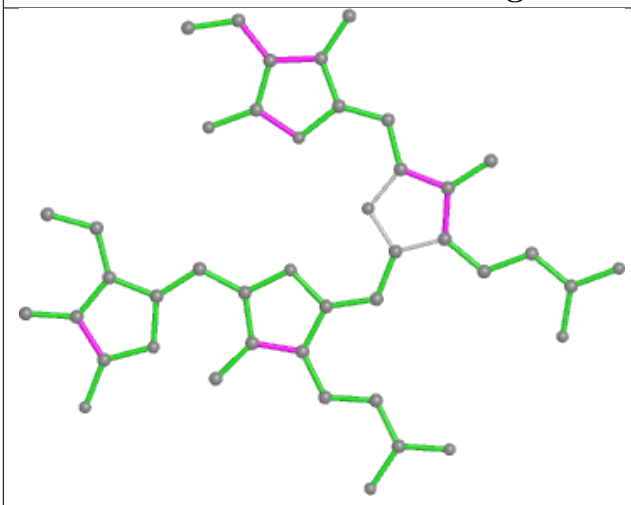


Rings

Ligand PEB A2 1003



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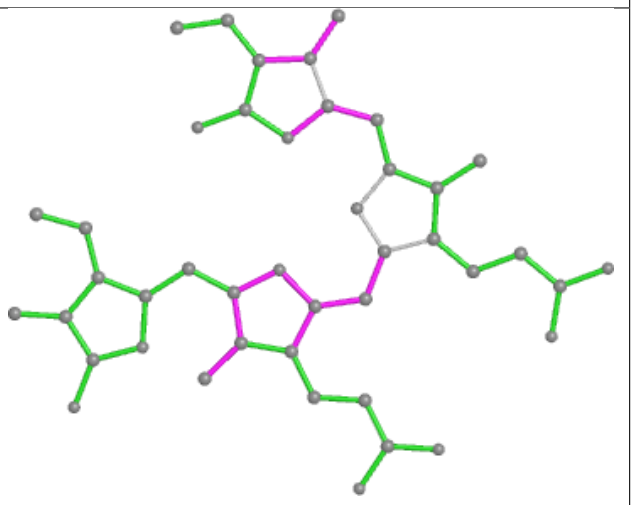

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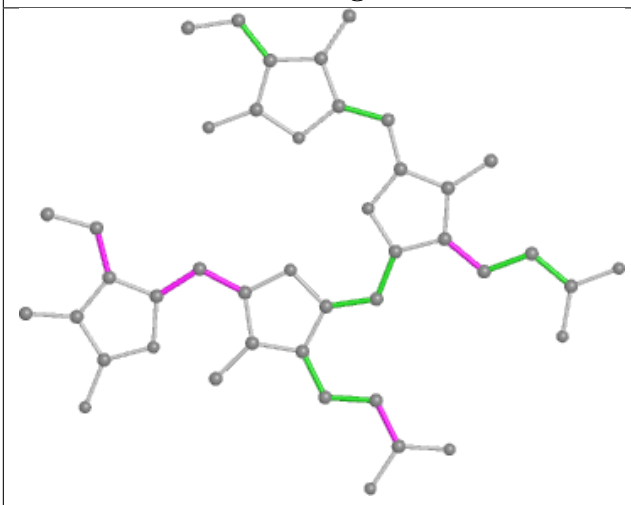

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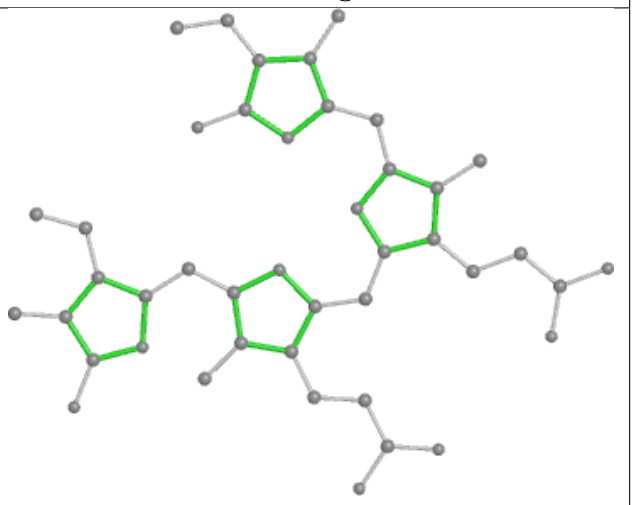

Rings

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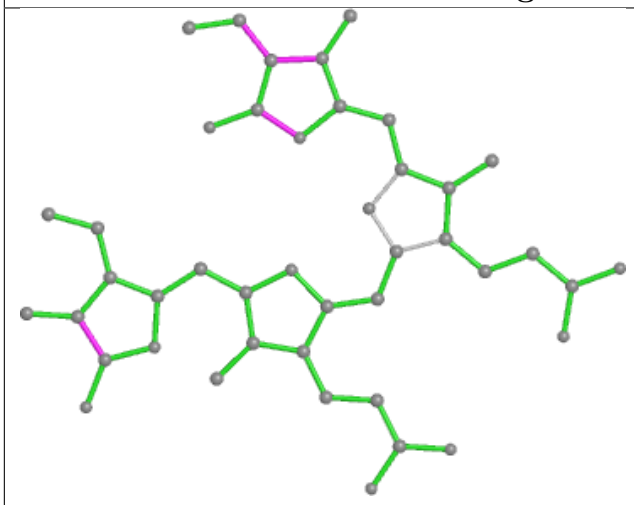

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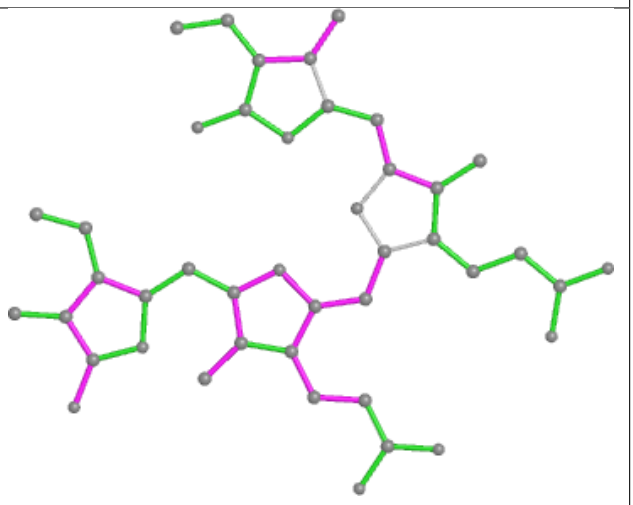

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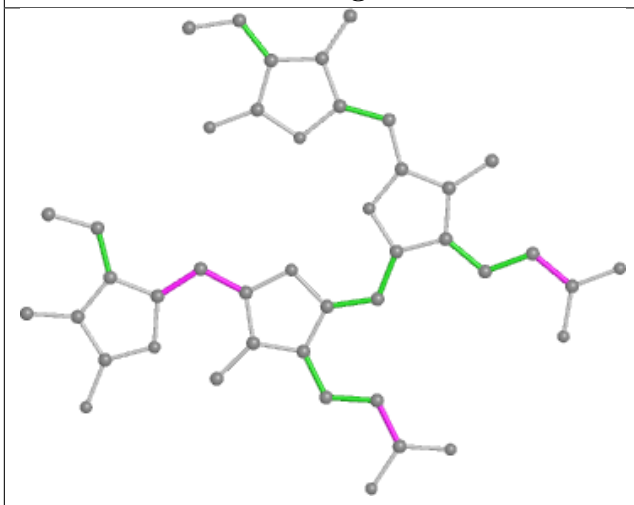

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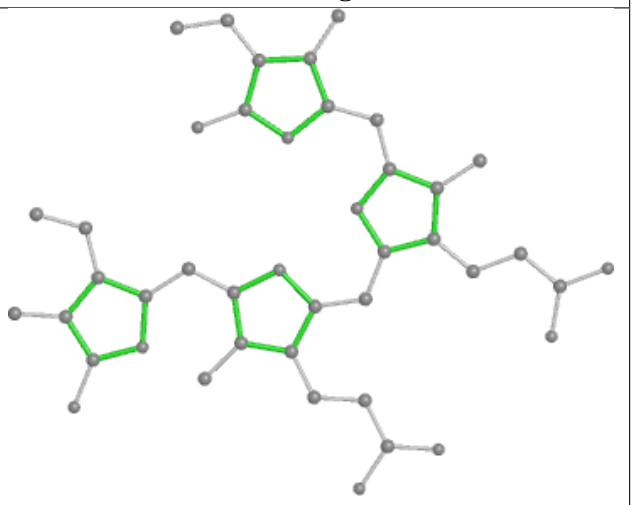

Rings

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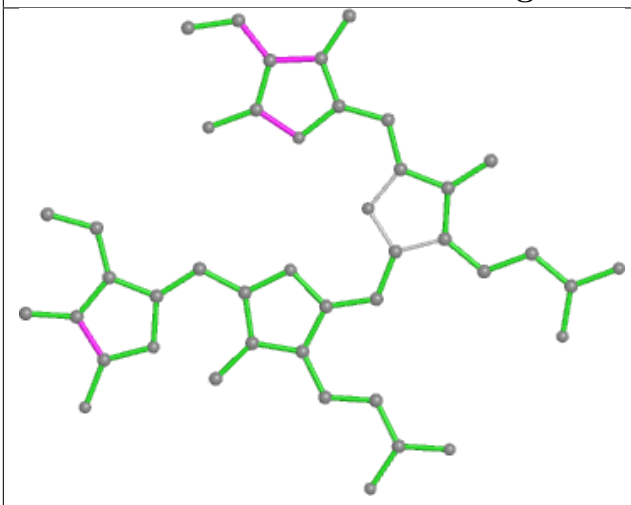

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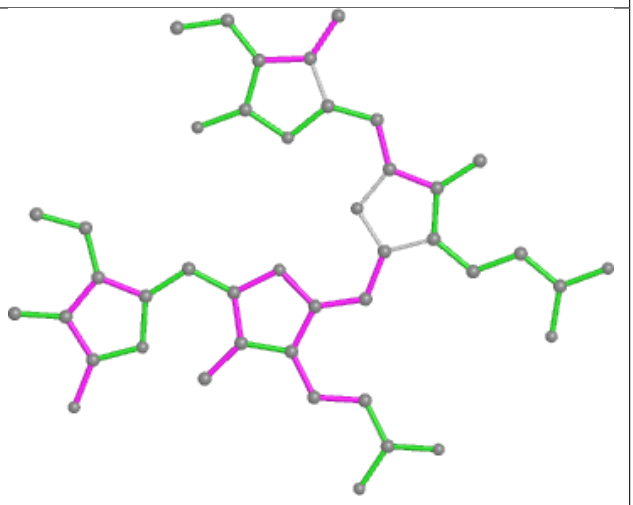

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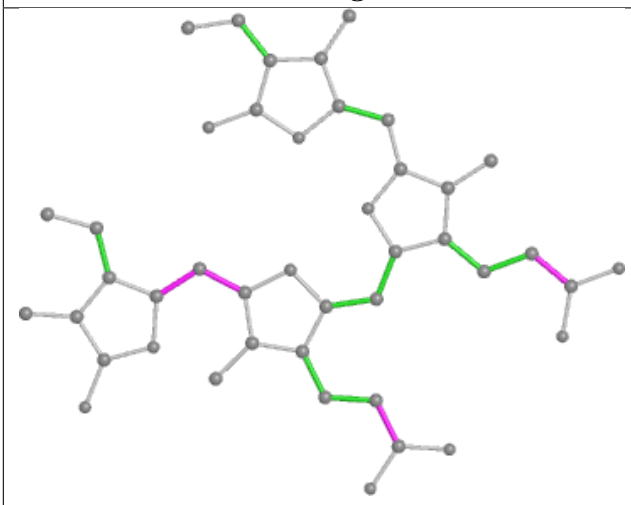

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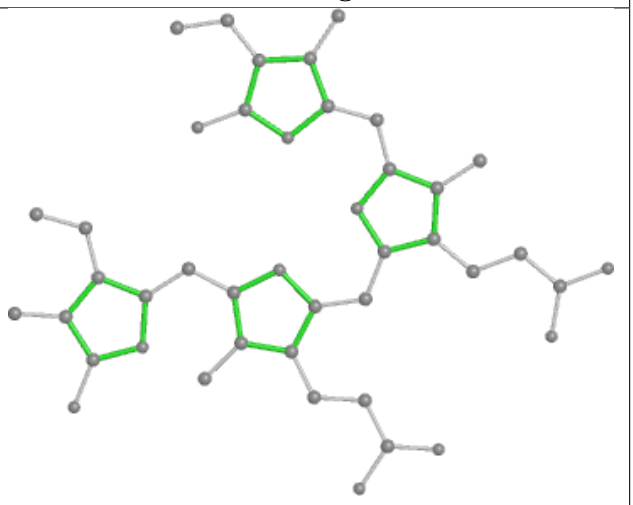

Rings

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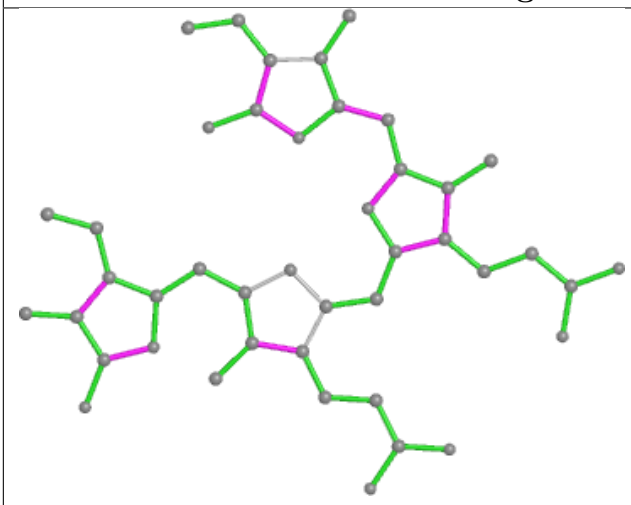

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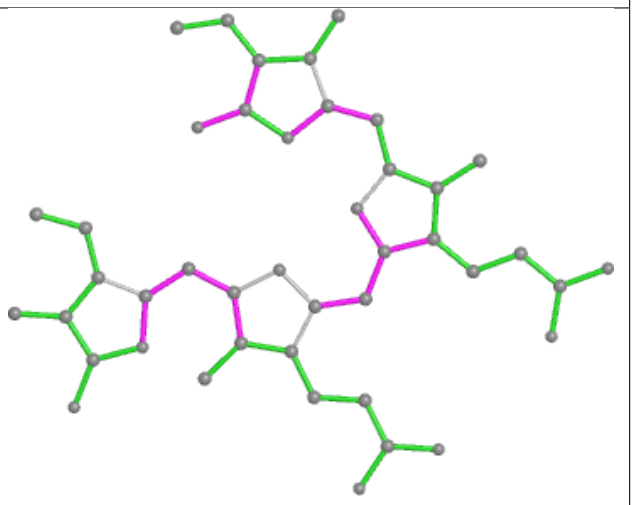

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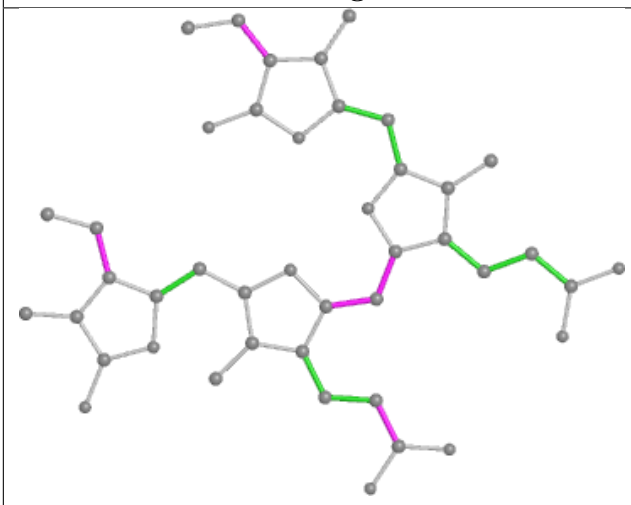

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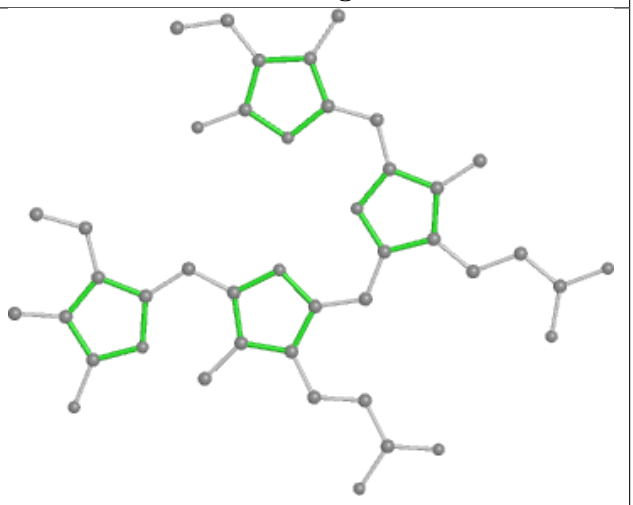

Rings

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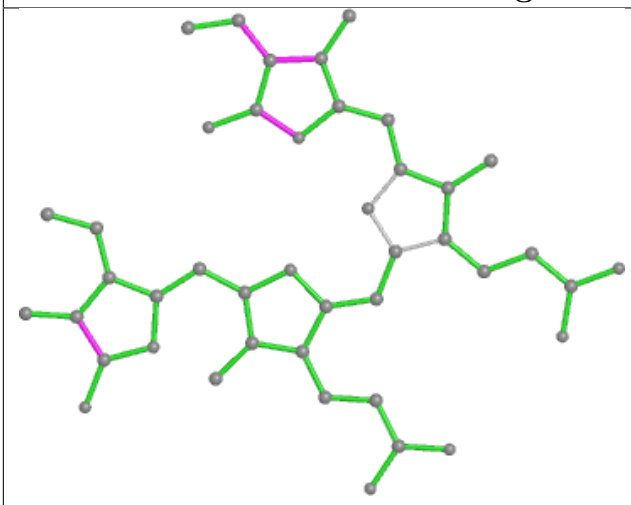

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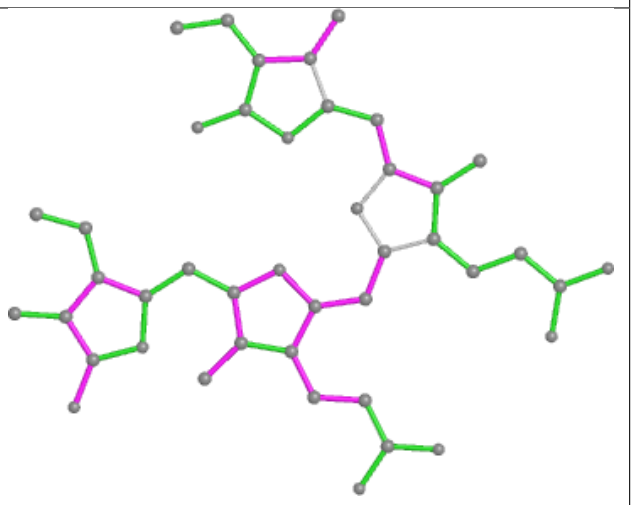

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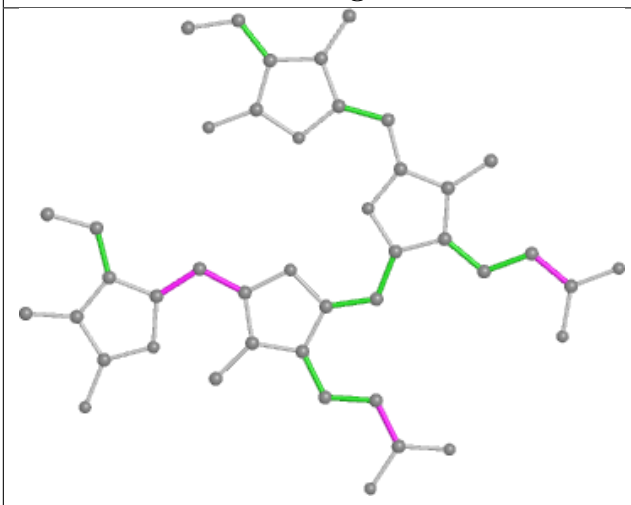

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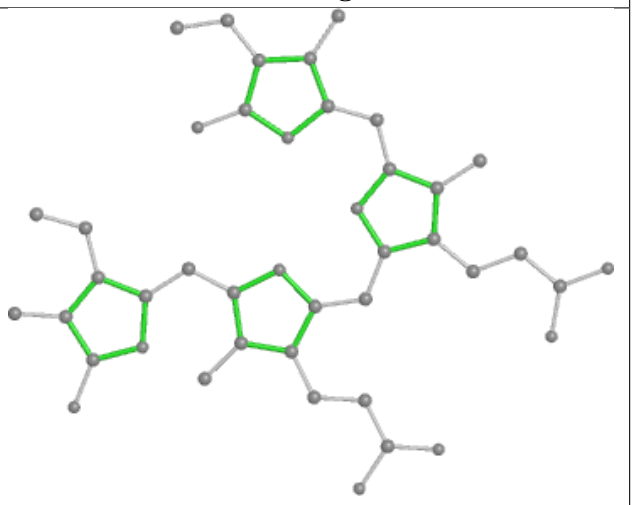

Rings

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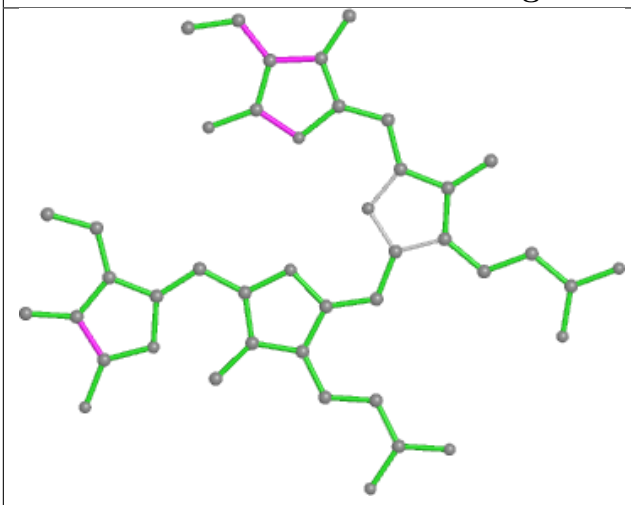

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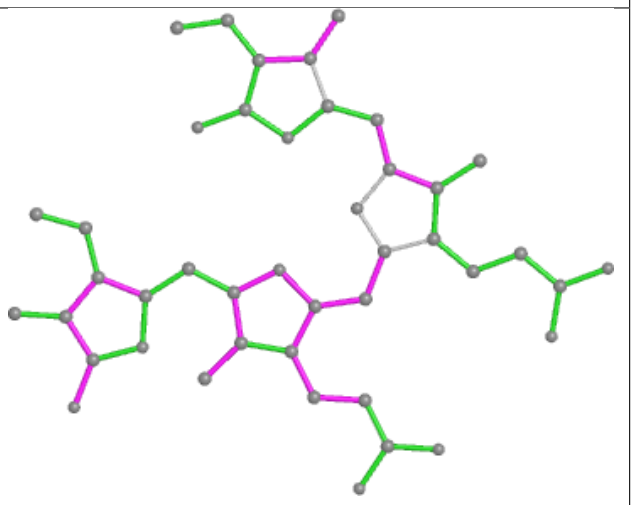

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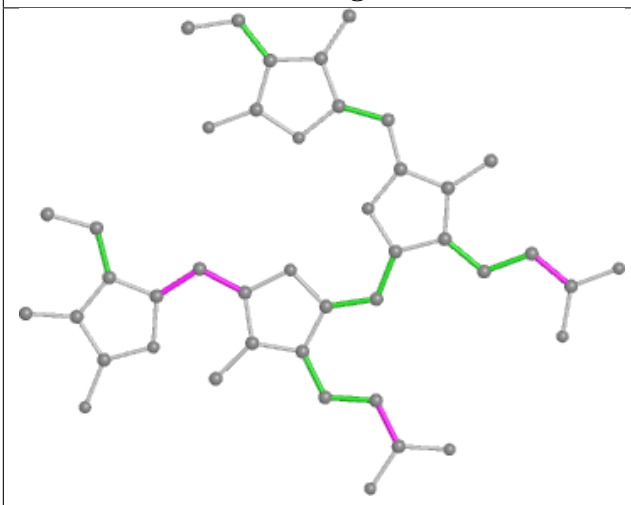

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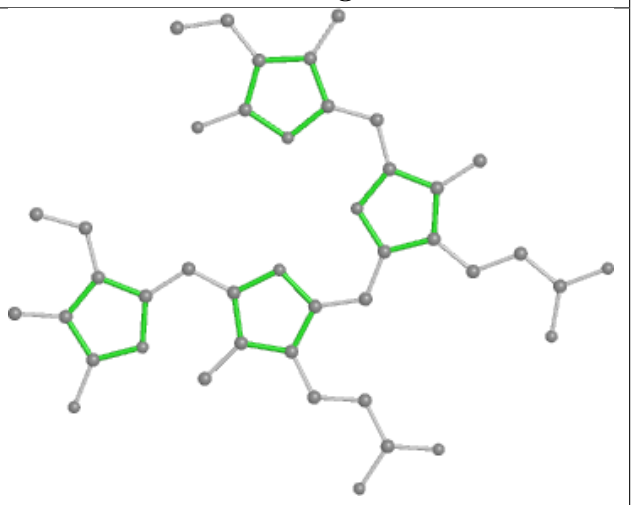

Rings

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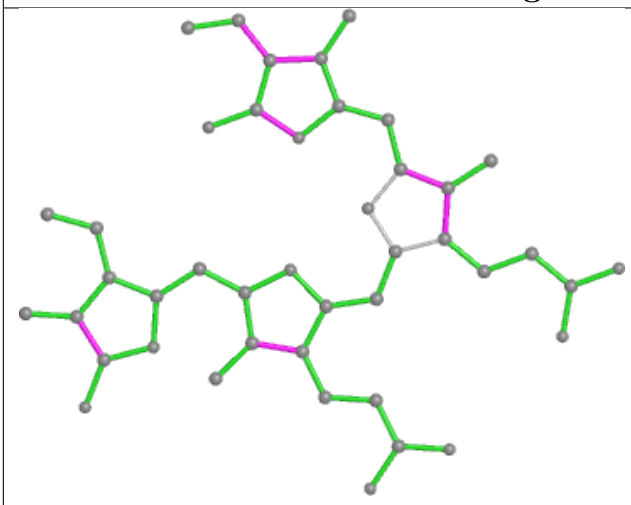

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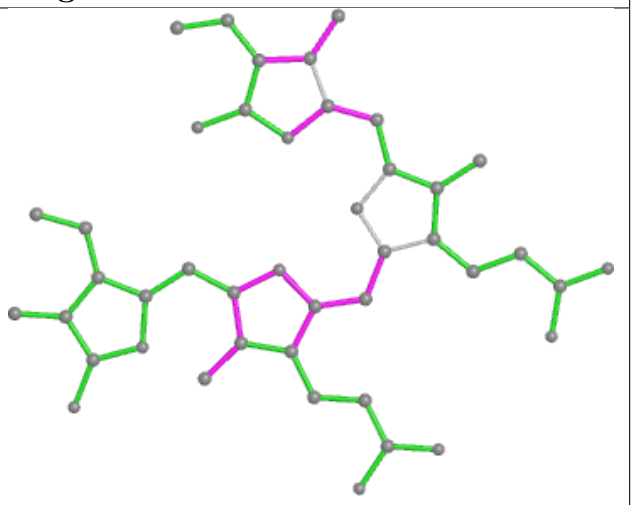

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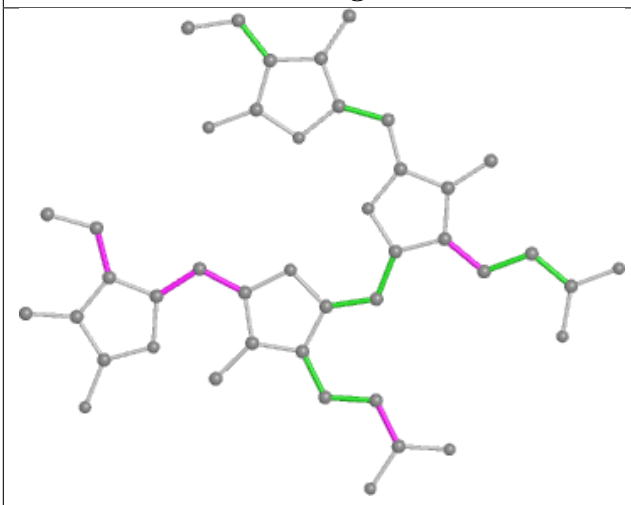

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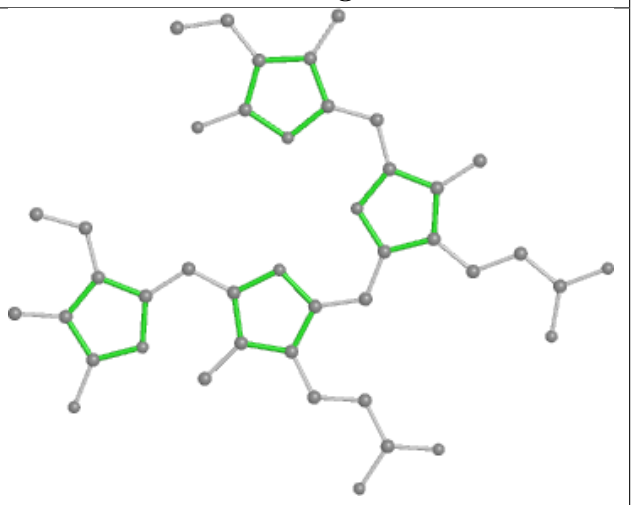

Rings

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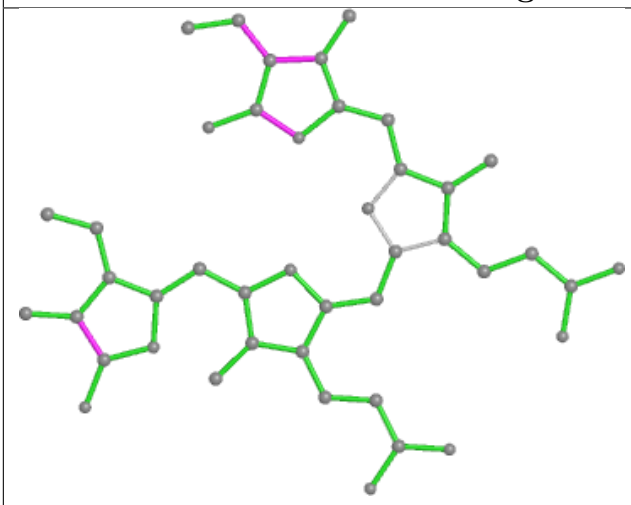

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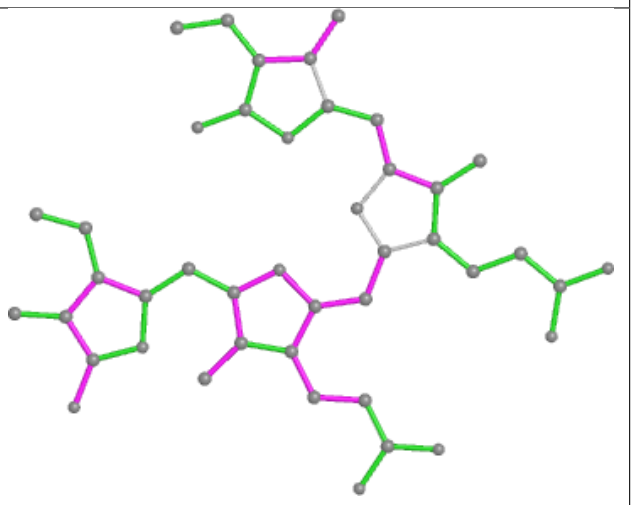

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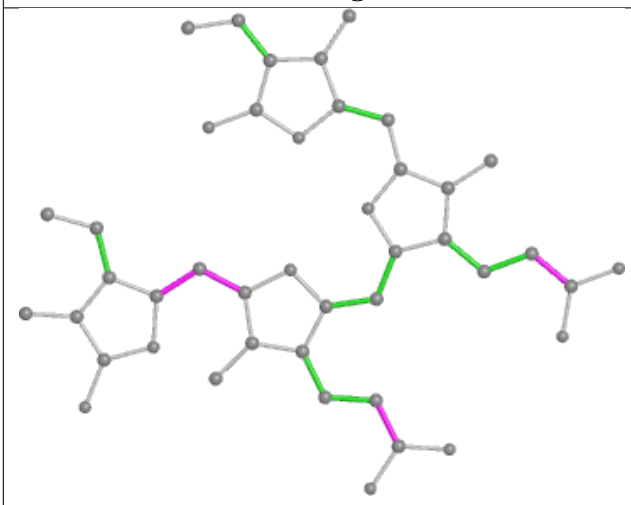

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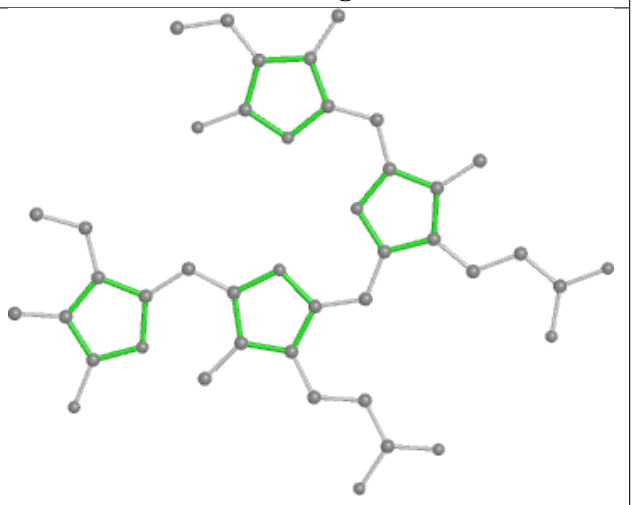
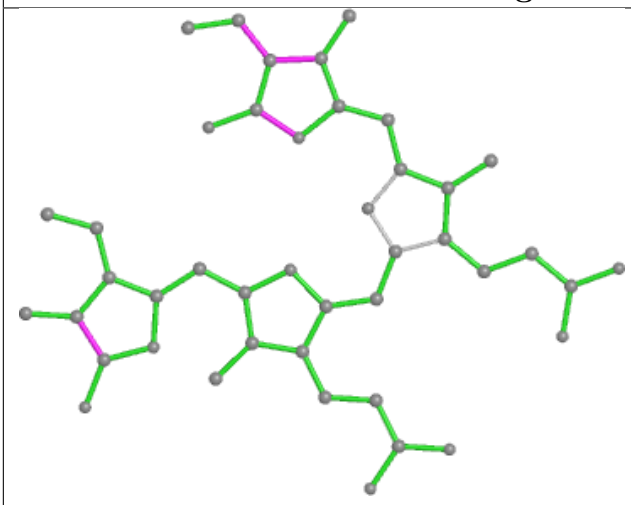


Rings

Ligand PEB Q5 201



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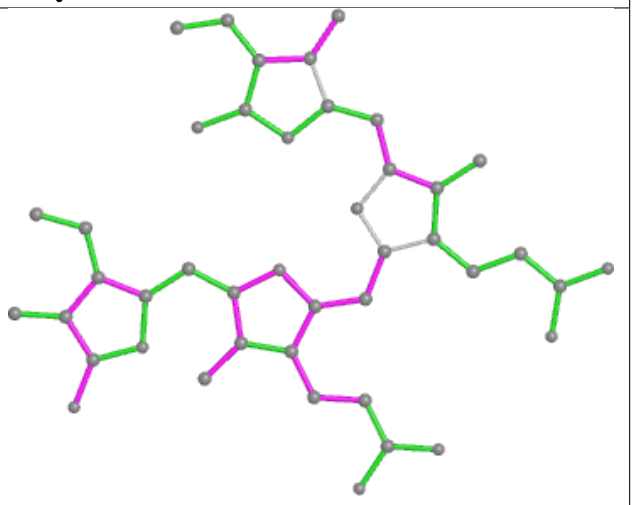

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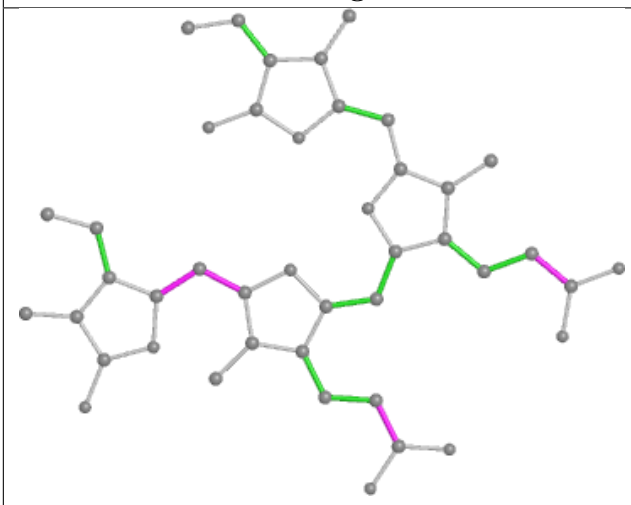

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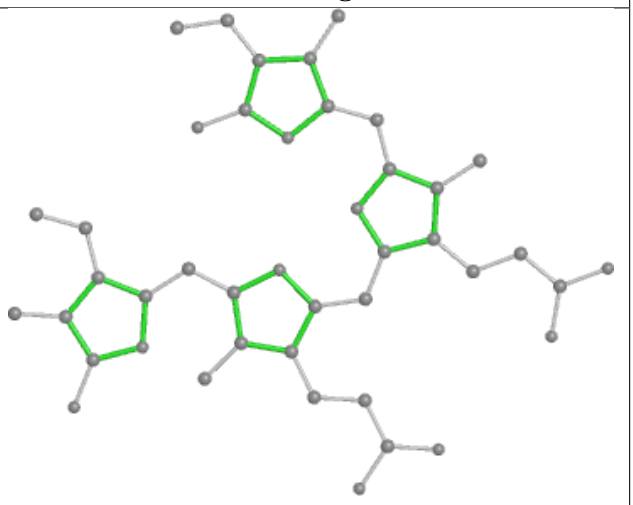

Rings

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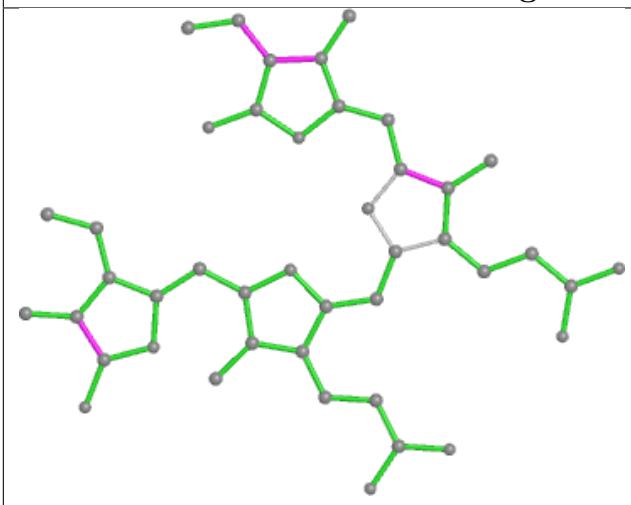
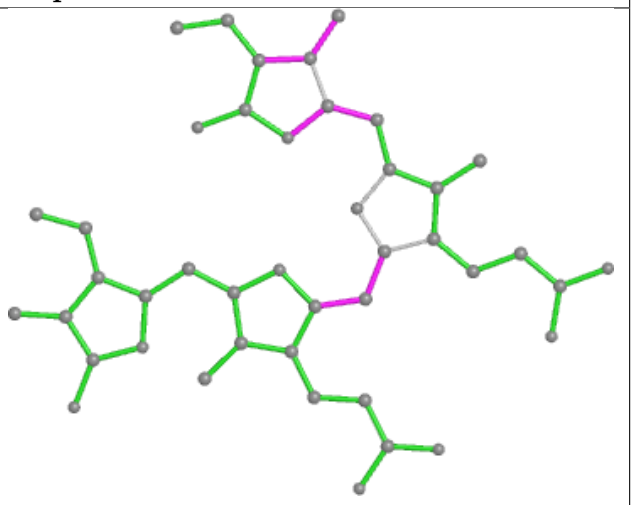
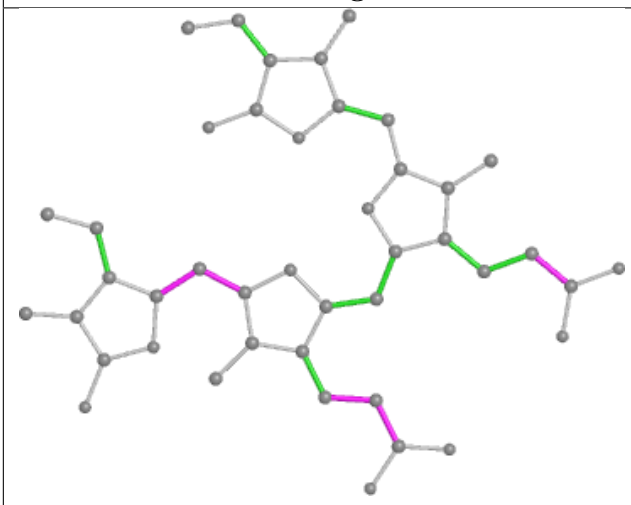


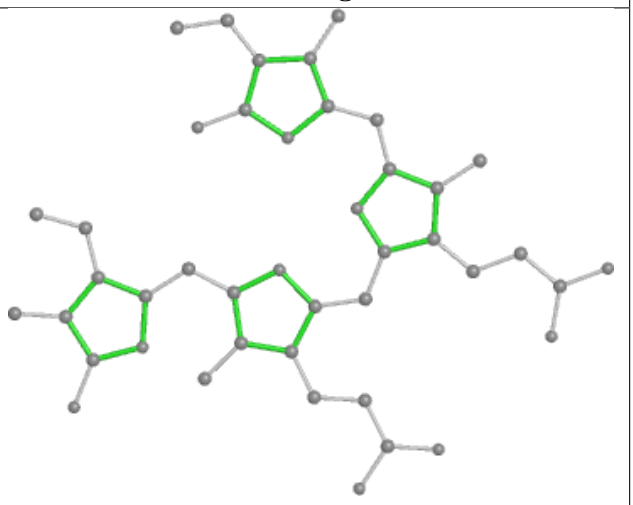
Bond lengths



Bond angles

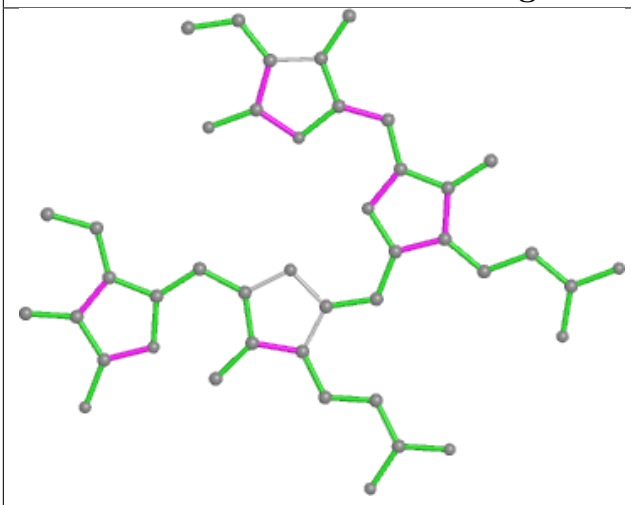


Torsions



Rings

Ligand PUB e7 203



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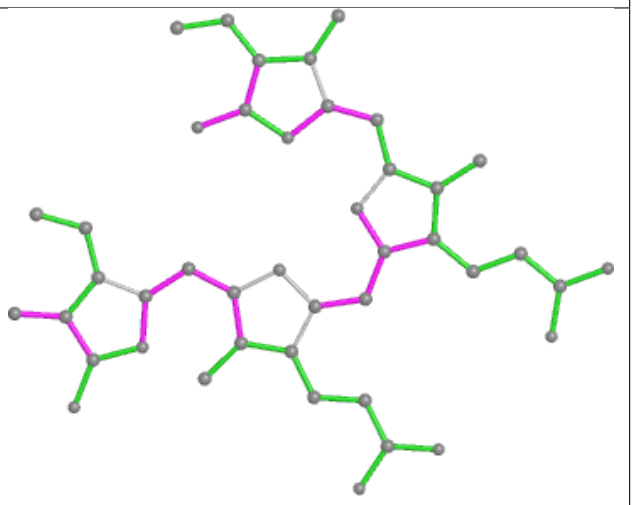

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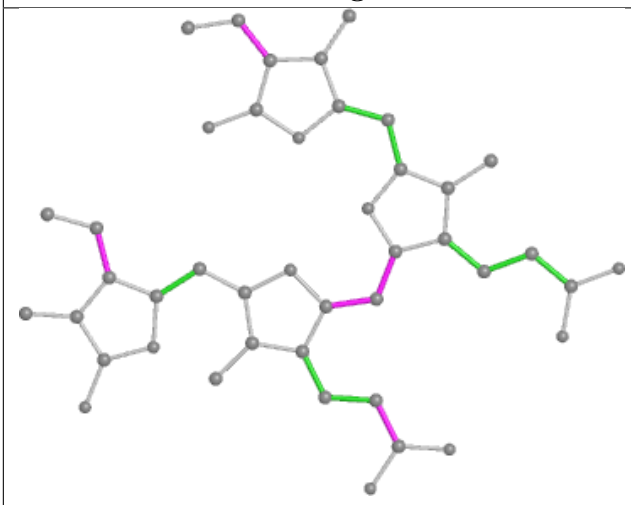

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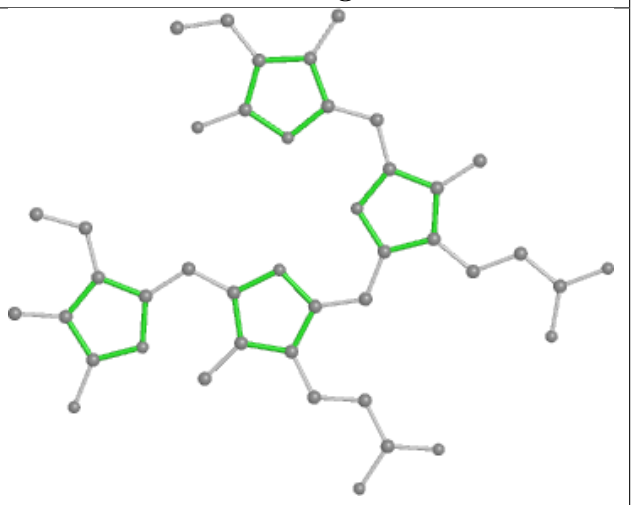
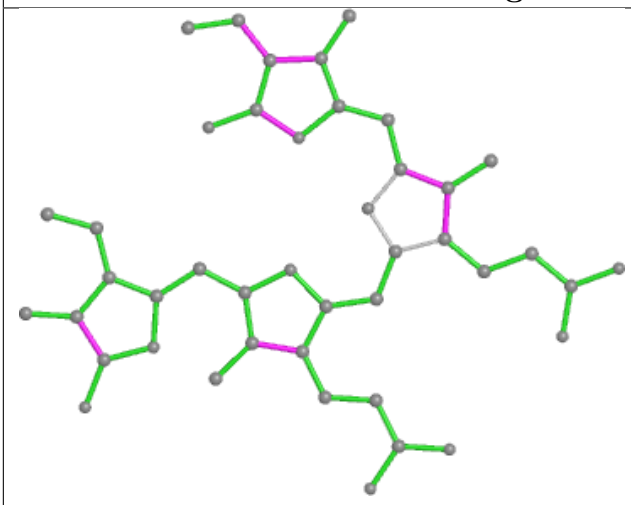


Rings

Ligand PEB kX 1002



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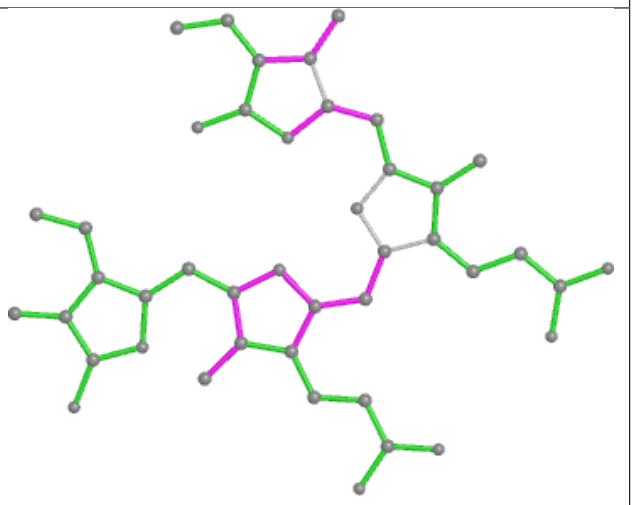

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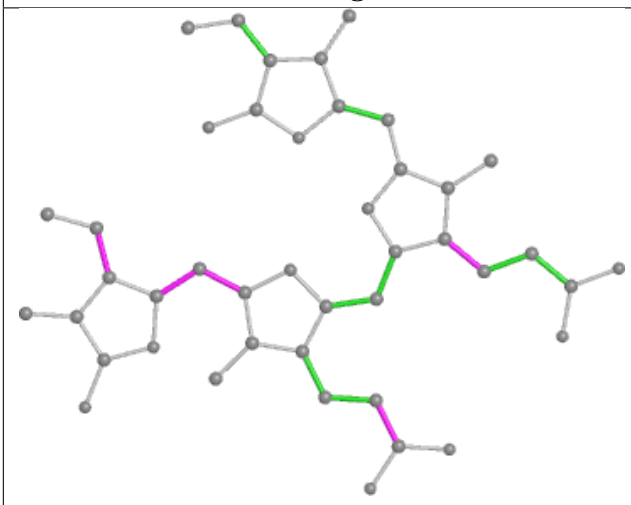

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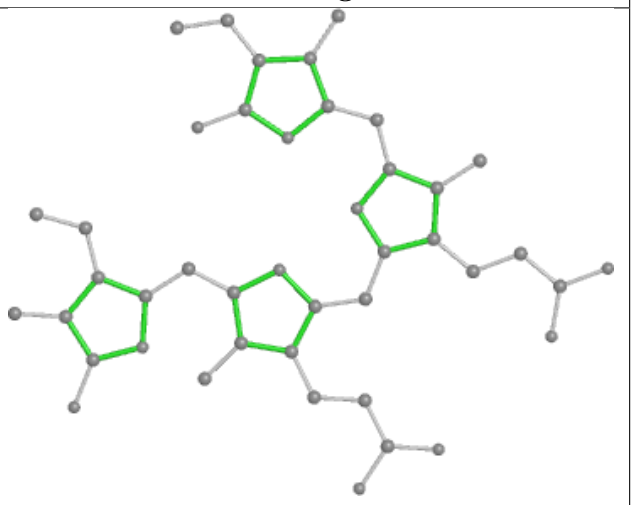
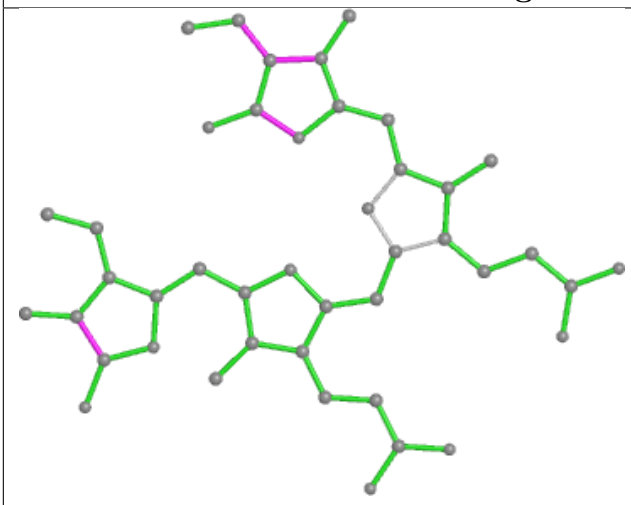


Rings

Ligand PEB dB 201



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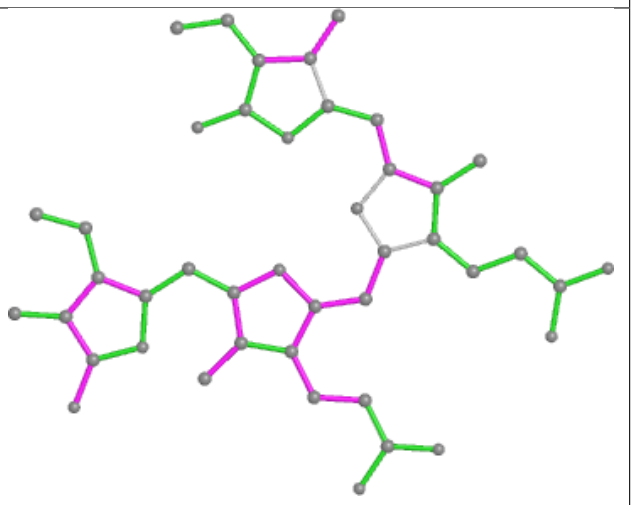
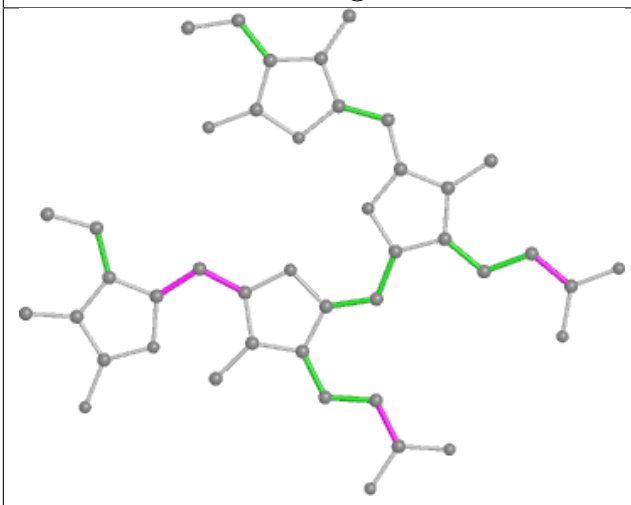


Bond angles



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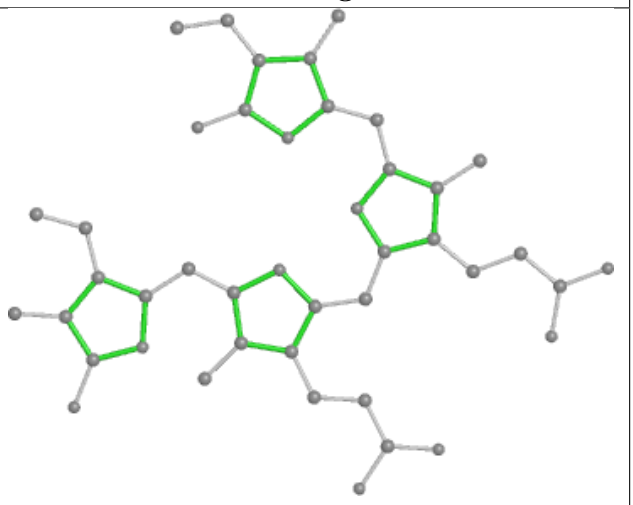
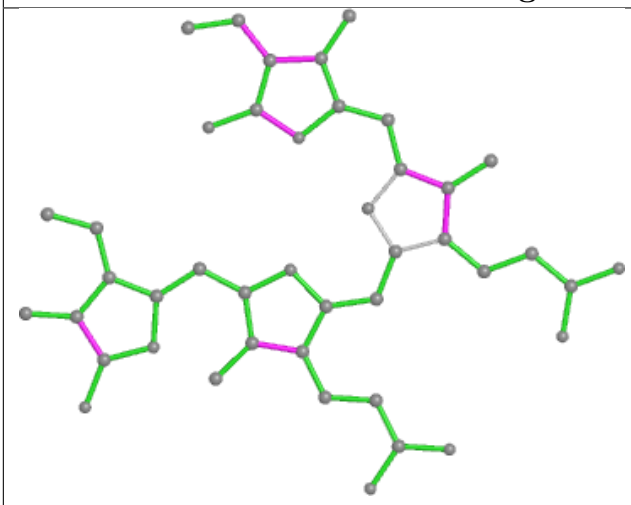


Rings

Ligand PEB n2 202



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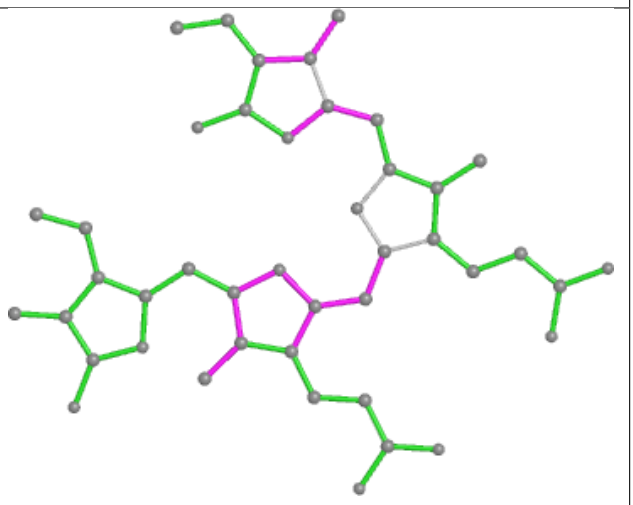

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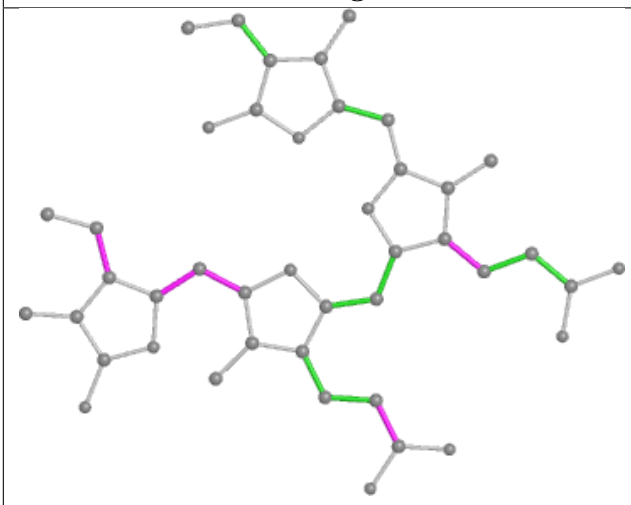

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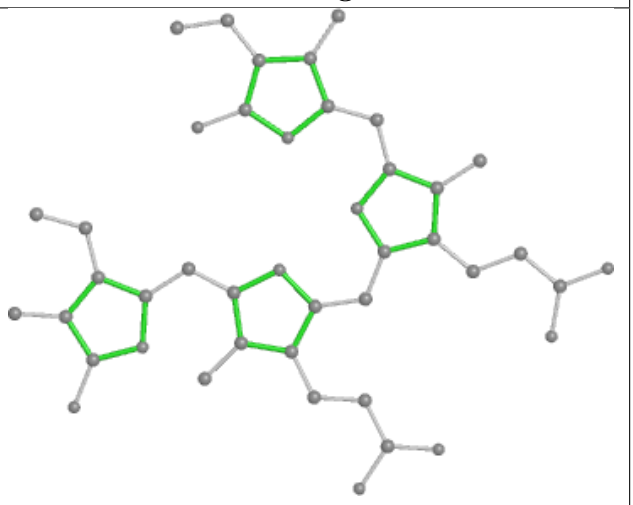
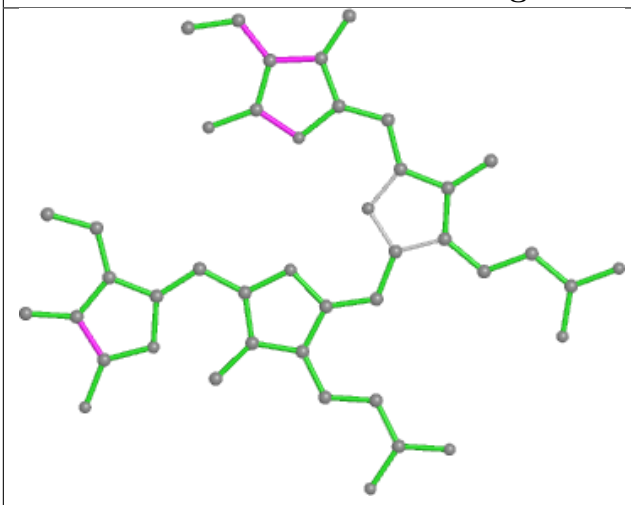


Rings

Ligand PEB b8 1003



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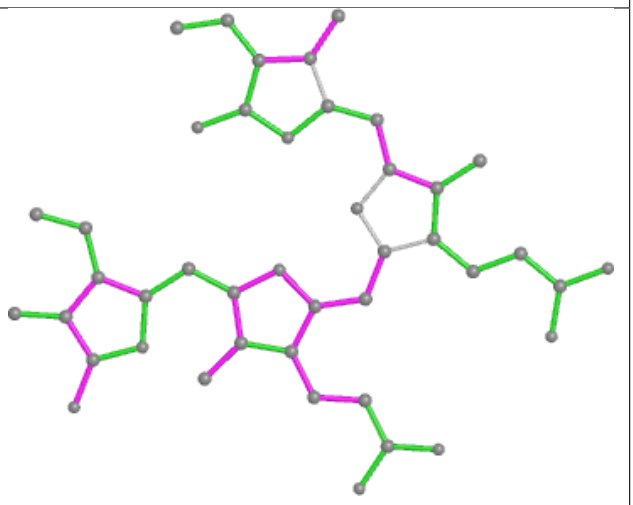

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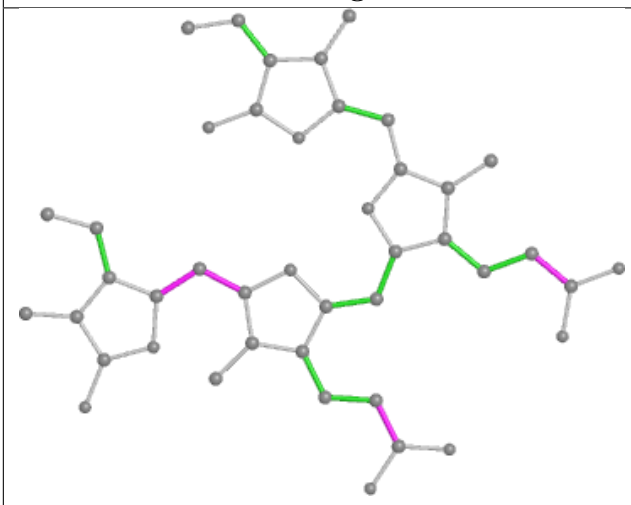

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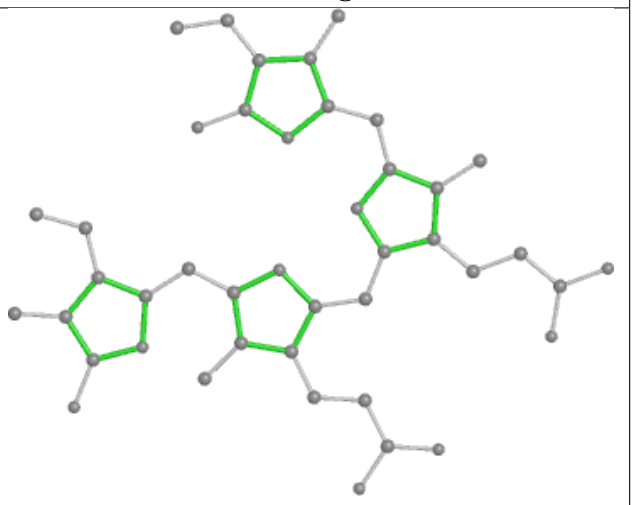
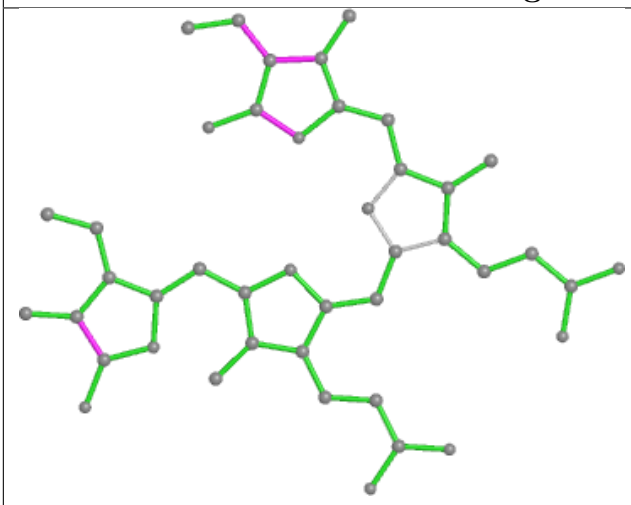


Rings

Ligand PEB l4 201



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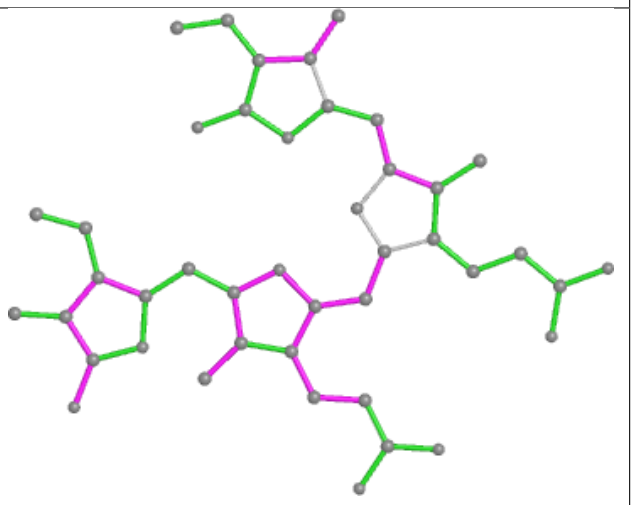

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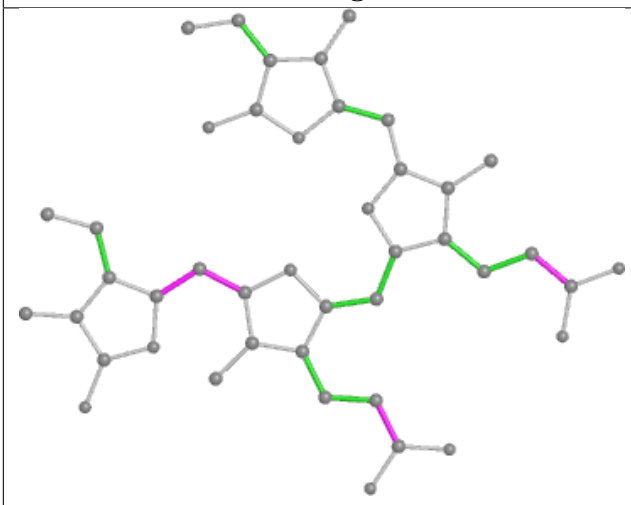

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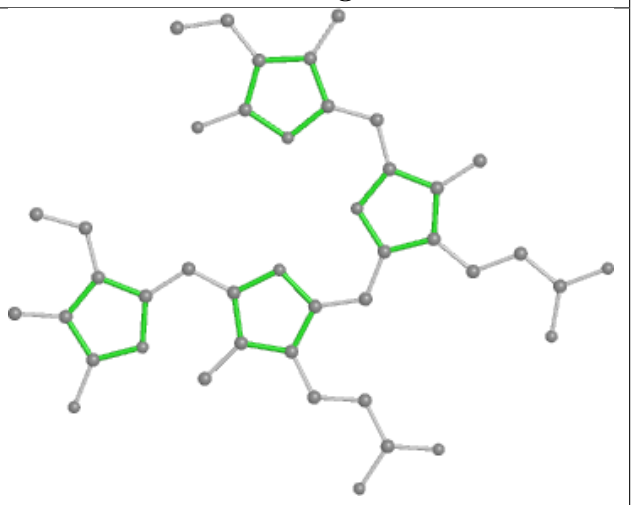
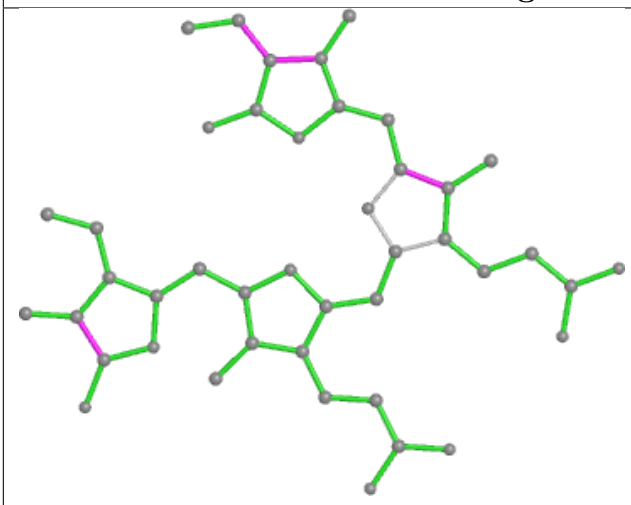


Rings

Ligand PEB db 202



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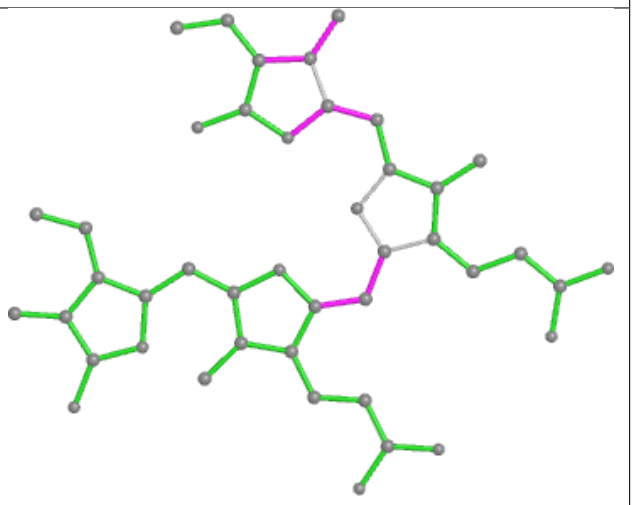

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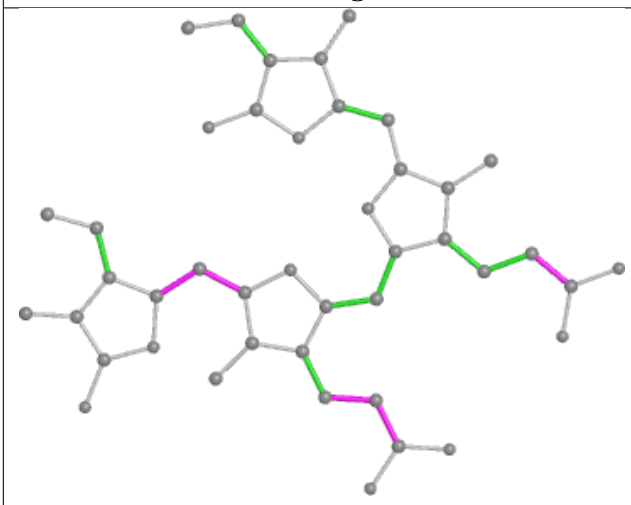

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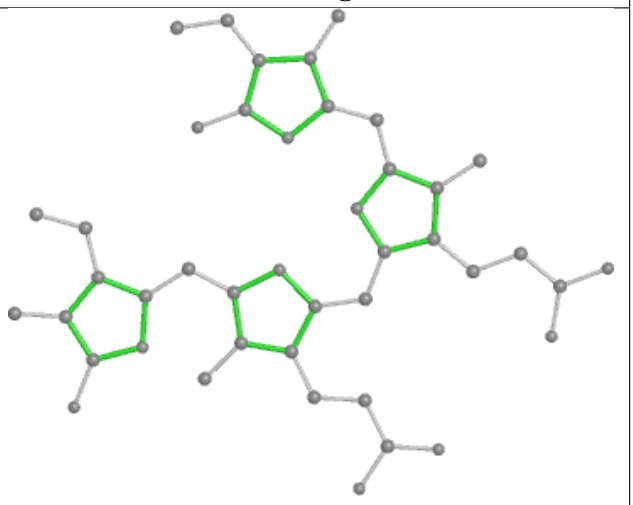
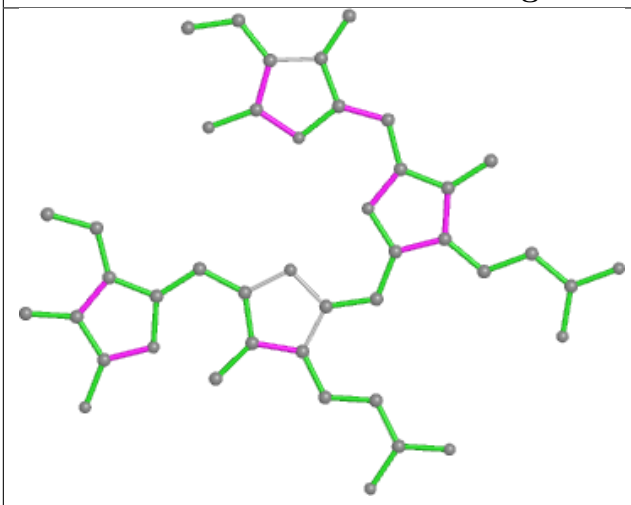


Rings

Ligand PUB lv 202



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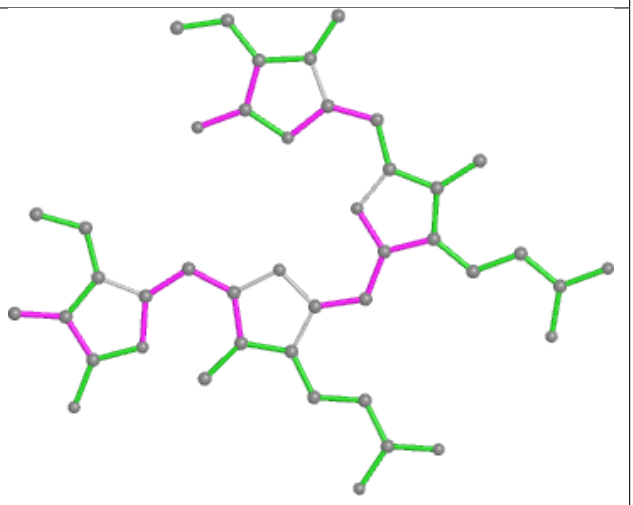

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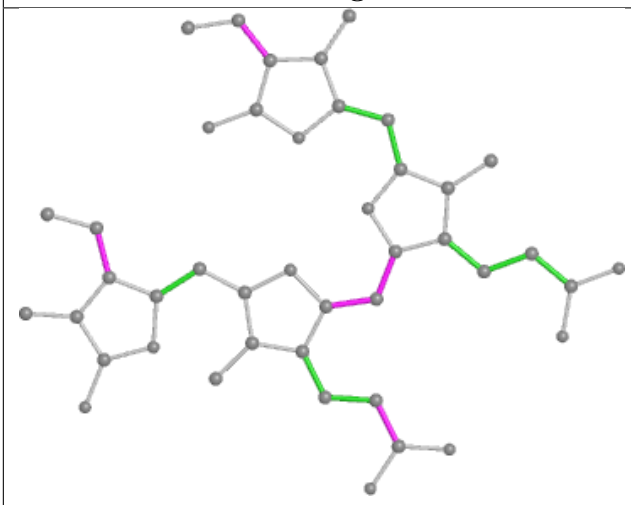

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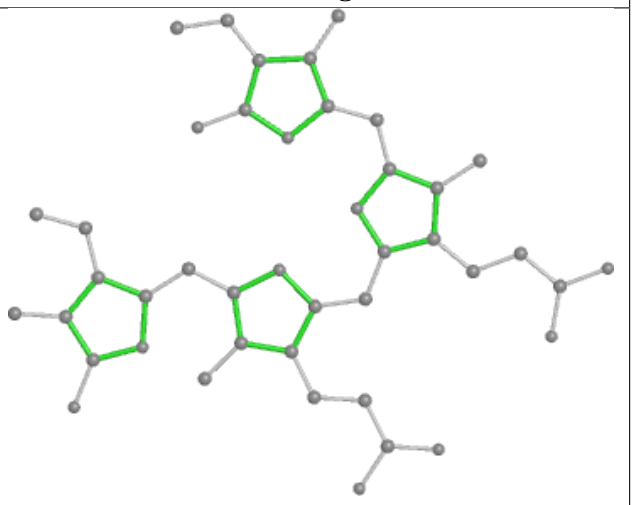
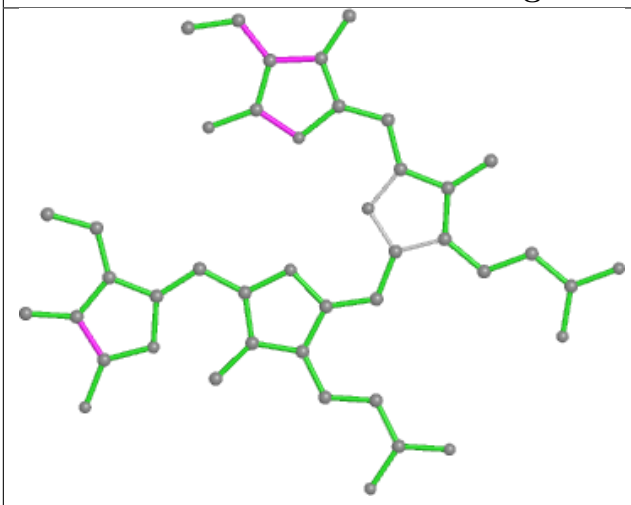


Rings

Ligand PEB i9 201



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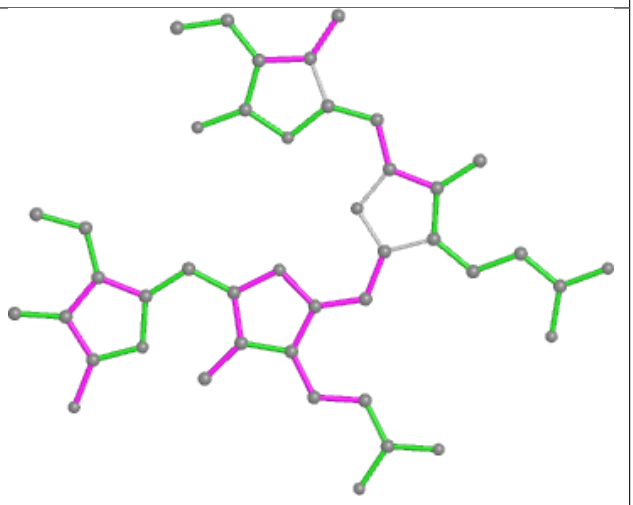
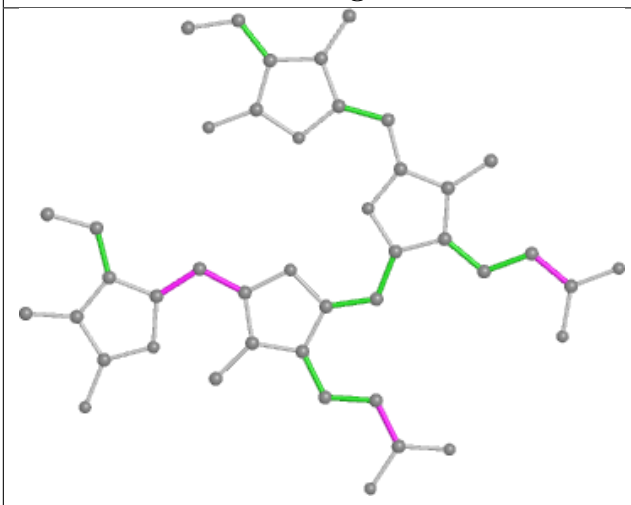


Bond angles



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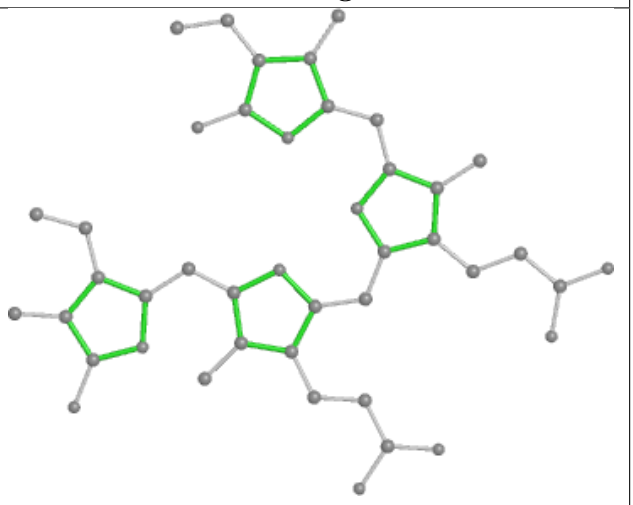
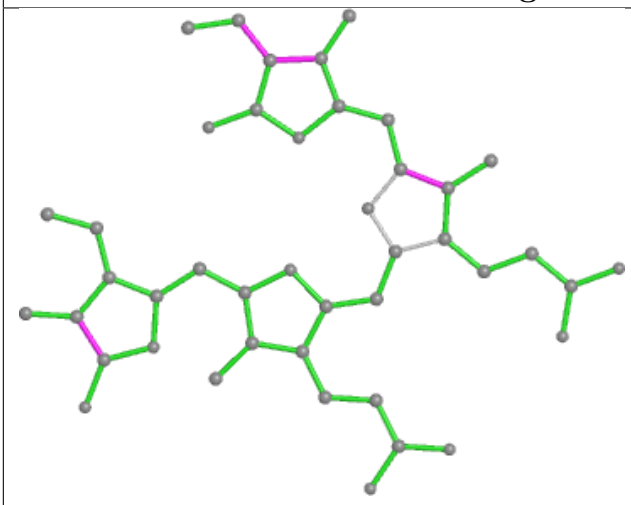


Rings

Ligand PEB y3 202



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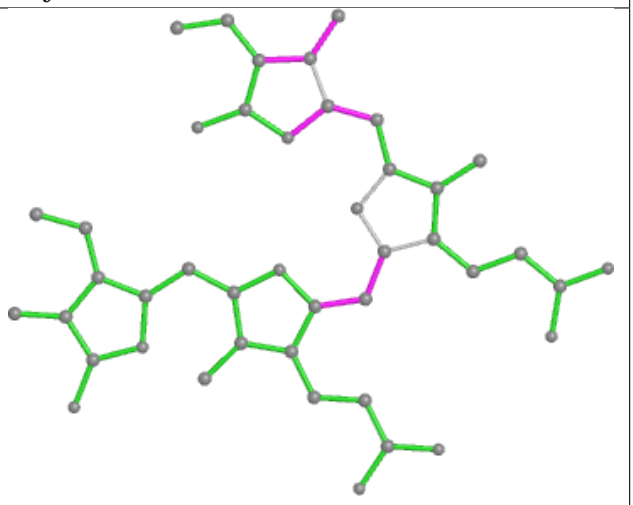

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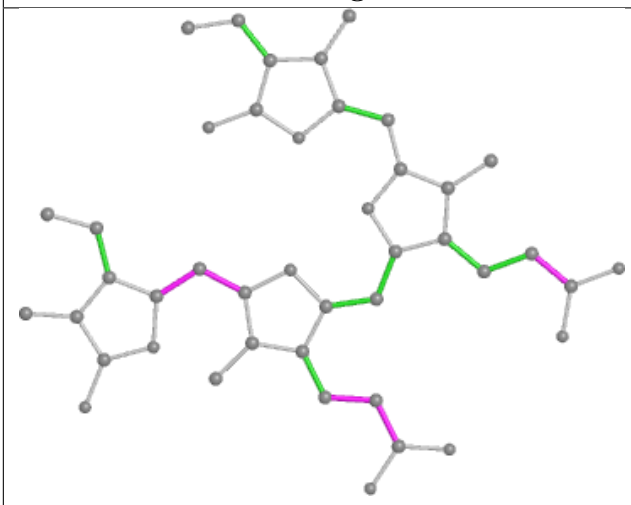

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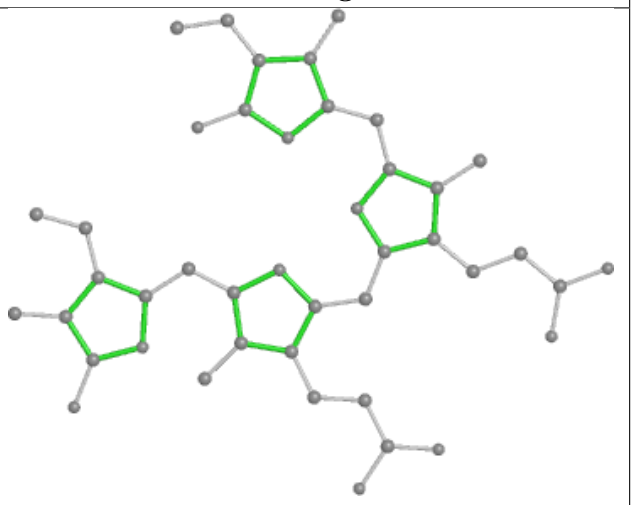
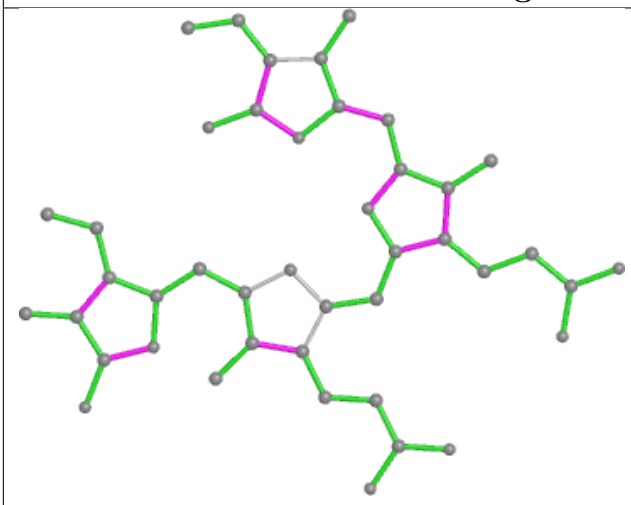


Rings

Ligand PUB cQ 202



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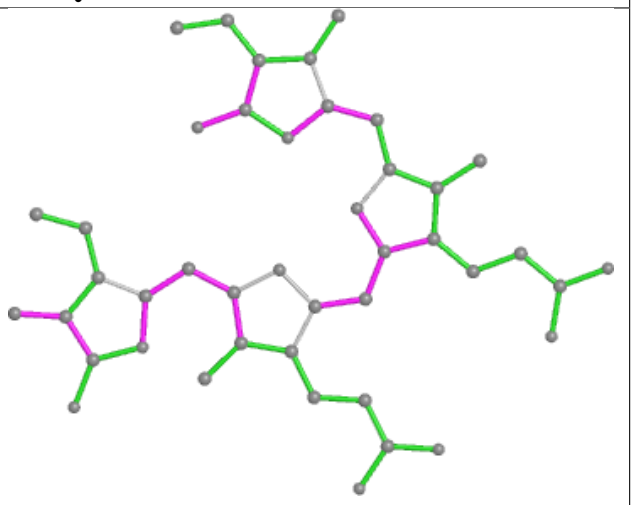

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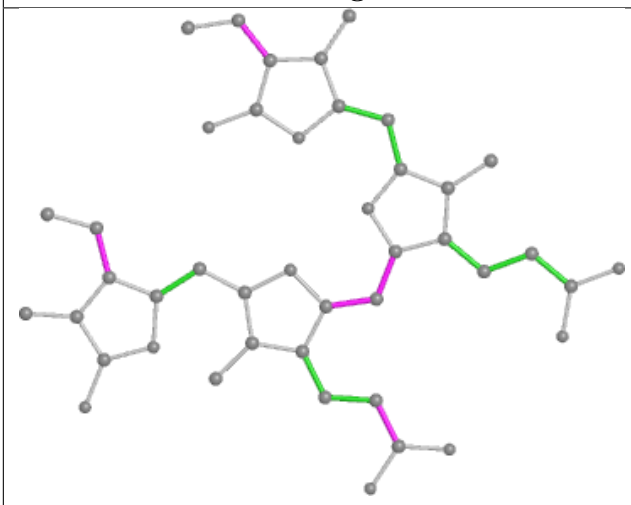

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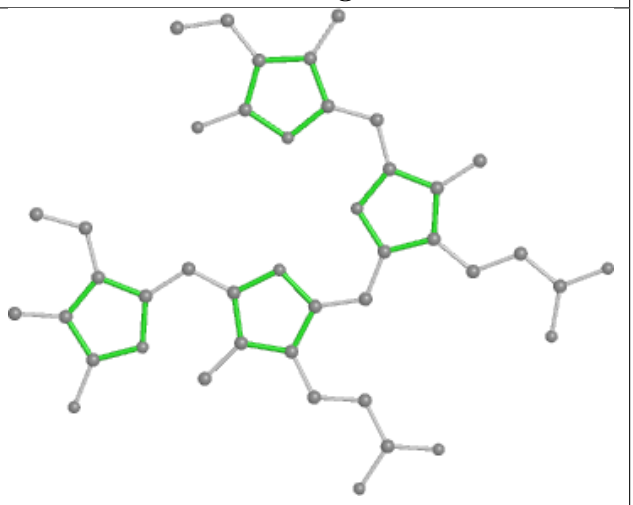
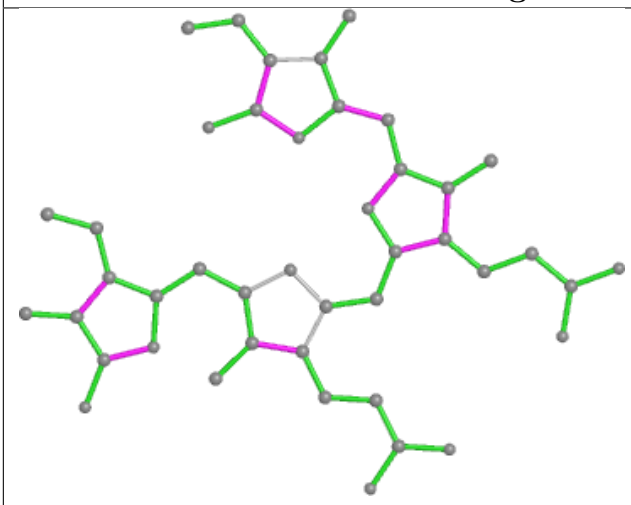


Rings

Ligand PUB a3 1005



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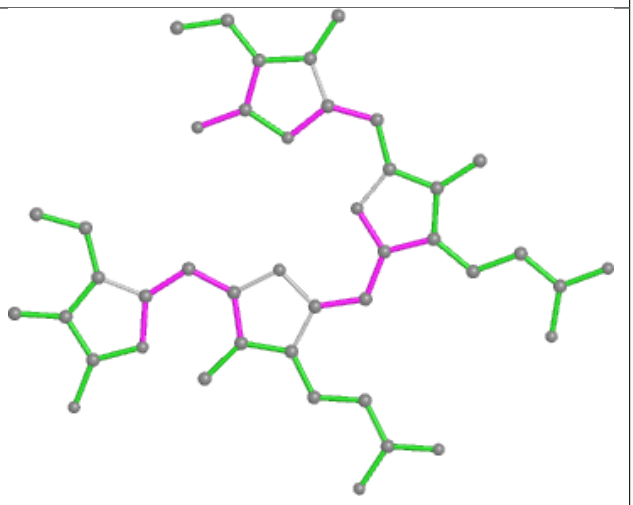
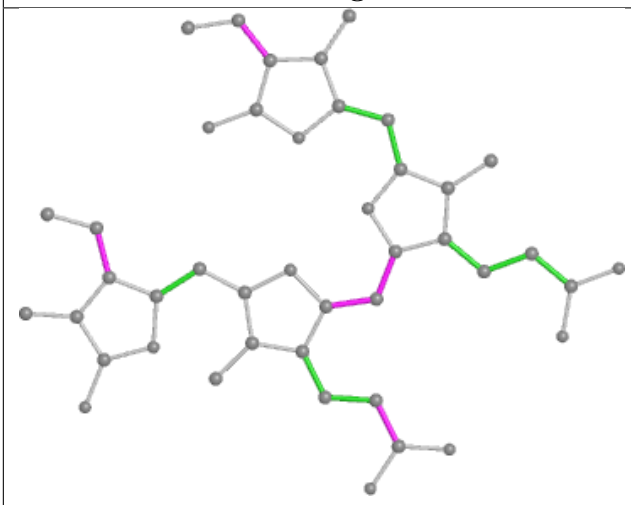


Bond angles



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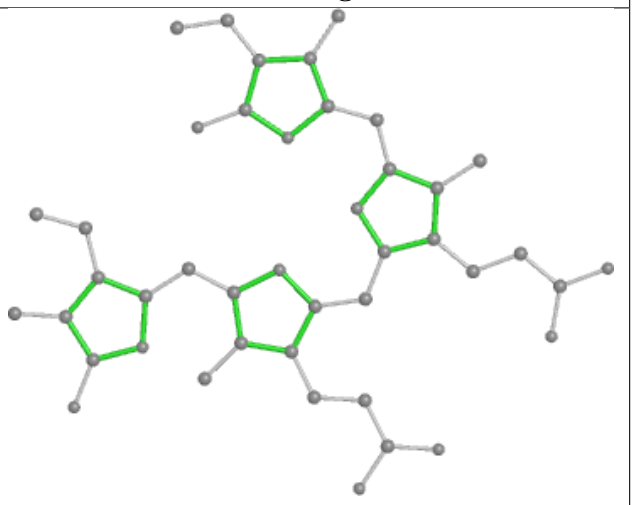
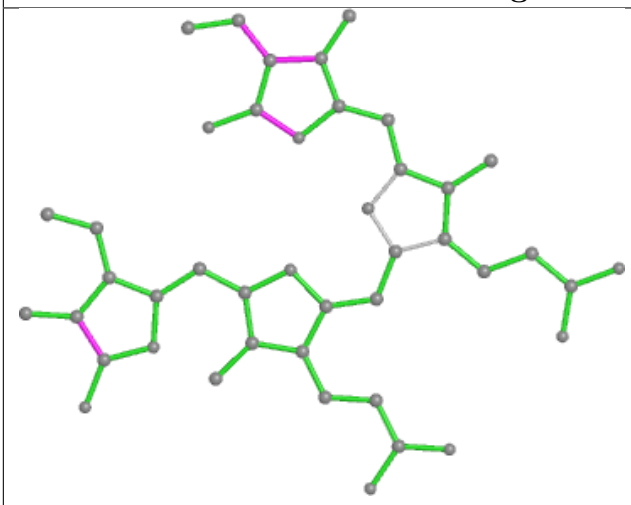


Rings

Ligand PEB W8 201



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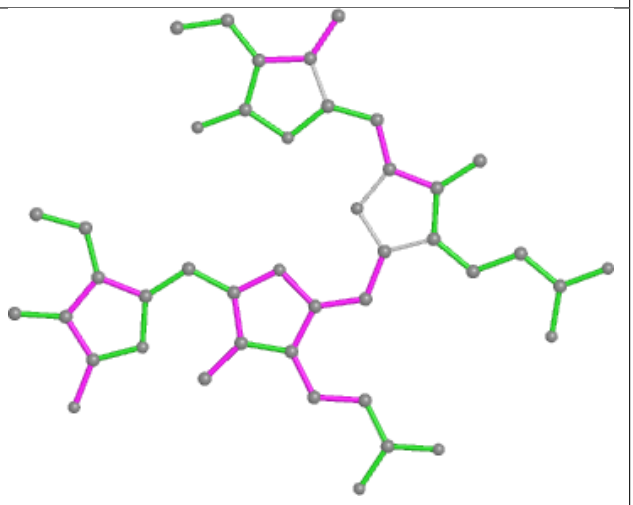
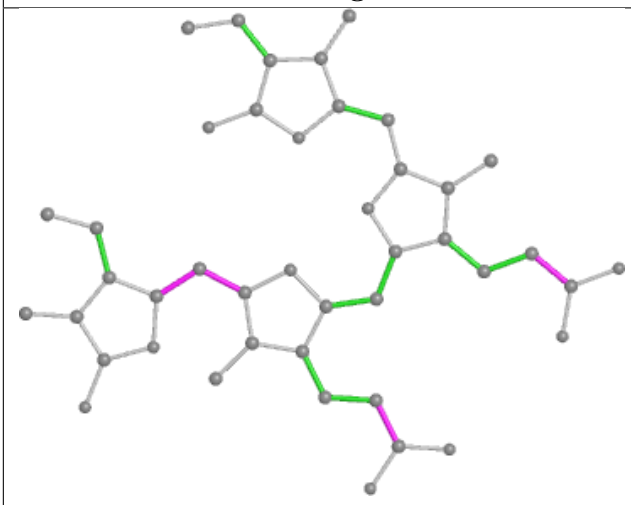
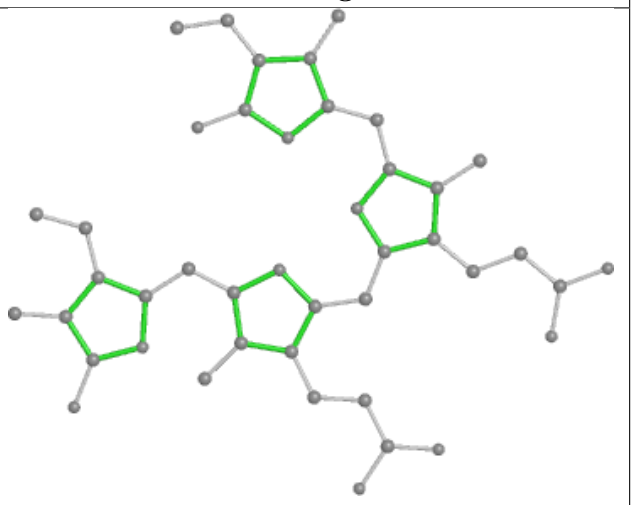


Bond angles

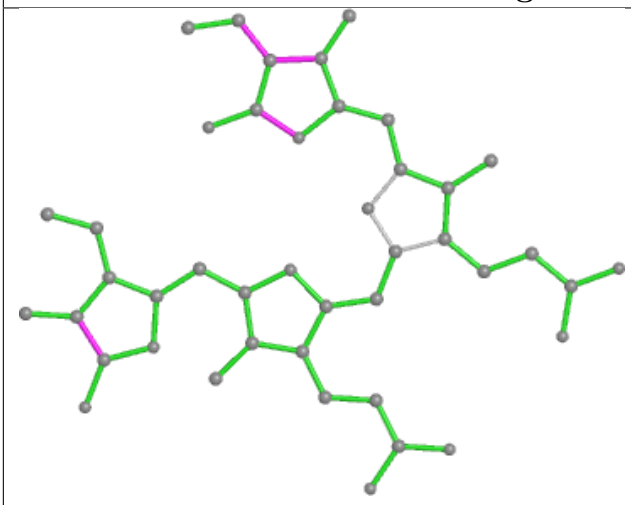


Torsions



Rings

Ligand PEB cU 201



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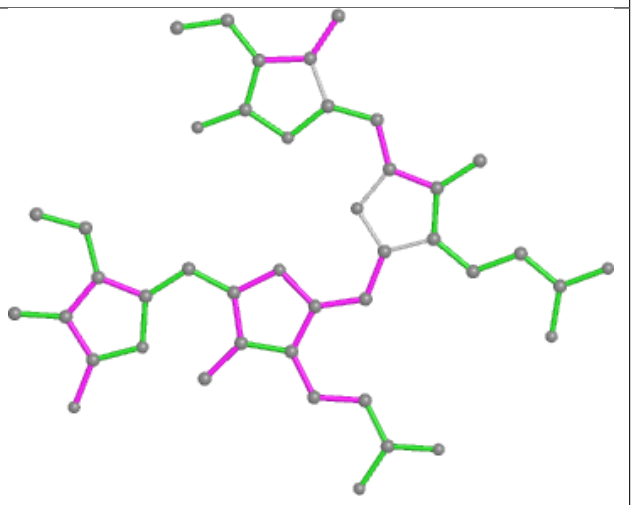

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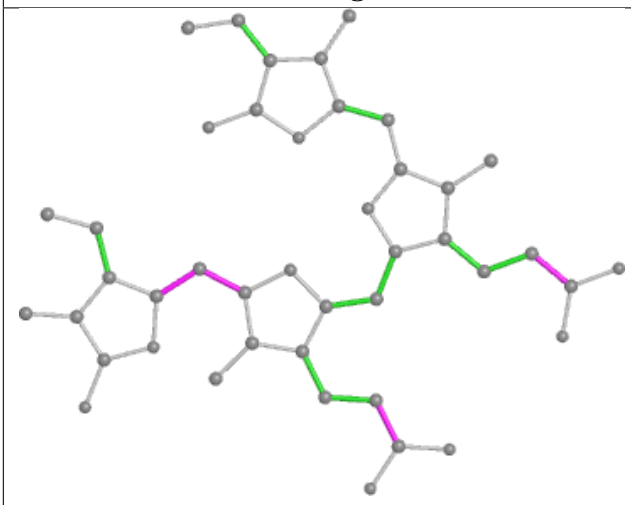

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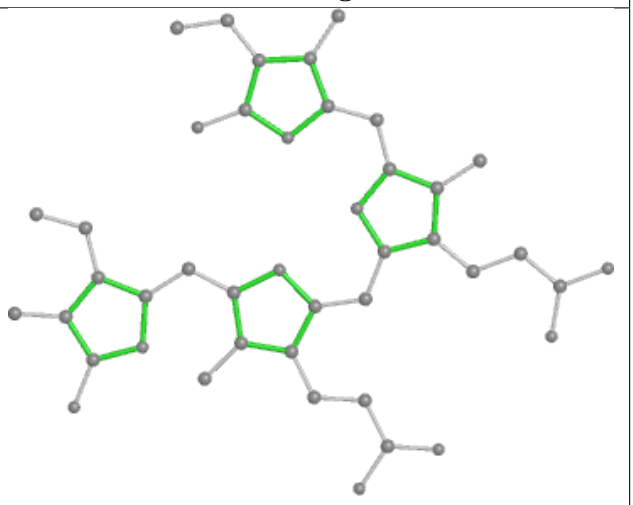
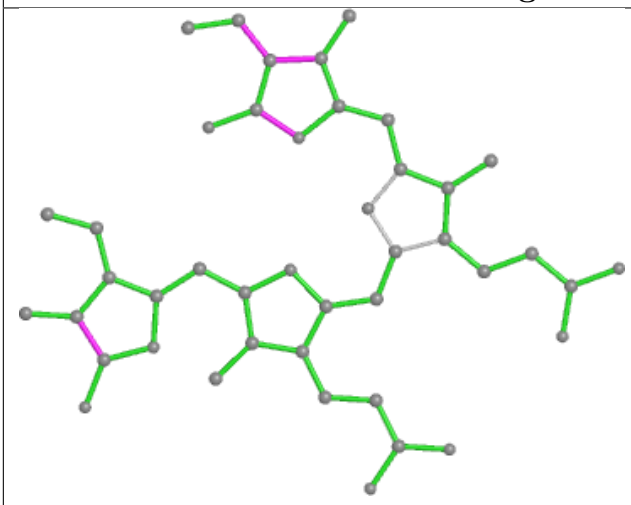


Rings

Ligand PEB p8 201



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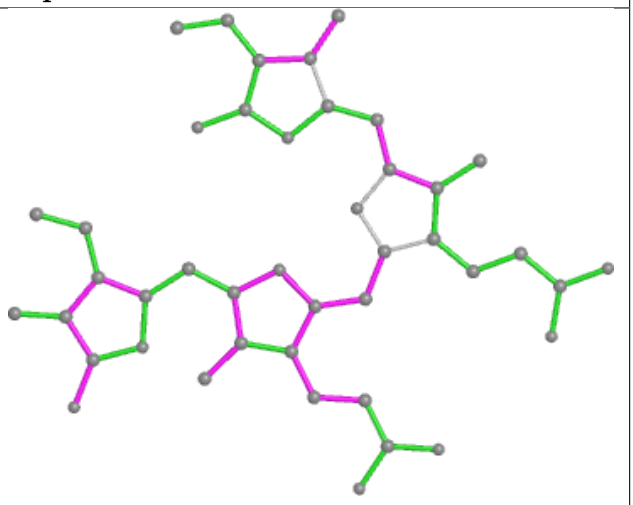

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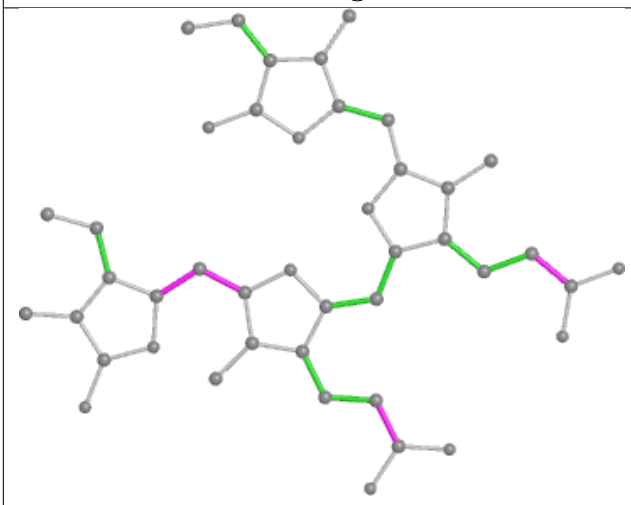

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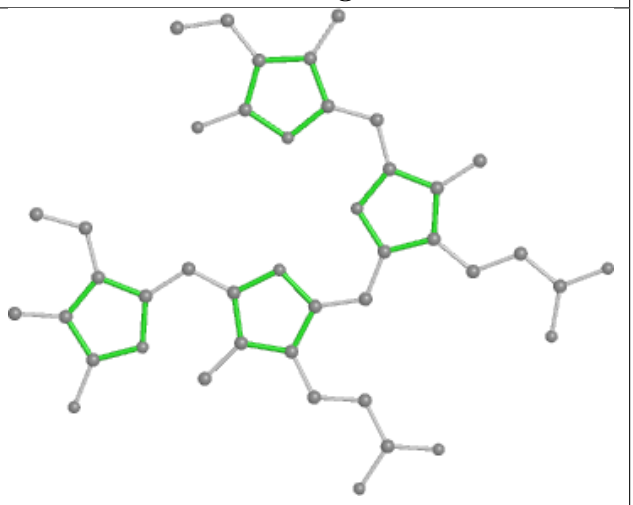
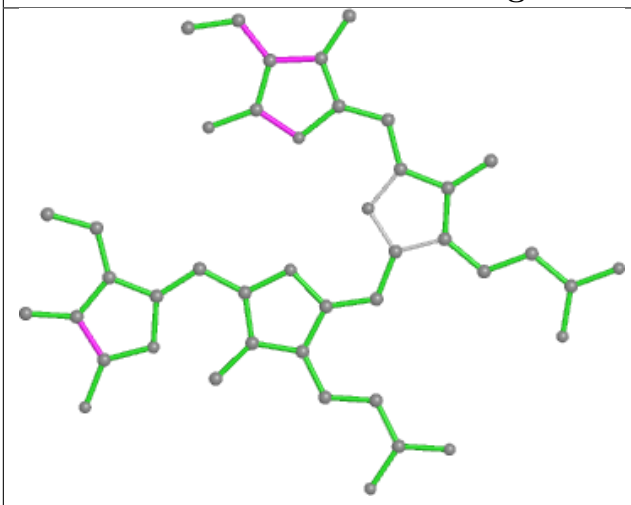


Rings

Ligand PEB cC 1003



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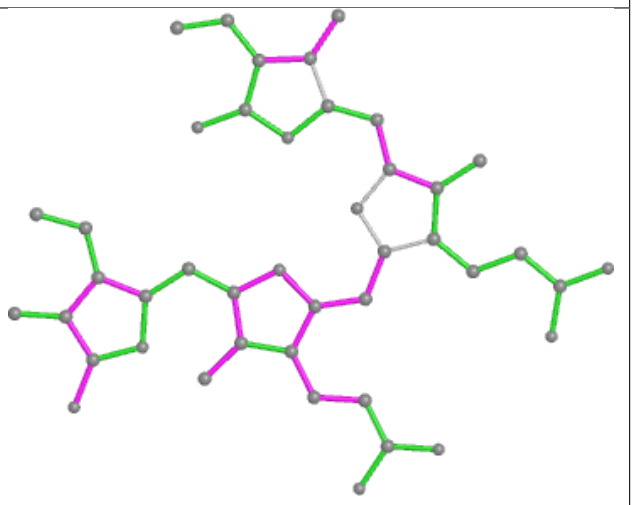
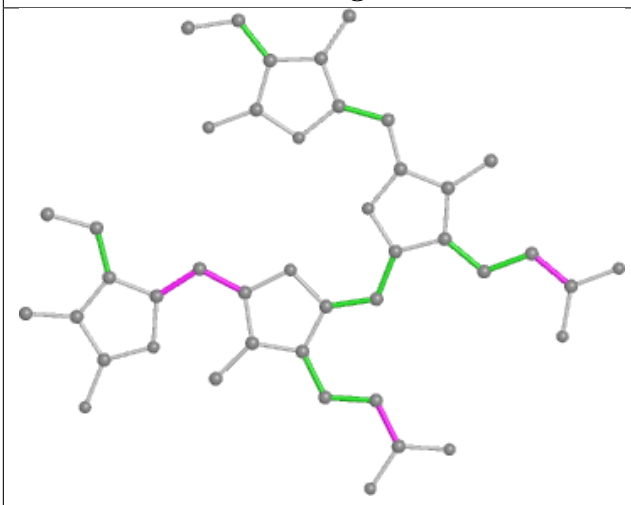


Bond angles



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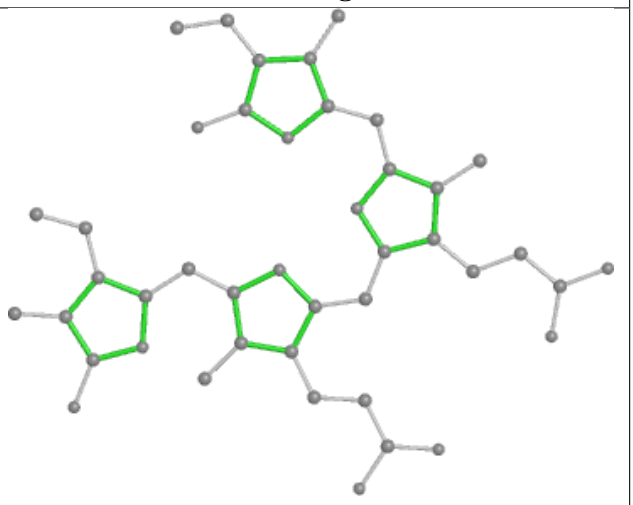
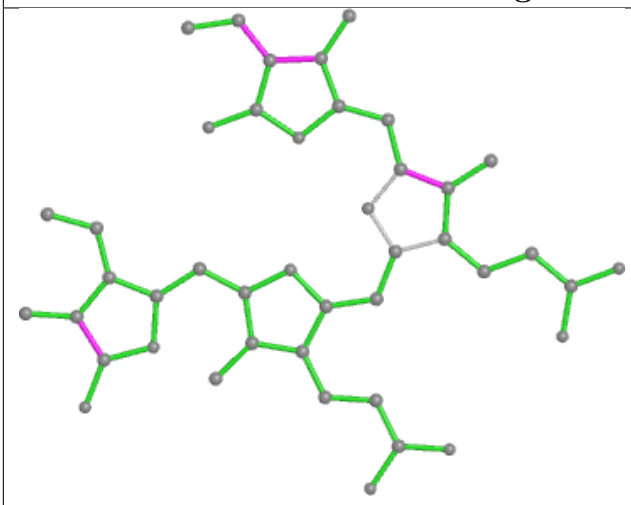


Rings

Ligand PEB hA 202



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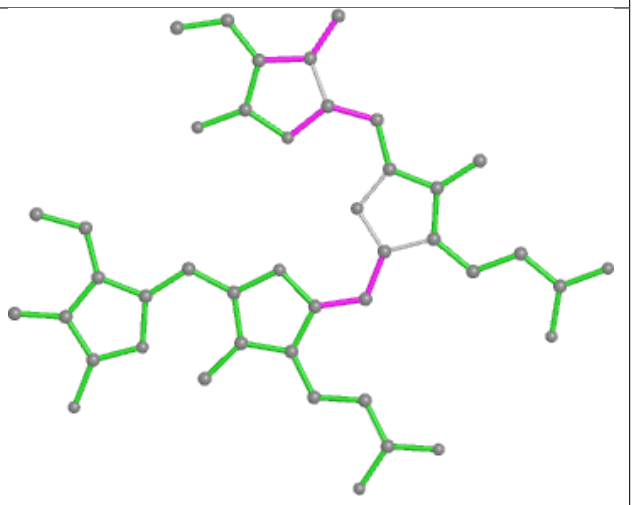

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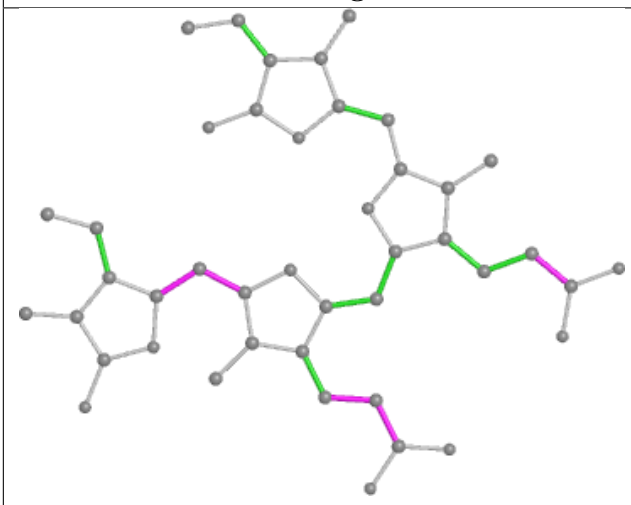

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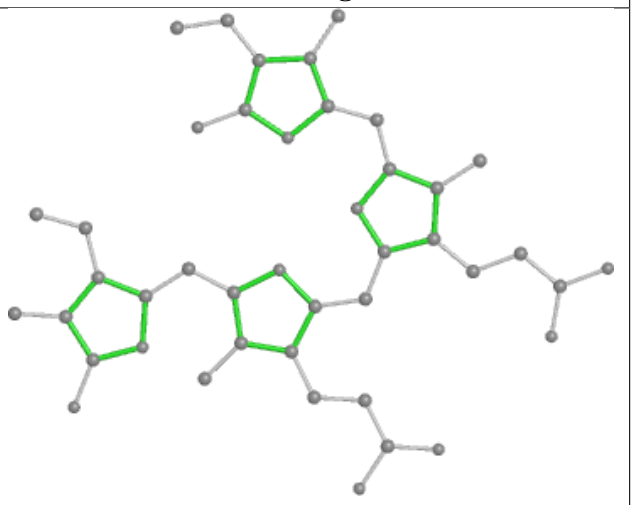
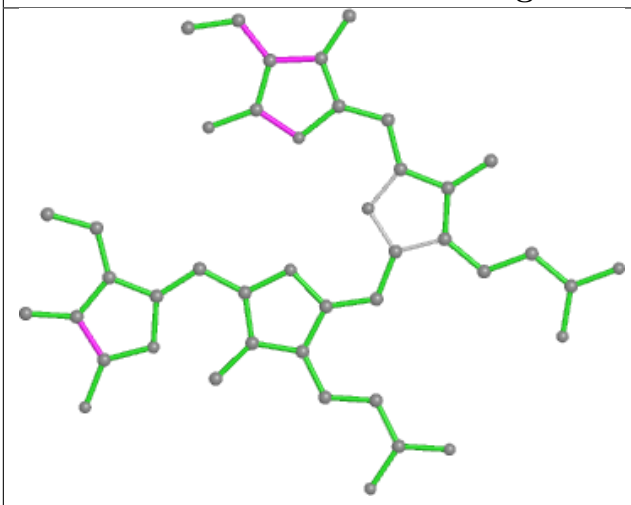


Rings

Ligand PEB eR 201



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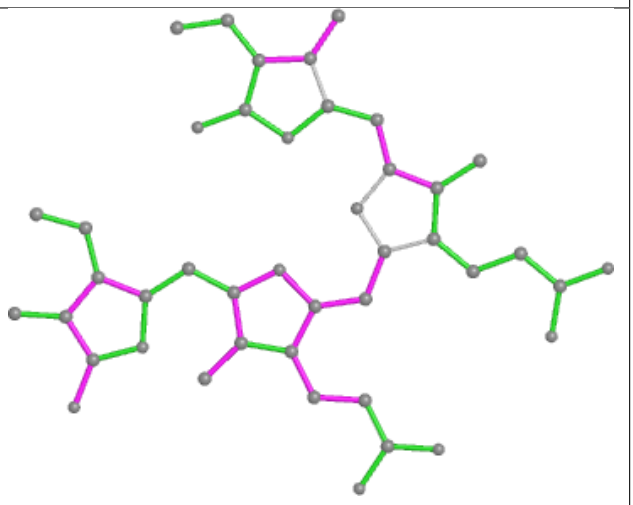

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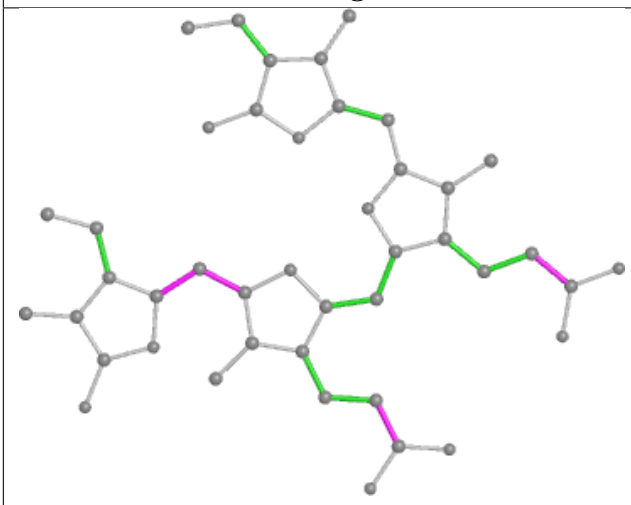

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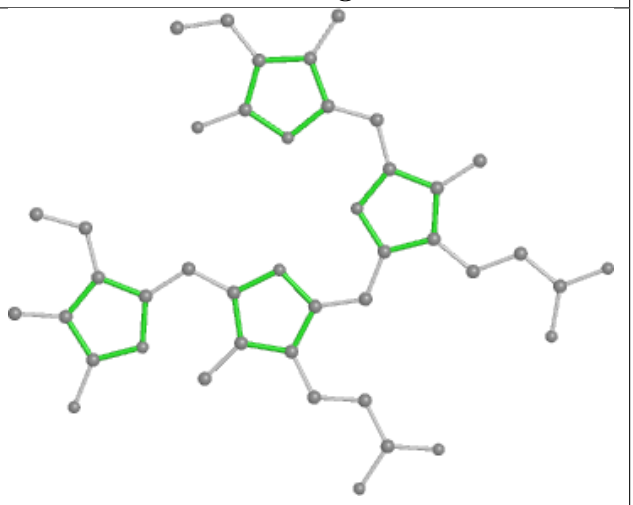
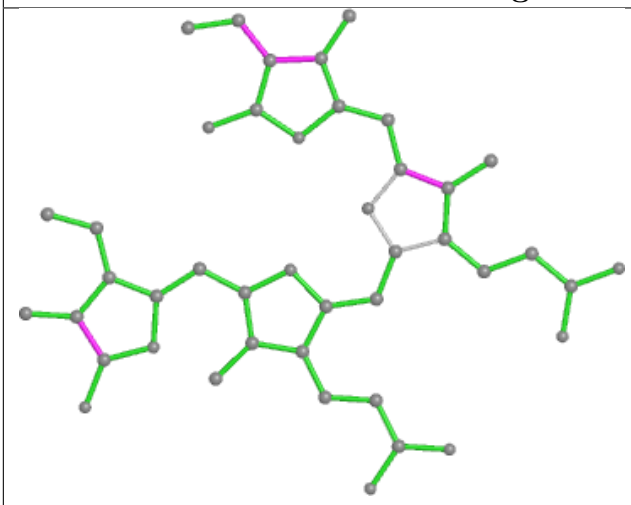


Rings

Ligand PEB M9 202



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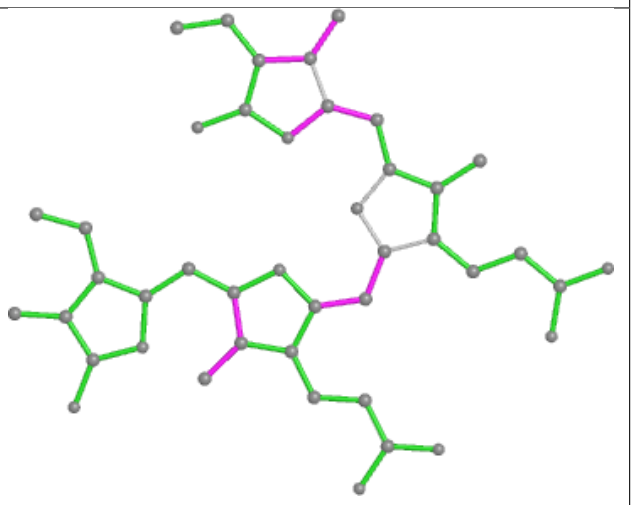

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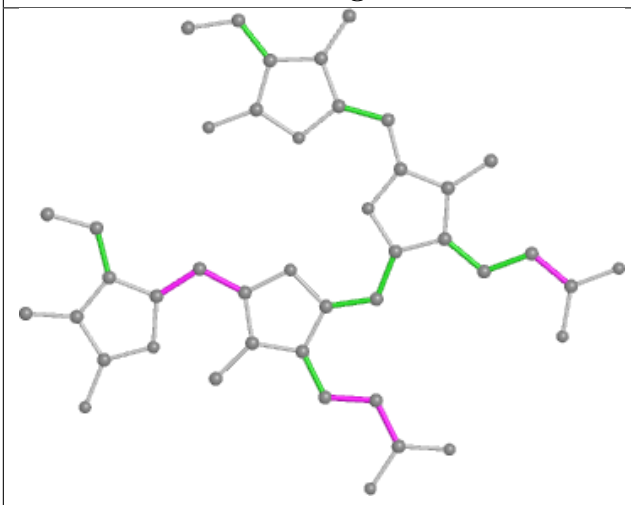

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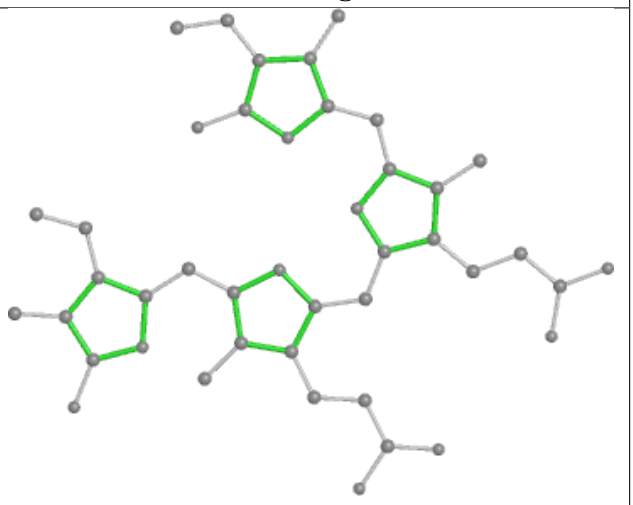
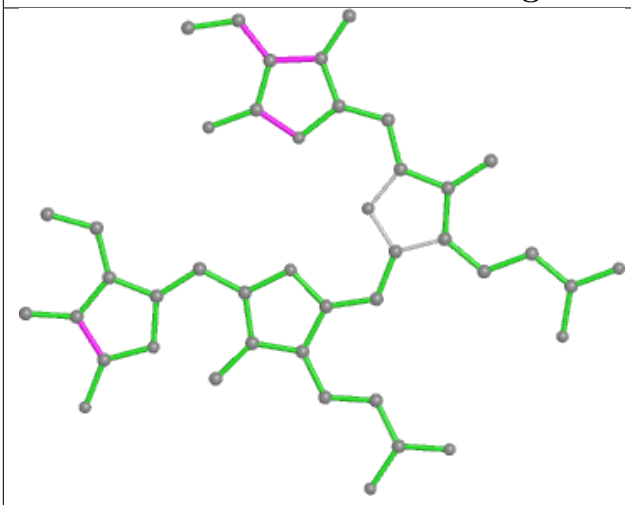


Rings

Ligand PEB at 201



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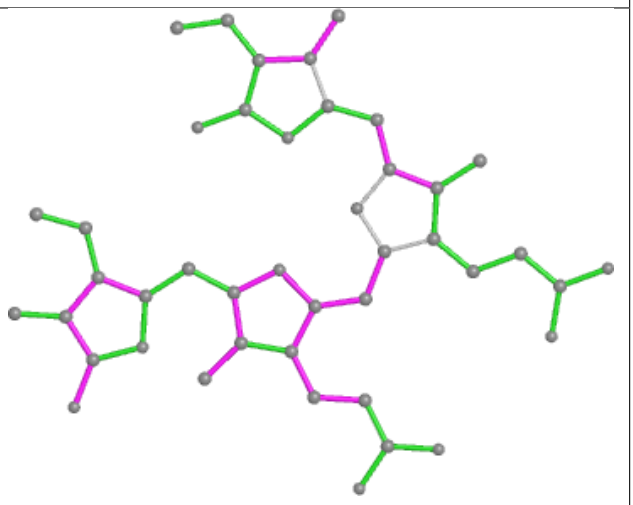

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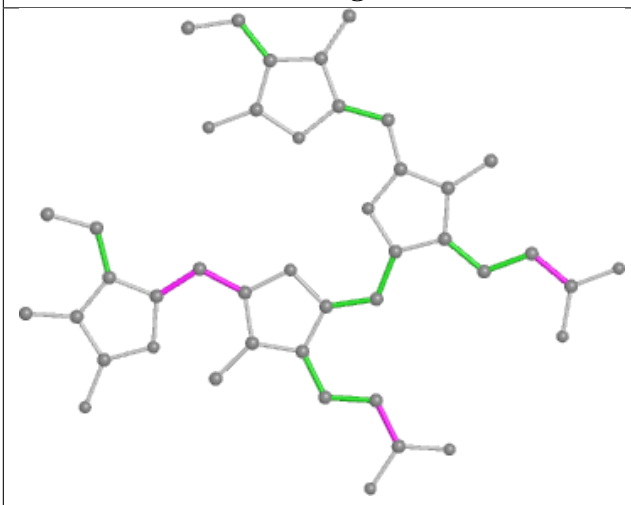

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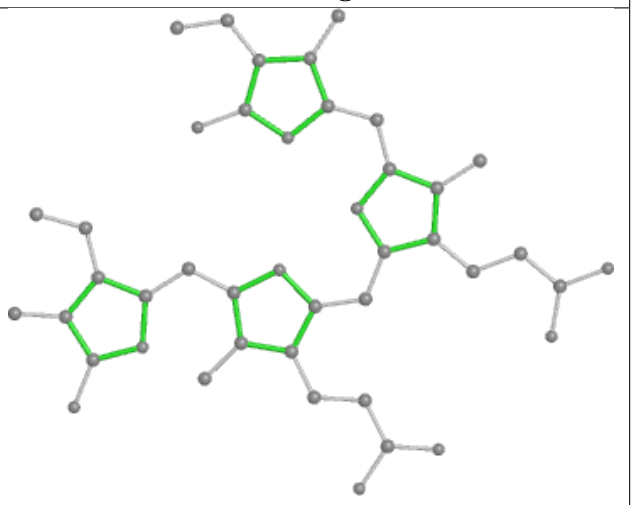
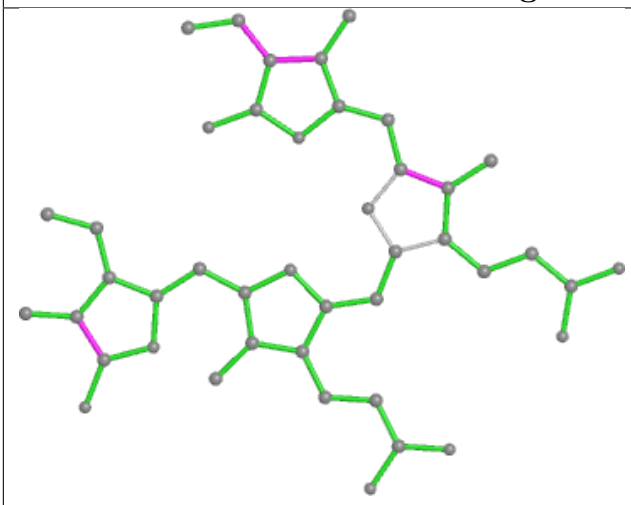


Rings

Ligand PEB lw 201



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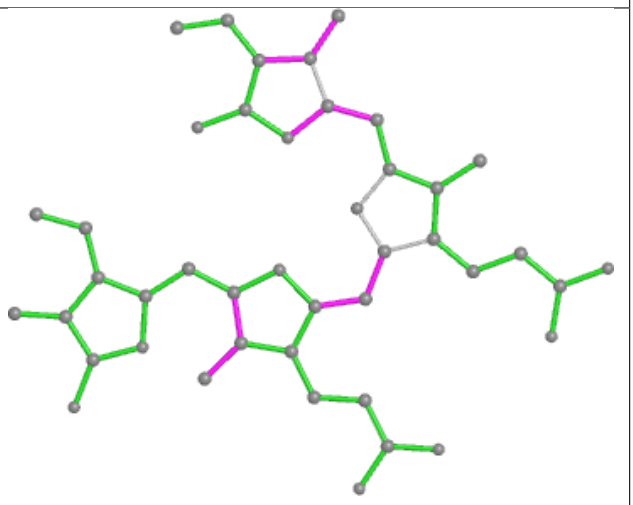

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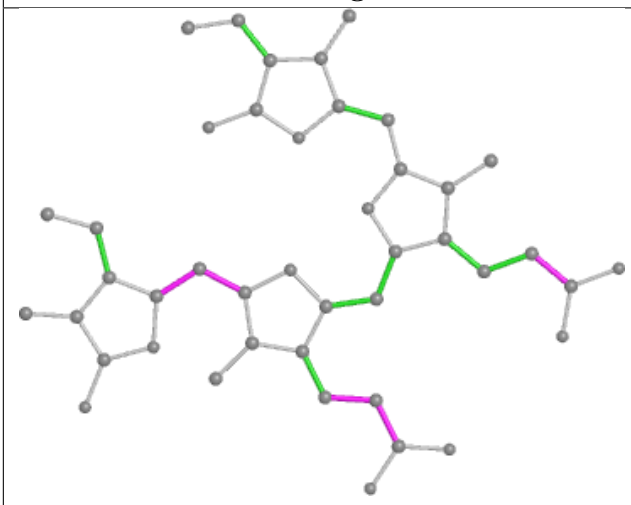

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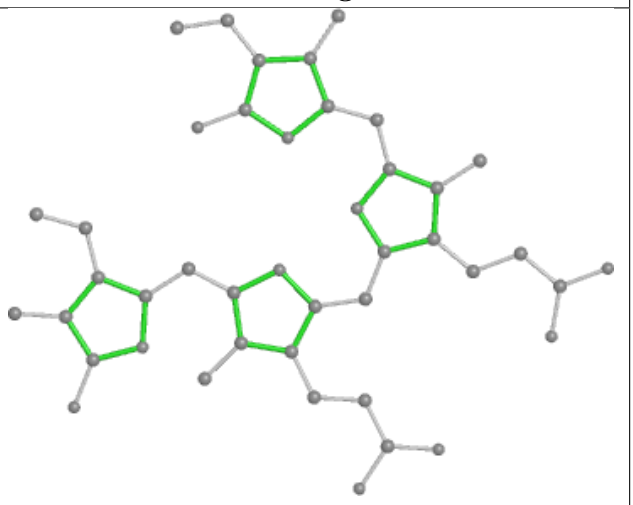
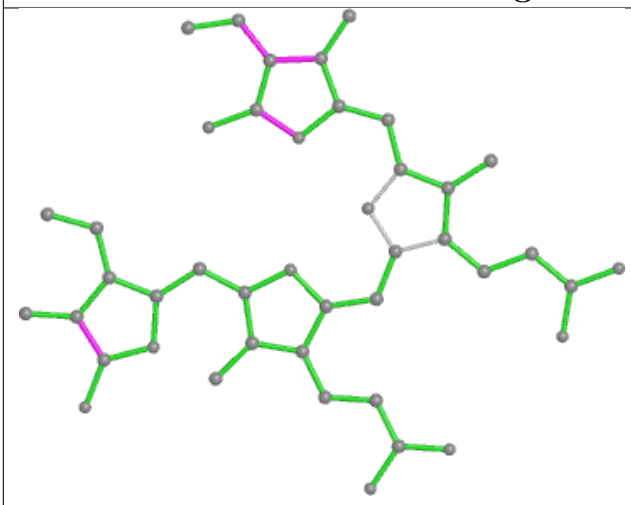


Rings

Ligand PEB jJ 1001



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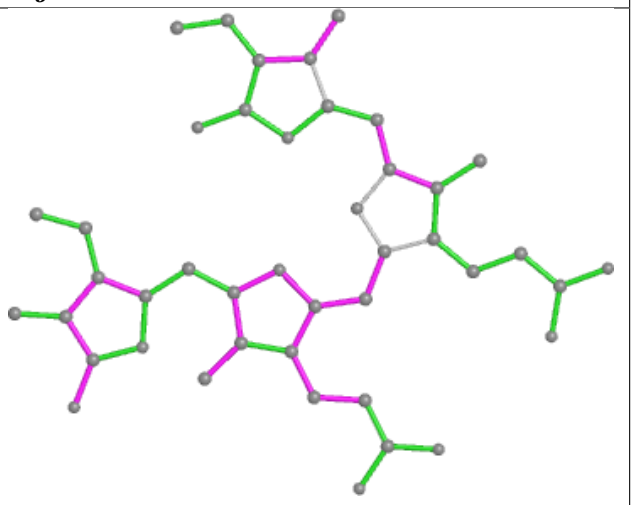

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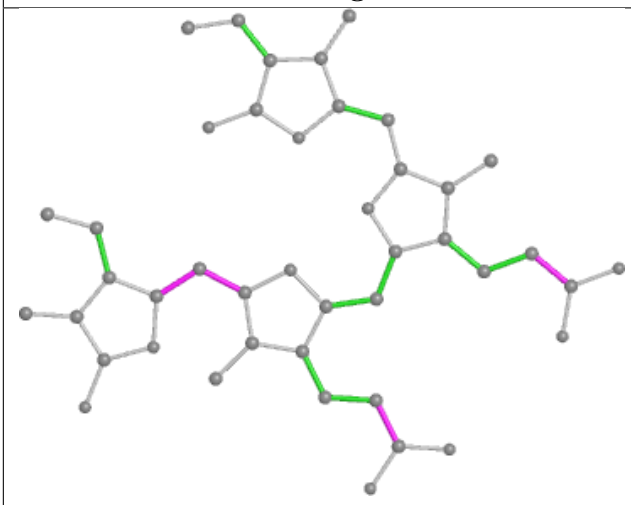

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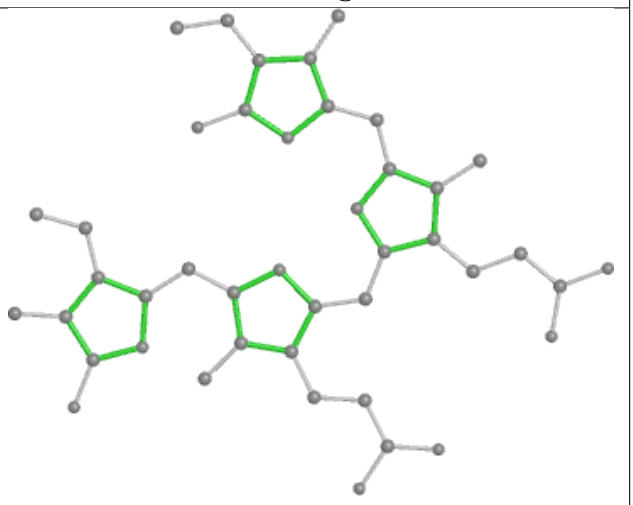
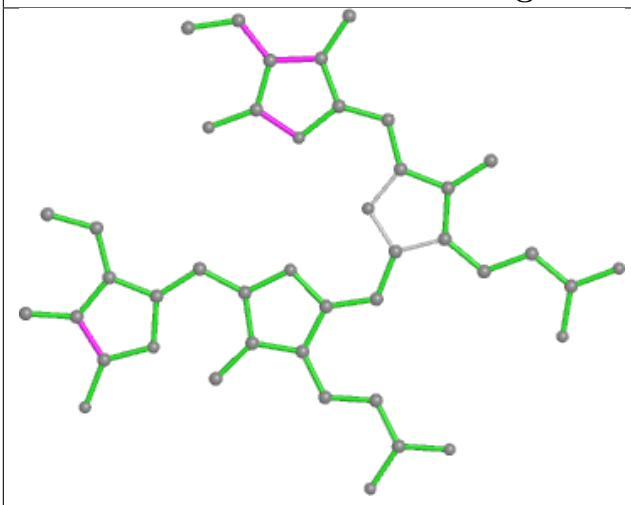


Rings

Ligand PEB B9 201



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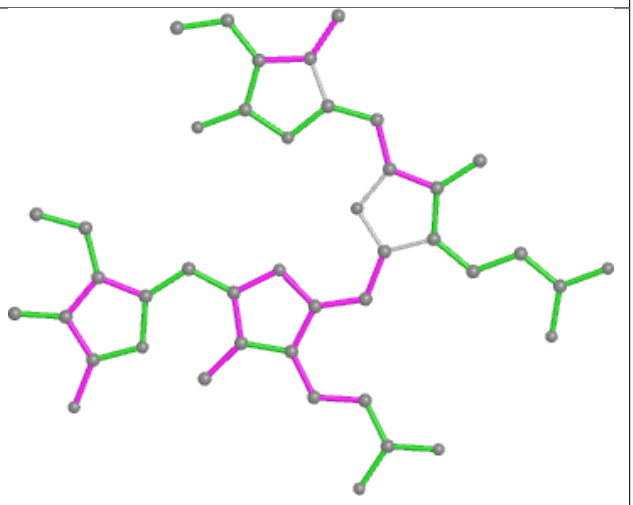
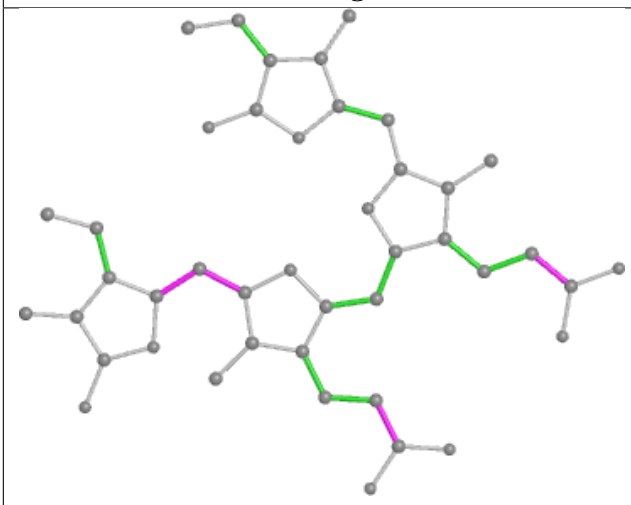


Bond angles



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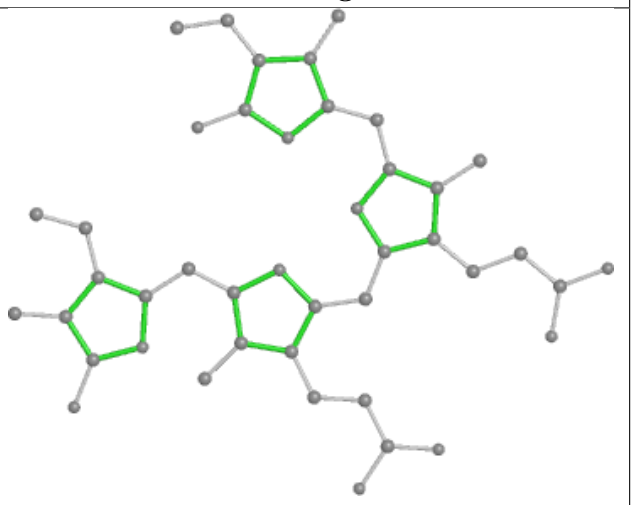
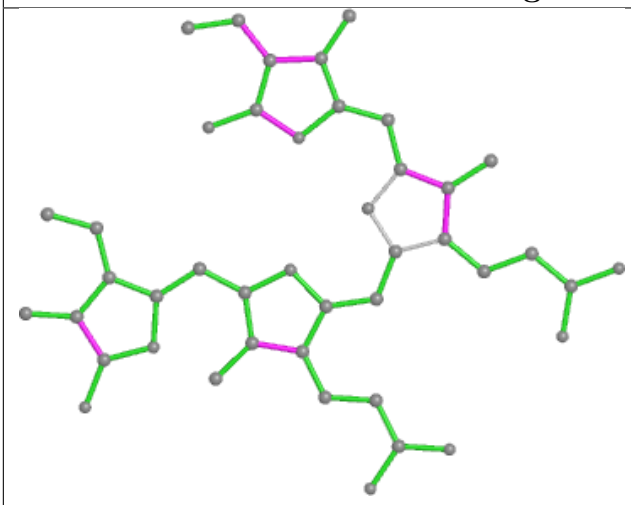


Rings

Ligand PEB f2 202



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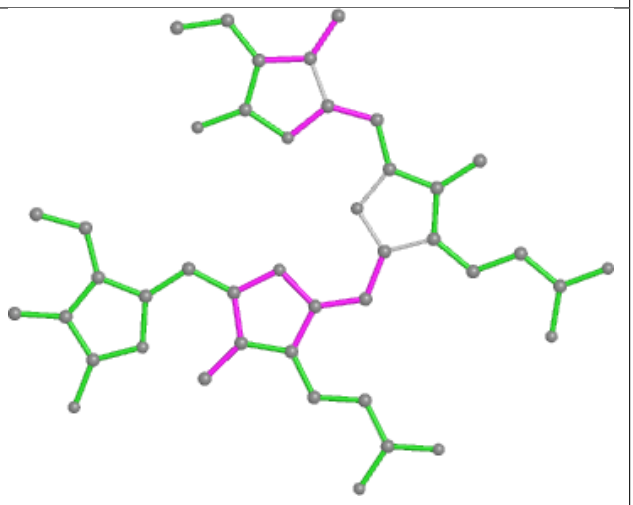
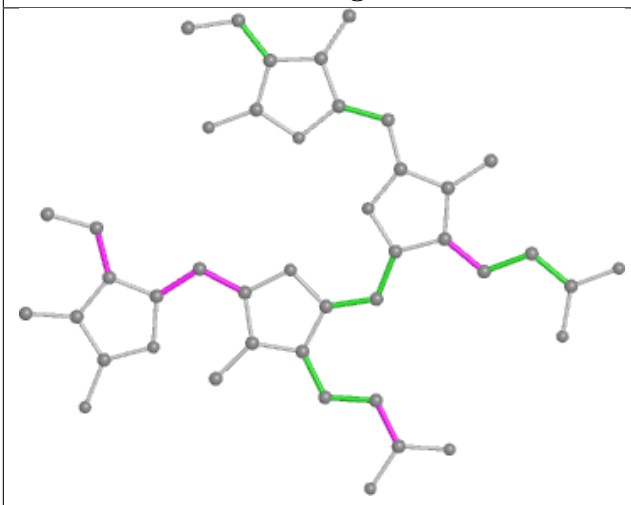


Bond angles



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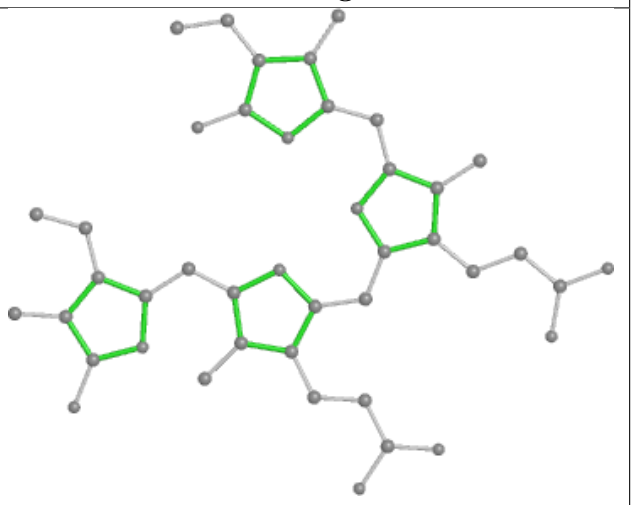
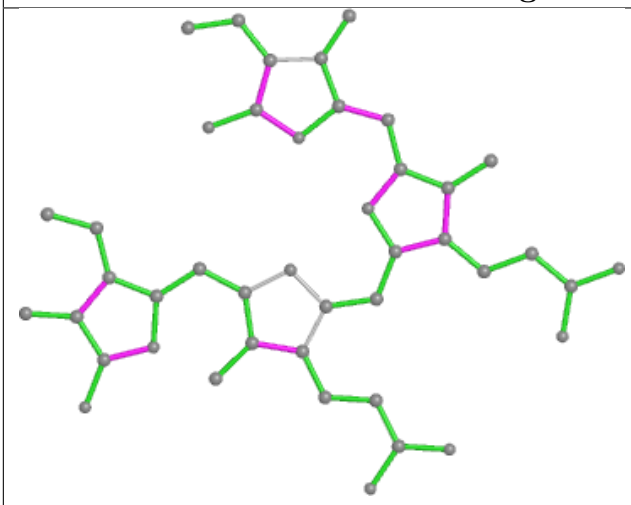


Rings

Ligand PUB r6 203



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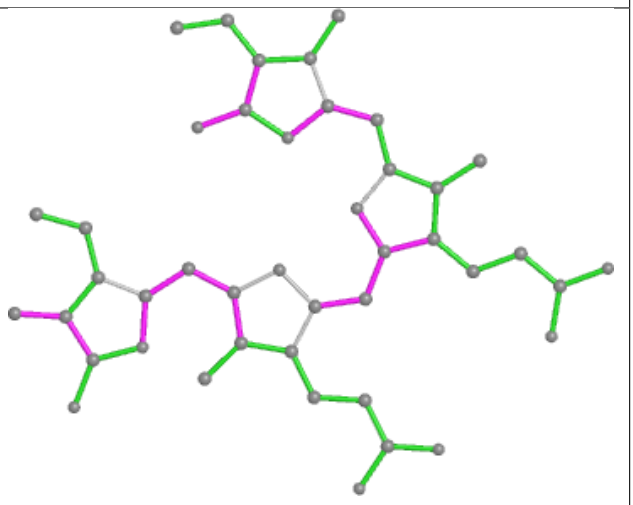
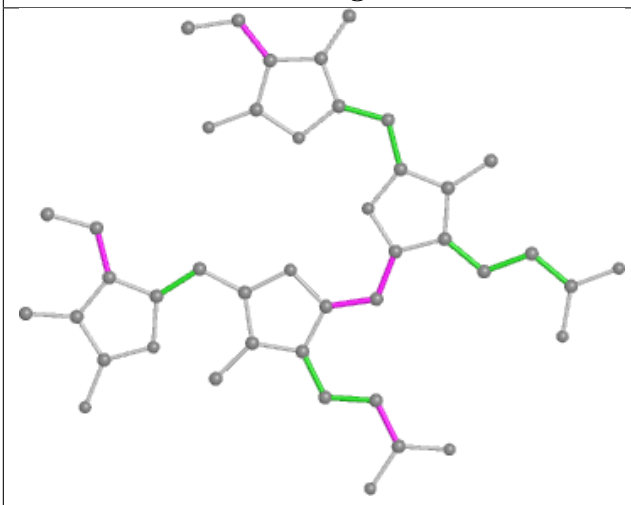


Bond angles



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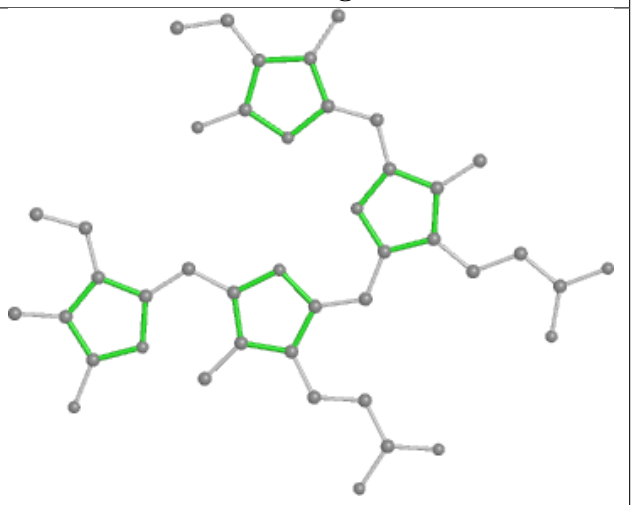
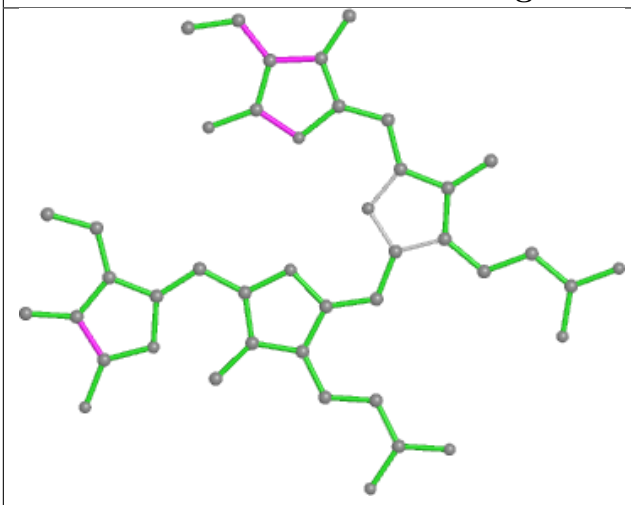


Rings

Ligand PEB bw 202



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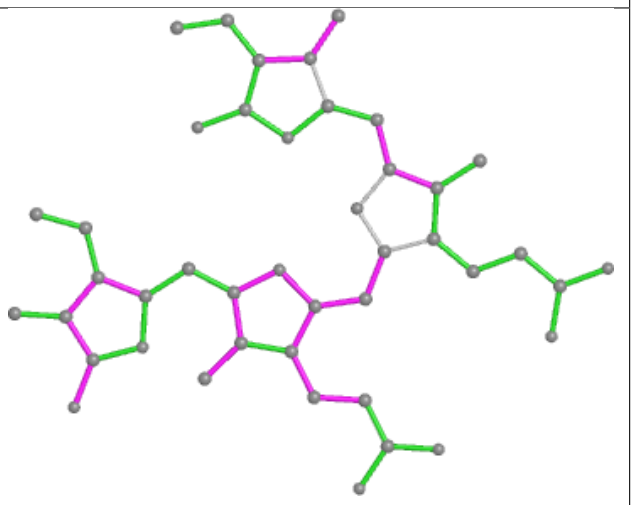
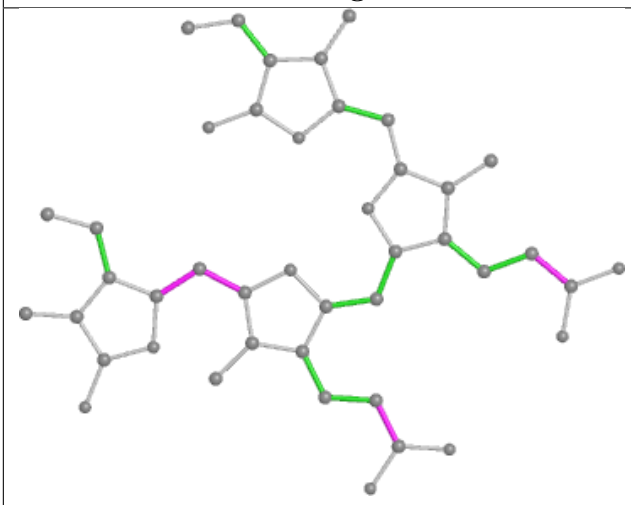
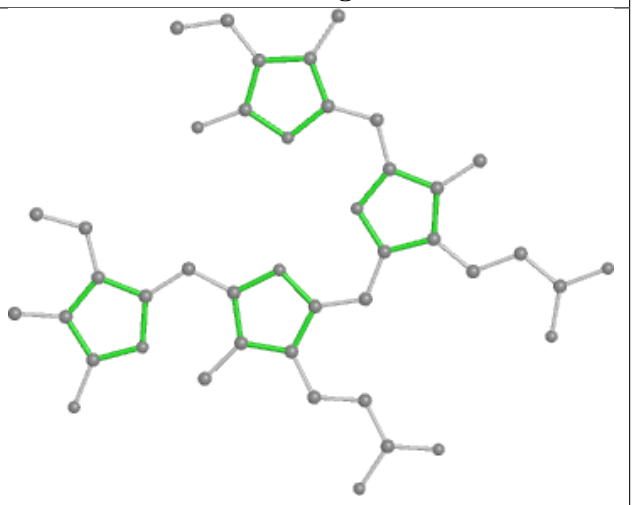


Bond angles

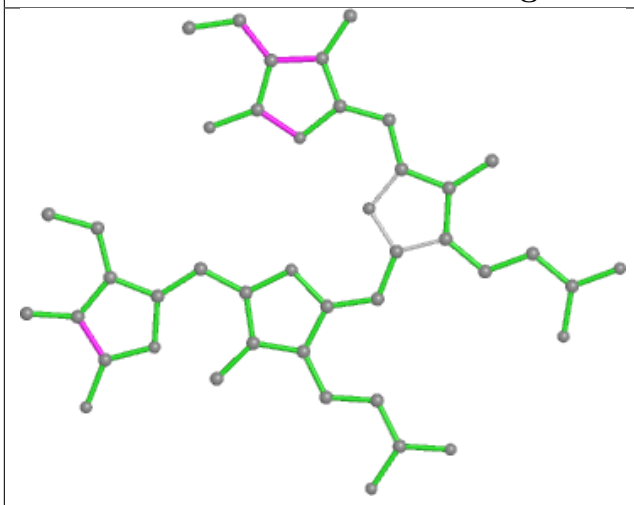


Torsions



Rings

Ligand PEB gy 301



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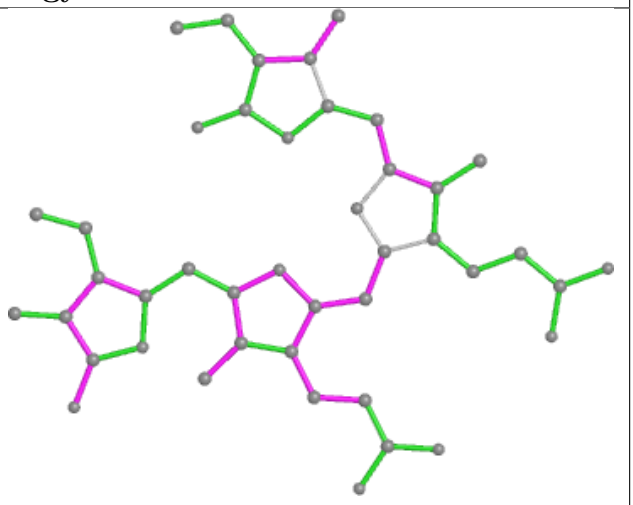

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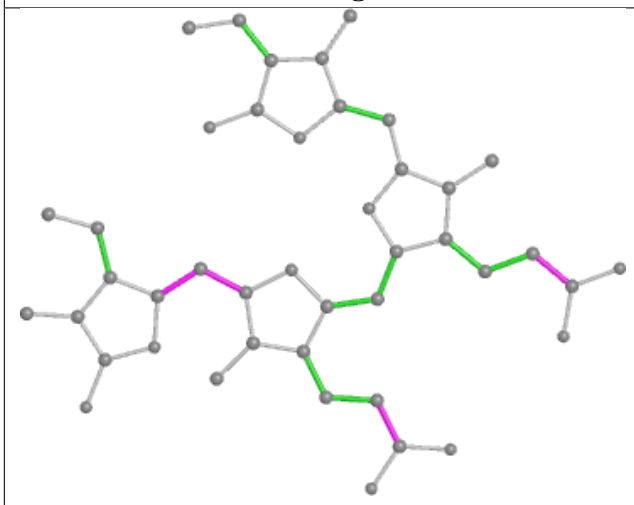

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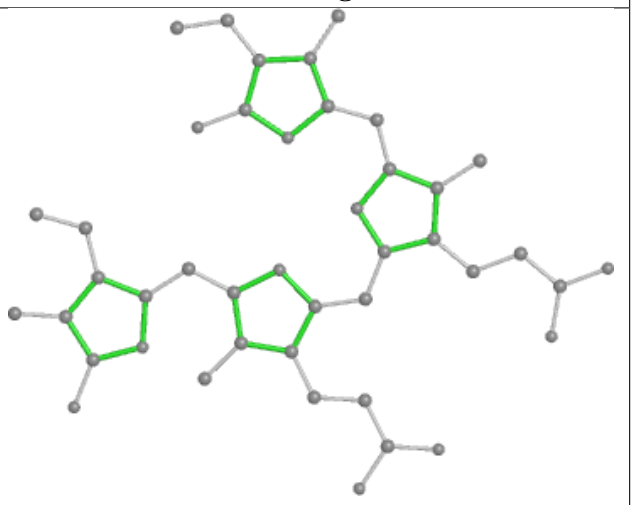
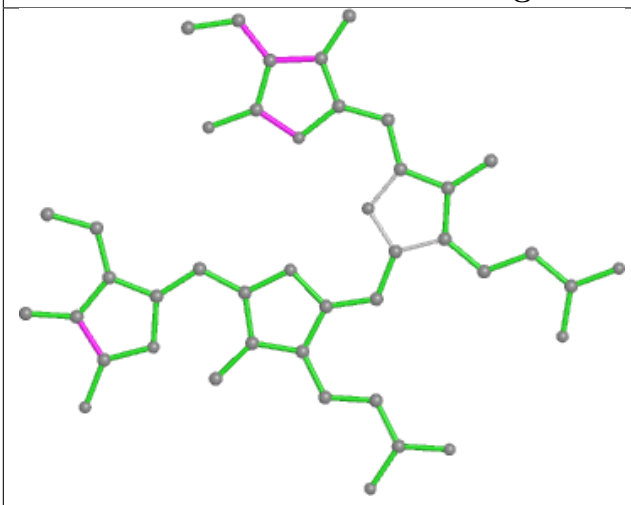


Rings

Ligand PEB hH 201



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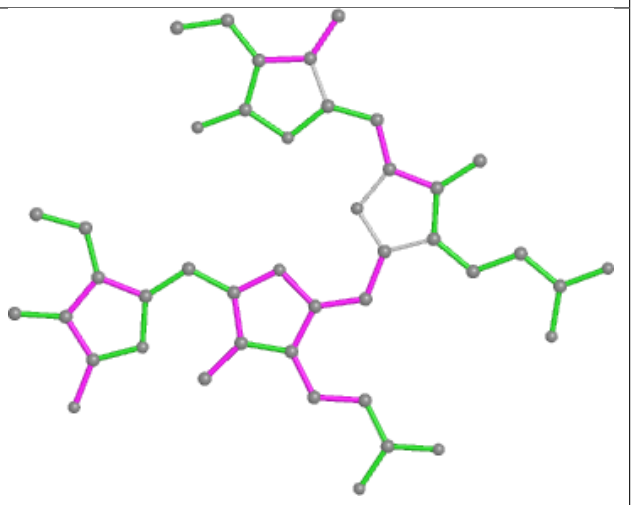

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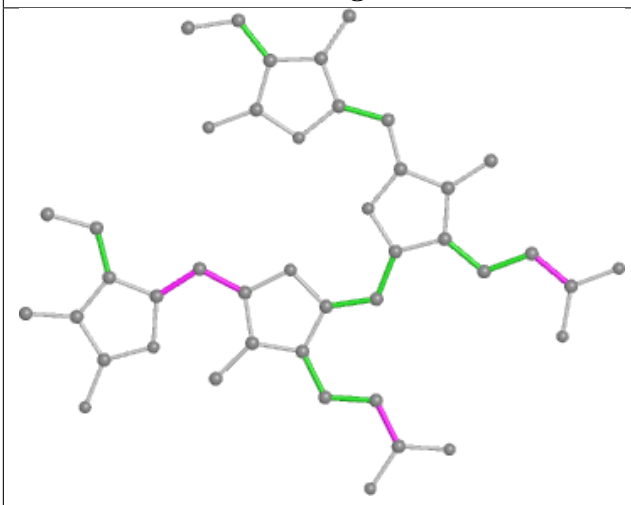

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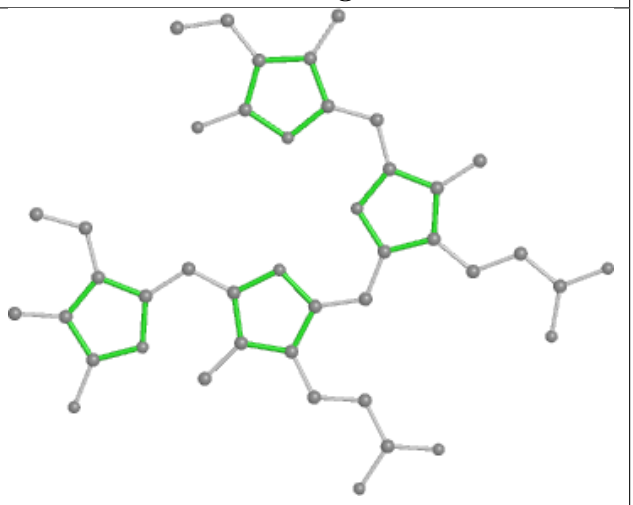
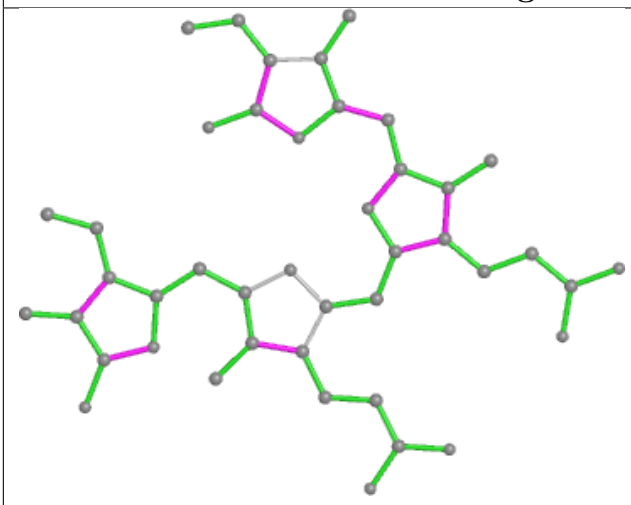


Rings

Ligand PUB J2 202



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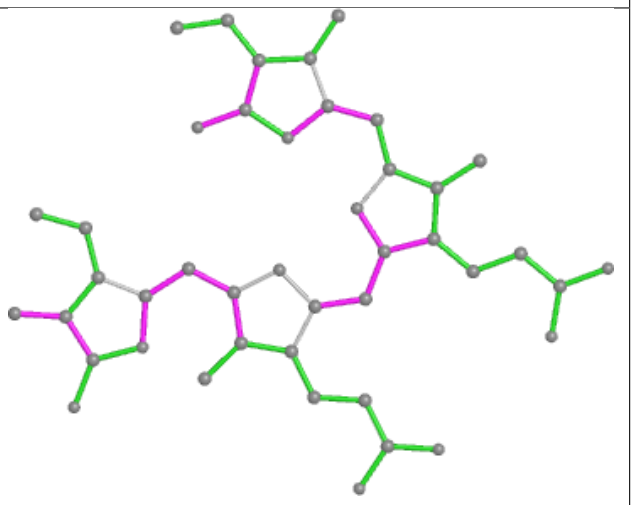

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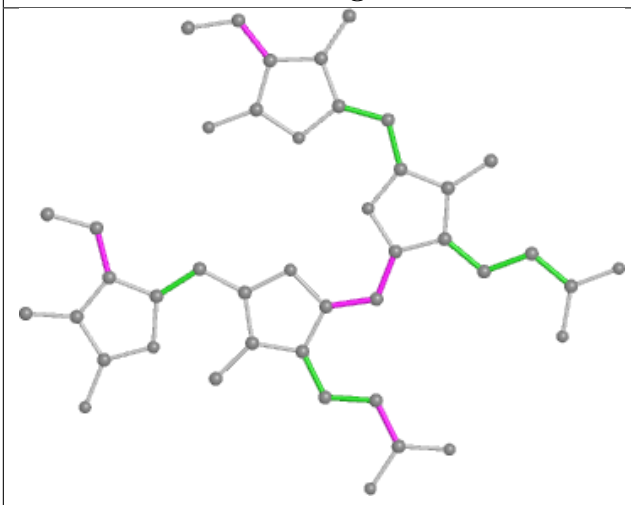

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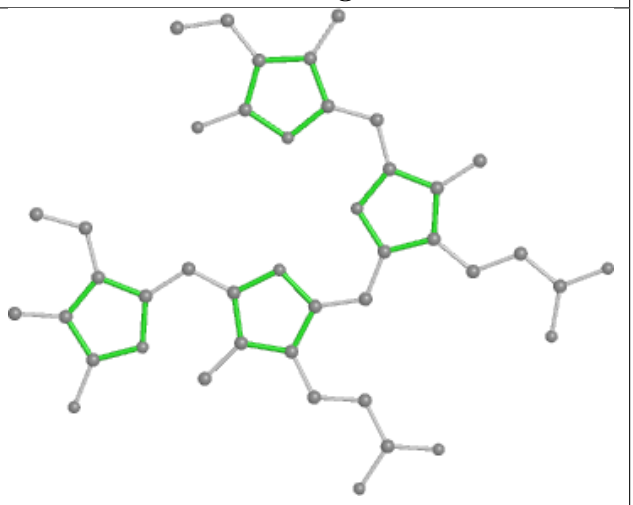
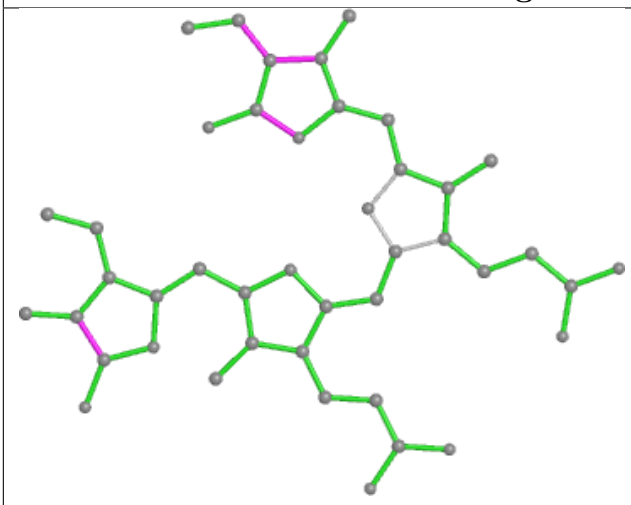


Rings

Ligand PEB Y4 201



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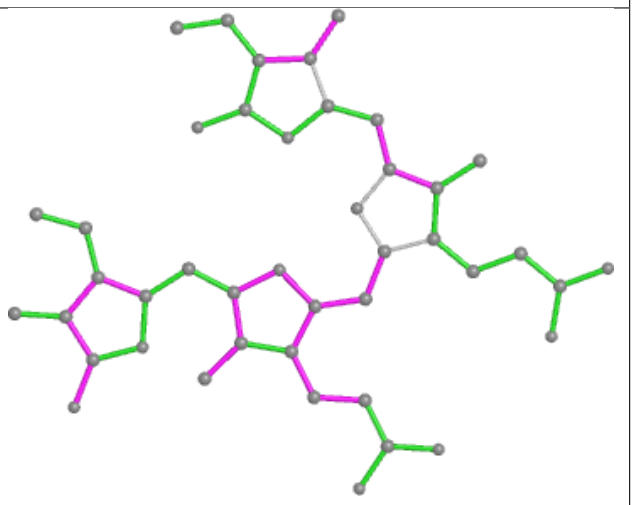
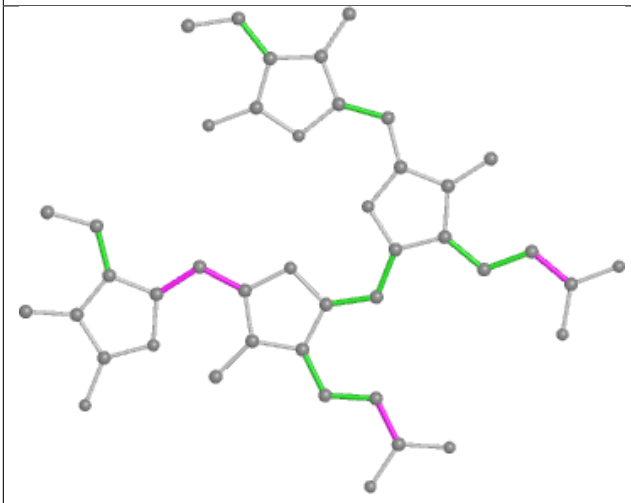


Bond angles



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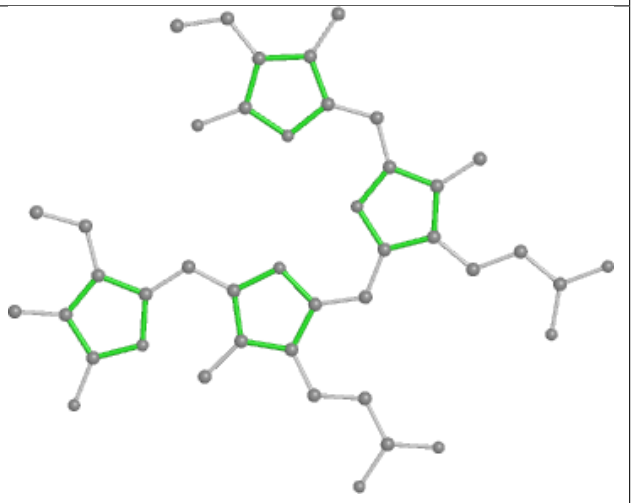
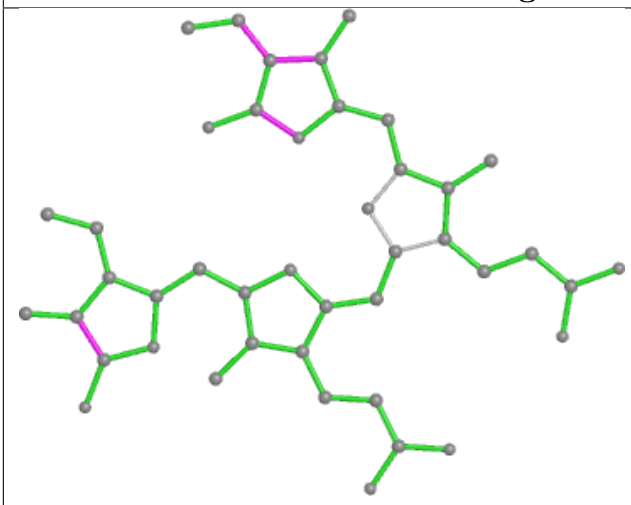


Rings

Ligand PEB u9 201



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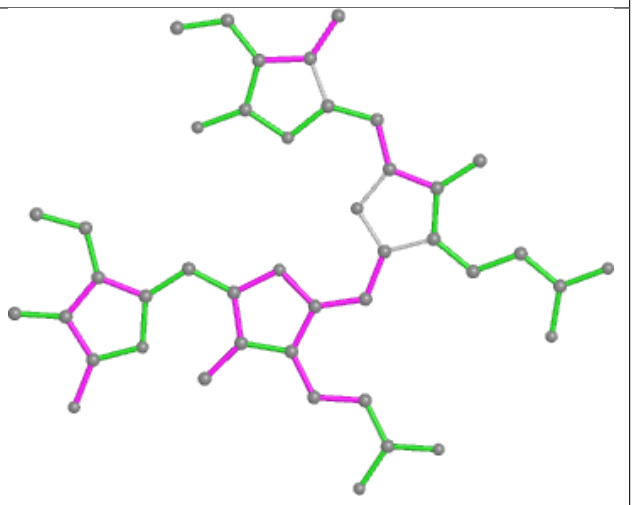

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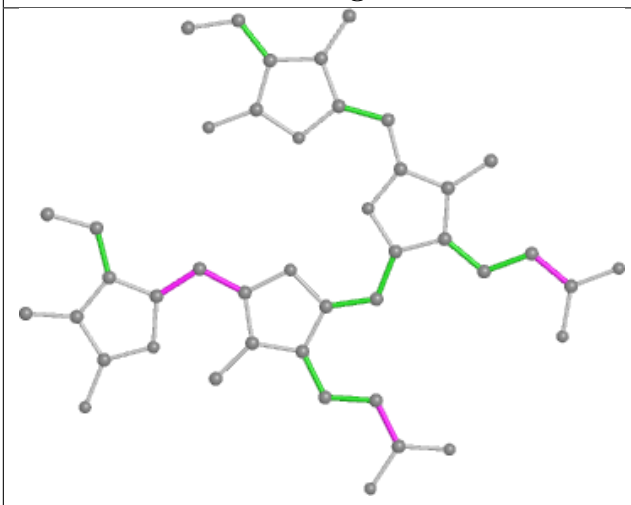

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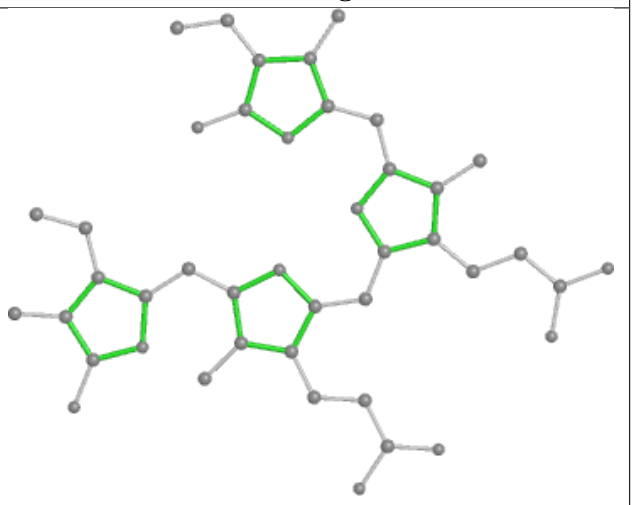

Rings

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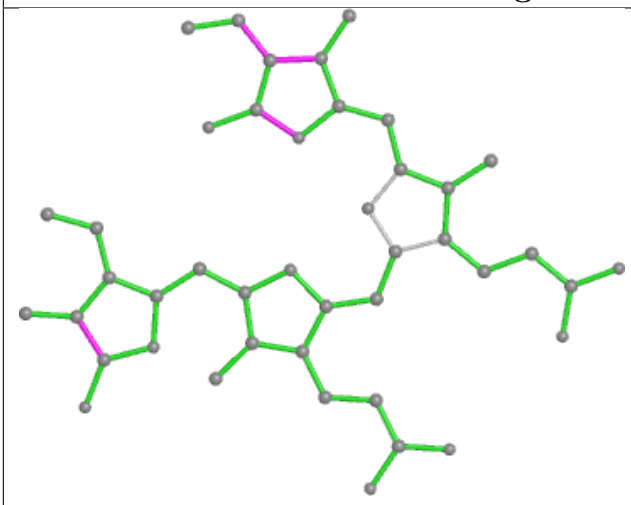

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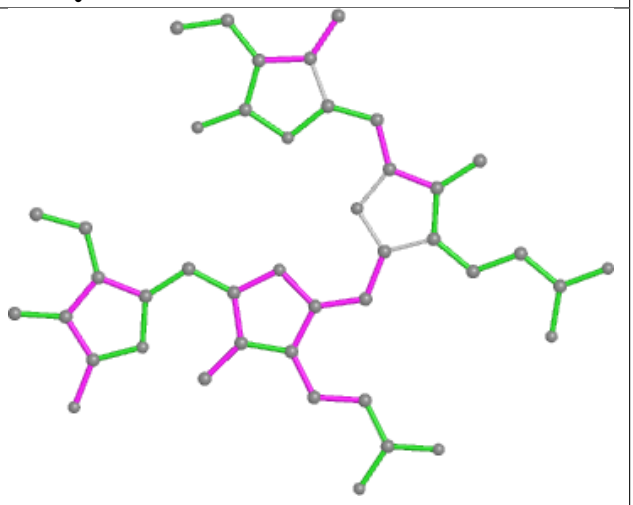

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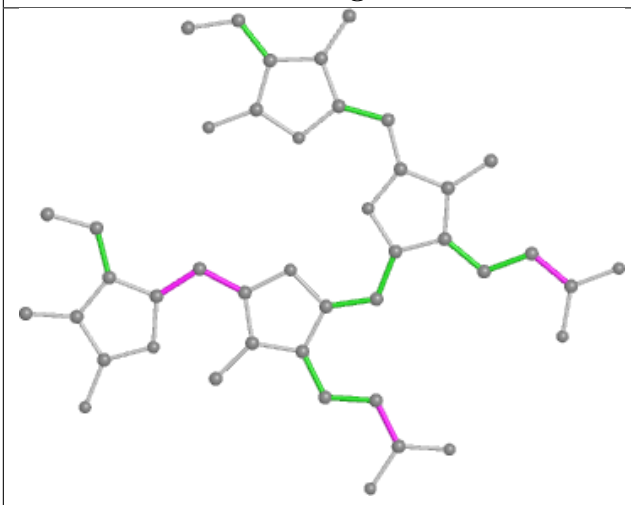

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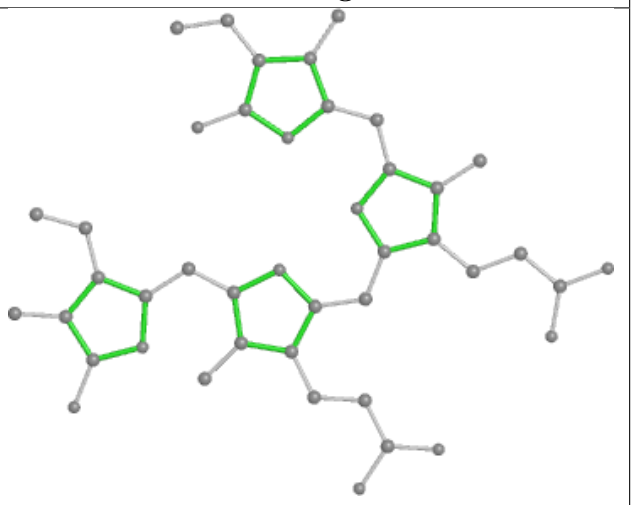
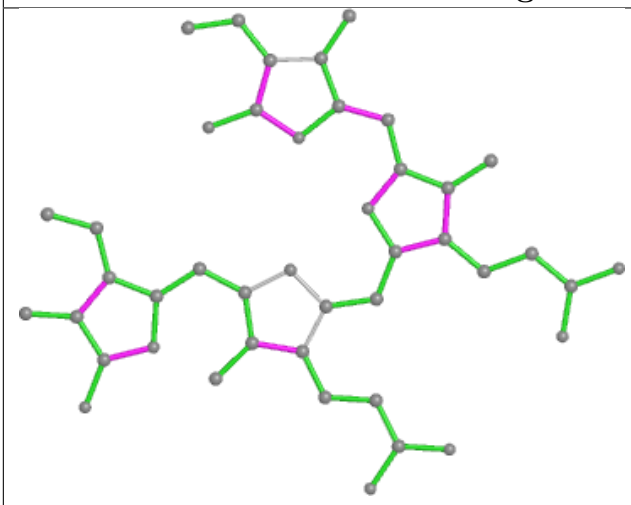


Rings

Ligand PUB d3 304



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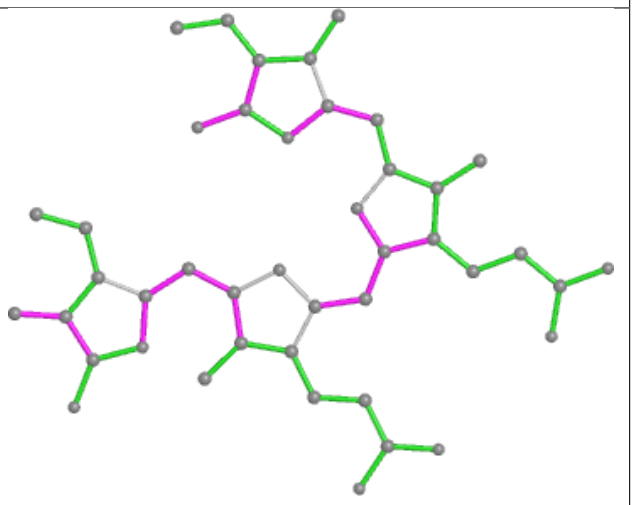

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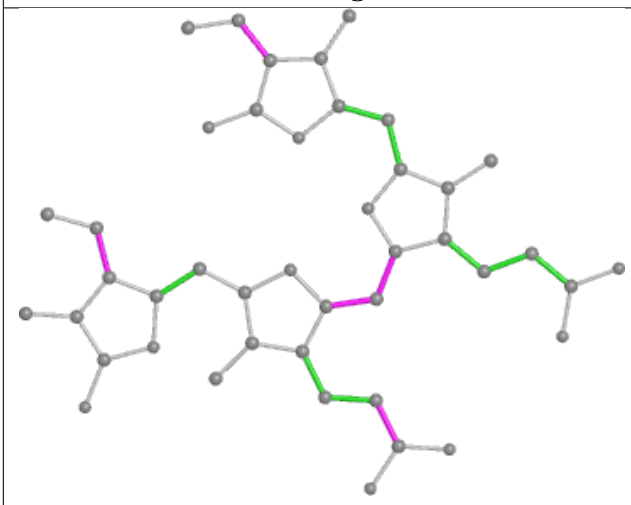

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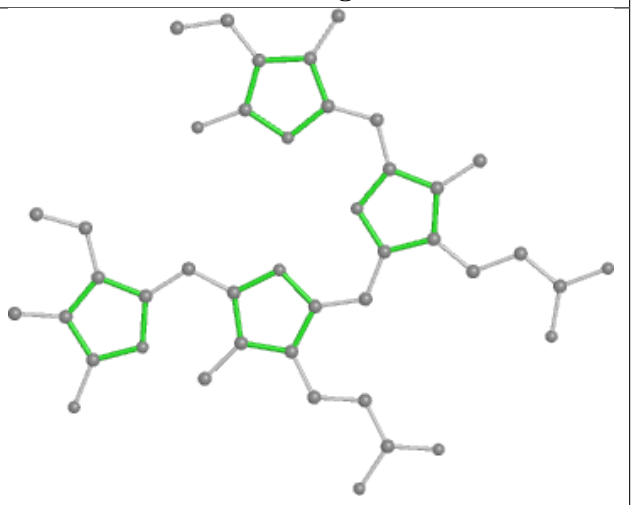
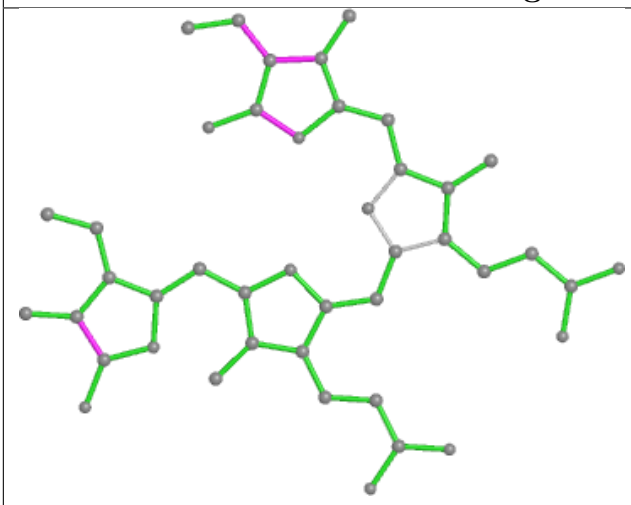


Rings

Ligand PEB l6 202



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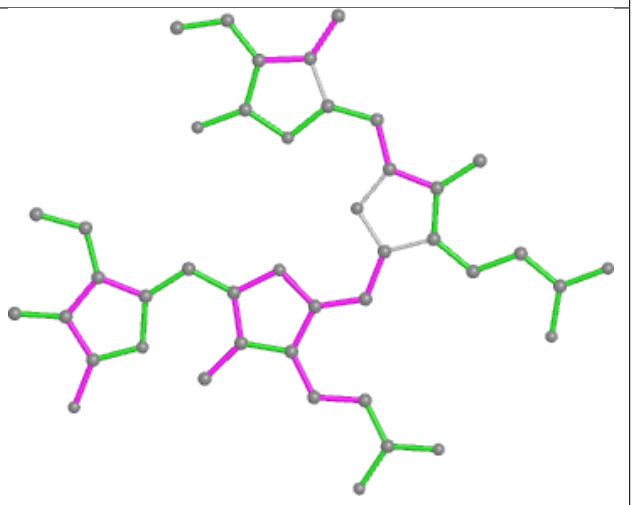

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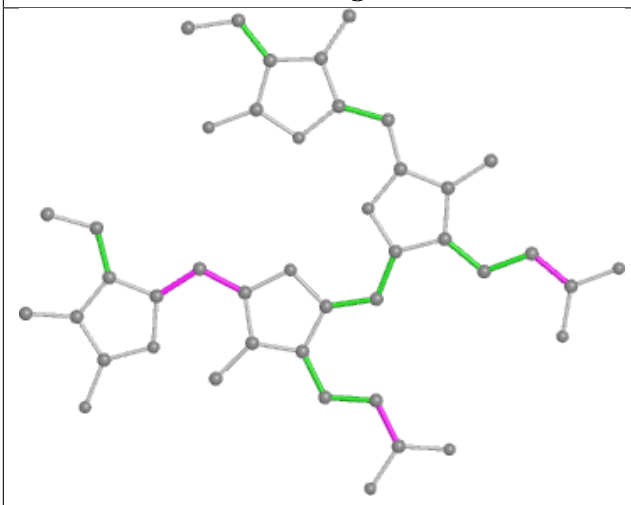

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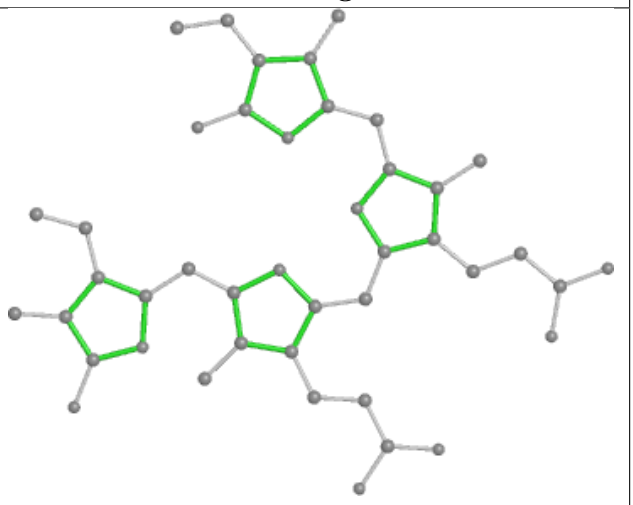
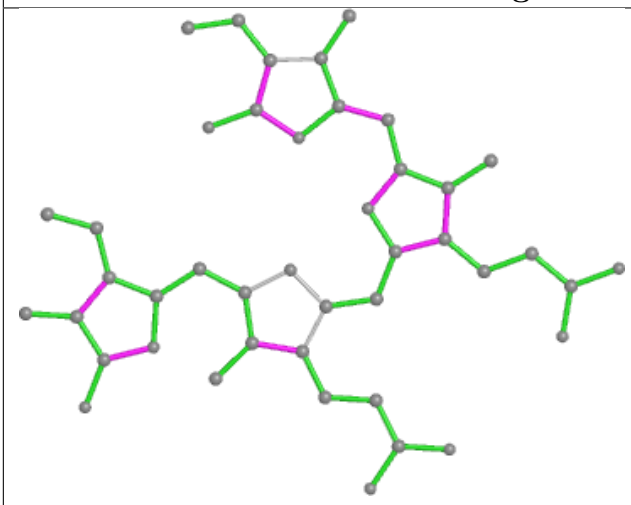


Rings

Ligand PUB hY 406



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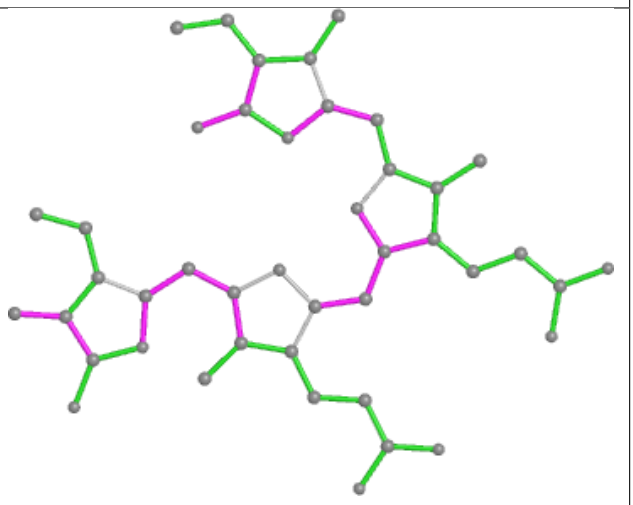

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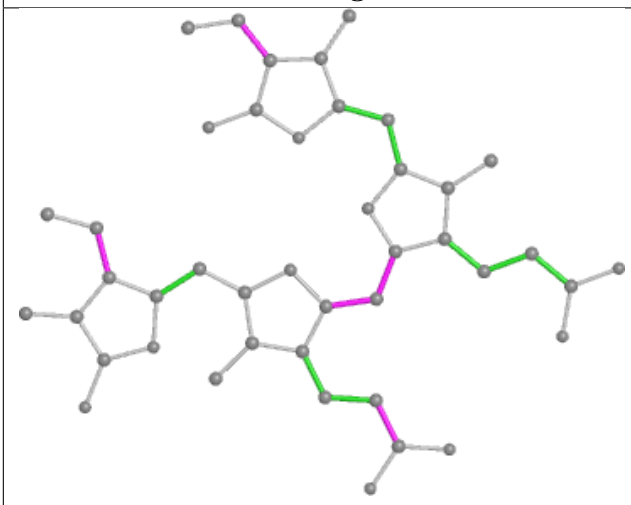

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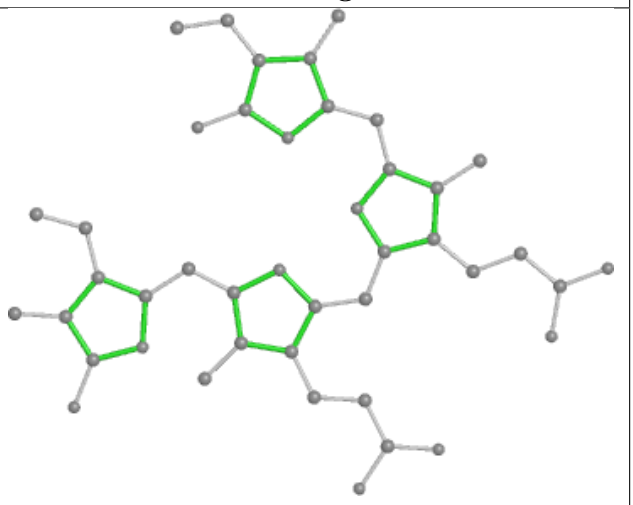
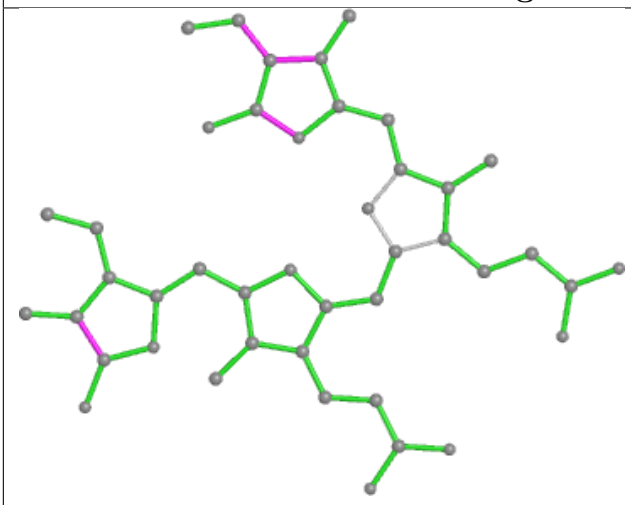


Rings

Ligand PEB T6 202



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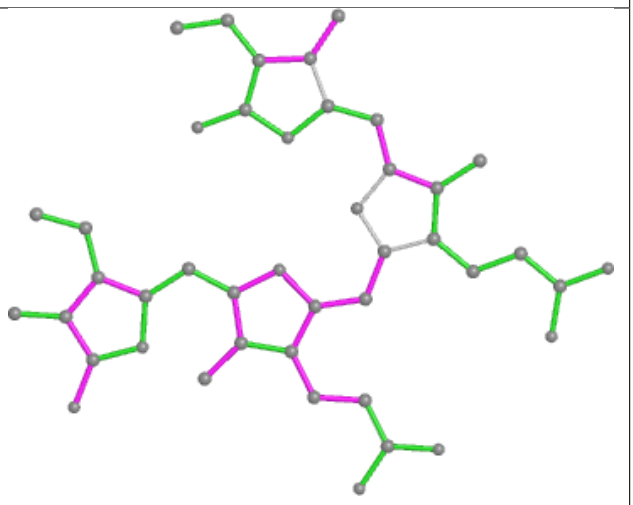

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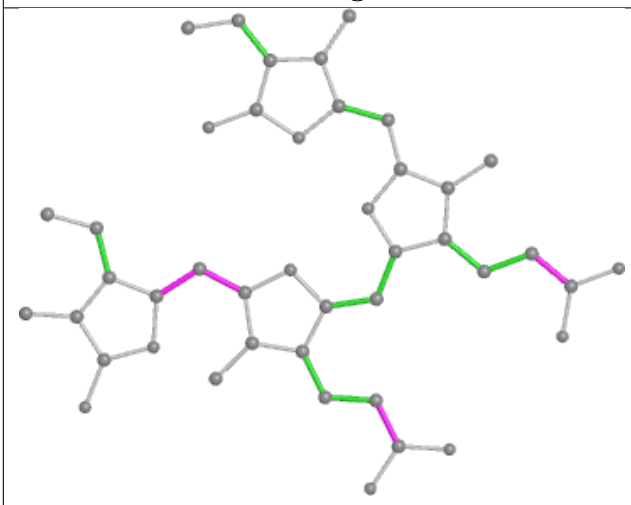

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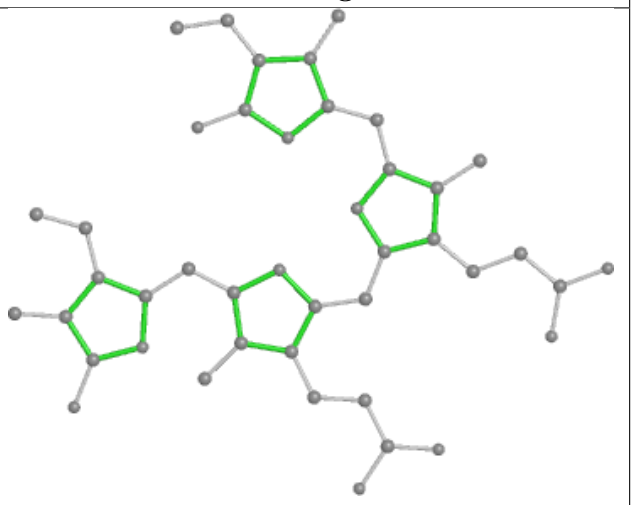
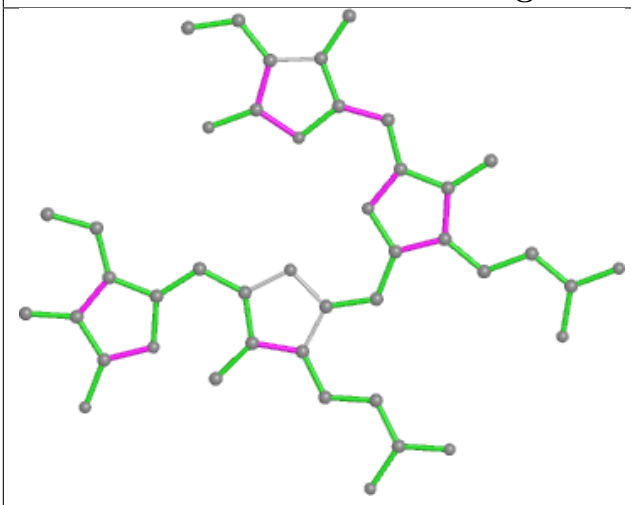


Rings

Ligand PUB aZ 305



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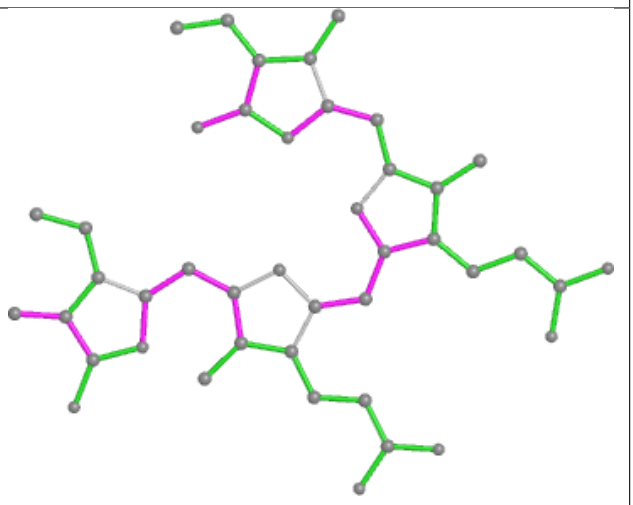

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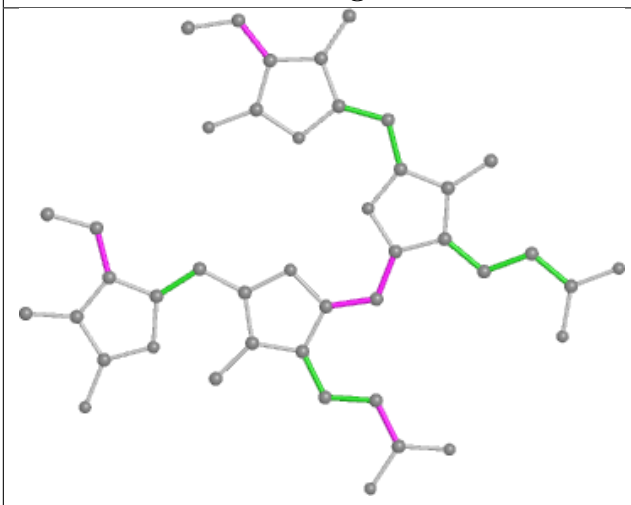

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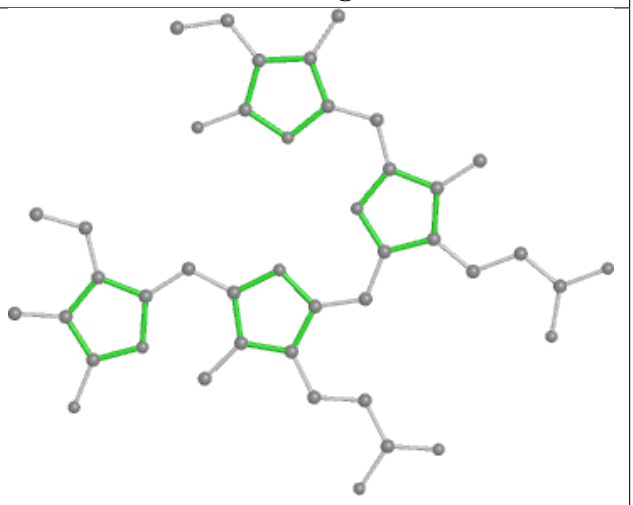
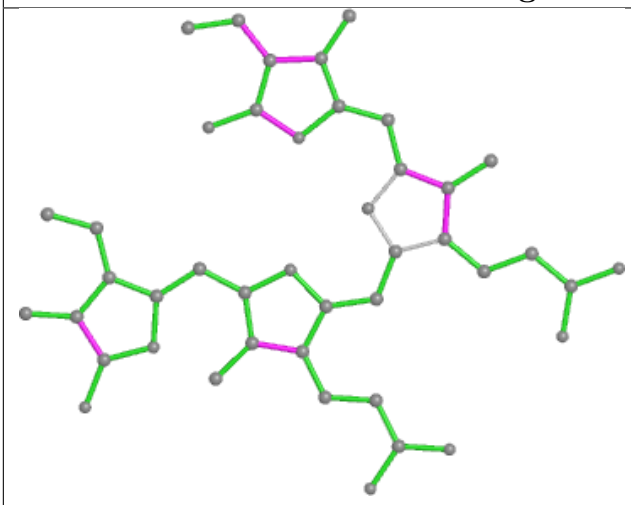


Rings

Ligand PEB h3 201



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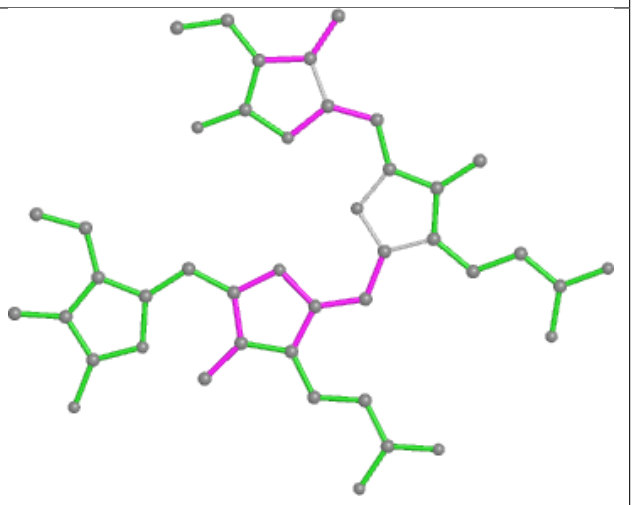

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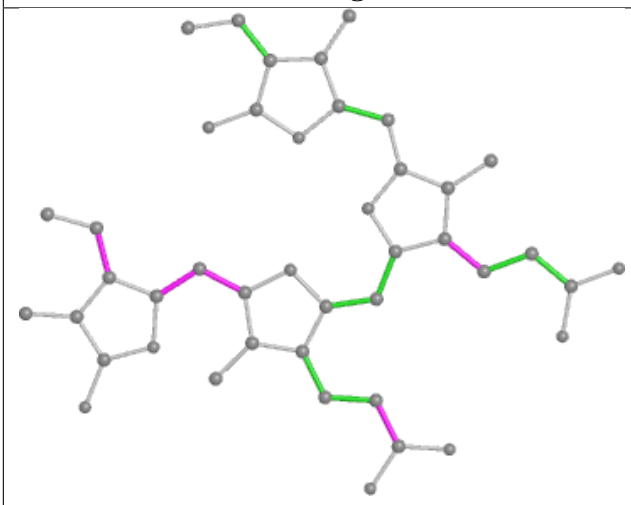

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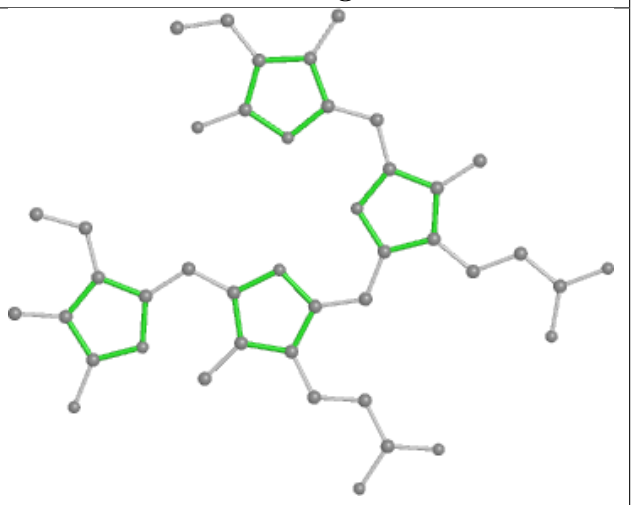
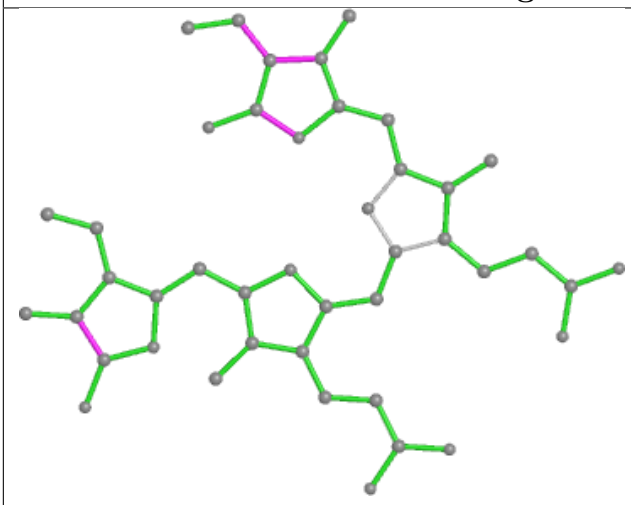


Rings

Ligand PEB E8 202



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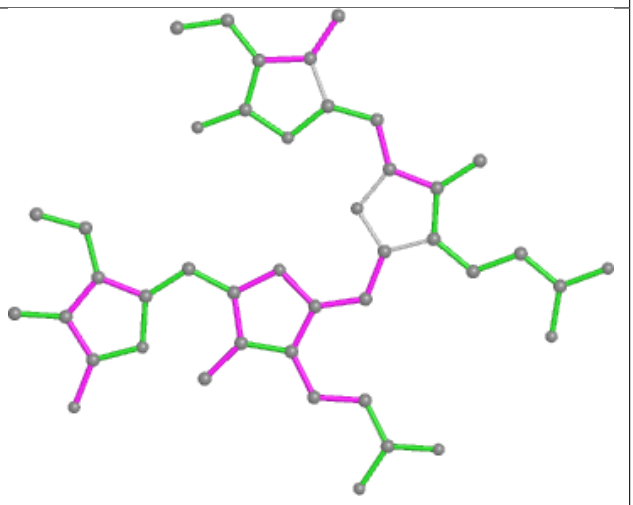
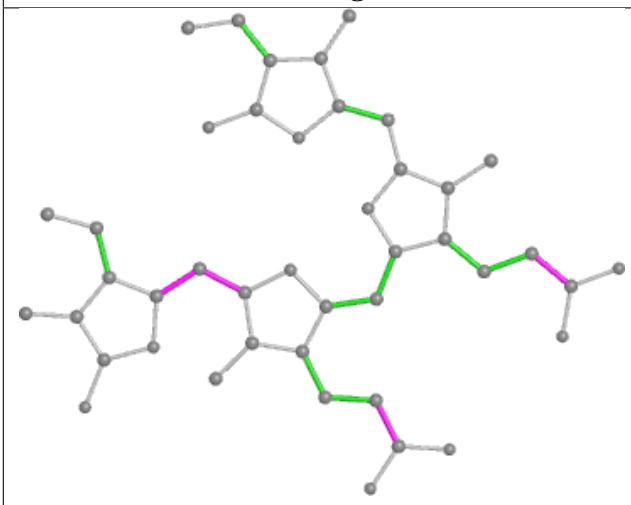


Bond angles



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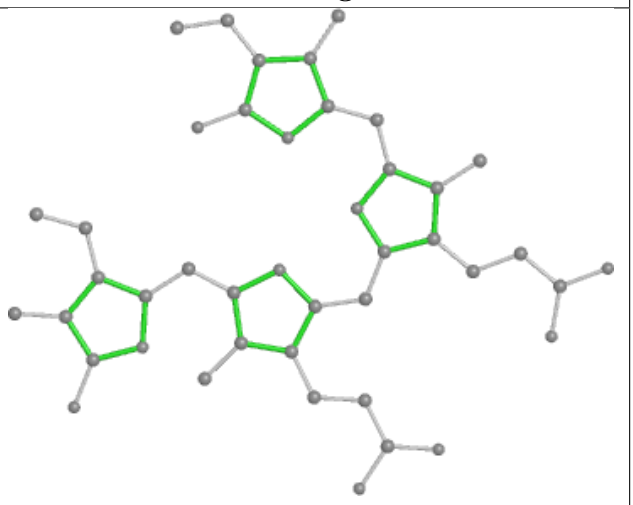
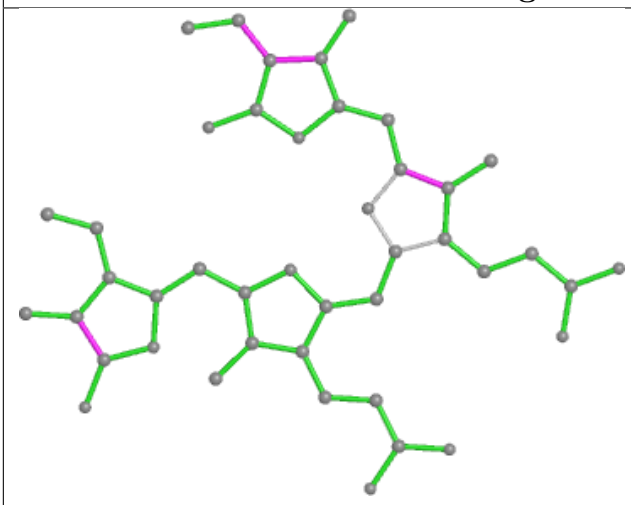
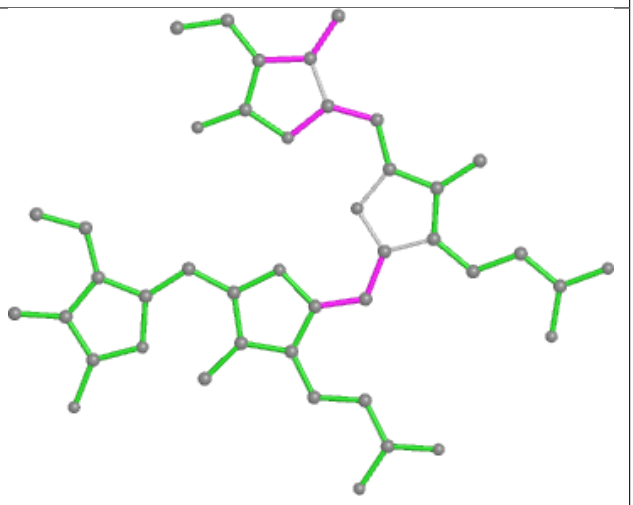


Rings

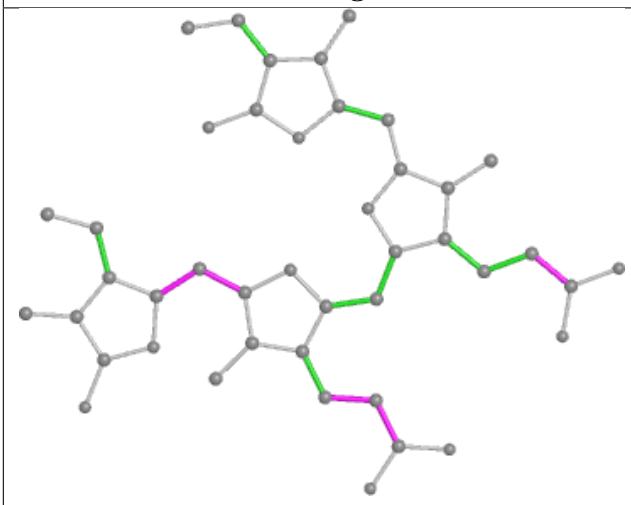
Ligand PEB u5 202



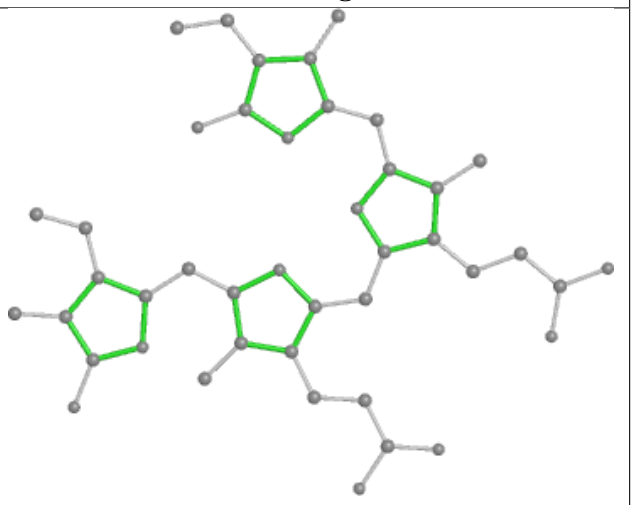
Bond lengths



Bond angles

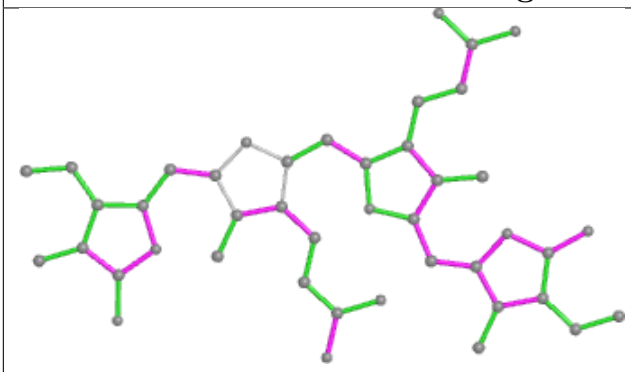


Torsions



Rings

Ligand CYC v1 201



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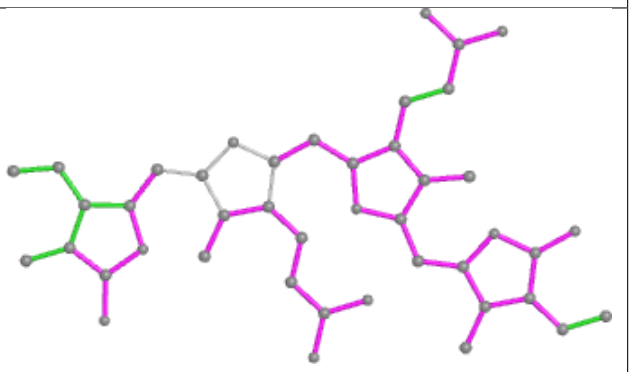

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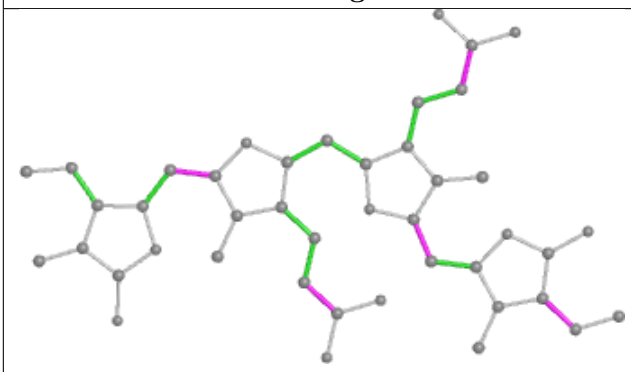

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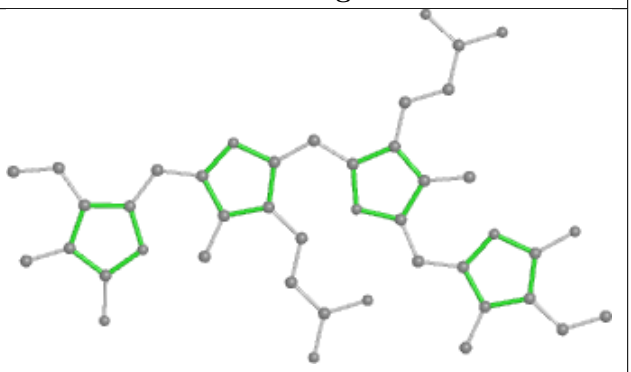
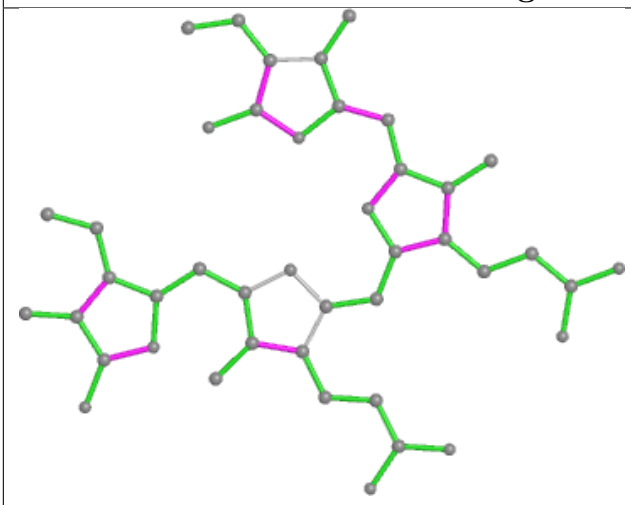


Rings

Ligand PUB en 203



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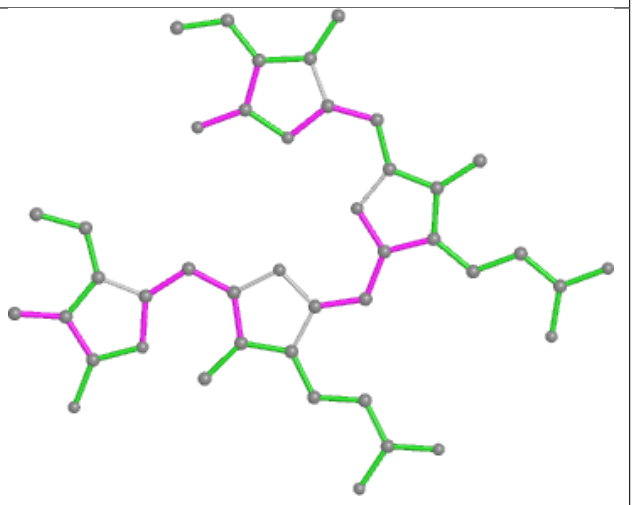

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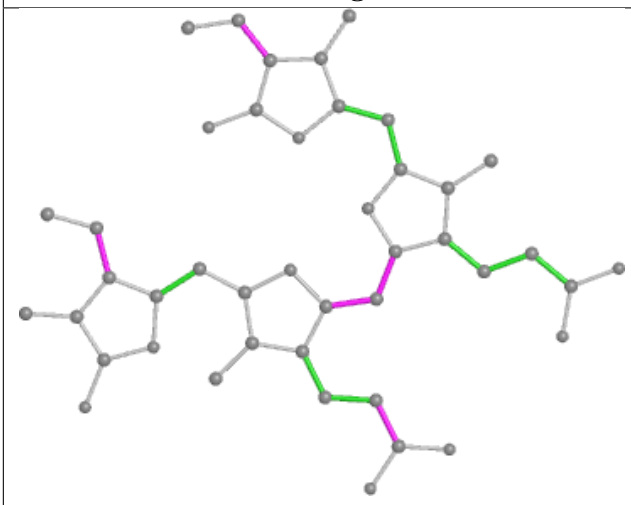

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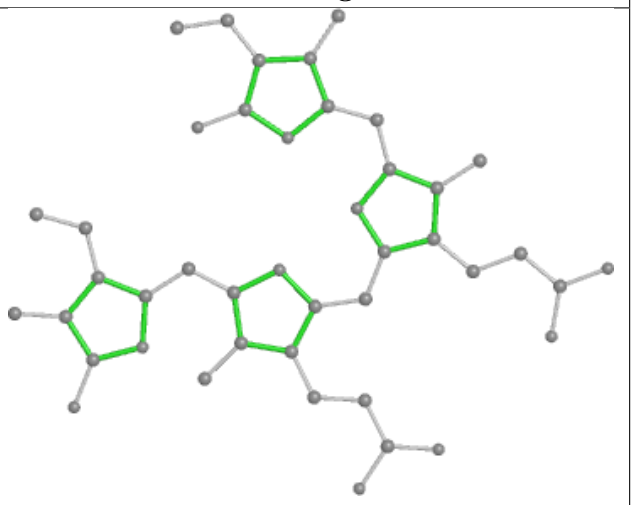
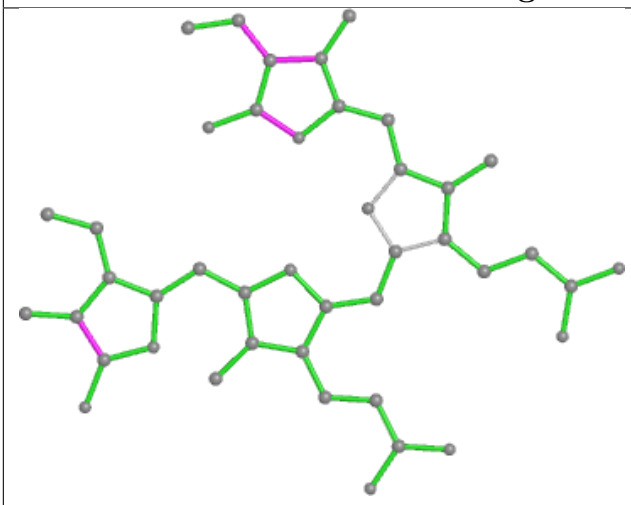


Rings

Ligand PEB L2 201



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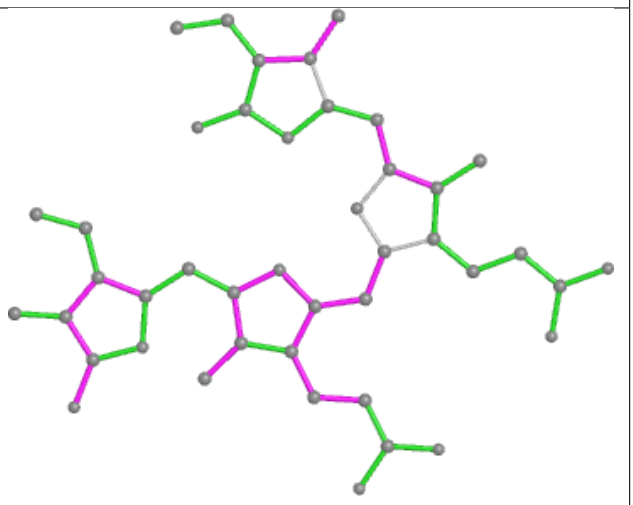

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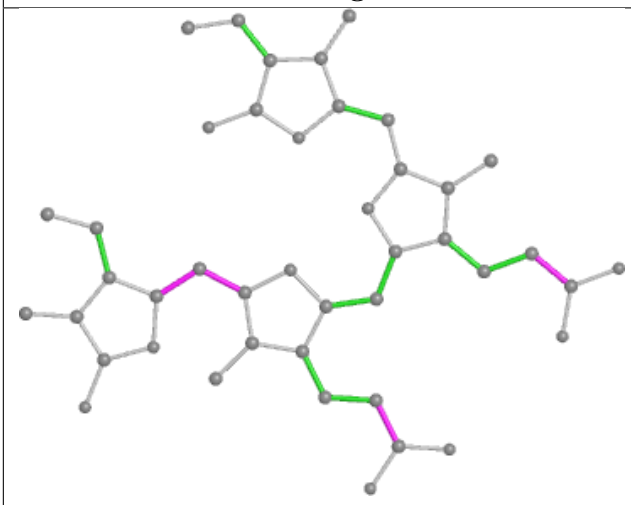

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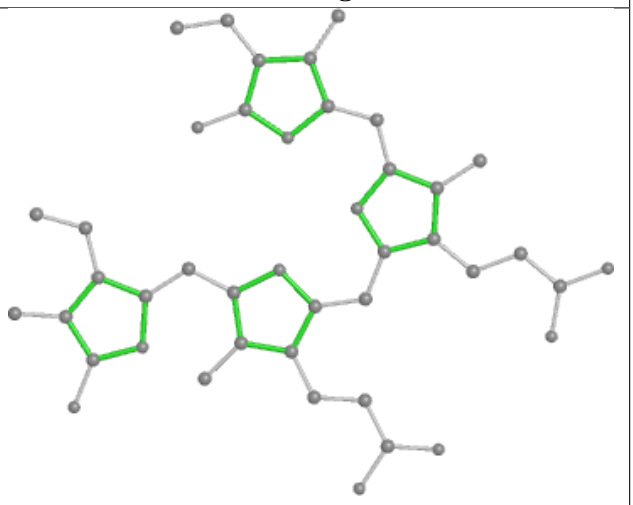

Rings

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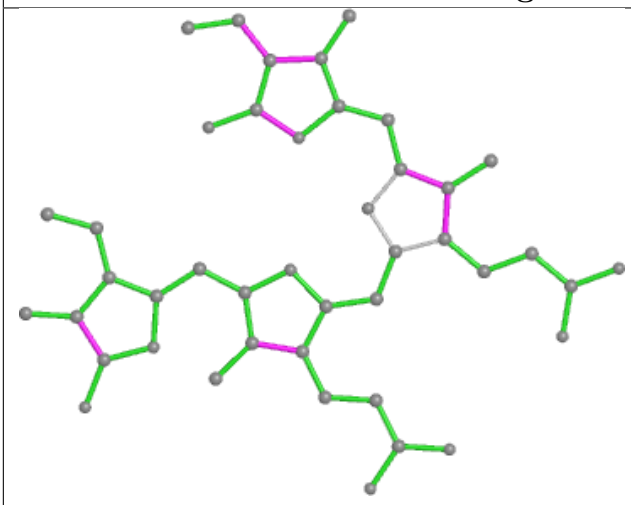

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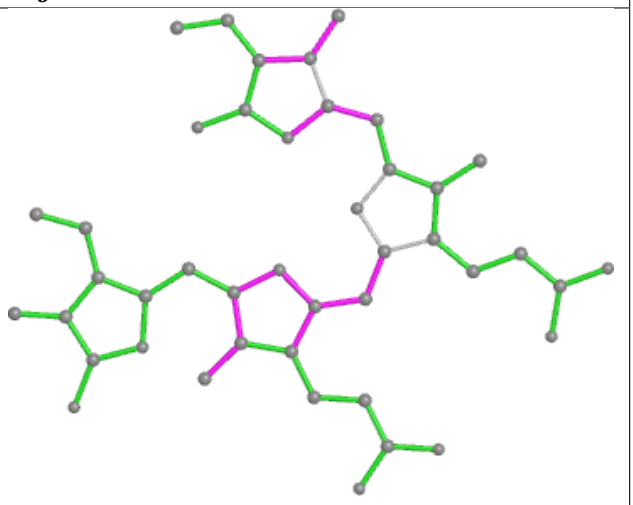

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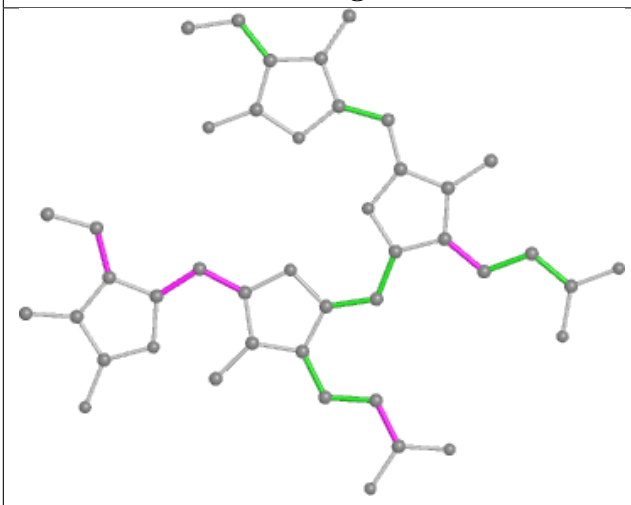

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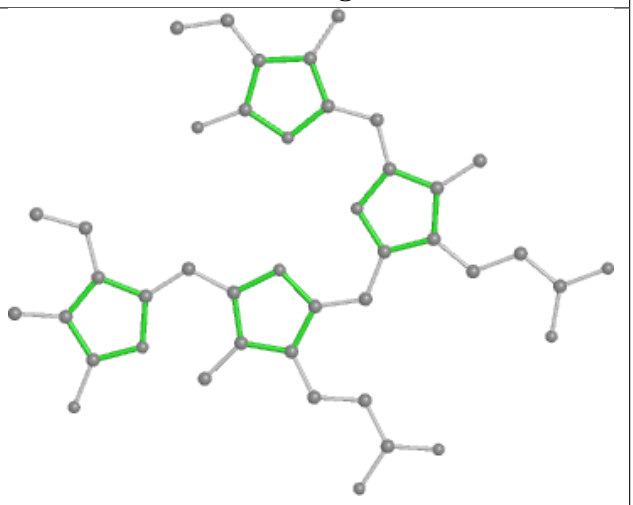

Rings

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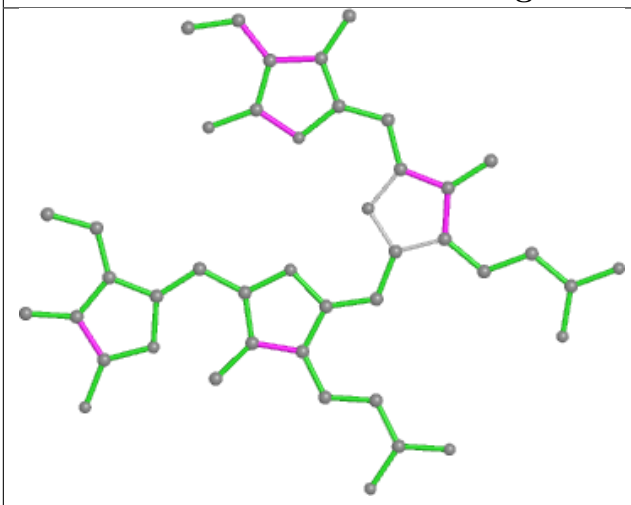

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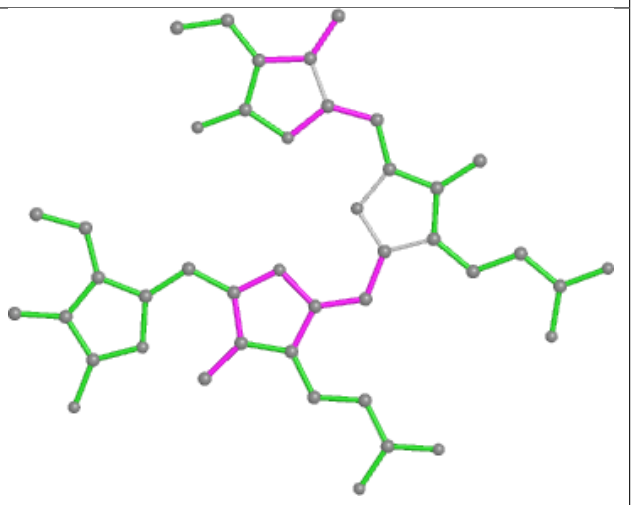

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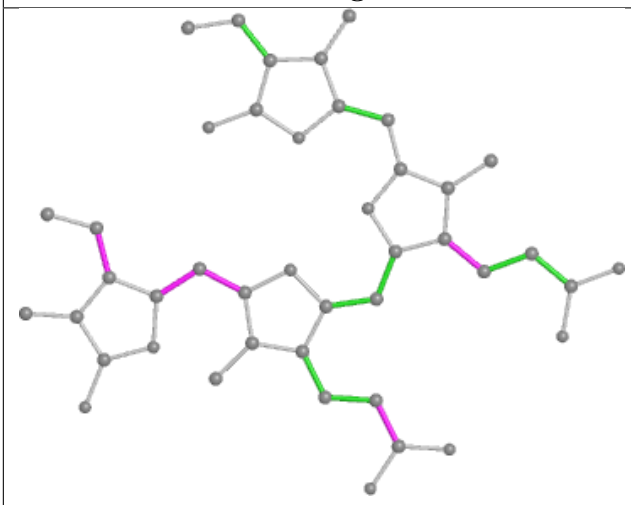

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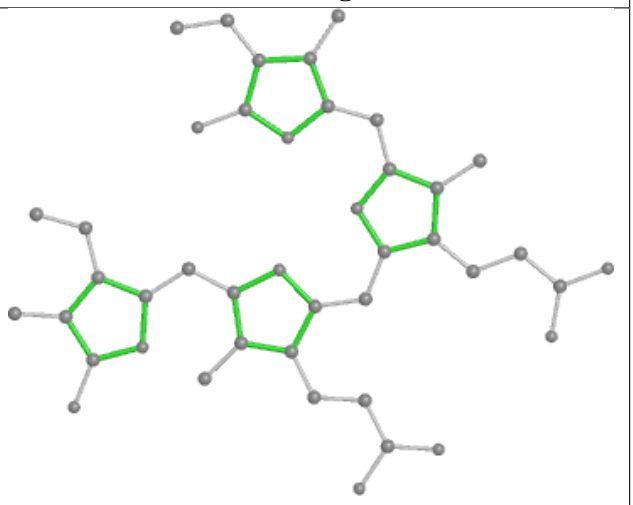

Rings

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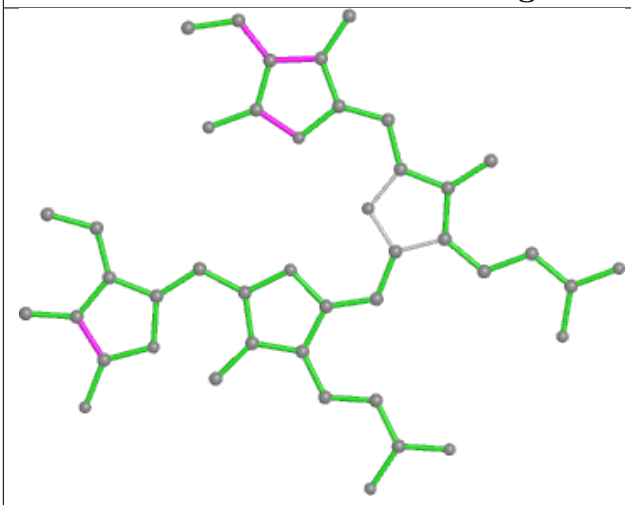

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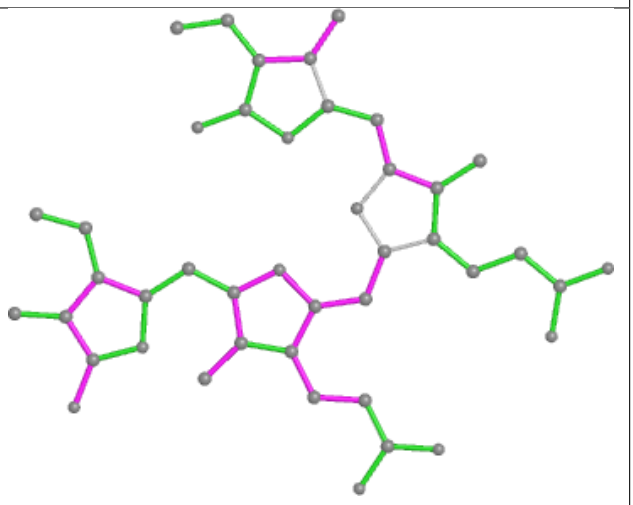

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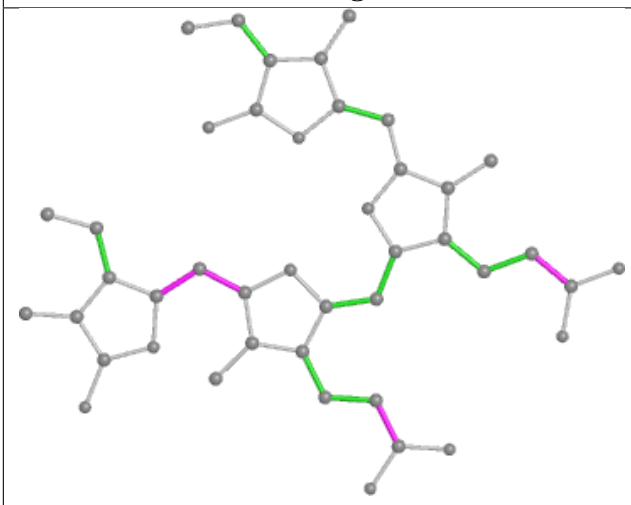

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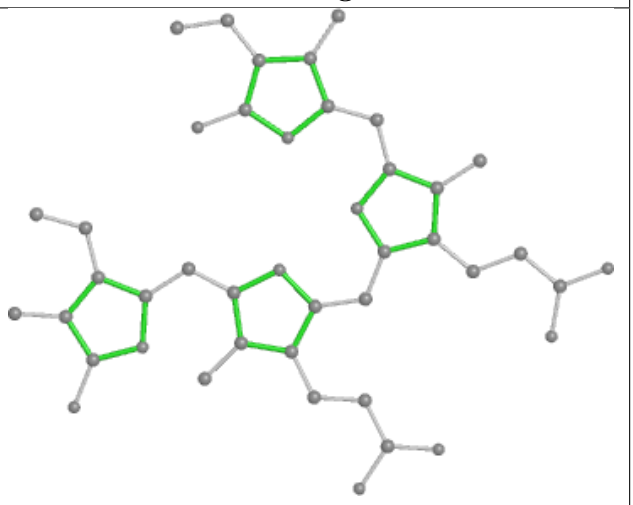

Rings

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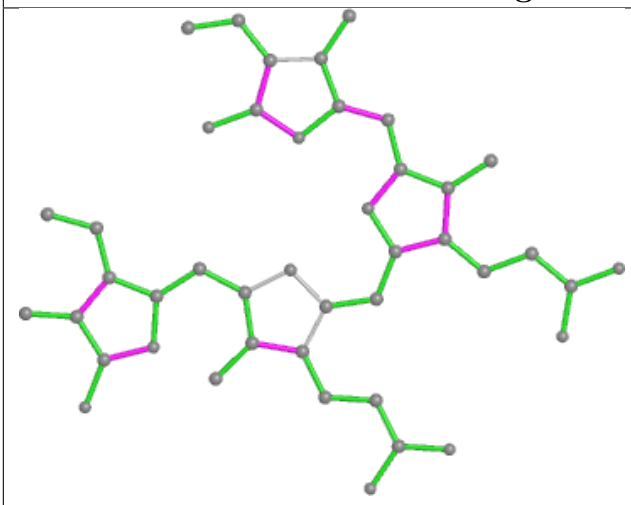

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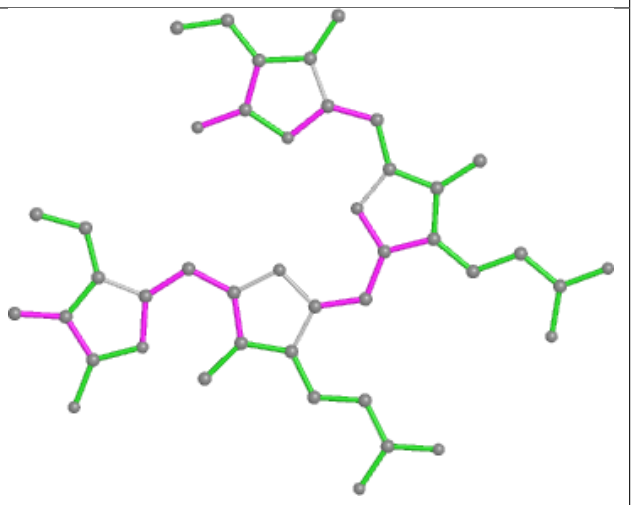

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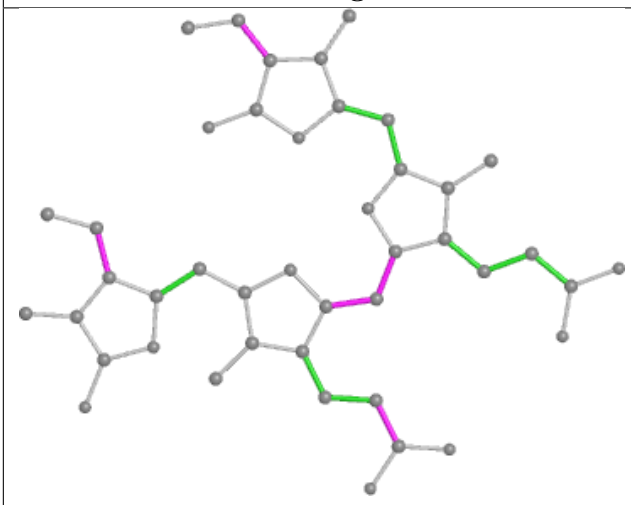

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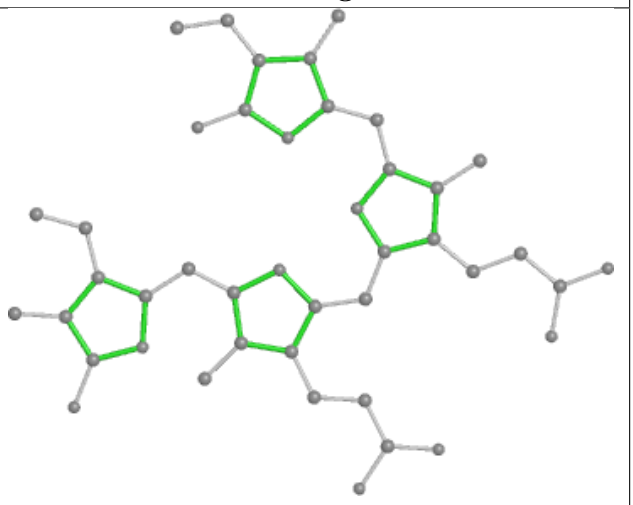

Rings

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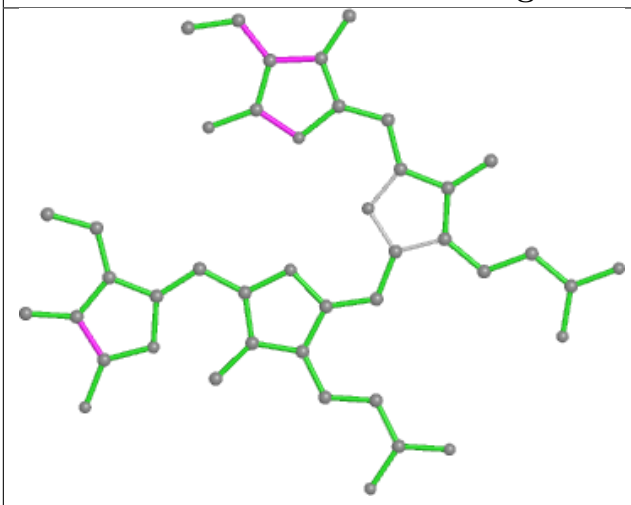

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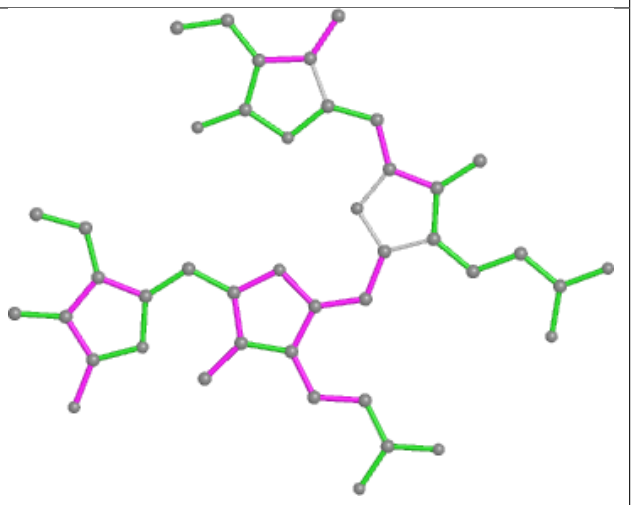

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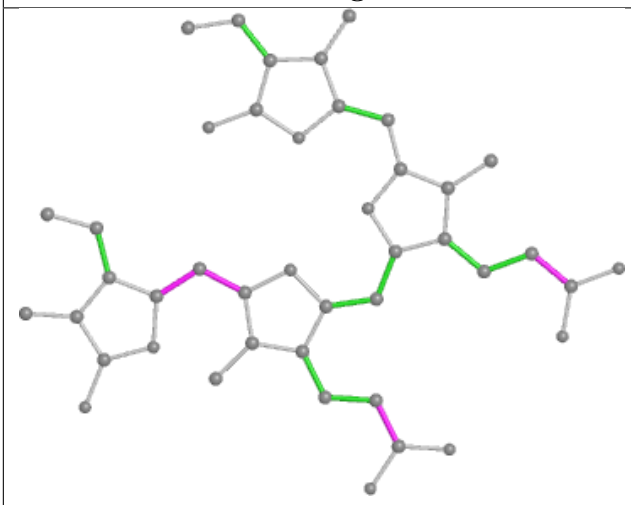

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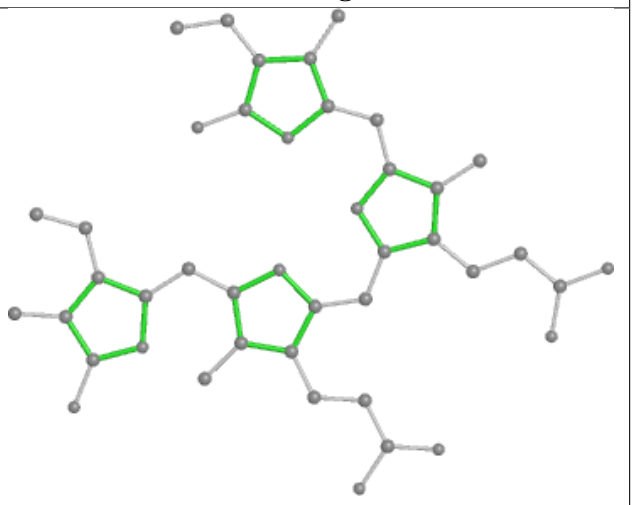

Rings

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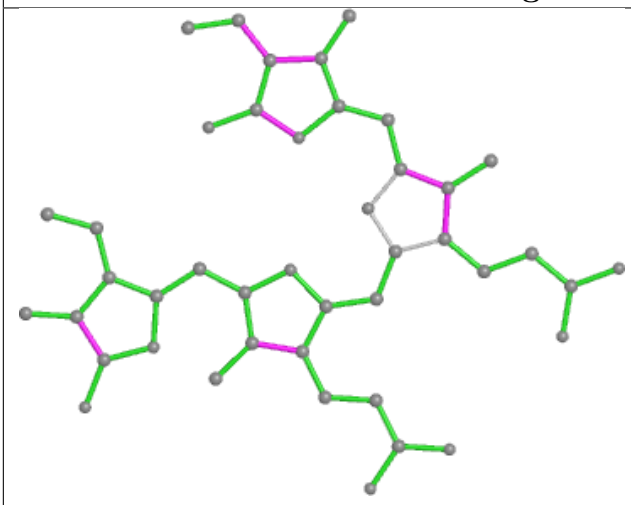

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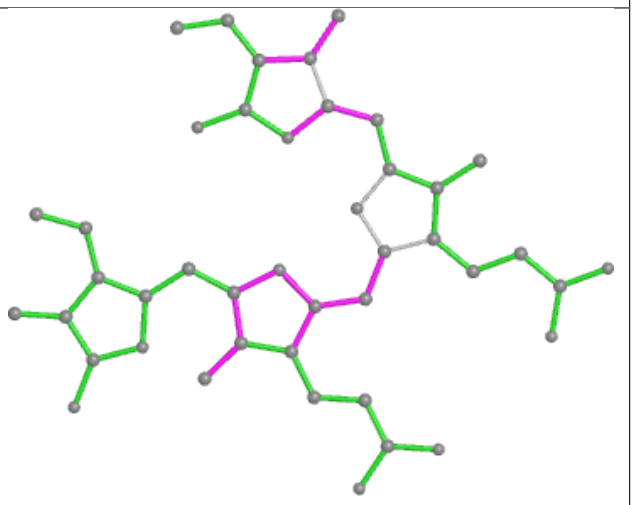

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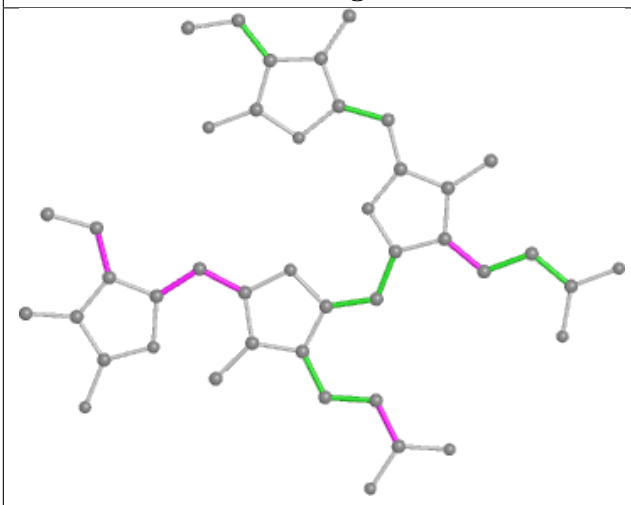

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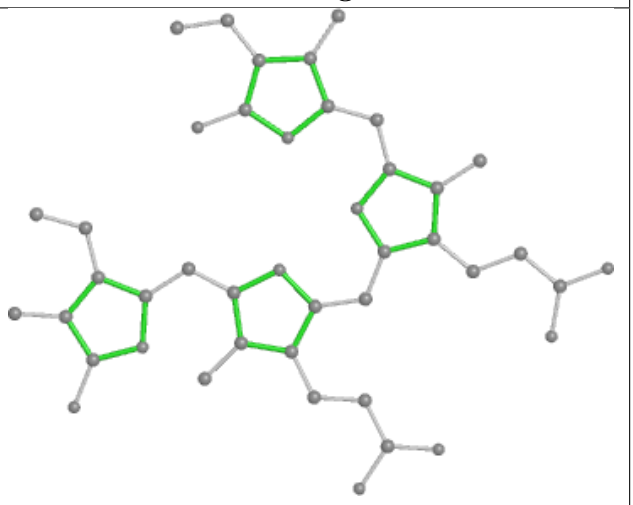

Rings

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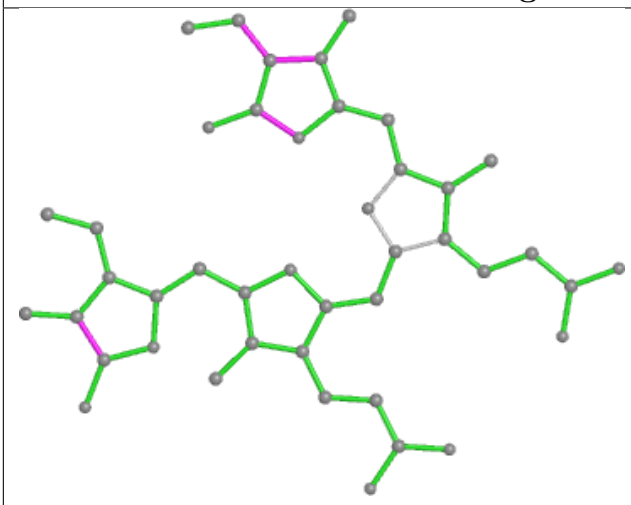

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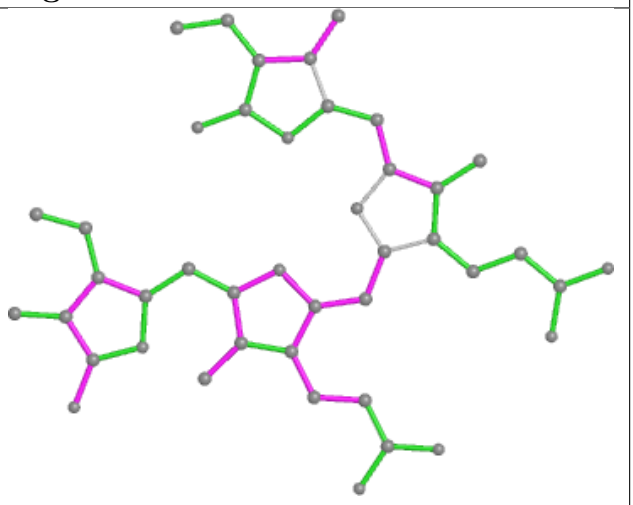

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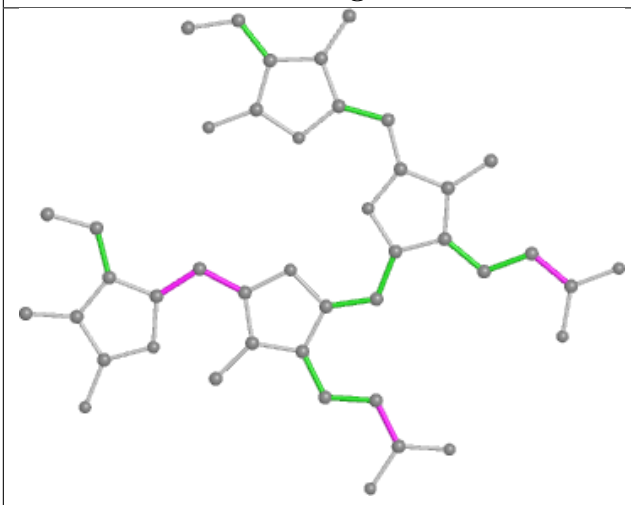

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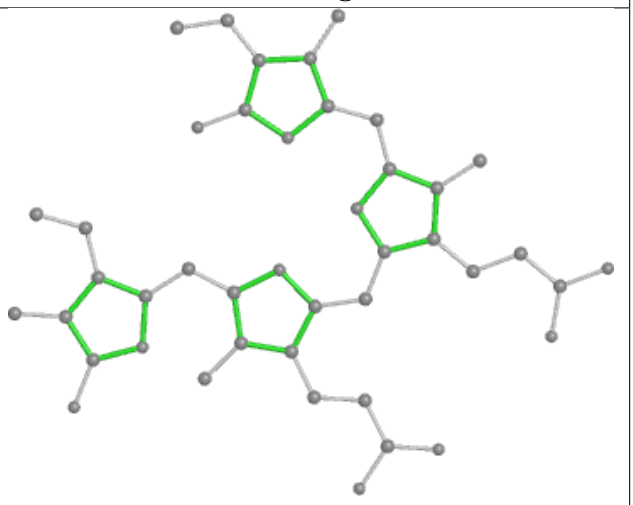

Rings

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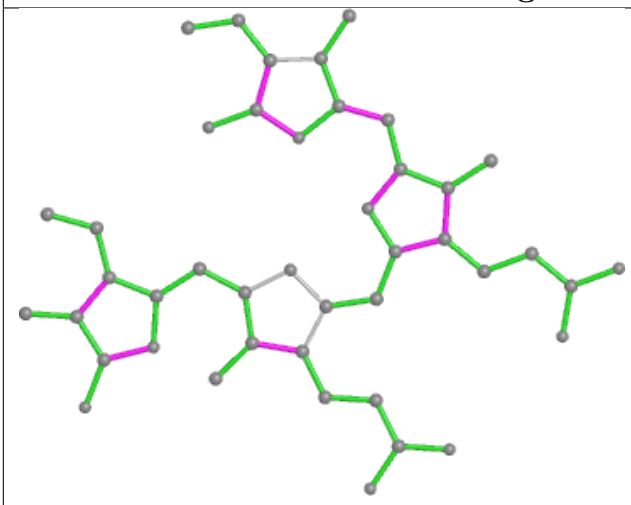

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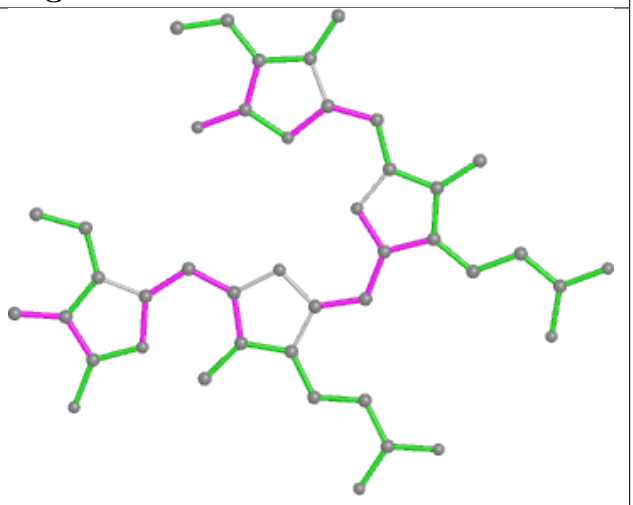

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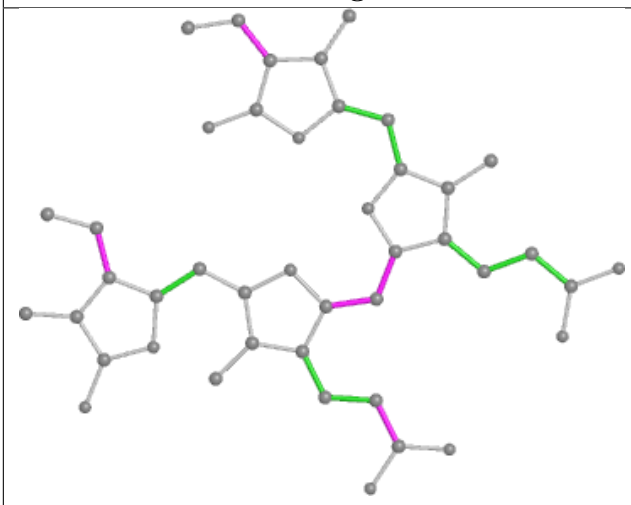

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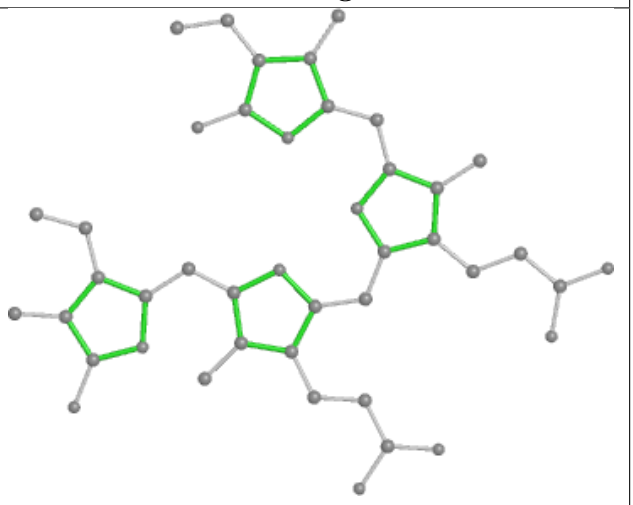
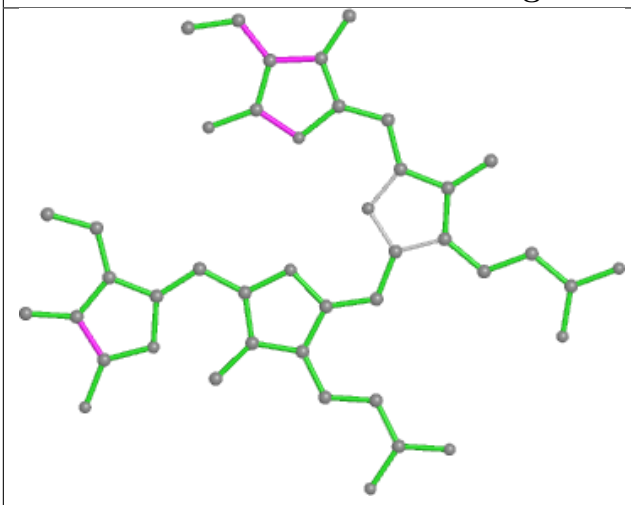


Rings

Ligand PEB eI 202



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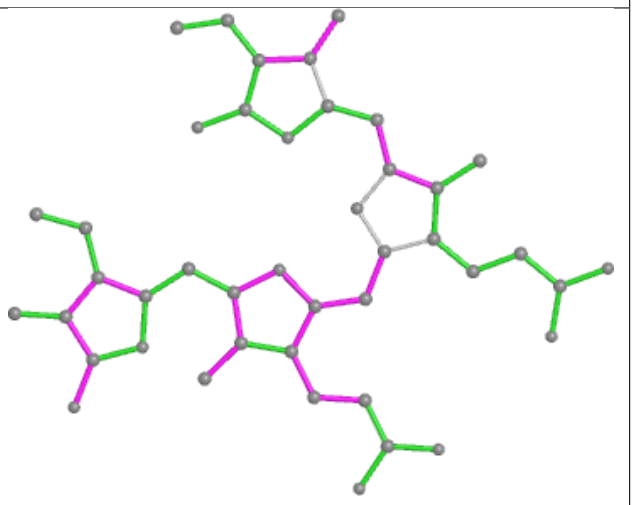

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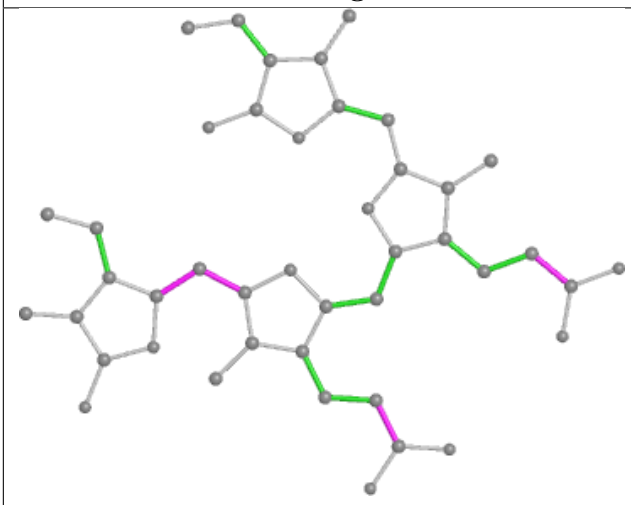

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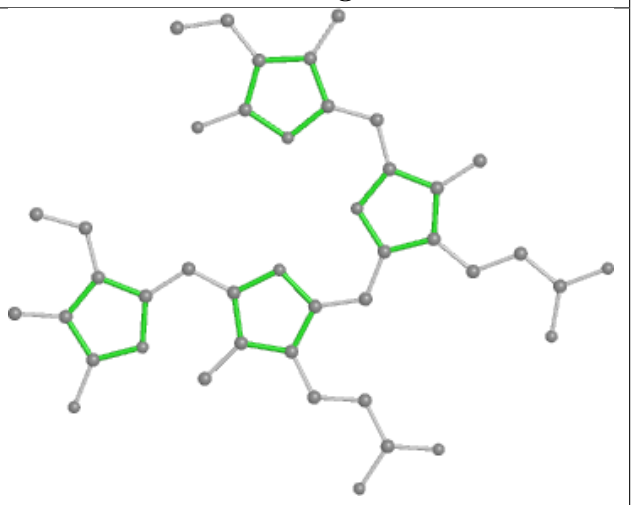
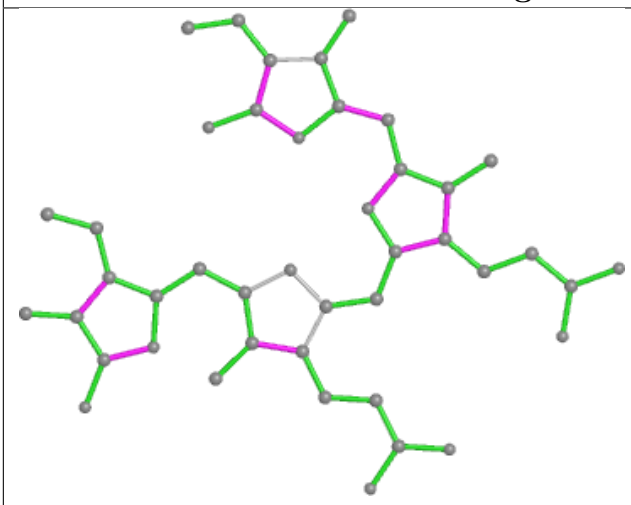
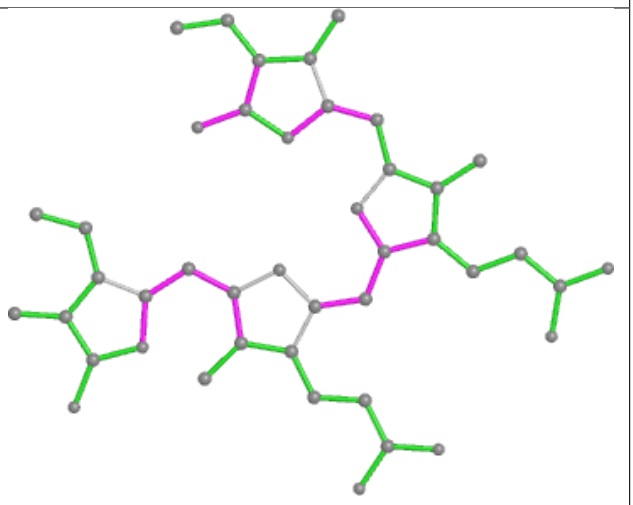


Rings

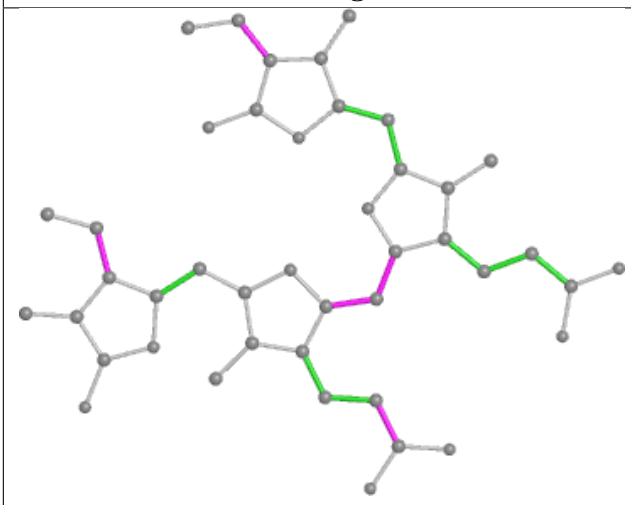
Ligand PUB aB 203



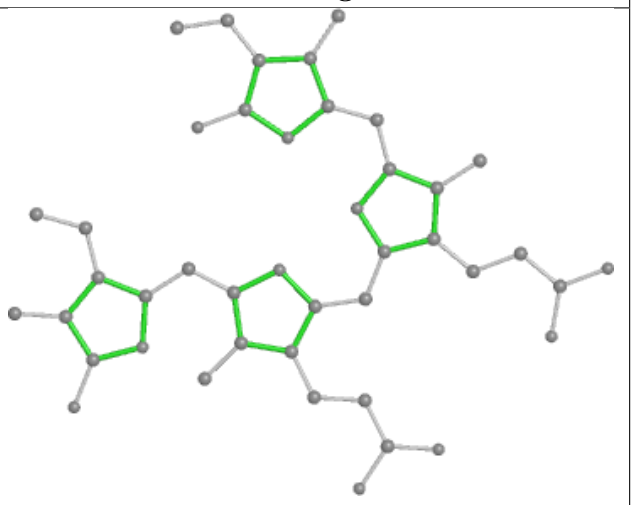
Bond lengths



Bond angles

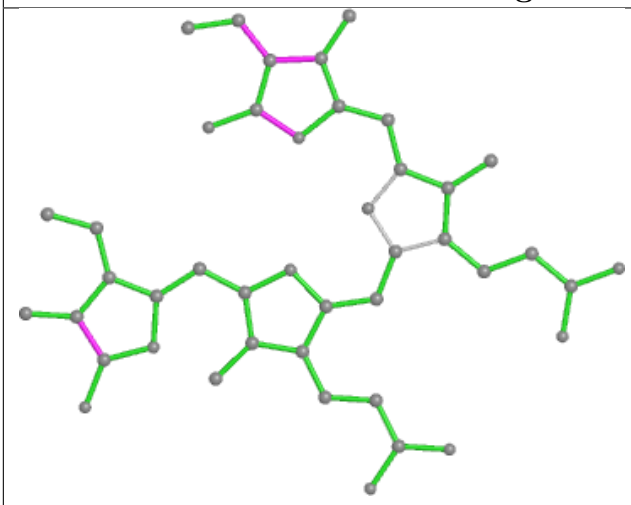


Torsions



Rings

Ligand PEB R9 201



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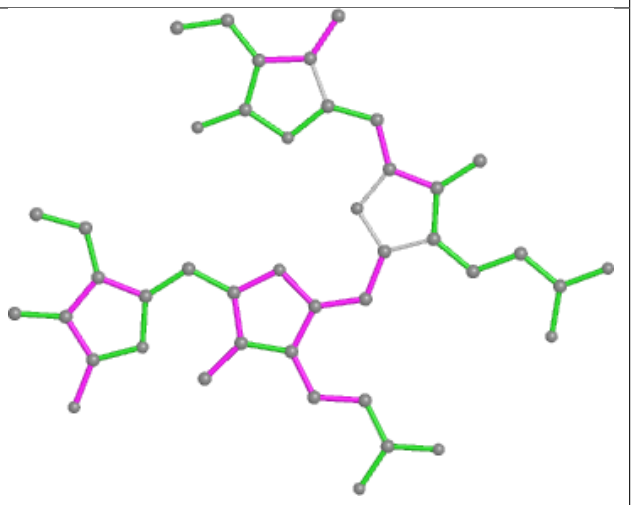

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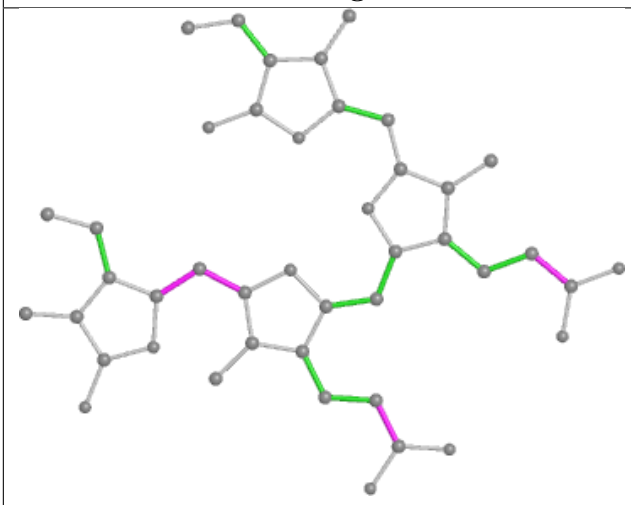

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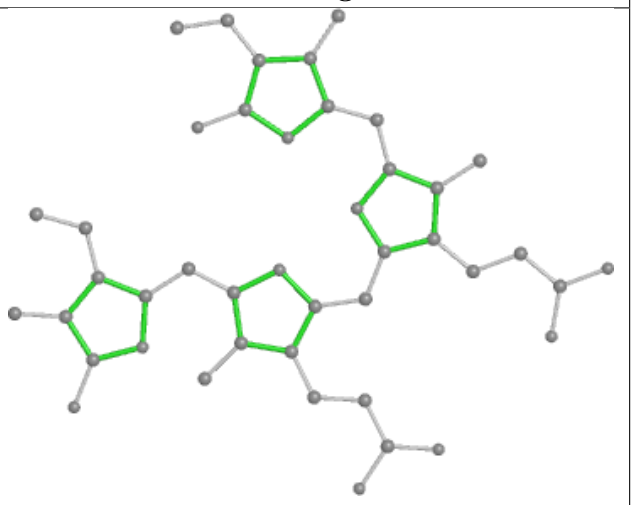
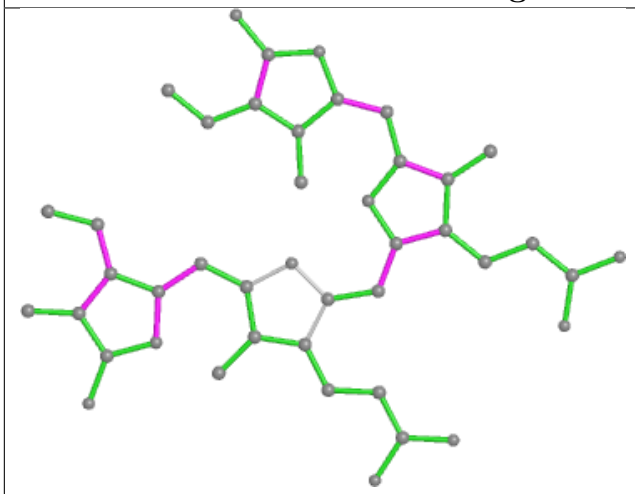


Rings

Ligand PVN ey 1004



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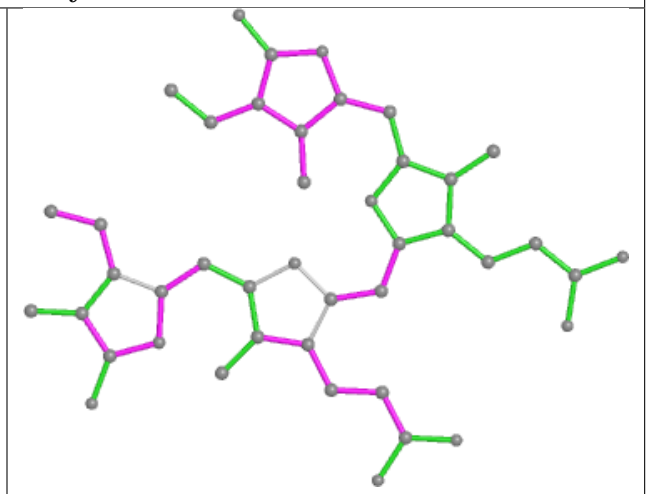

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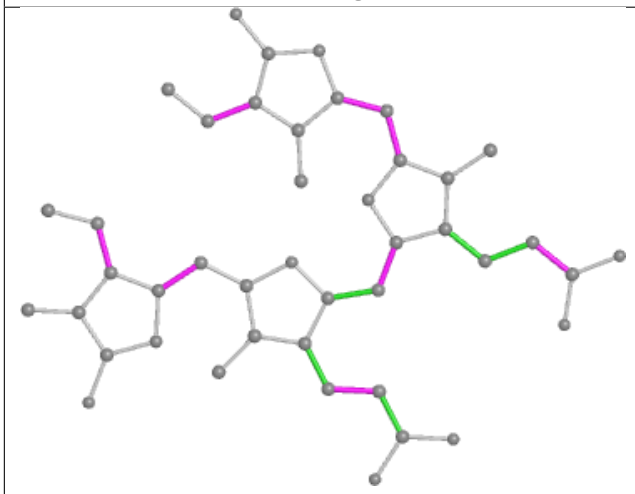

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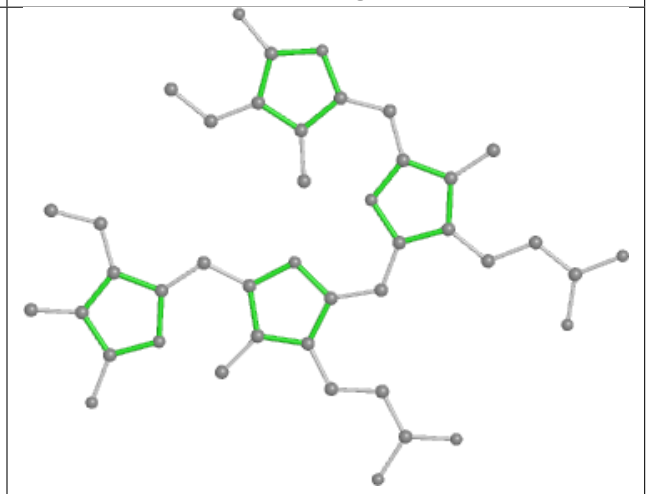
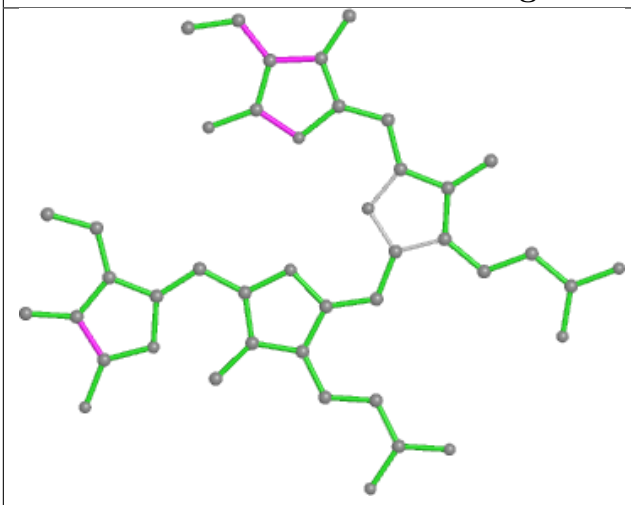


Rings

Ligand PEB v3 201



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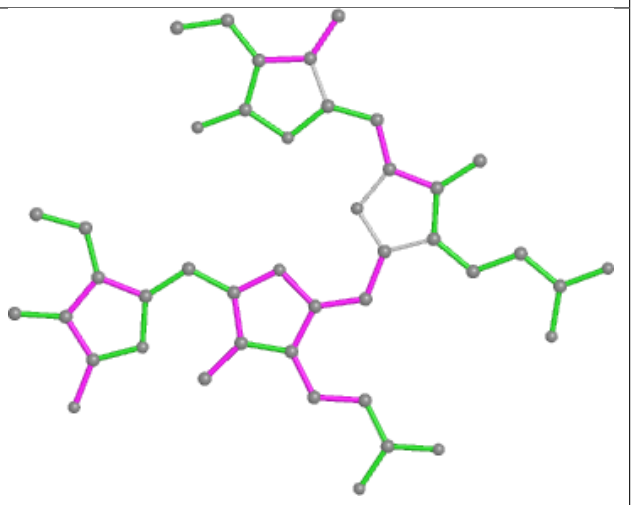

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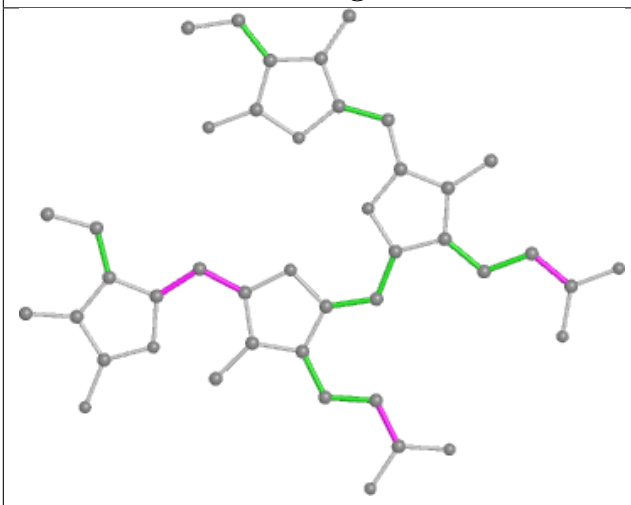

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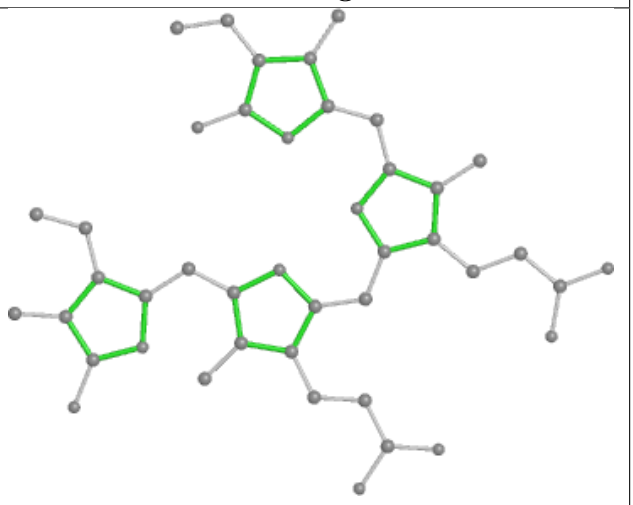

Rings

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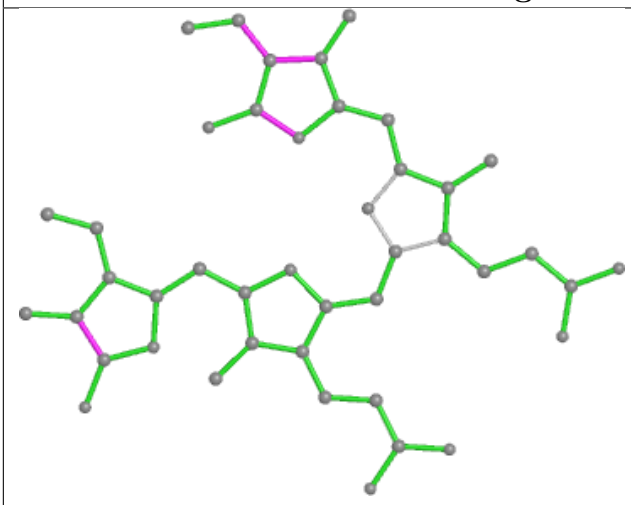

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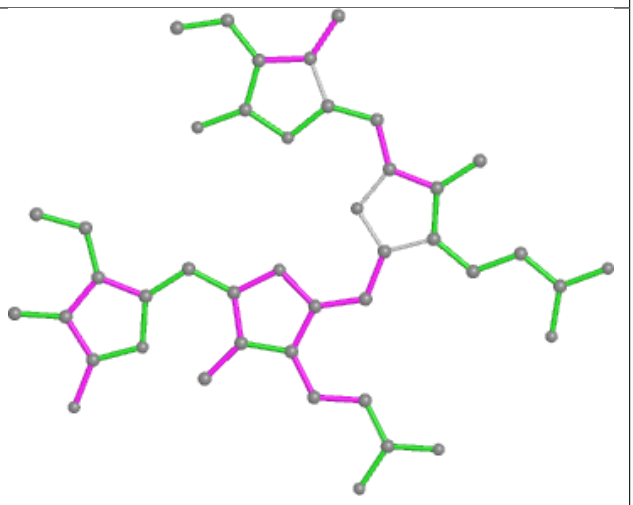

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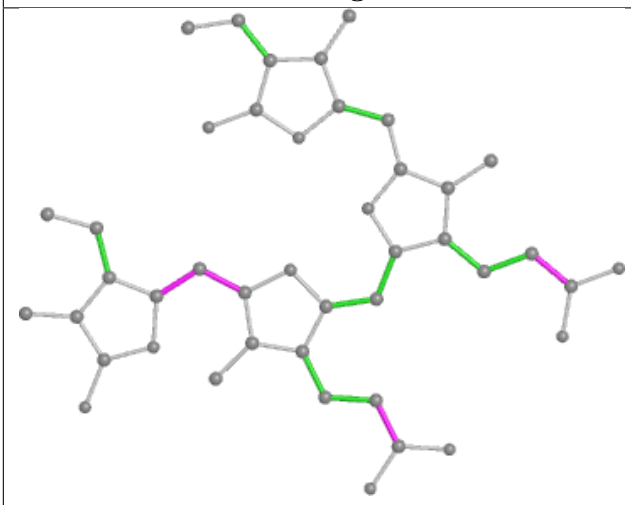

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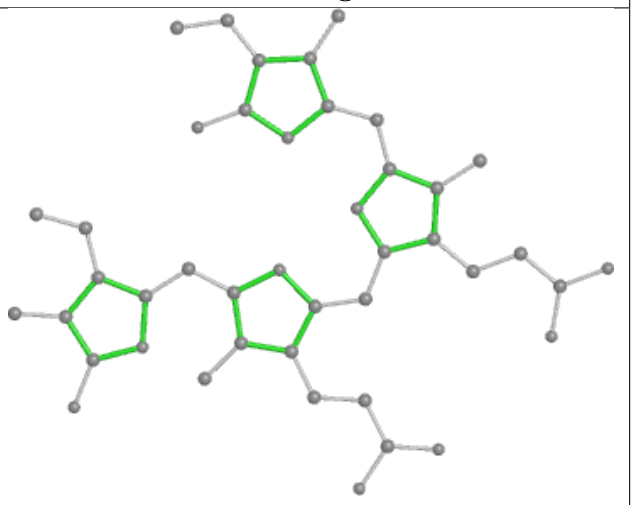
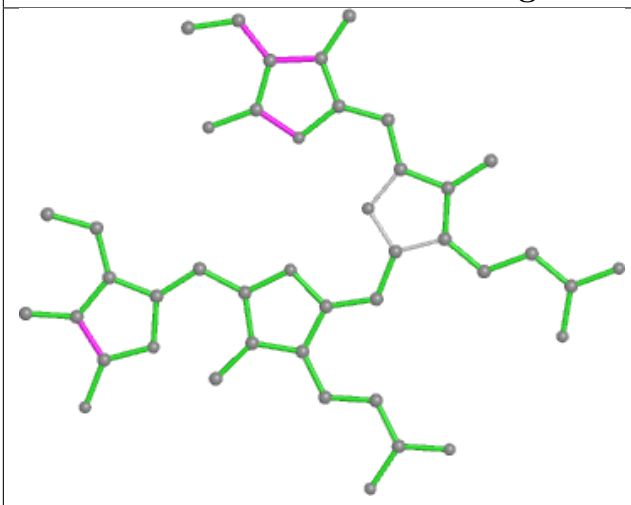


Rings

Ligand PEB gu 201



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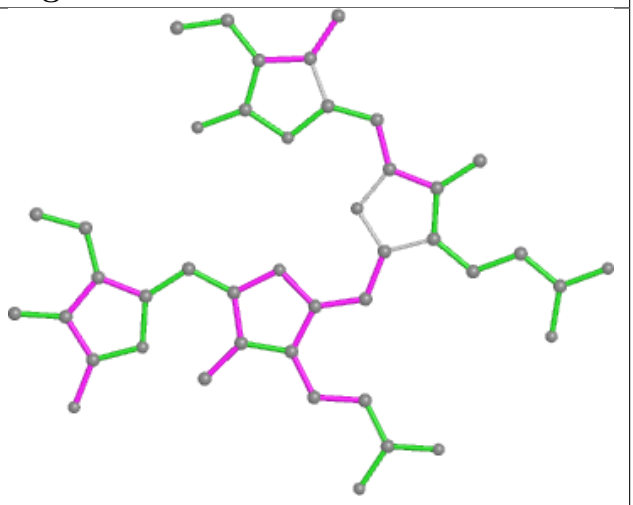

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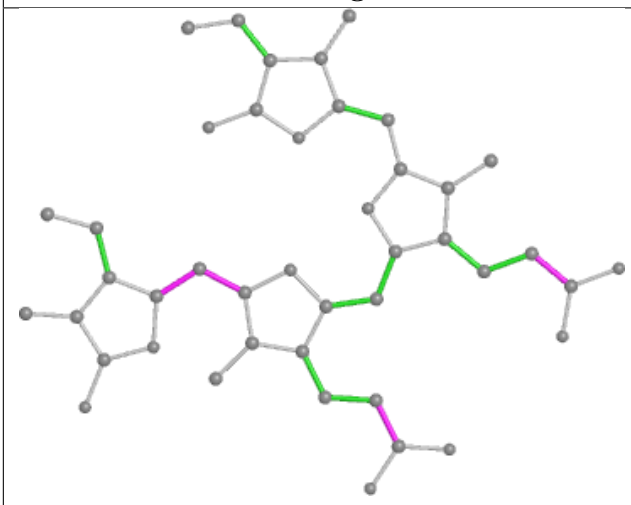

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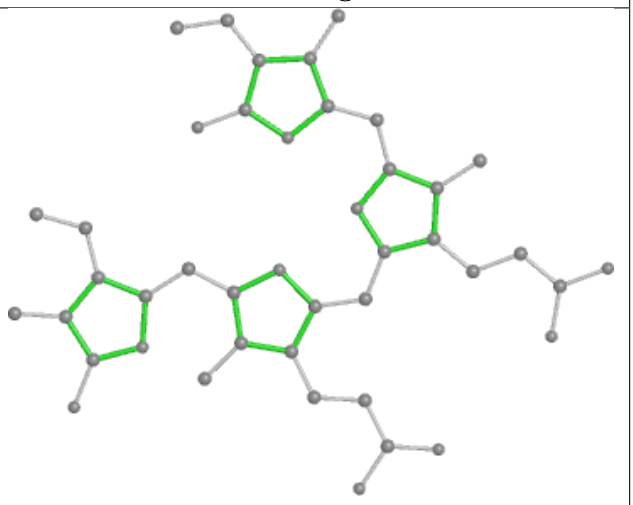
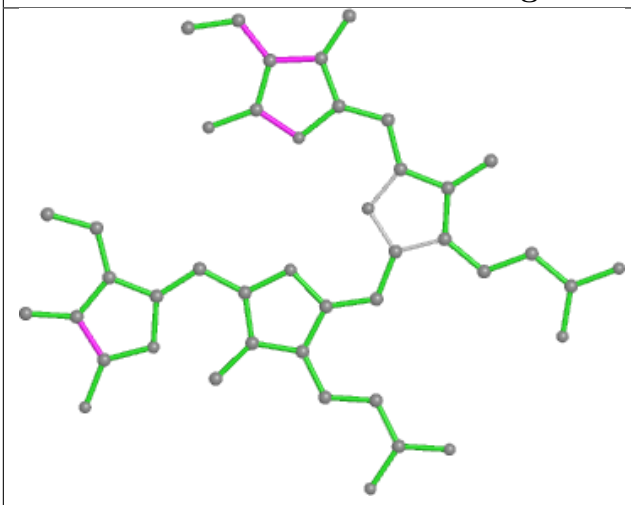


Rings

Ligand PEB z6 201



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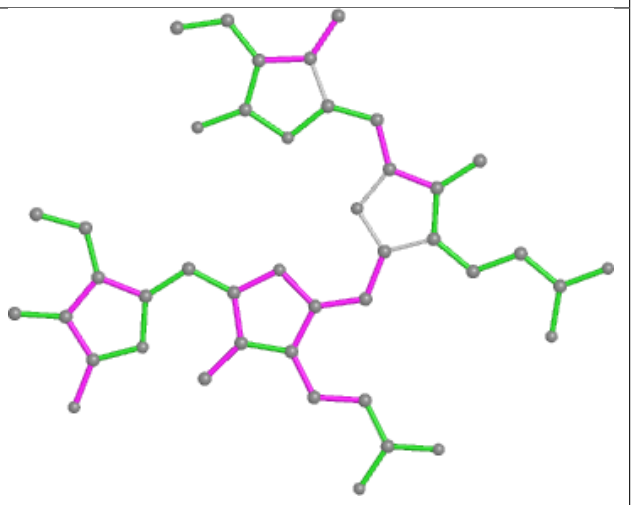

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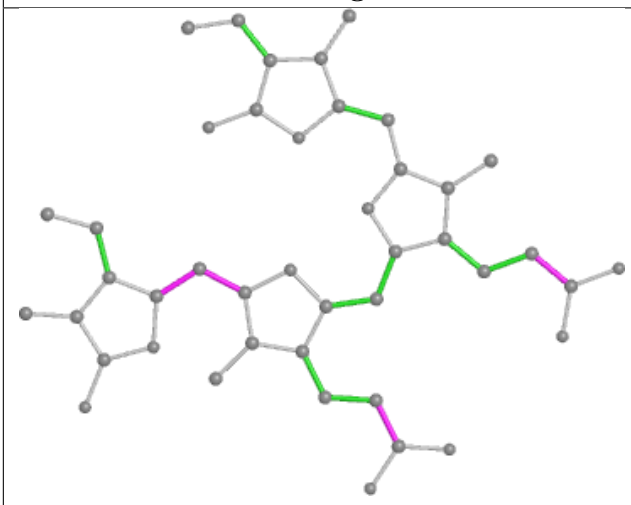

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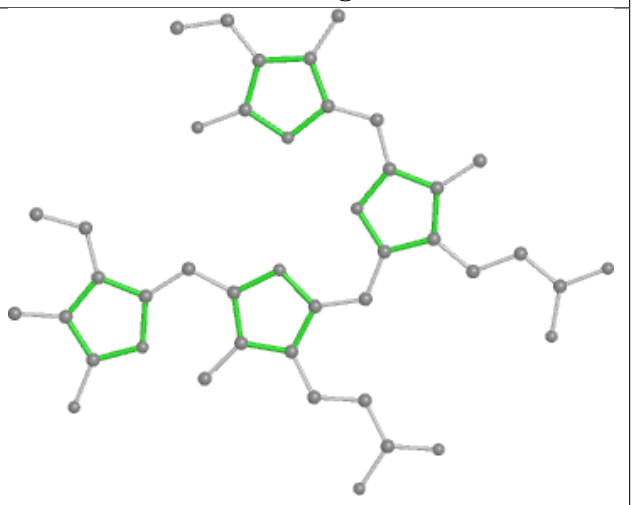

Rings

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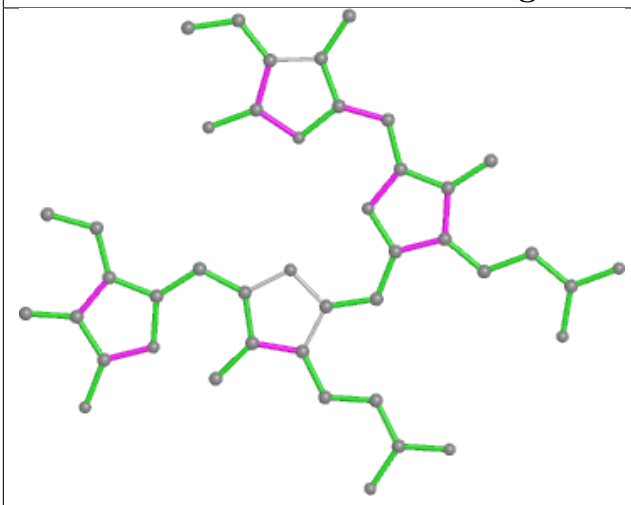

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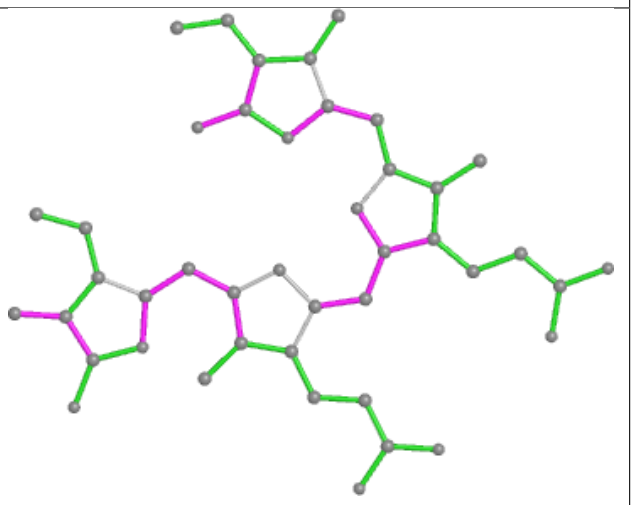

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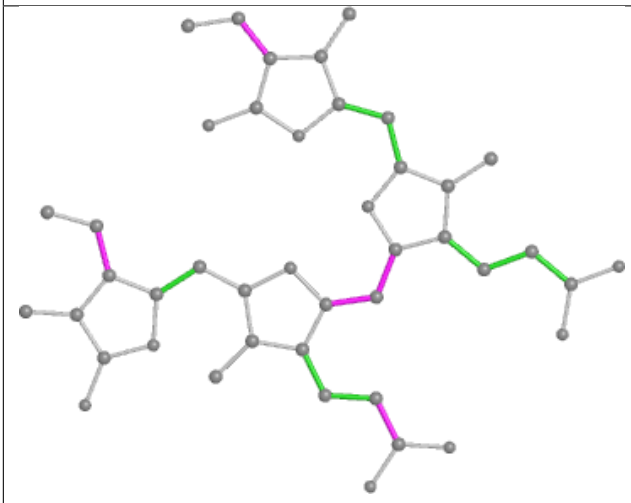

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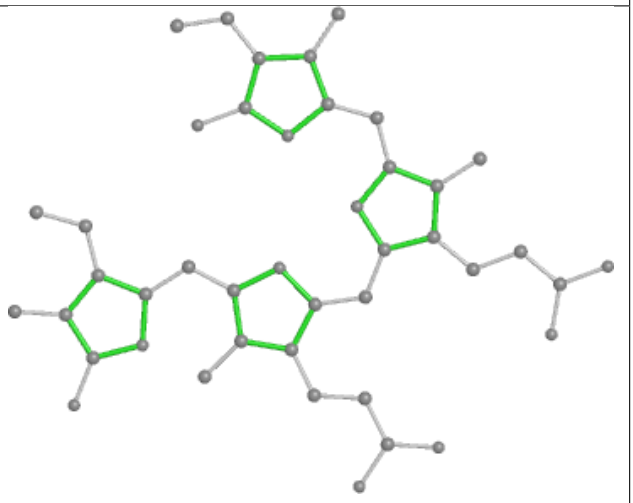

Rings

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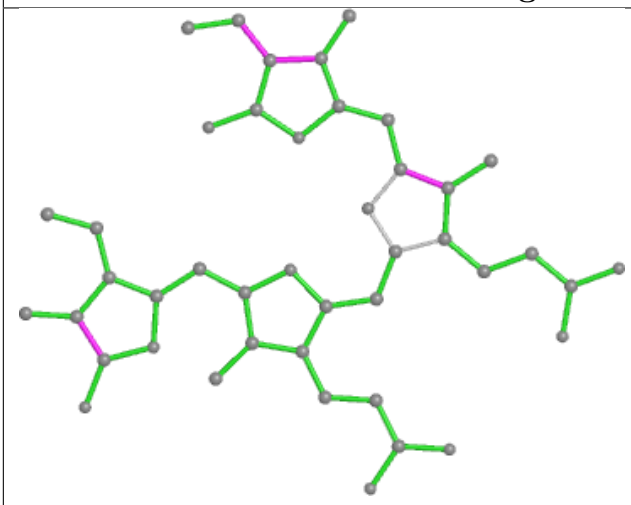

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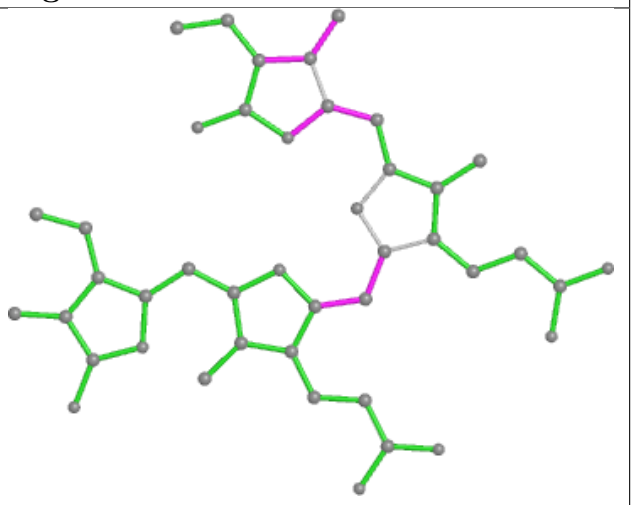

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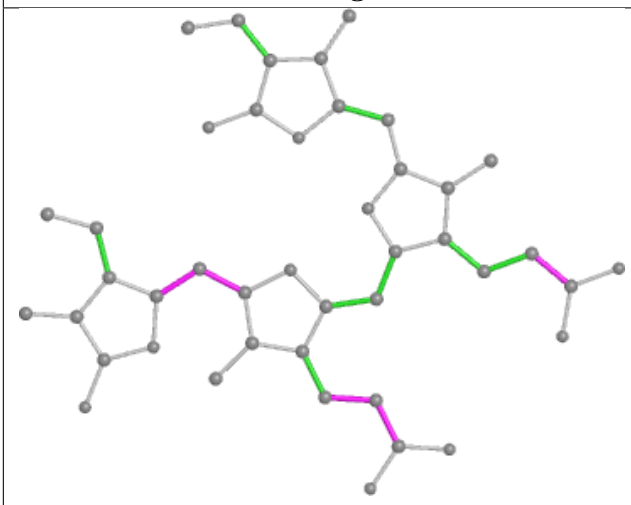

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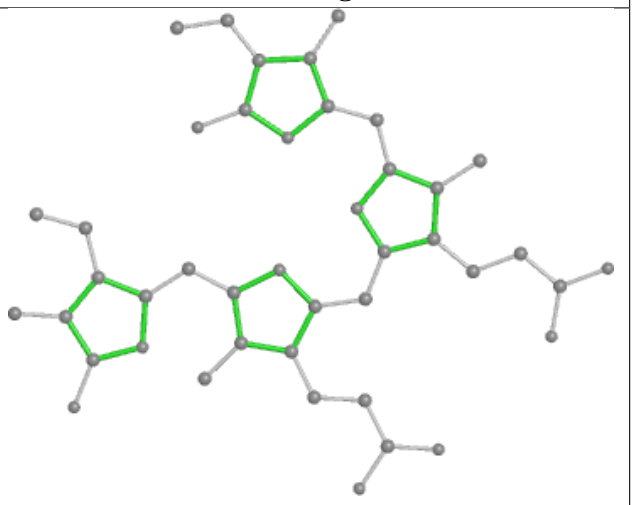

Rings

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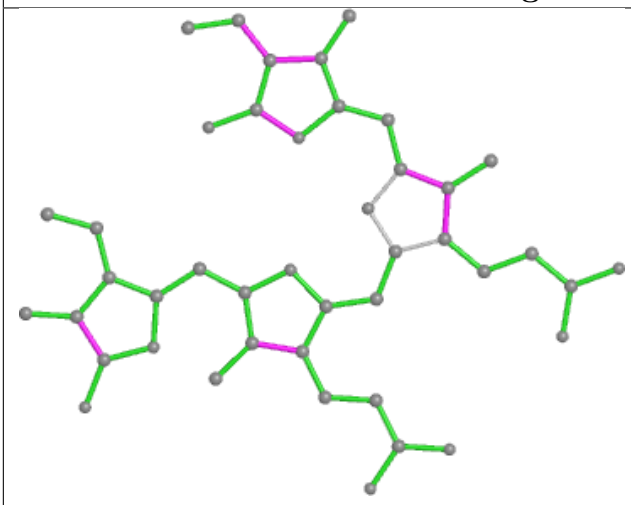

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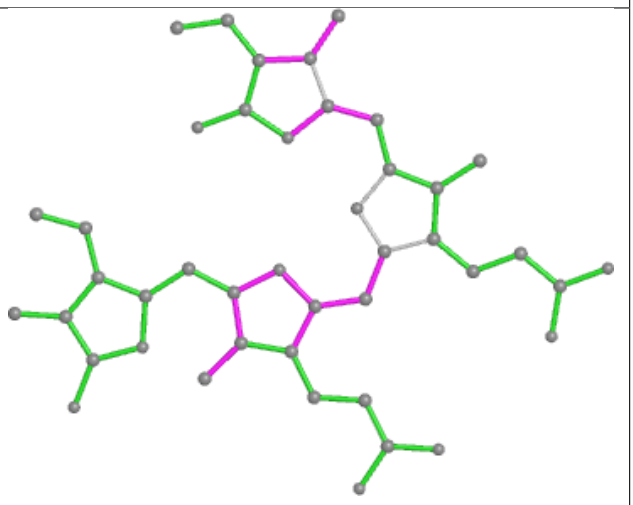

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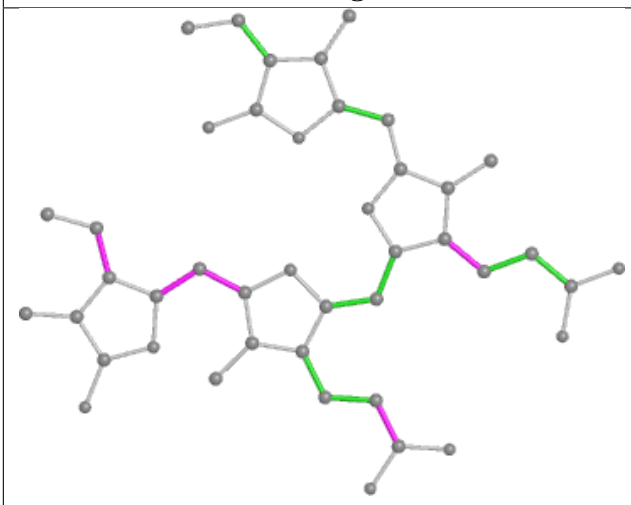

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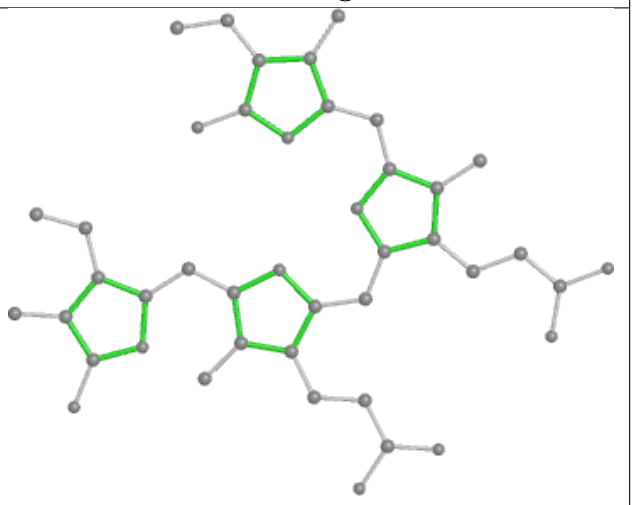
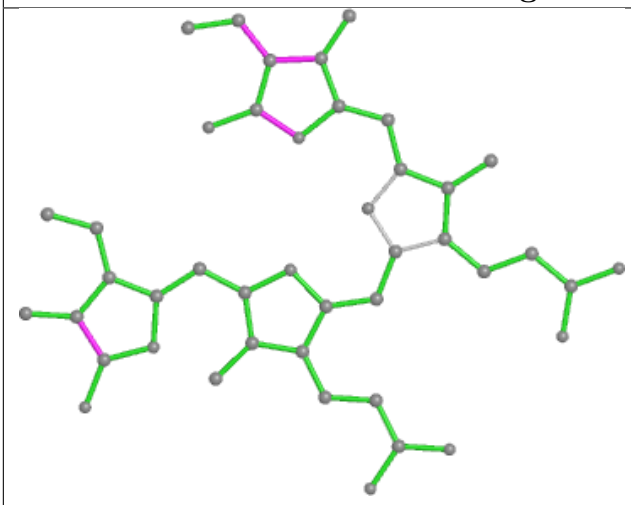


Rings

Ligand PEB o7 201



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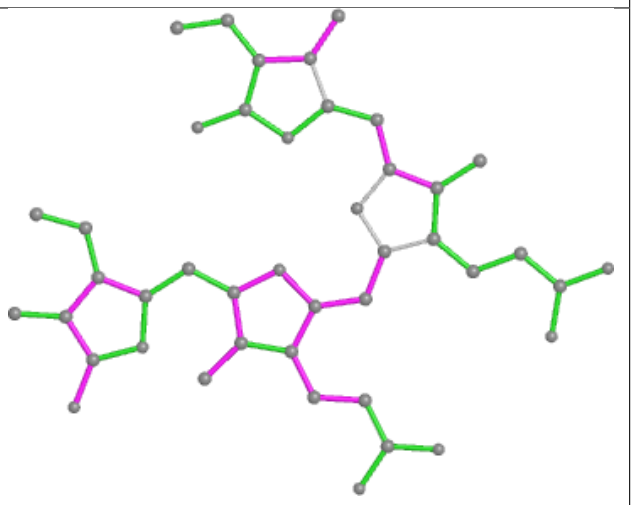

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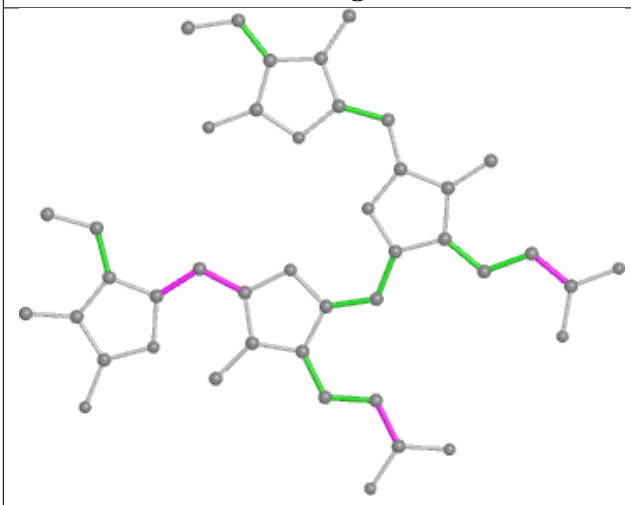

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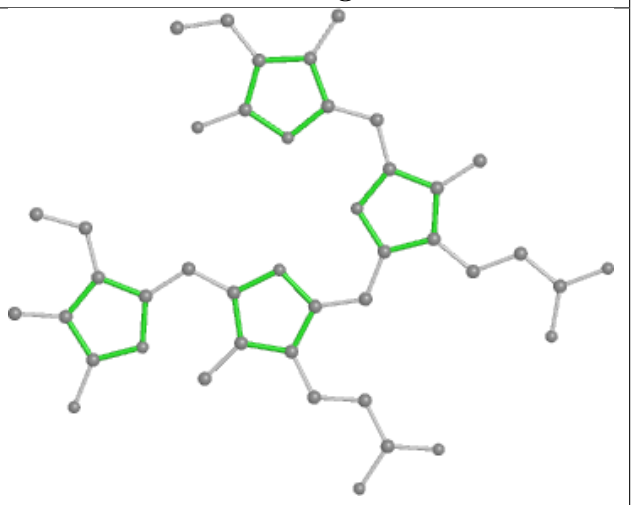
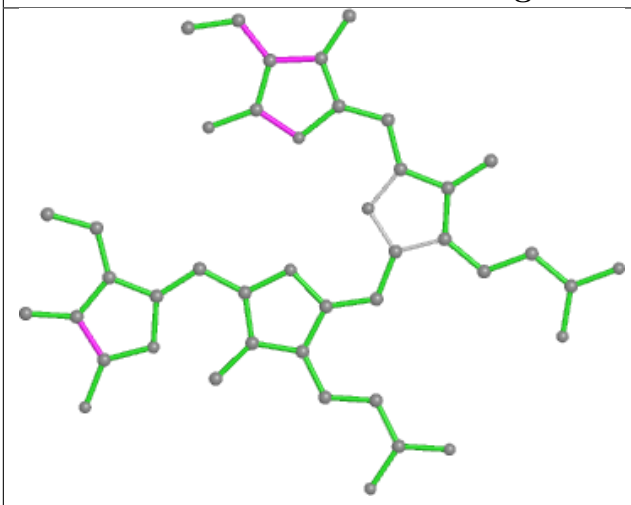


Rings

Ligand PEB dR 202



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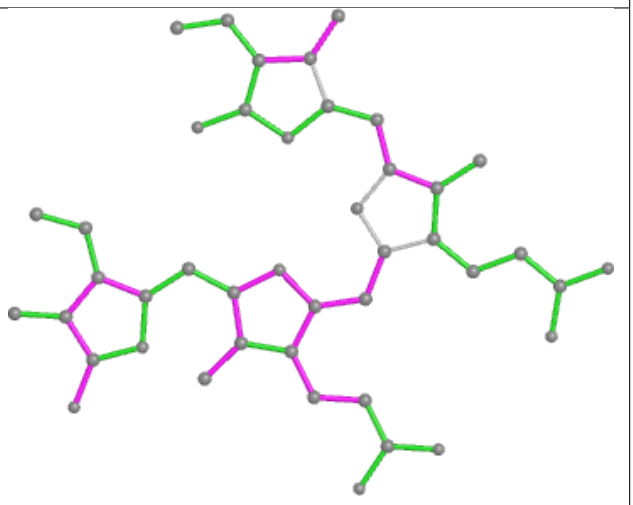

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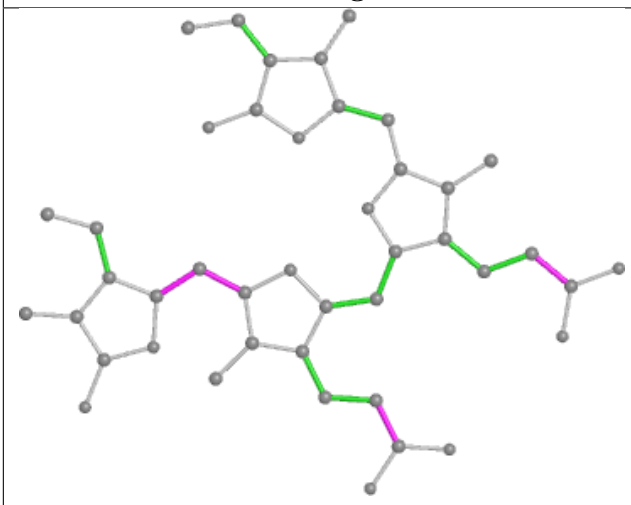

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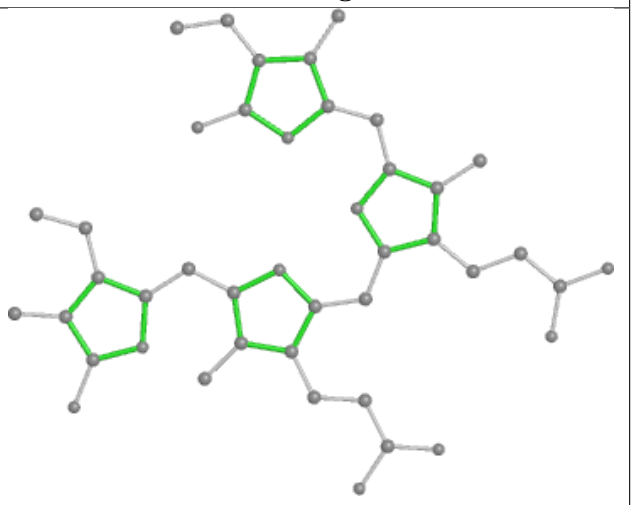
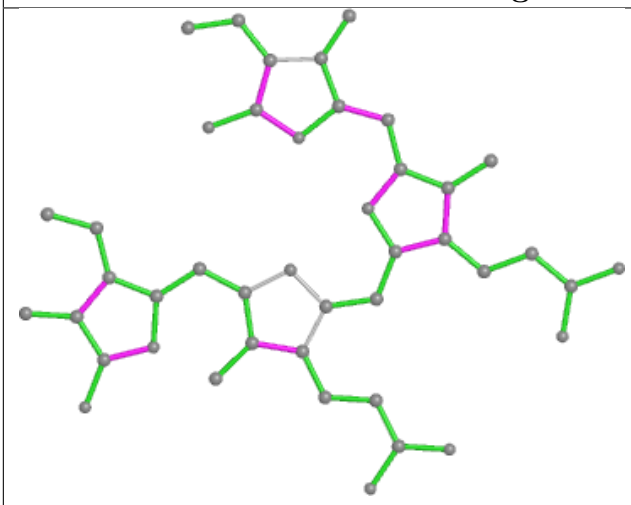


Rings

Ligand PUB hN 203



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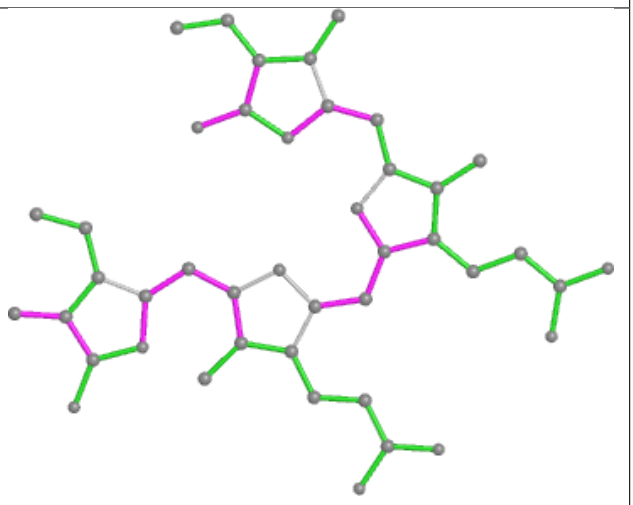

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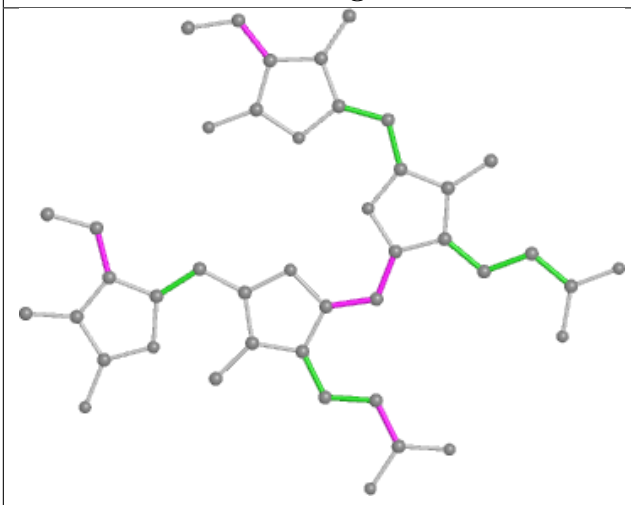

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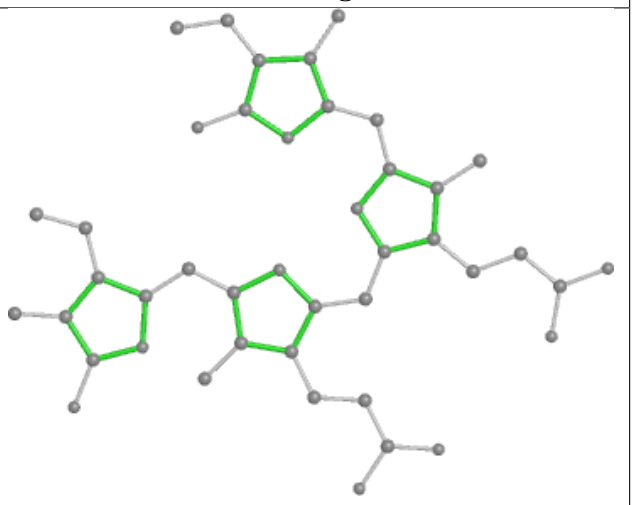
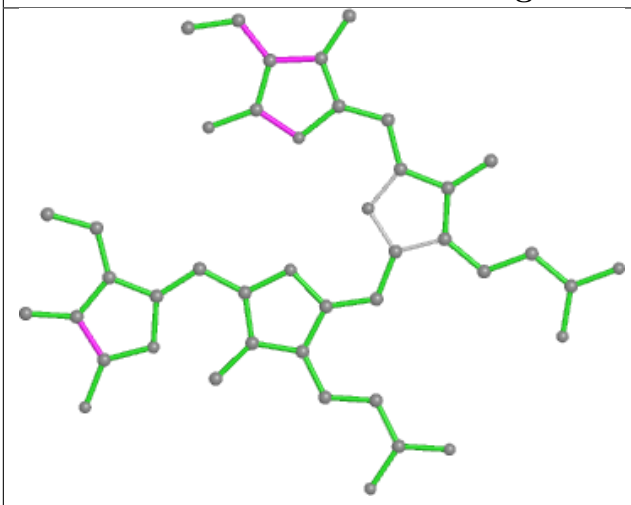


Rings

Ligand PEB A9 201



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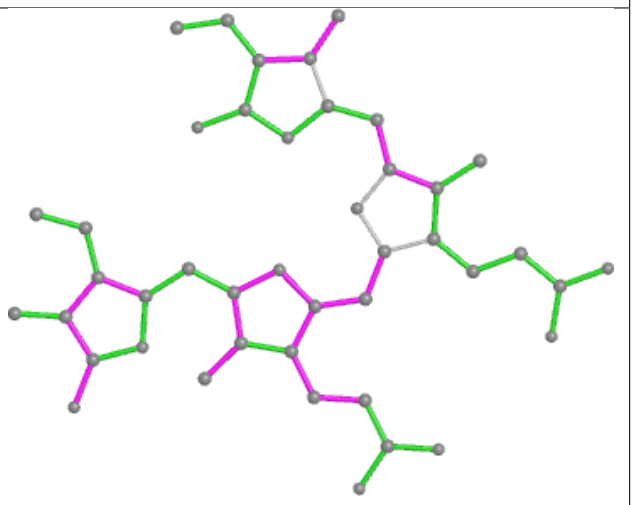
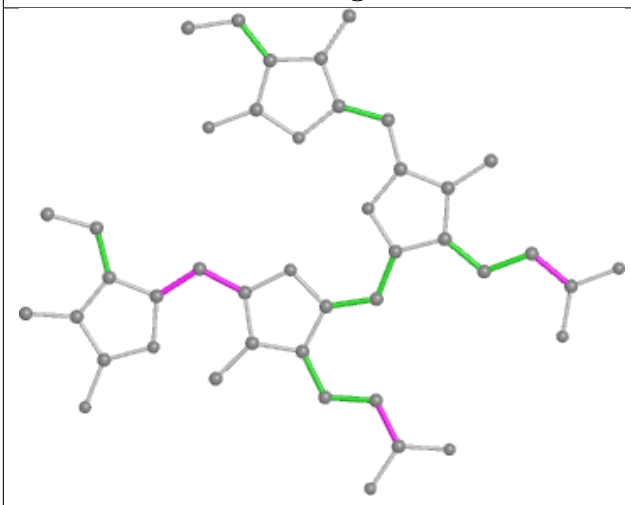
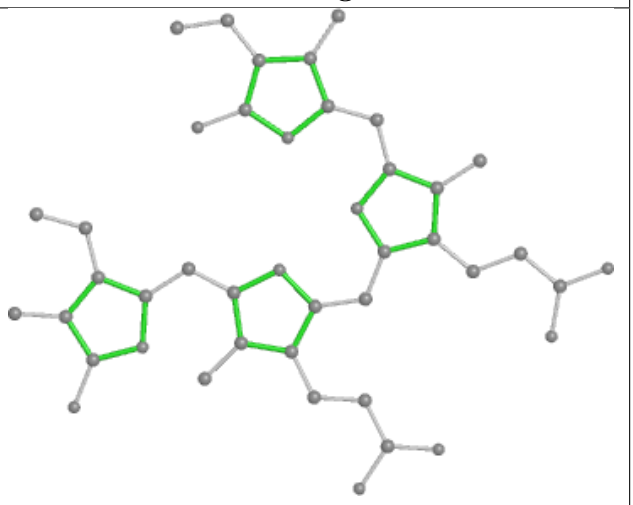


Bond angles

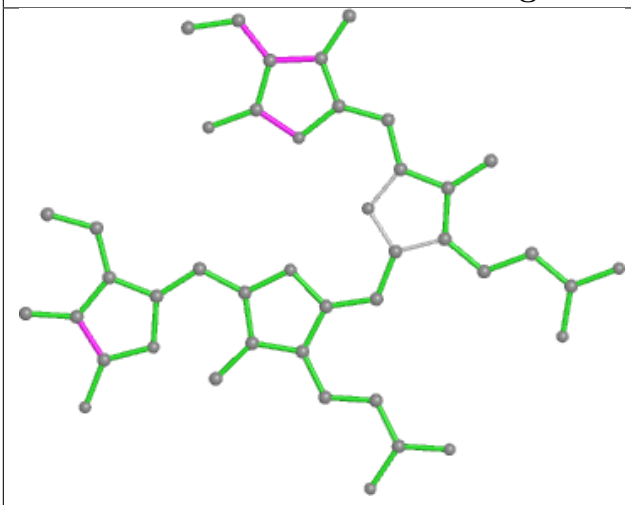


Torsions



Rings

Ligand PEB q2 201



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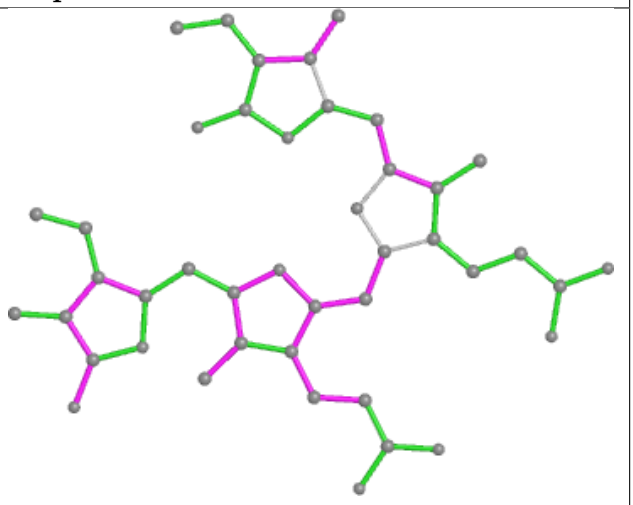

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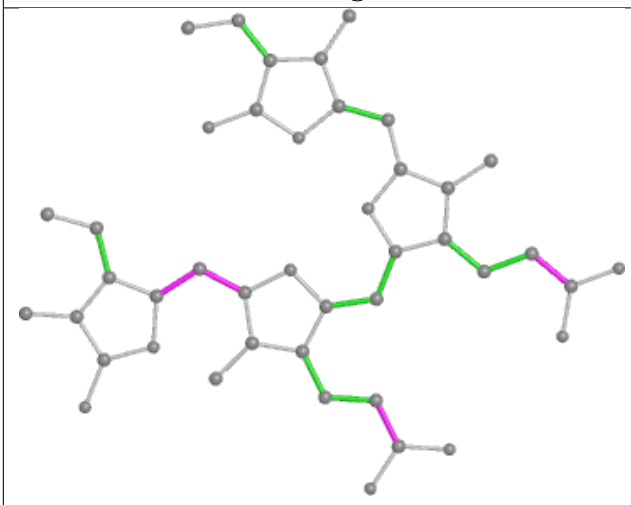

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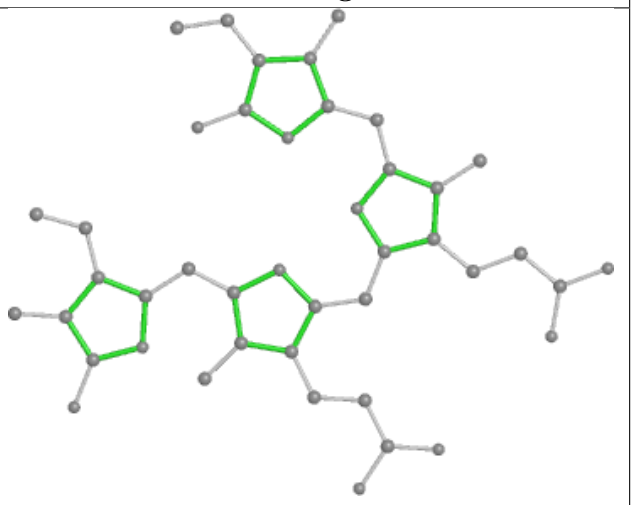
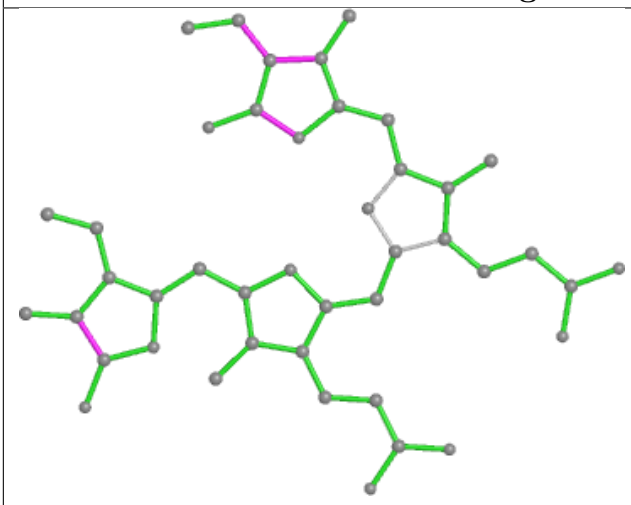


Rings

Ligand PEB k8 201



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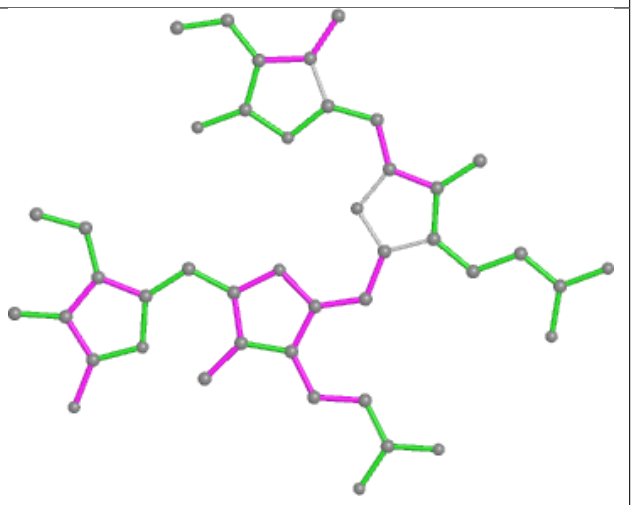

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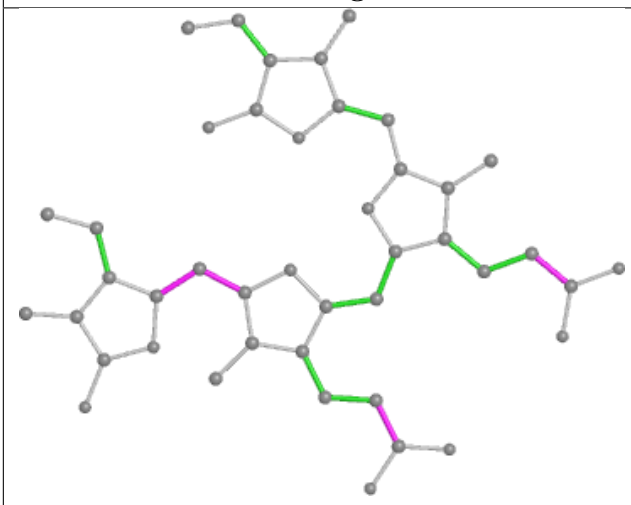

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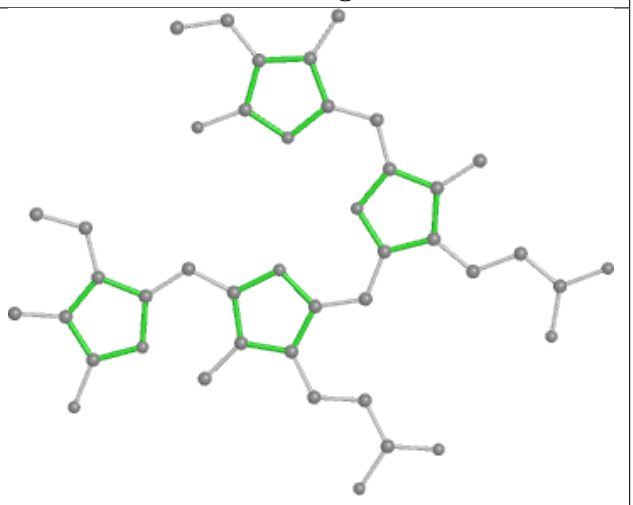
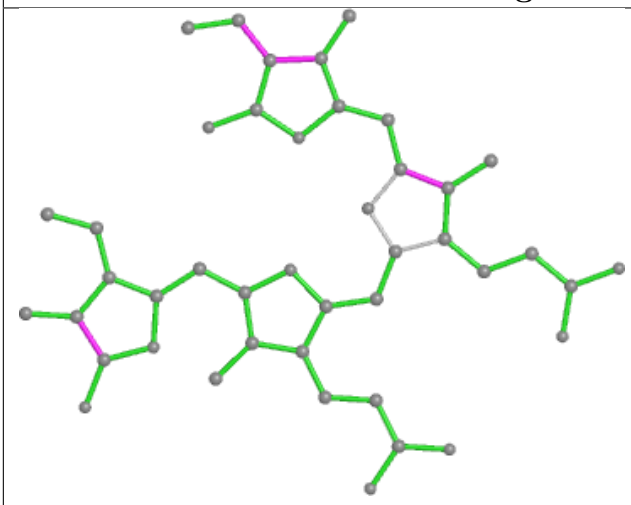


Rings

Ligand PEB Y9 301



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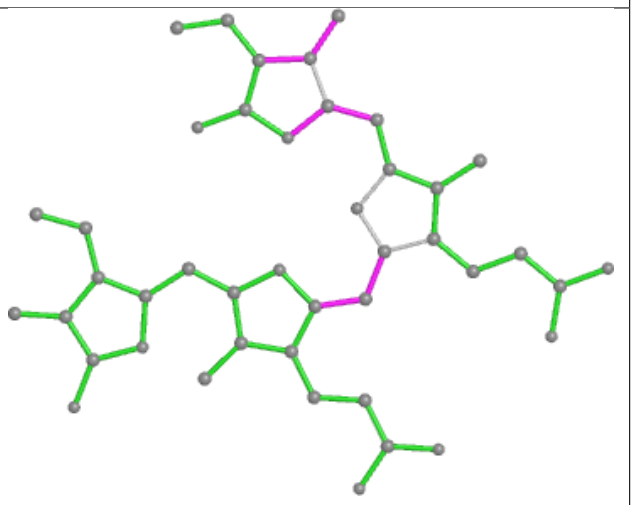

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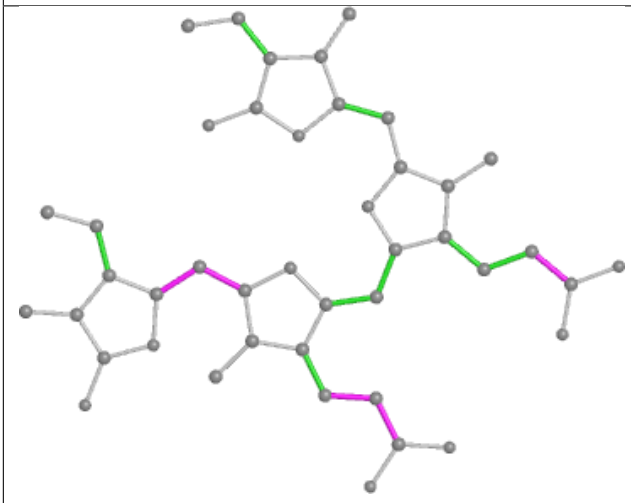

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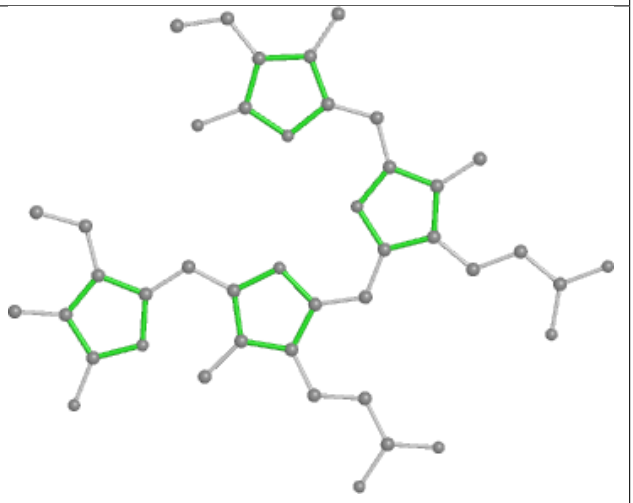
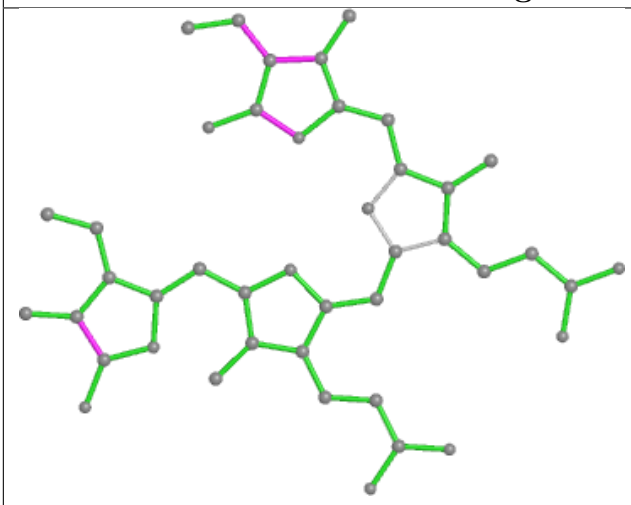


Rings

Ligand PEB G4 202



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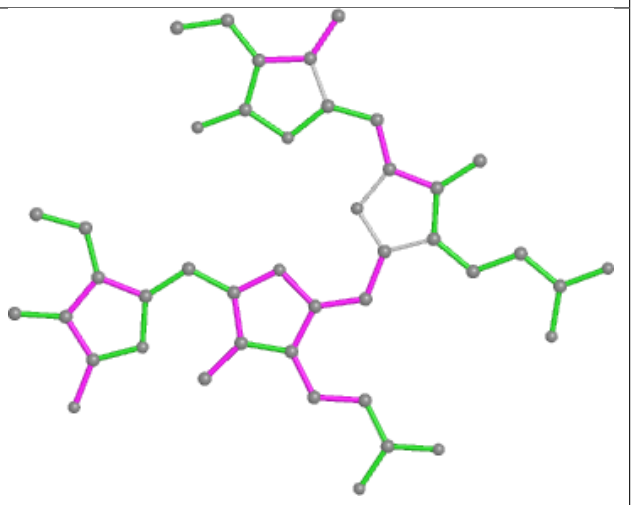

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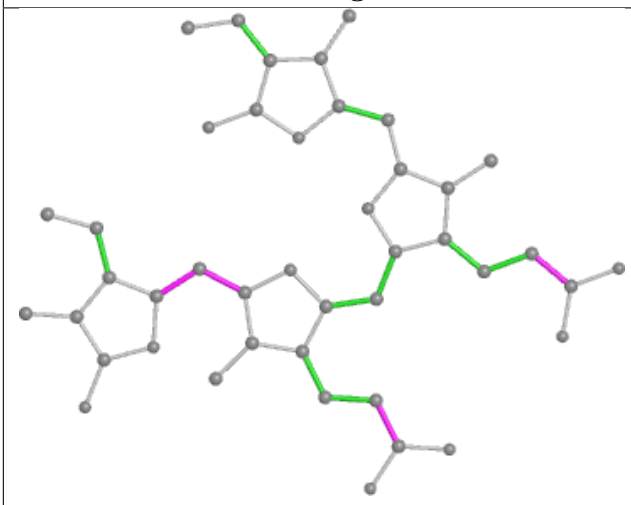

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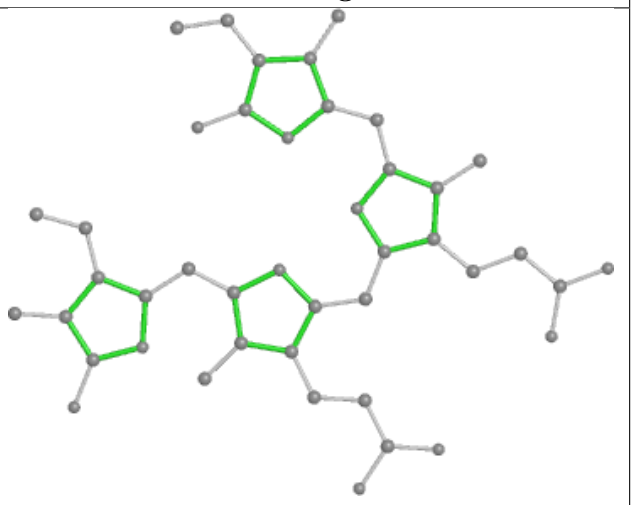
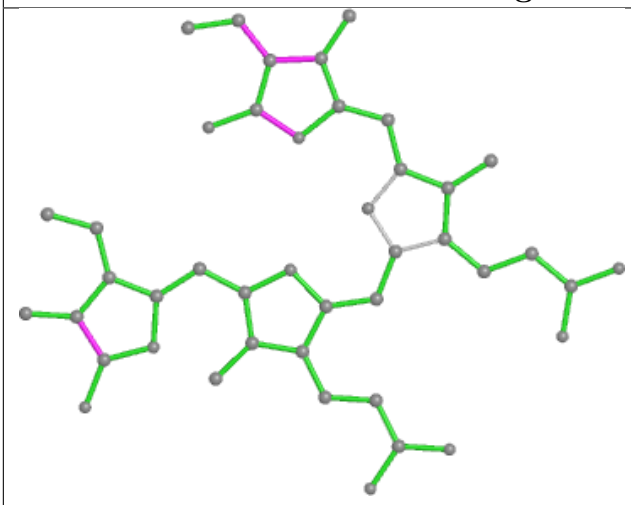


Rings

Ligand PEB D2 302



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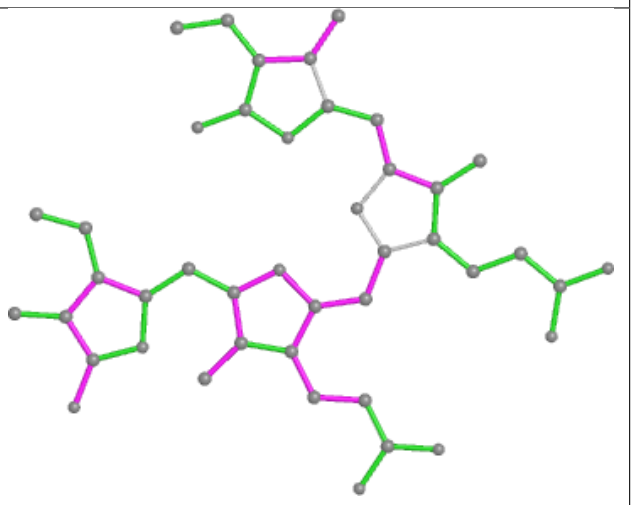

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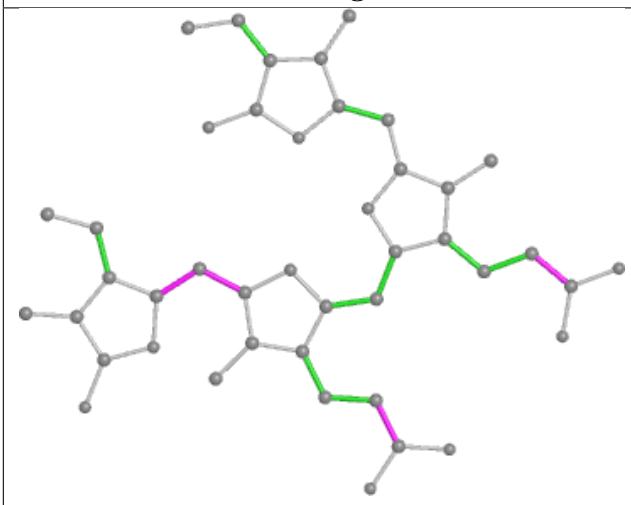

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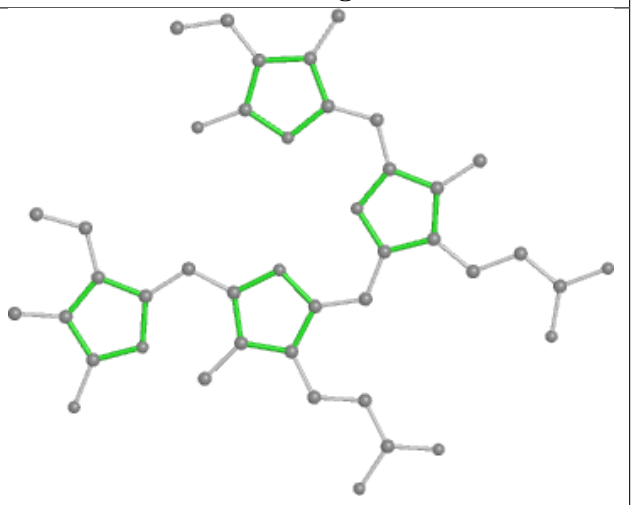

Rings

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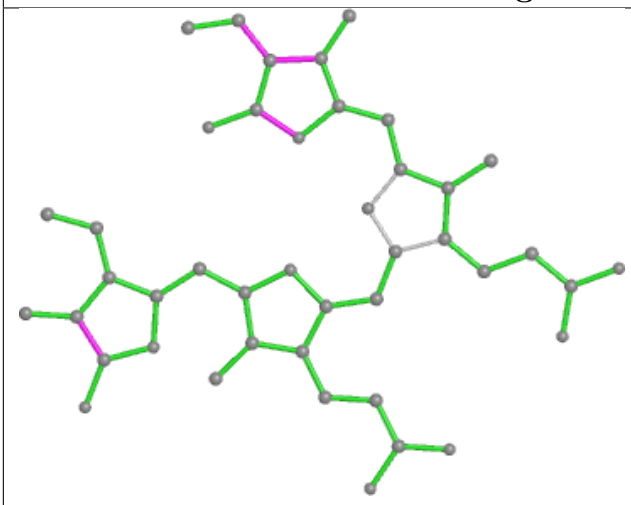

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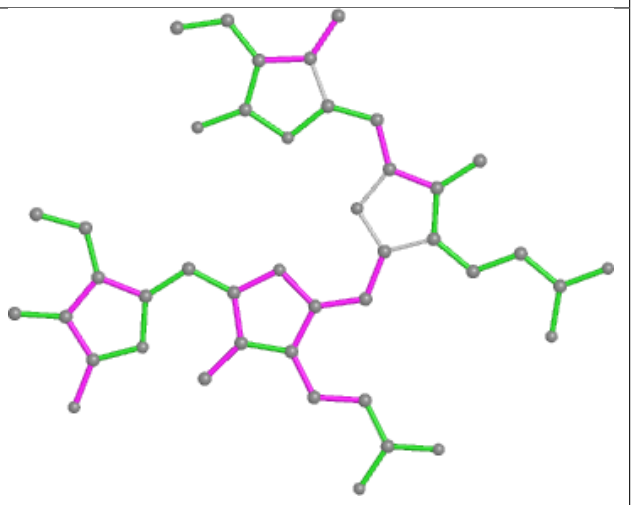

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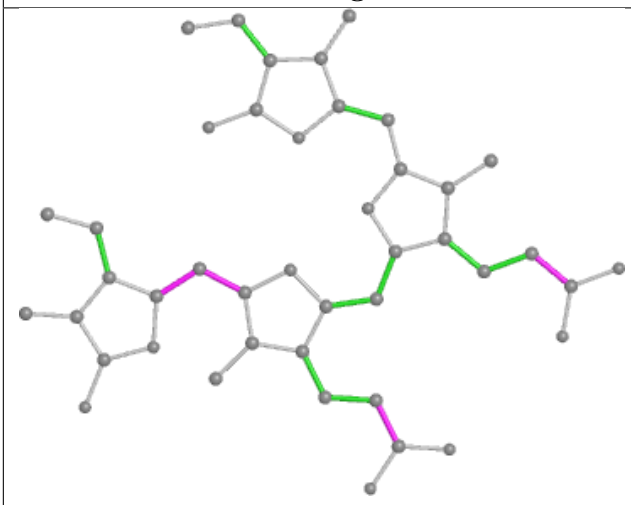

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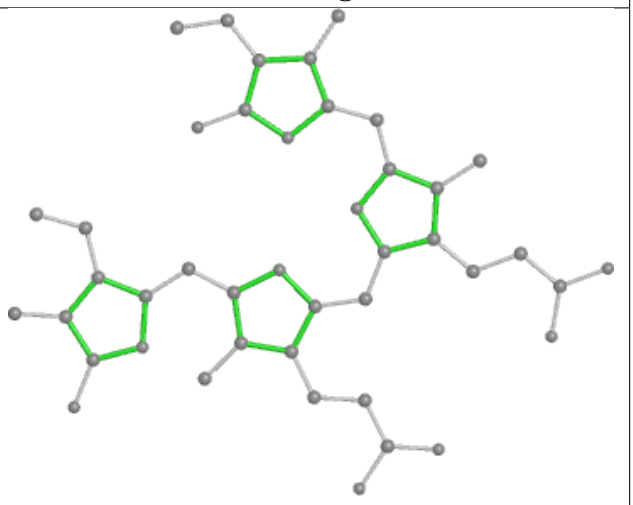

Rings

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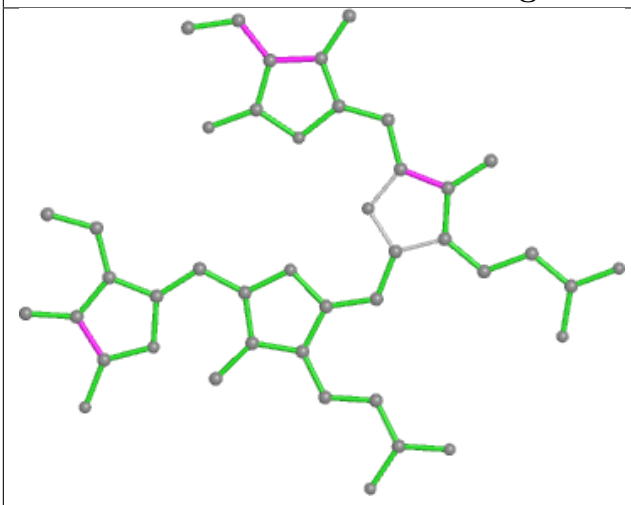

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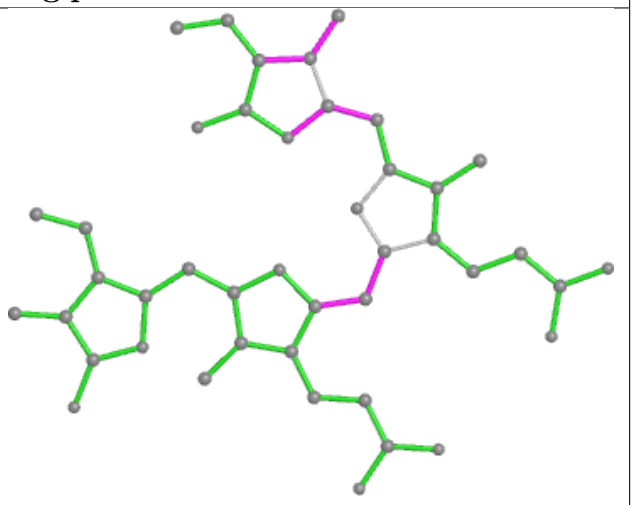

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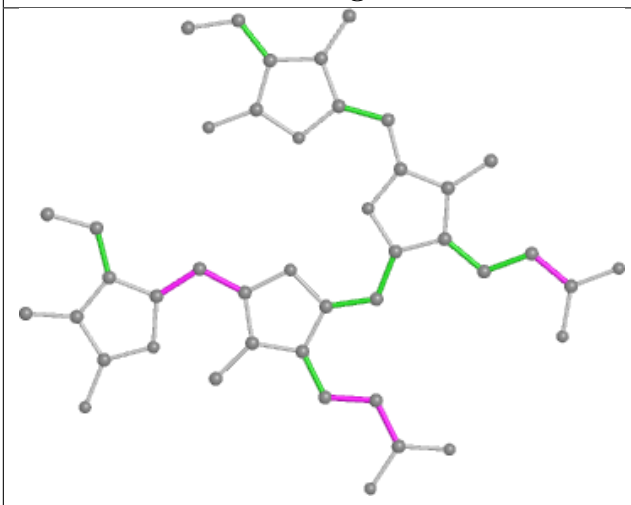

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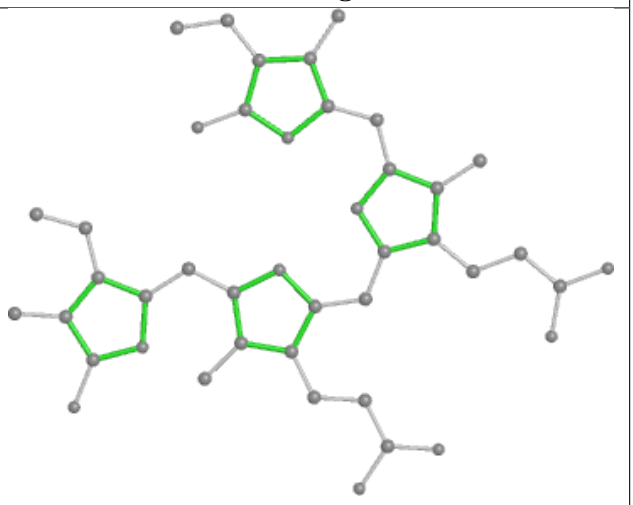
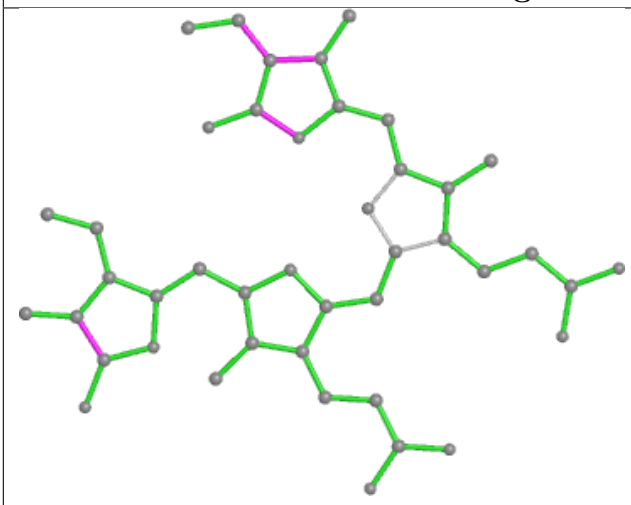


Rings

Ligand PEB bN 201



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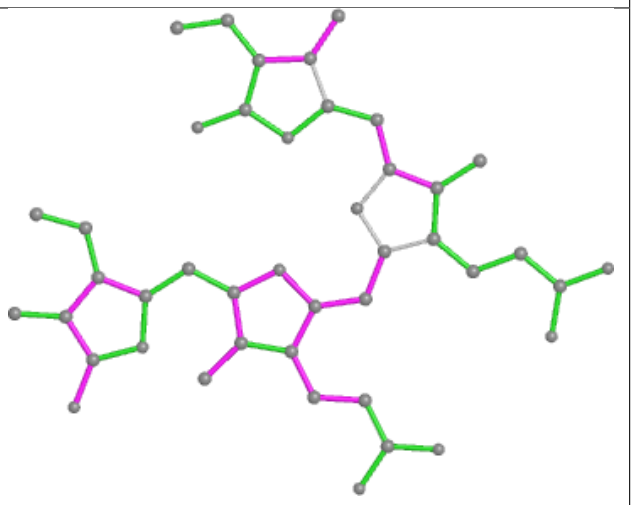
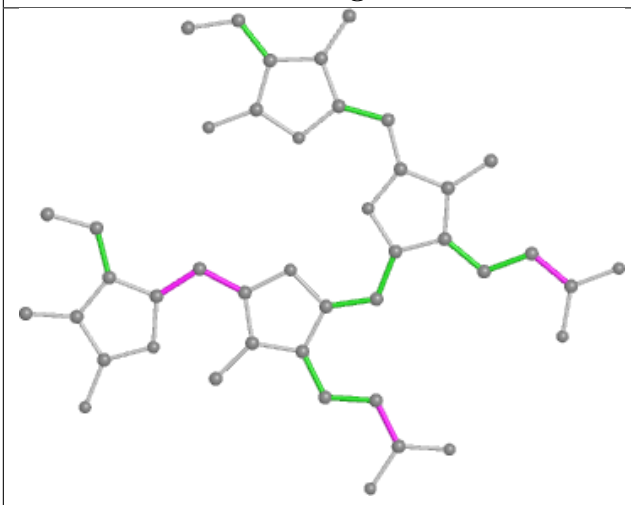


Bond angles



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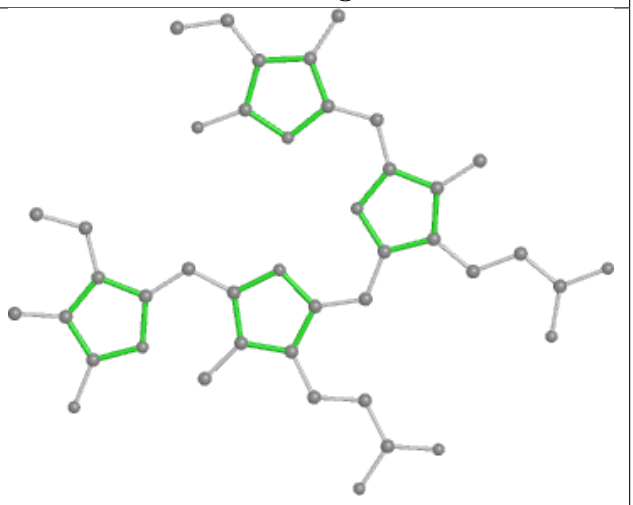
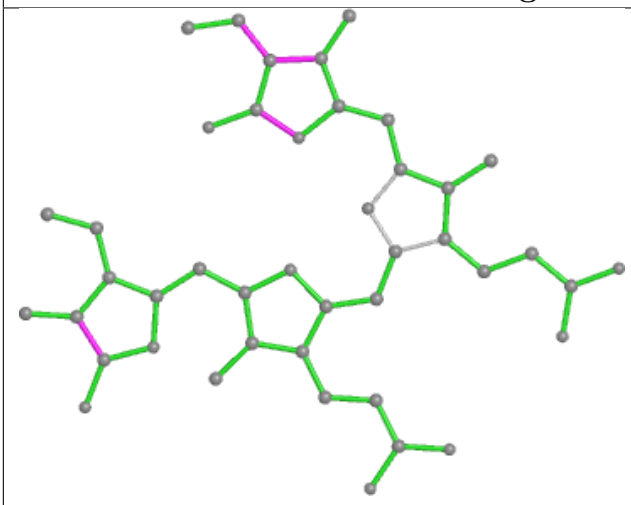


Rings

Ligand PEB q6 201



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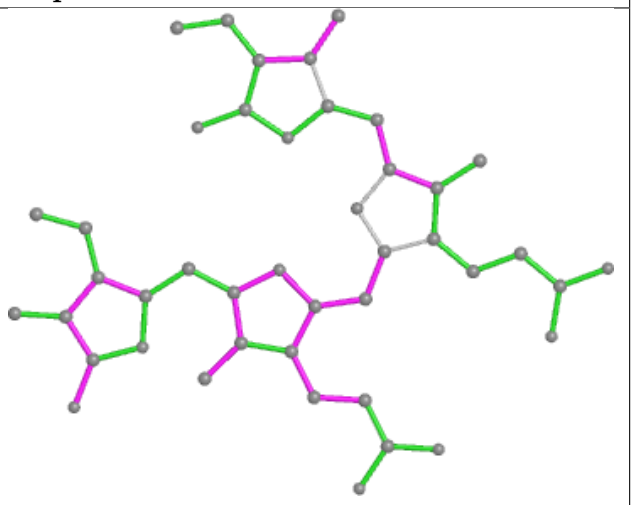

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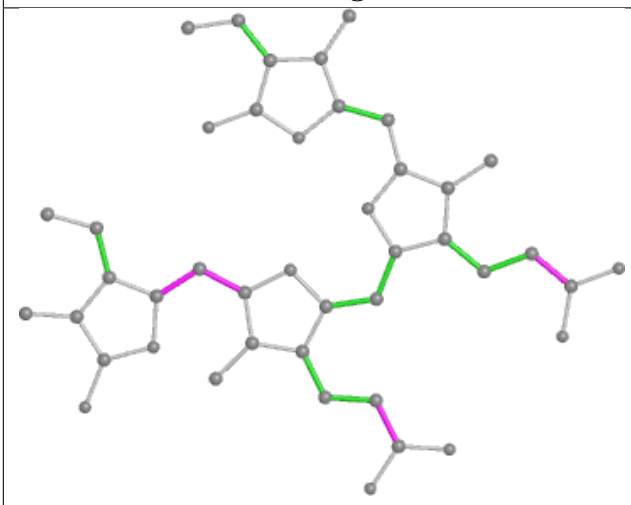

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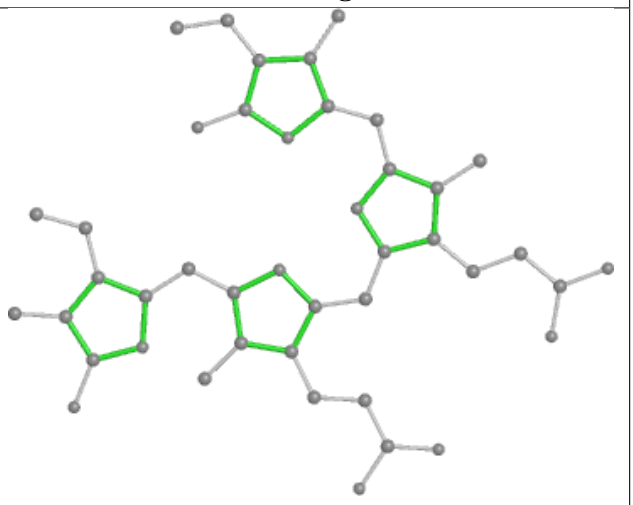
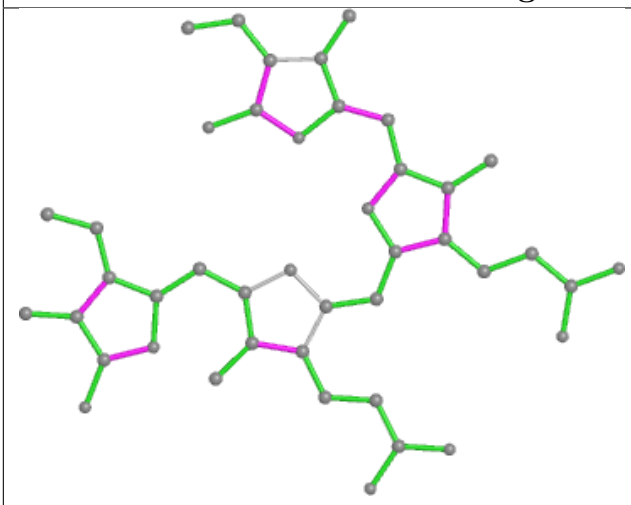


Rings

Ligand PUB a6 203



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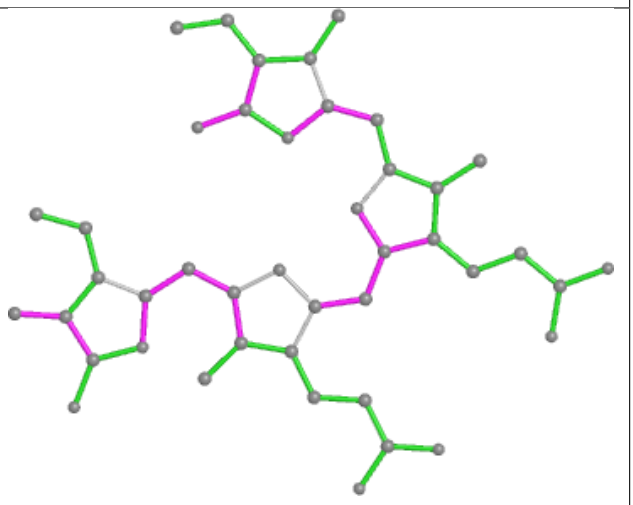

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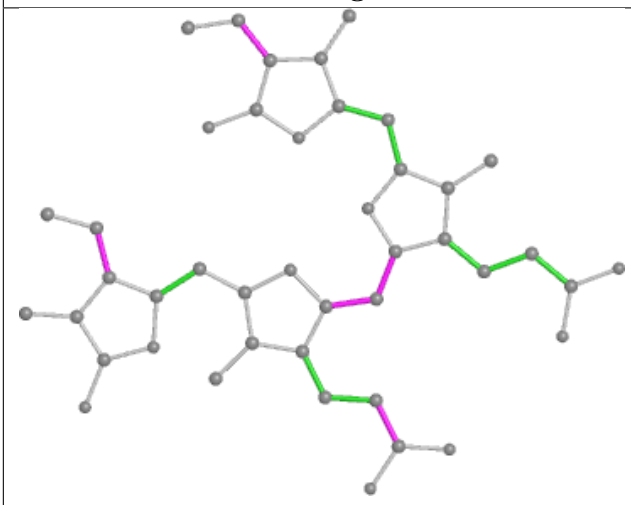

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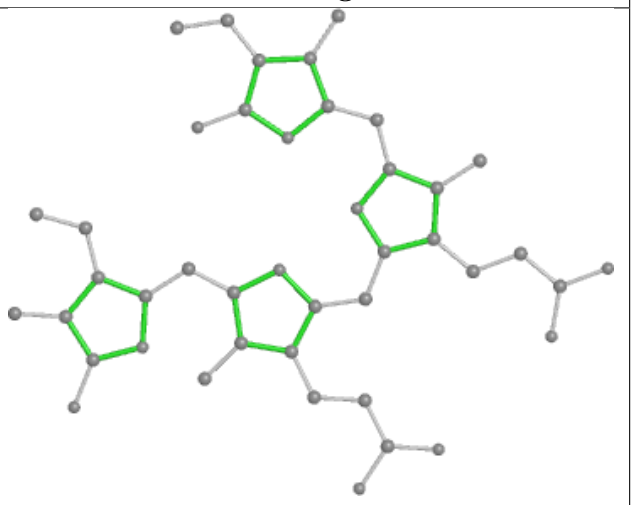
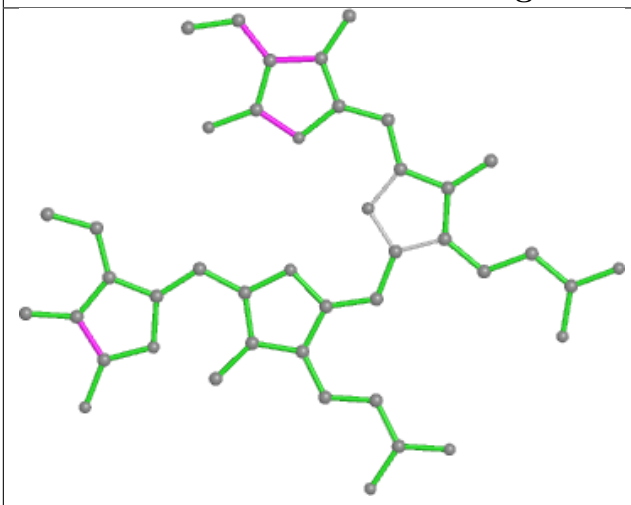


Rings

Ligand PEB aY 402



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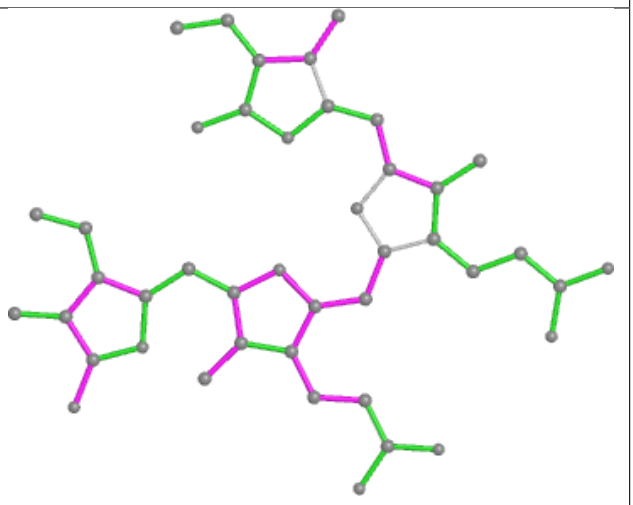

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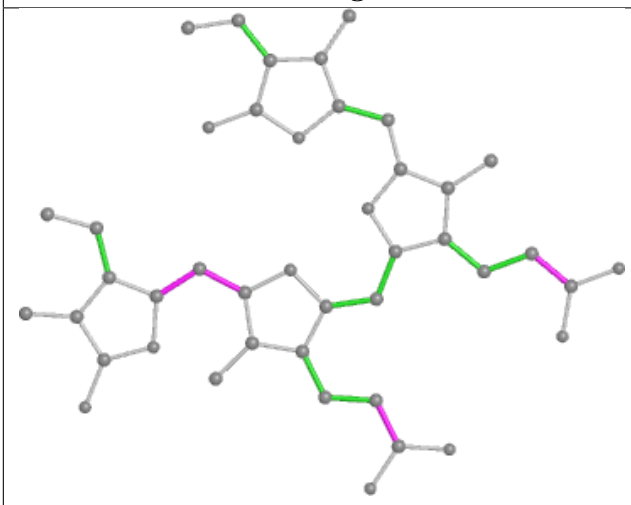

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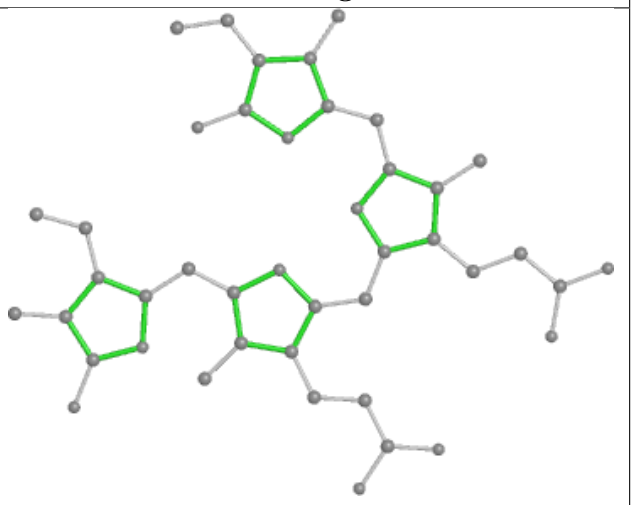
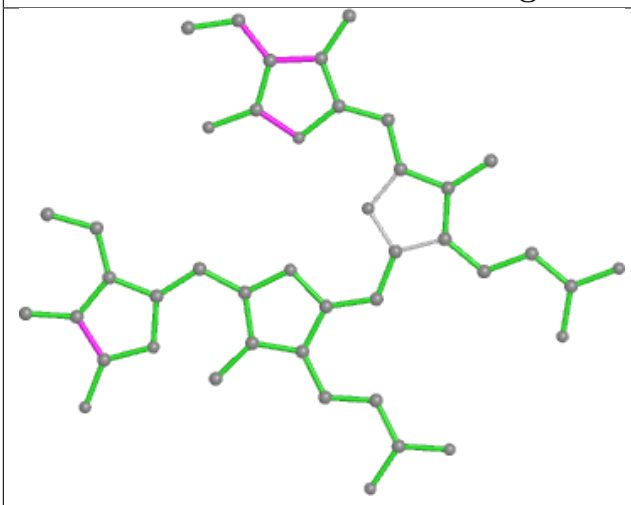


Rings

Ligand PEB x8 202



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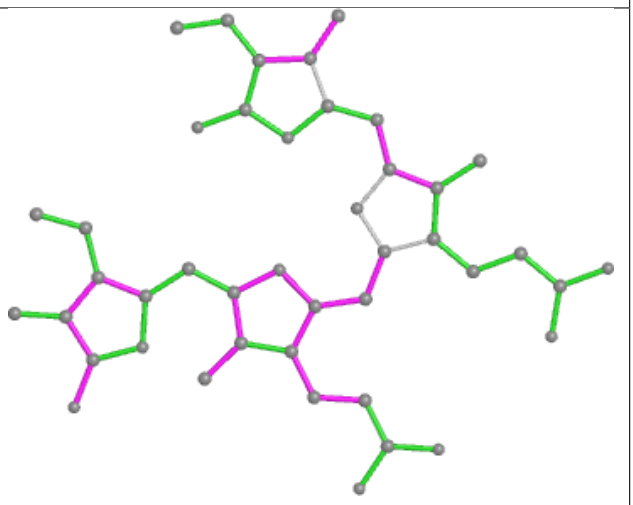

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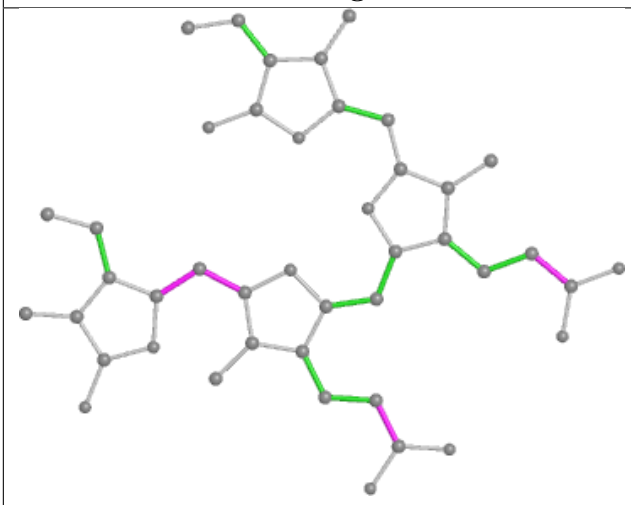

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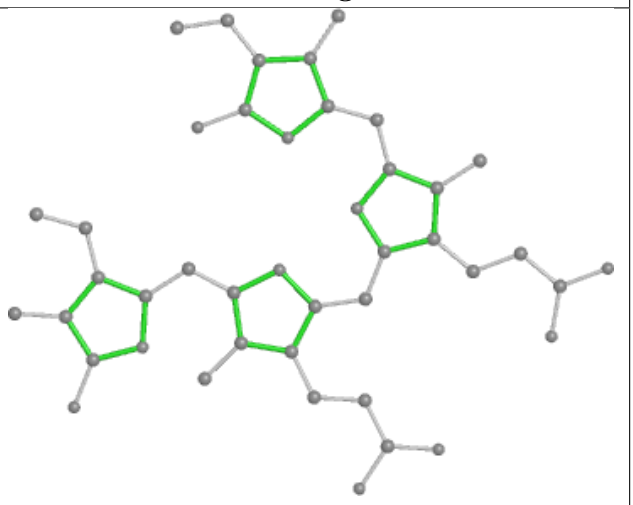
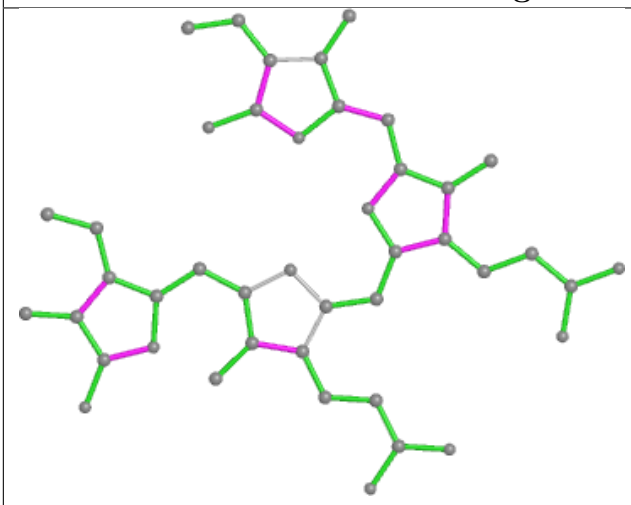


Rings

Ligand PUB Y9 304



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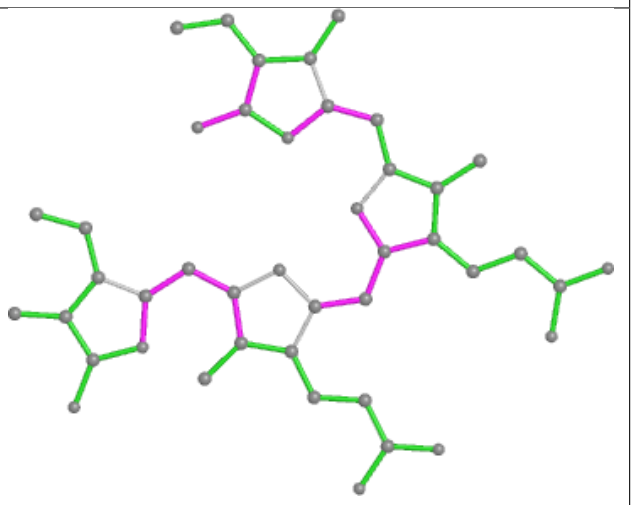
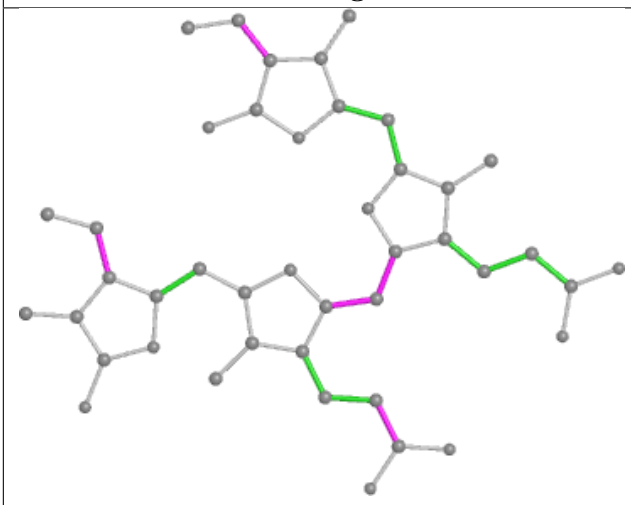
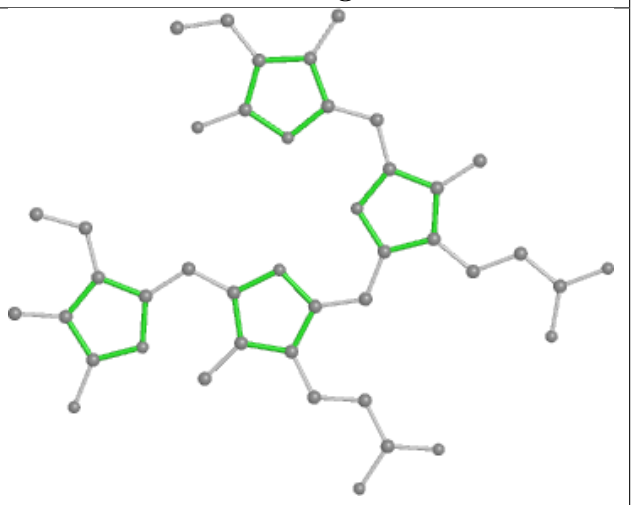


Bond angles

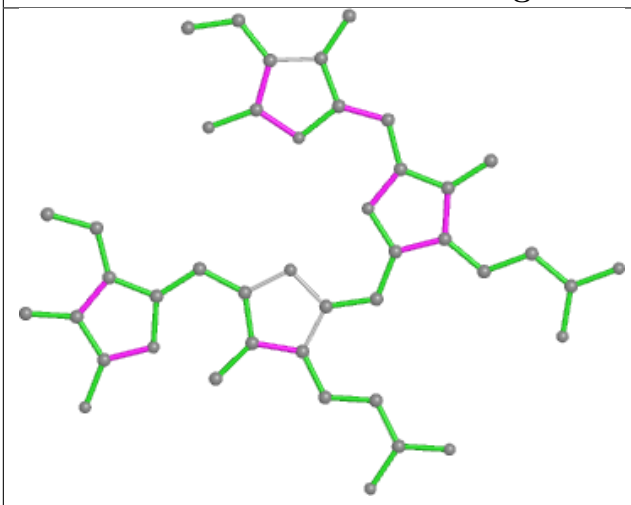


Torsions



Rings

Ligand PUB R4 203



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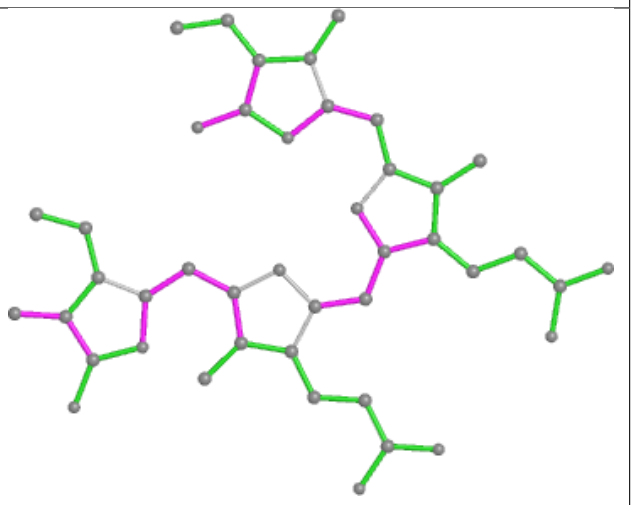

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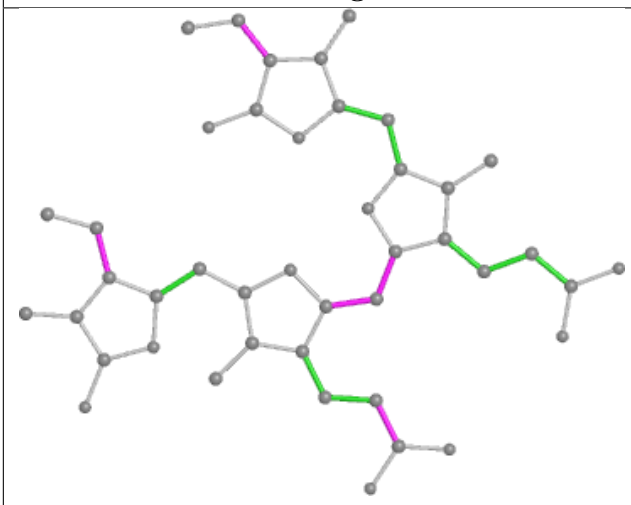

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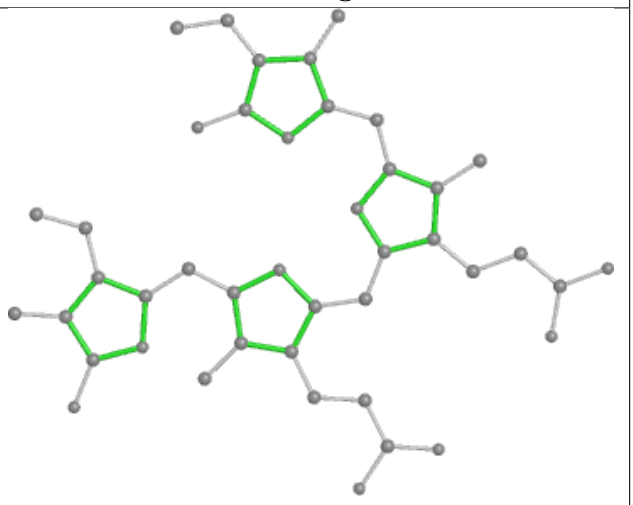
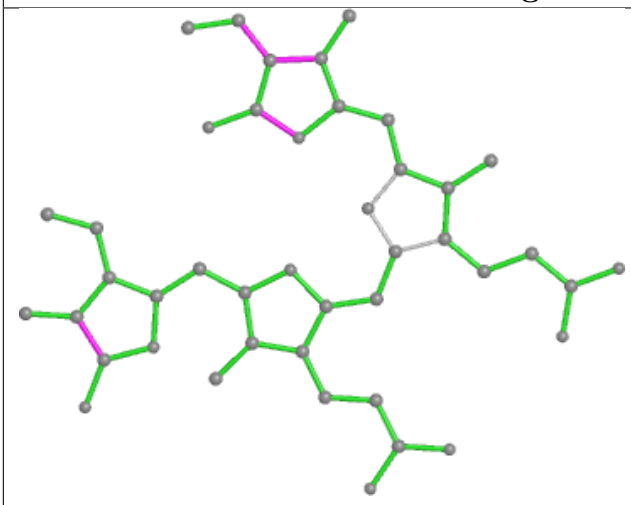


Rings

Ligand PEB s2 202



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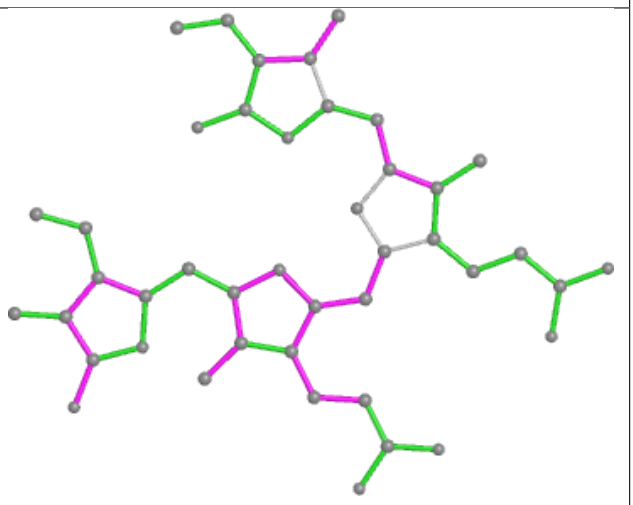

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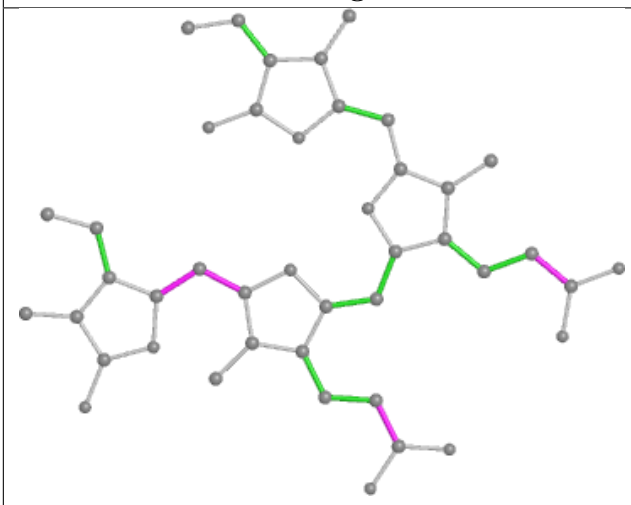

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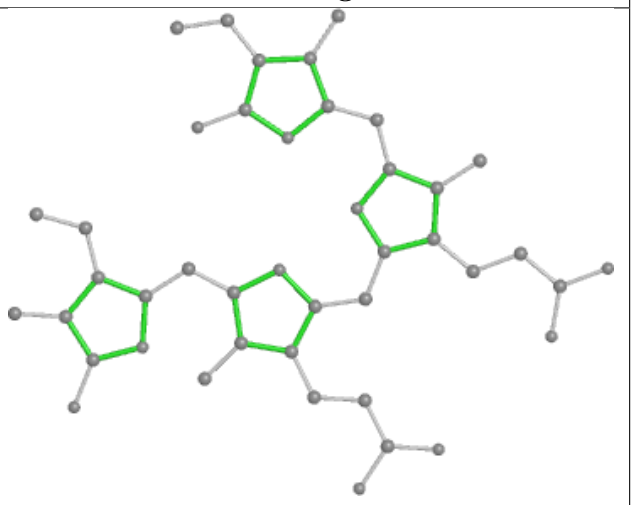
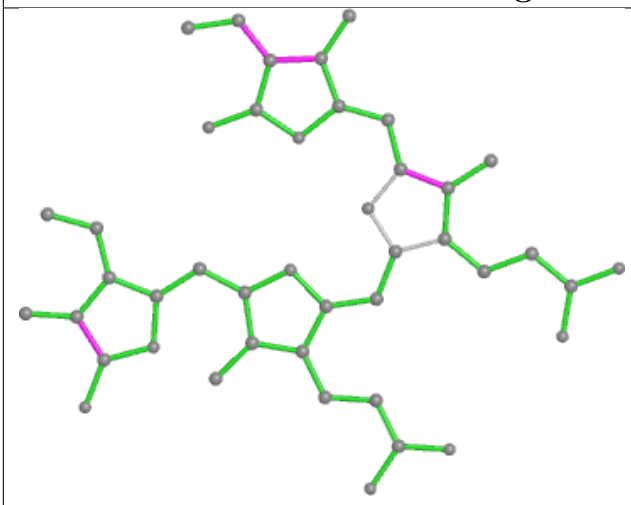


Rings

Ligand PEB G6 202



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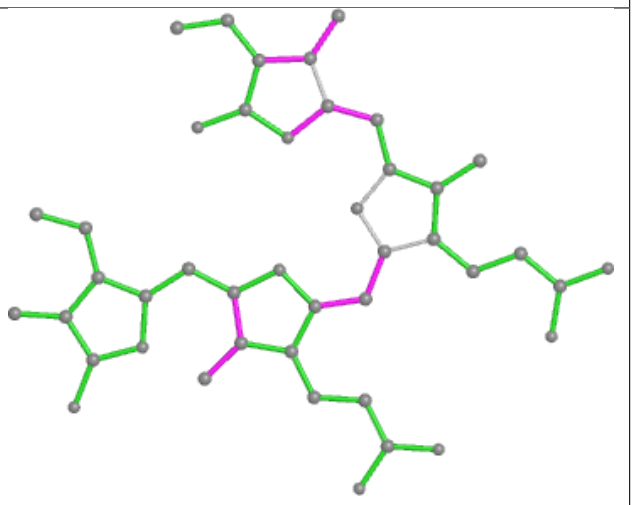

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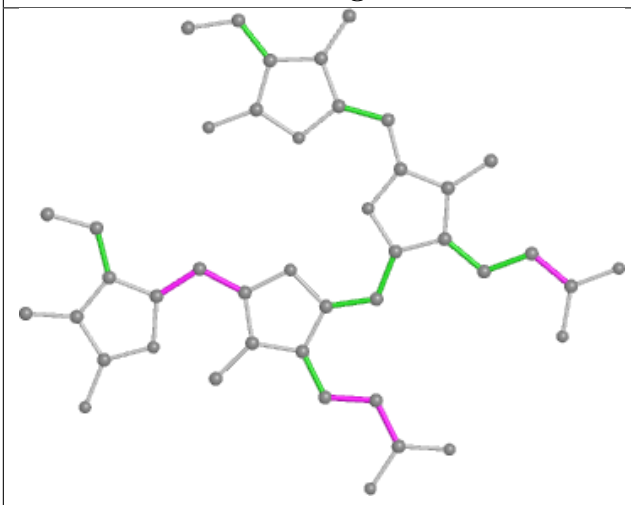

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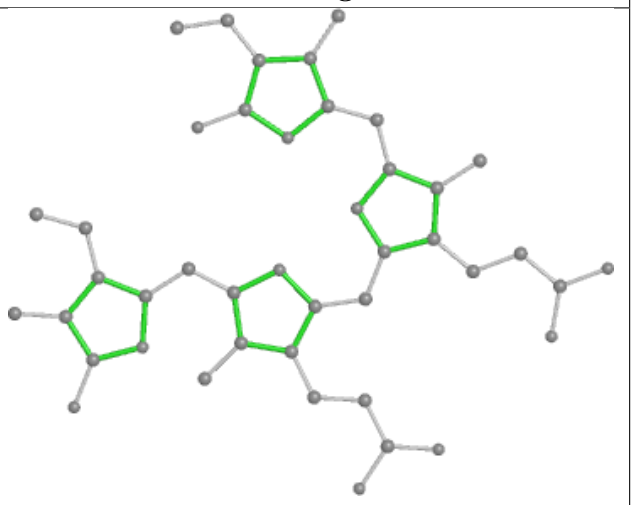
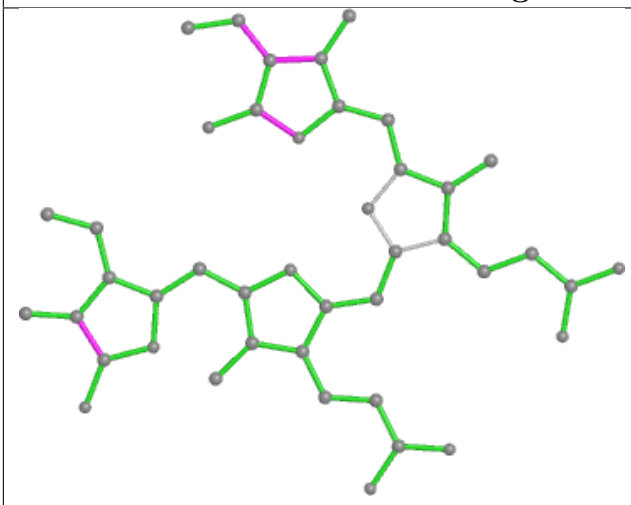


Rings

Ligand PEB c6 1001



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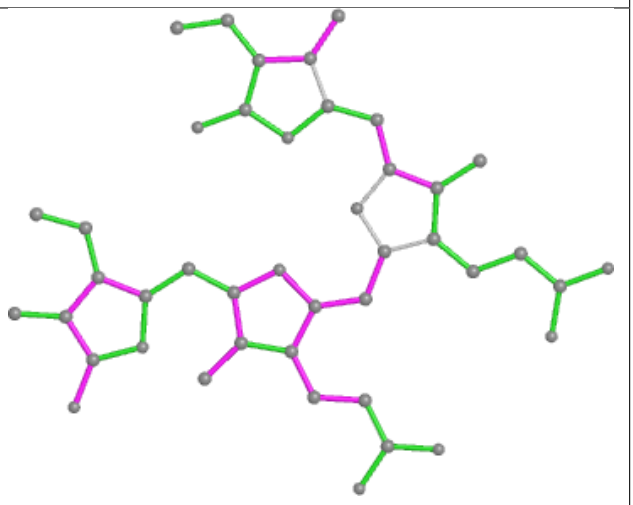

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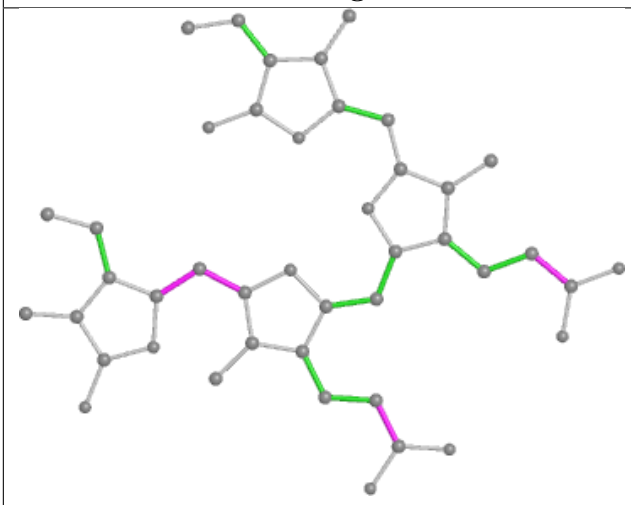

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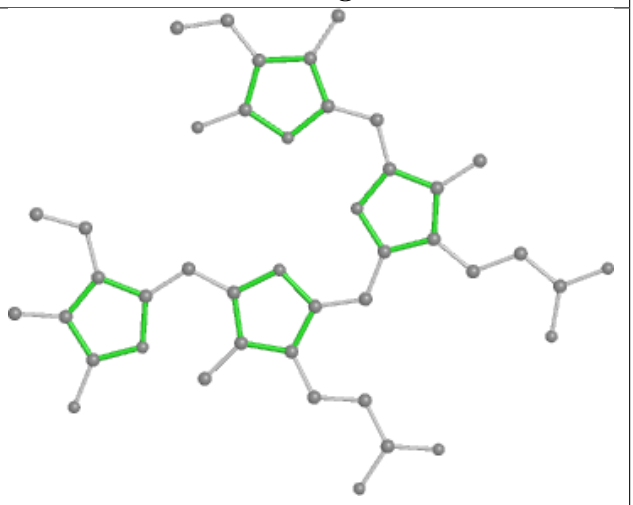

Rings

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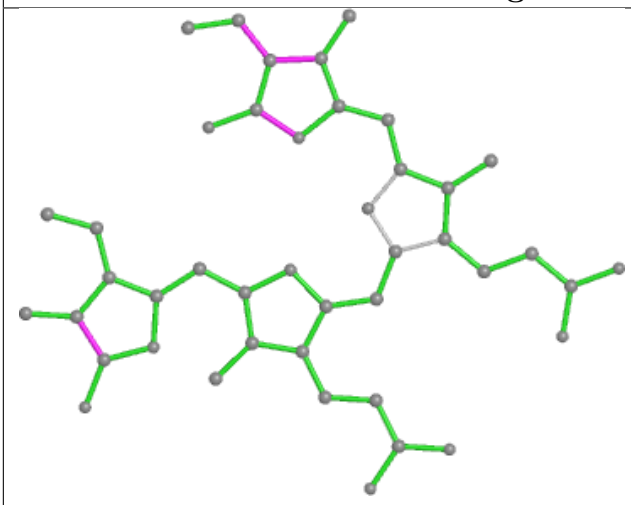

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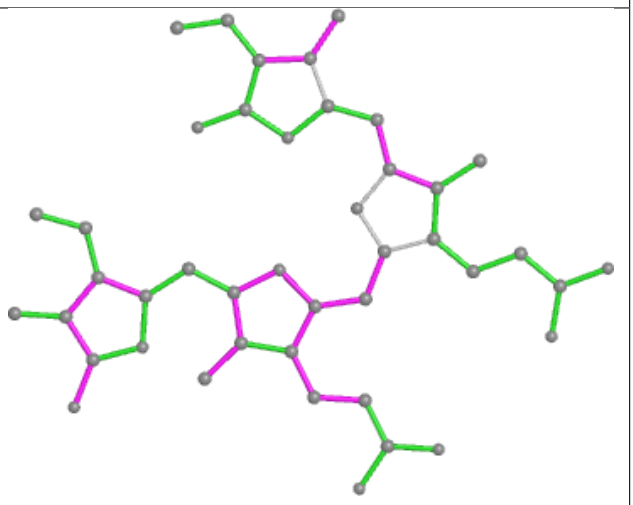

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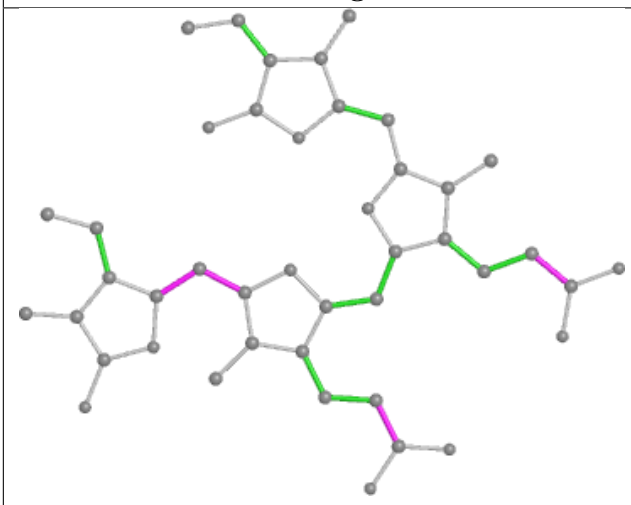

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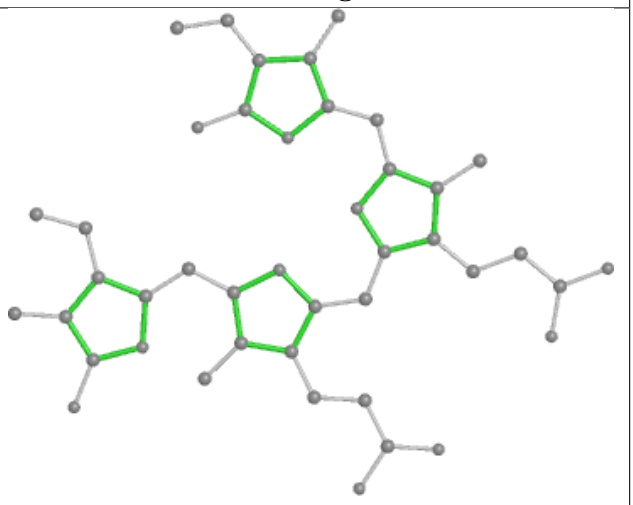
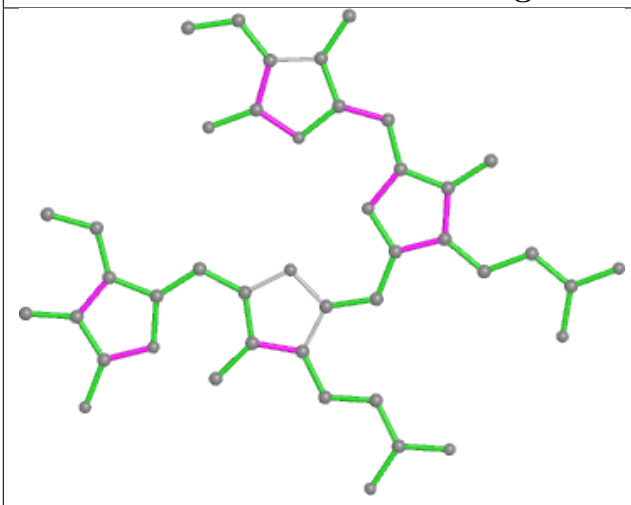


Rings

Ligand PUB T9 203



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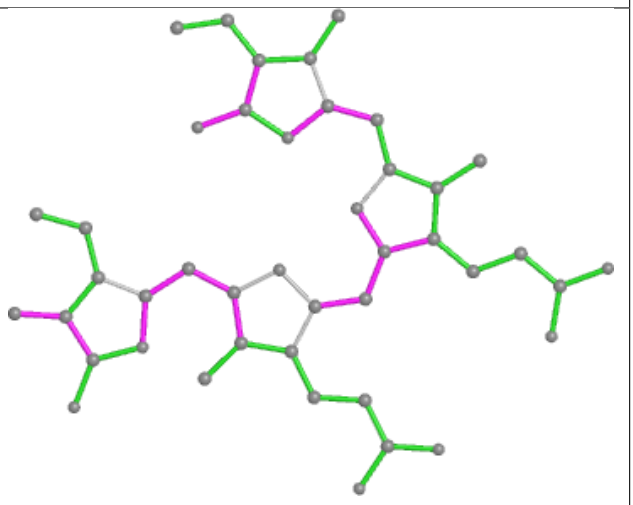

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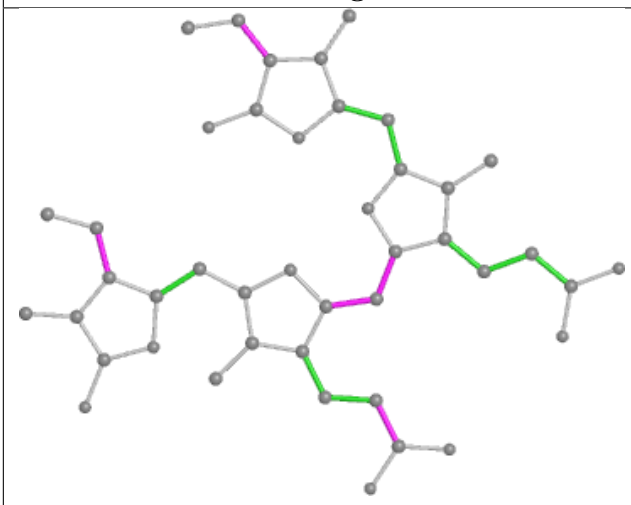

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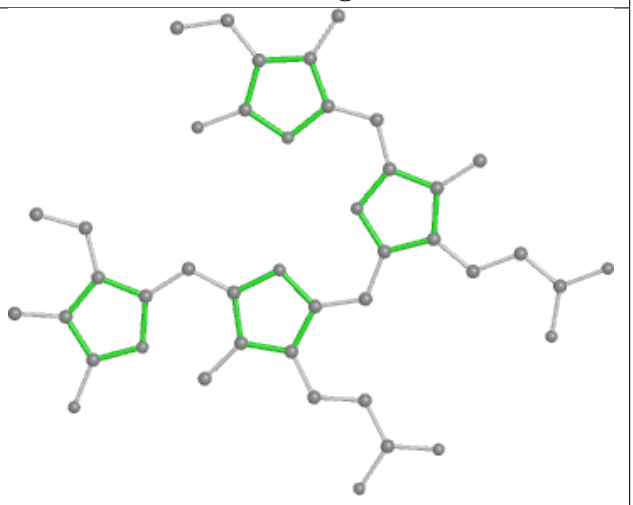
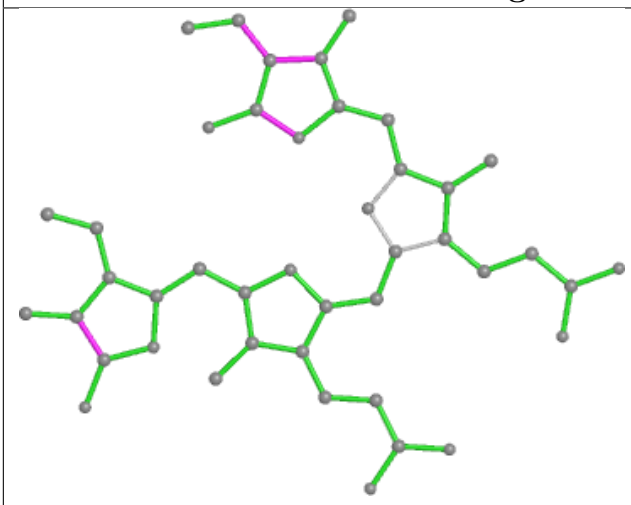


Rings

Ligand PEB F8 1001



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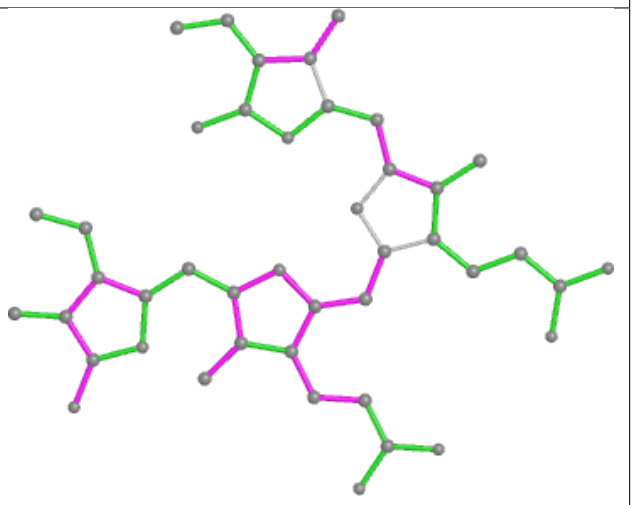

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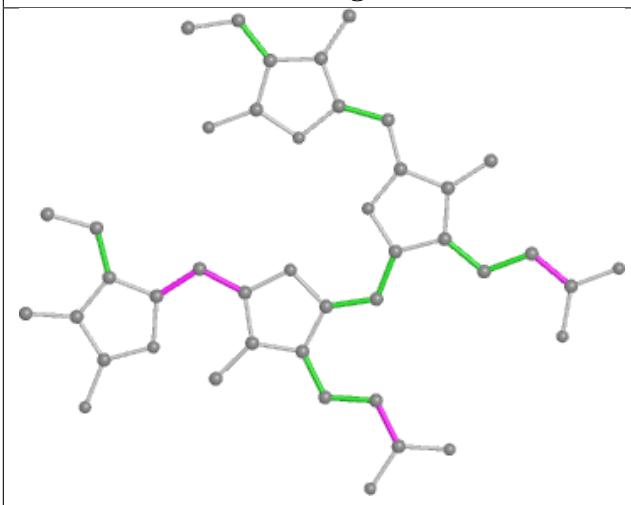

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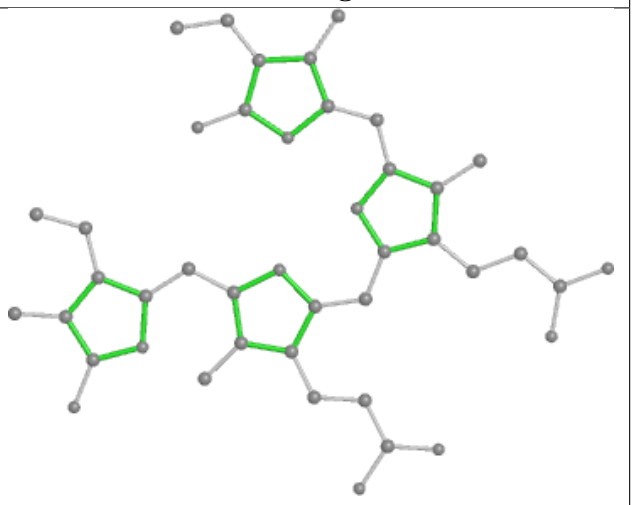
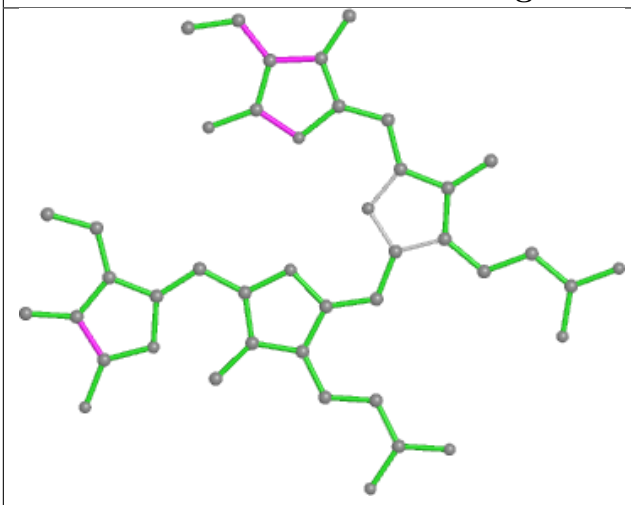


Rings

Ligand PEB A8 201



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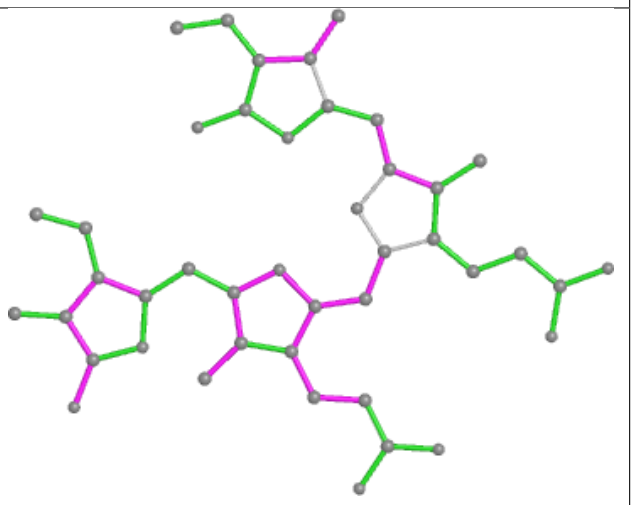

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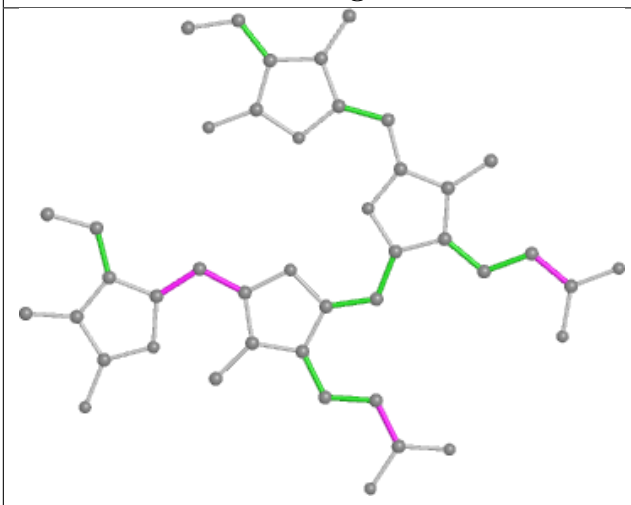

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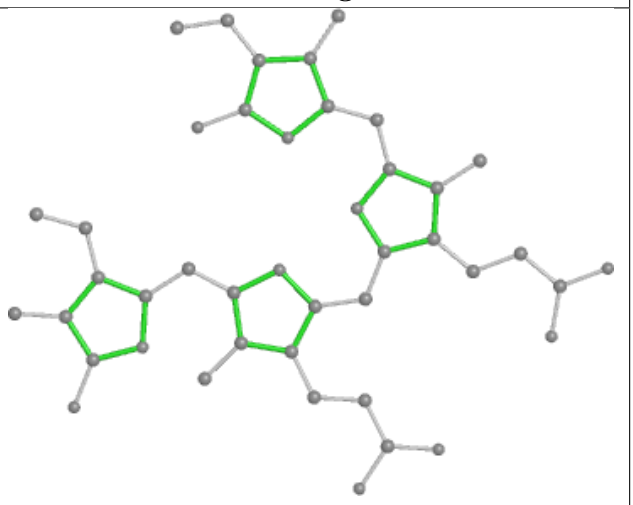
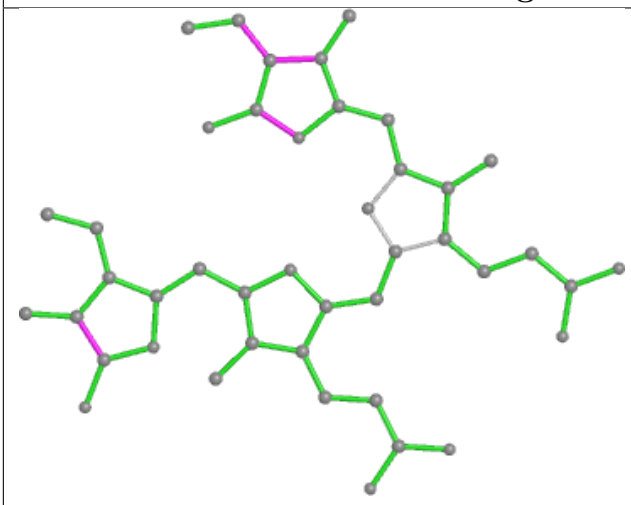


Rings

Ligand PEB ew 301



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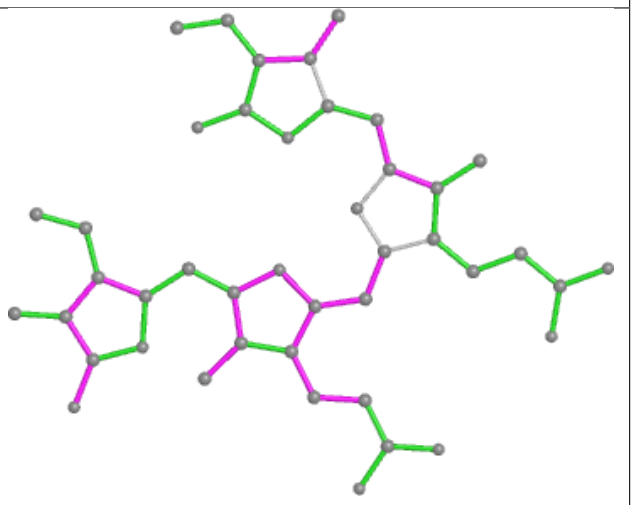

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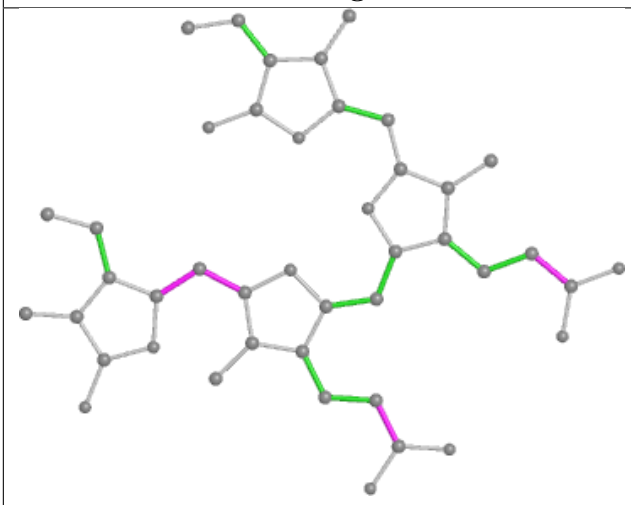

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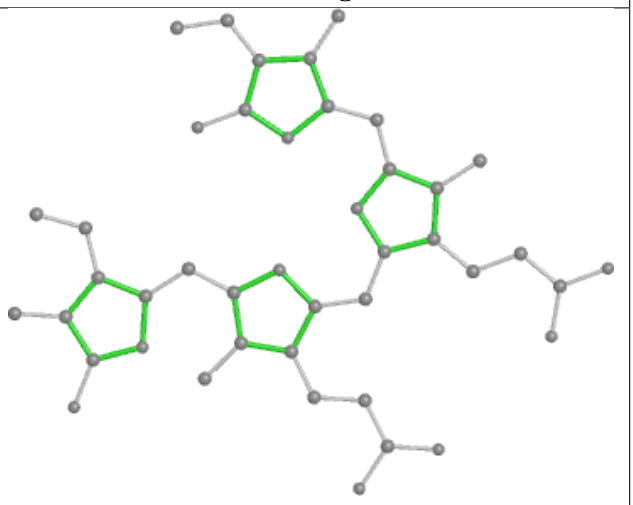

Rings

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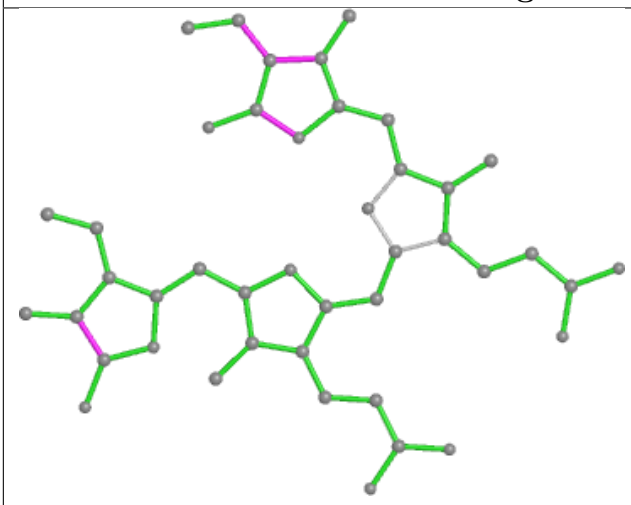

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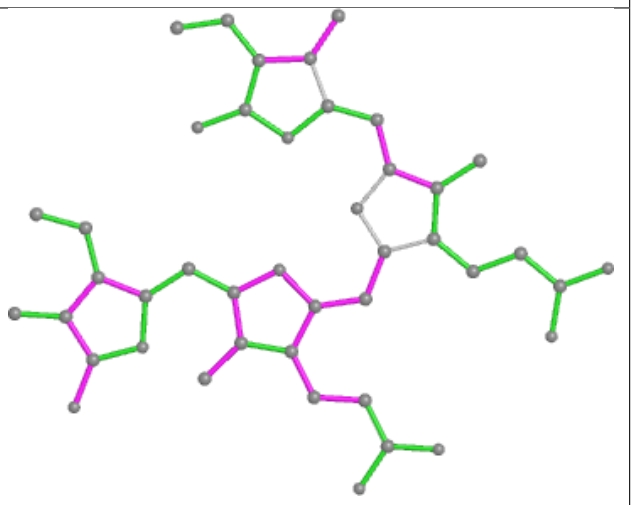

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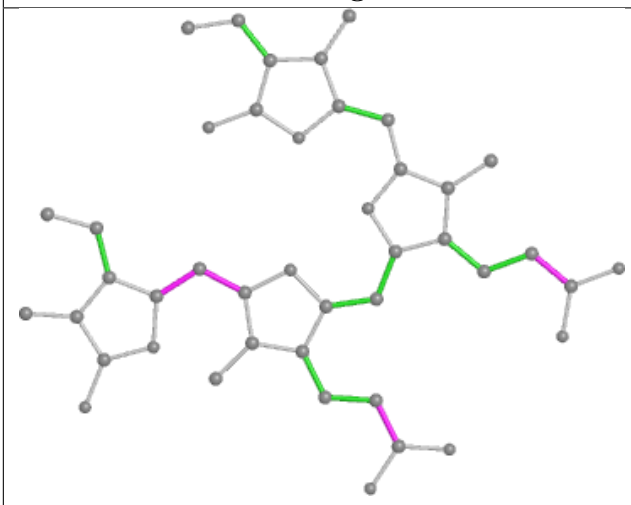

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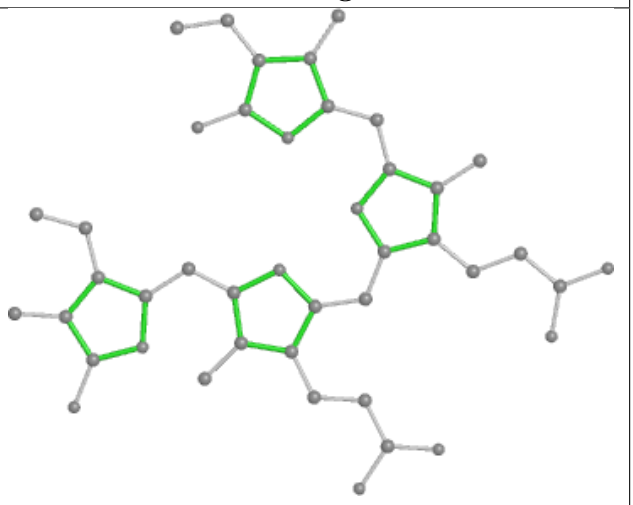
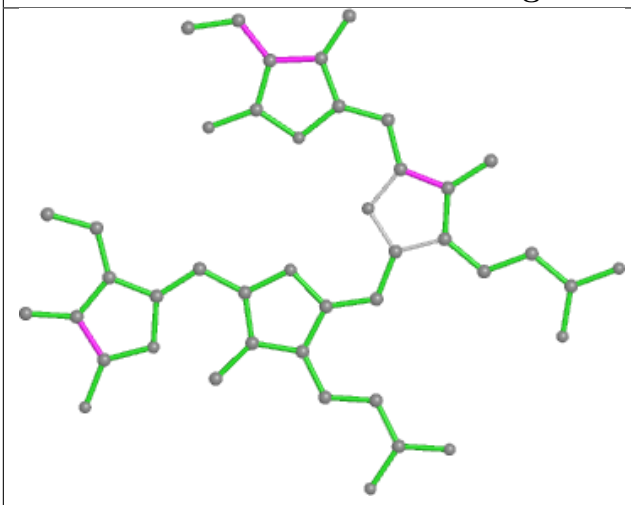


Rings

Ligand PEB ld 201



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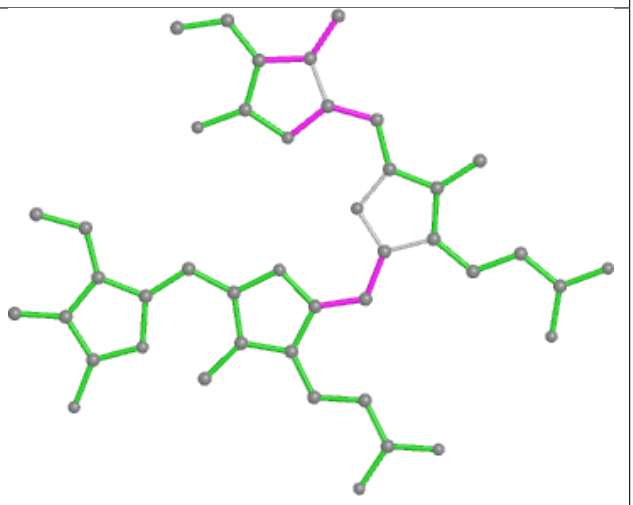

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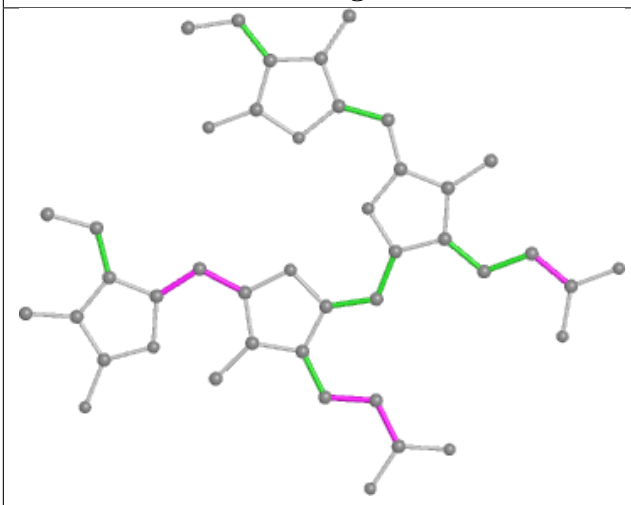

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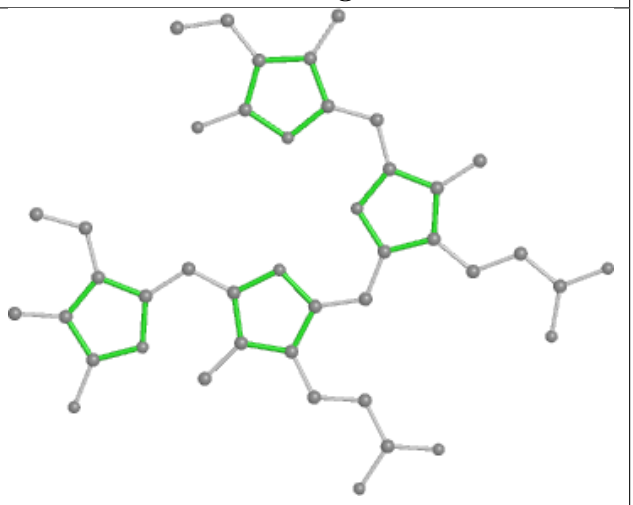
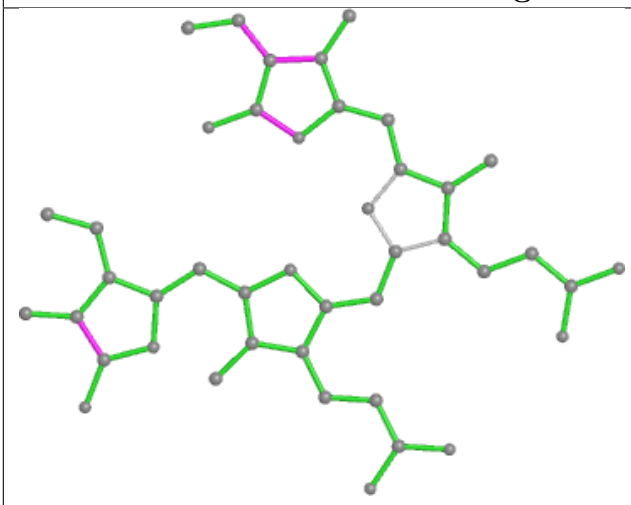


Rings

Ligand PEB m2 202



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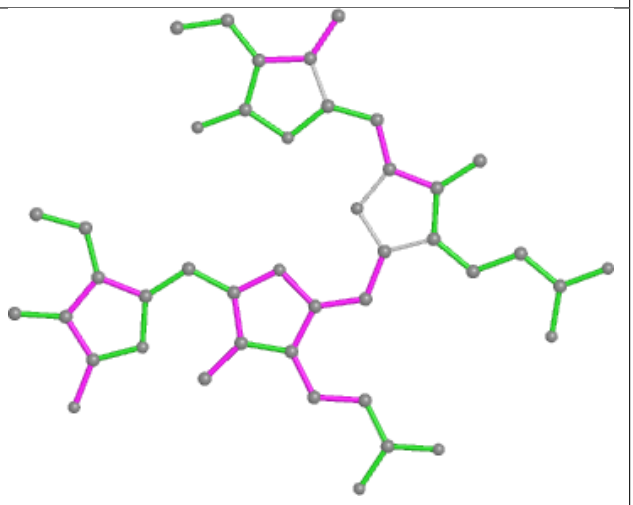

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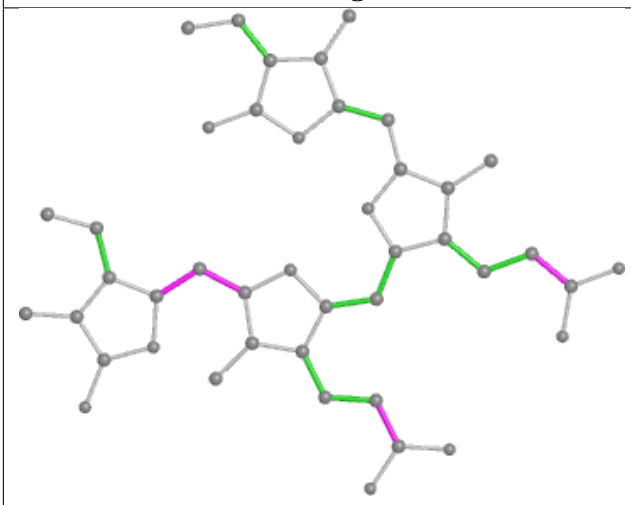

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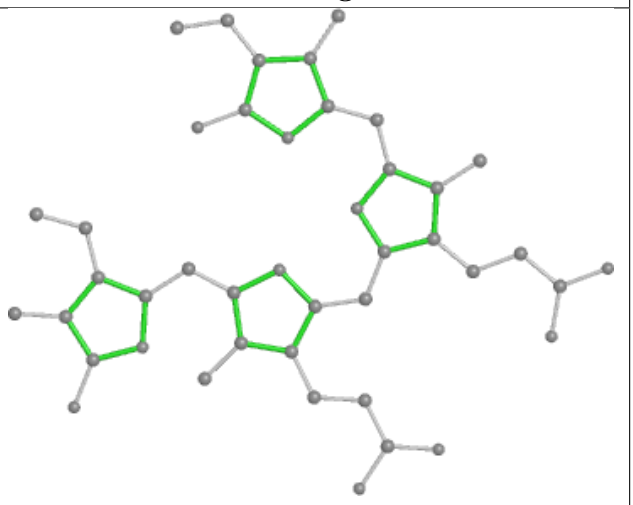
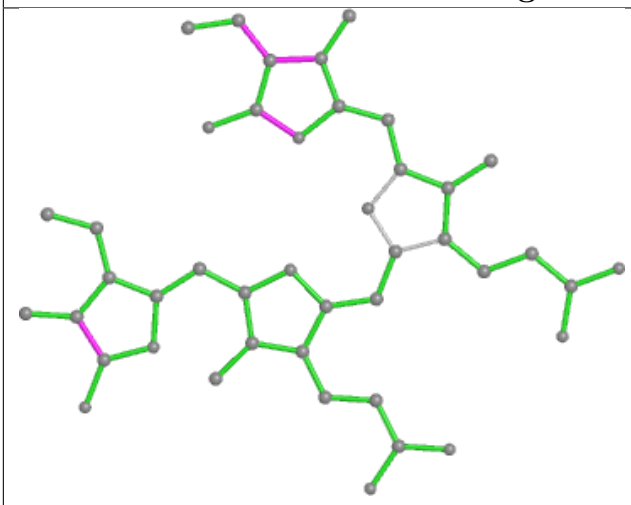


Rings

Ligand PEB L5 201



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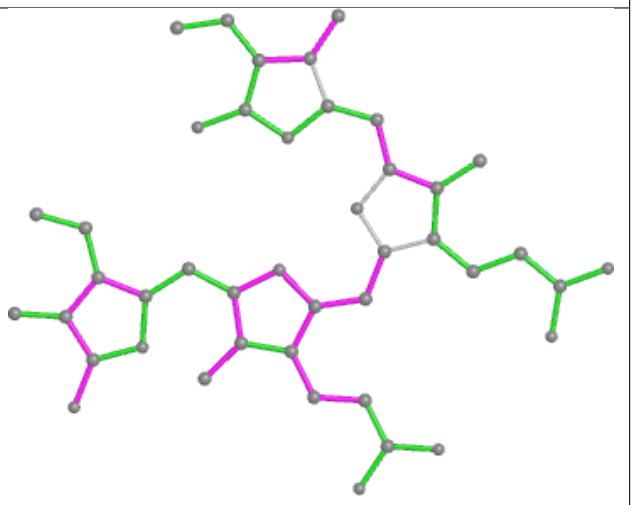
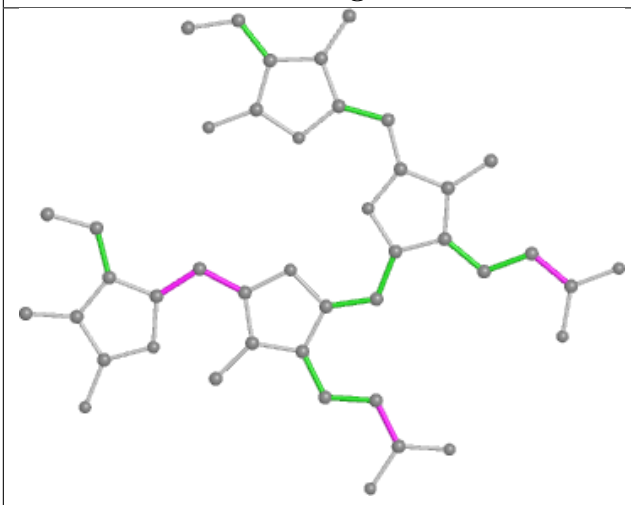


Bond angles



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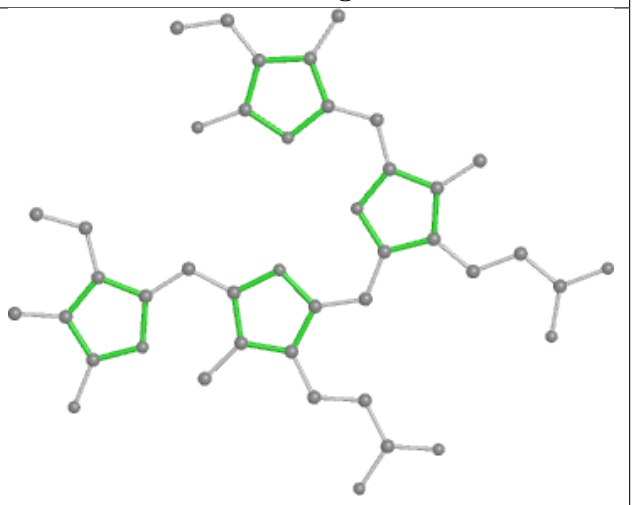
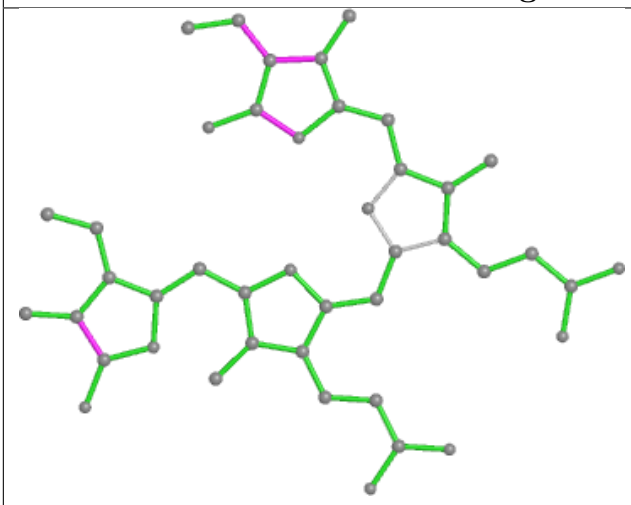


Rings

Ligand PEB J8 202



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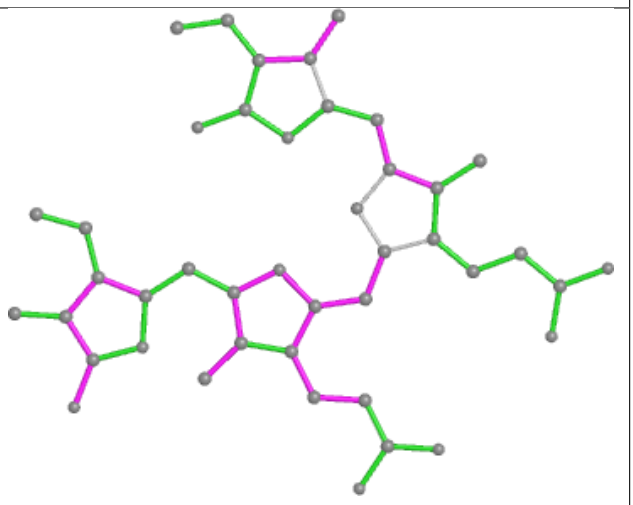
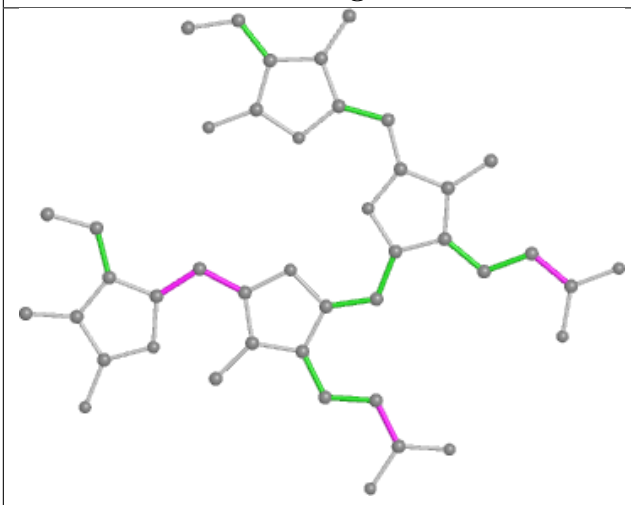
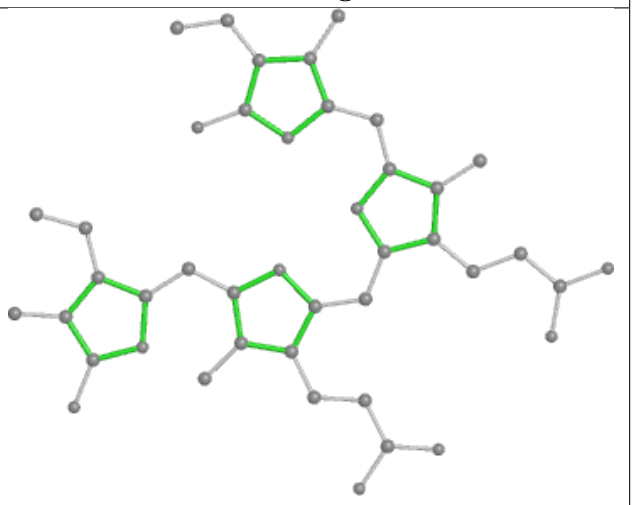


Bond angles

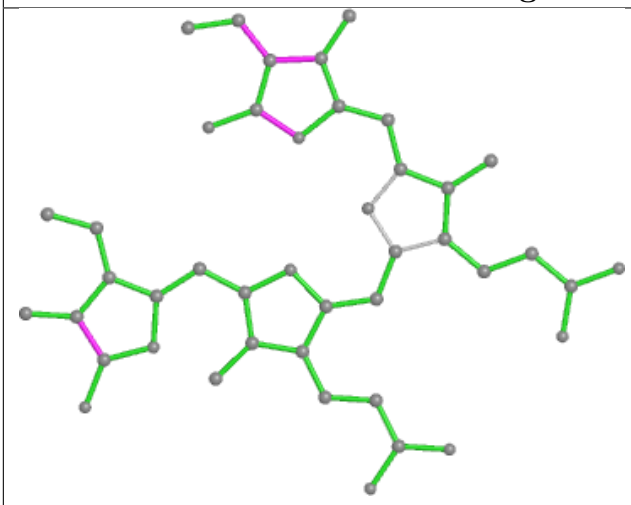


Torsions



Rings

Ligand PEB y8 201



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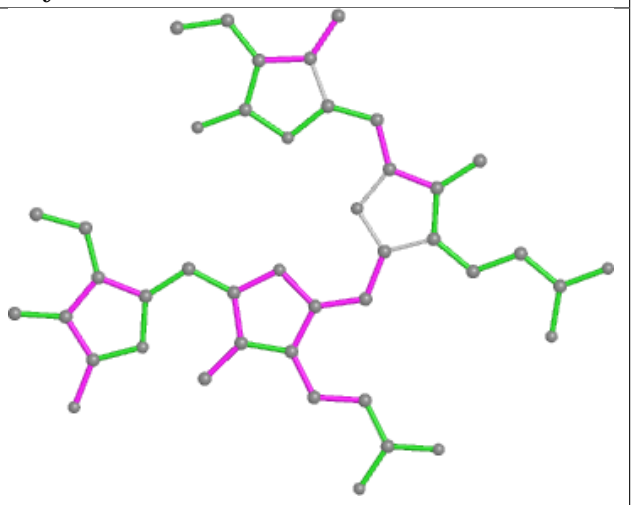

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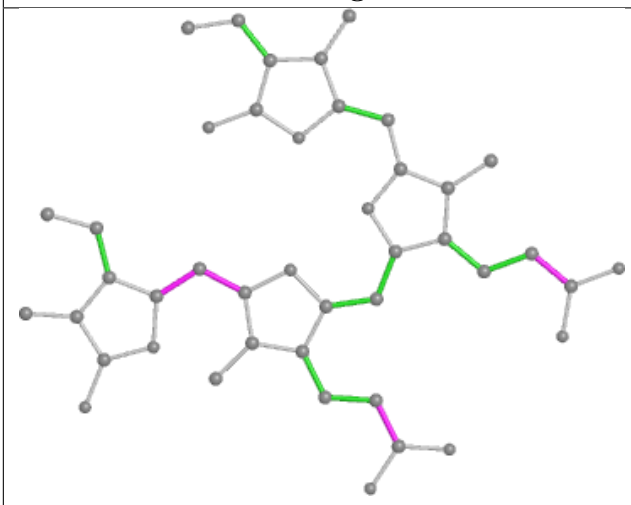

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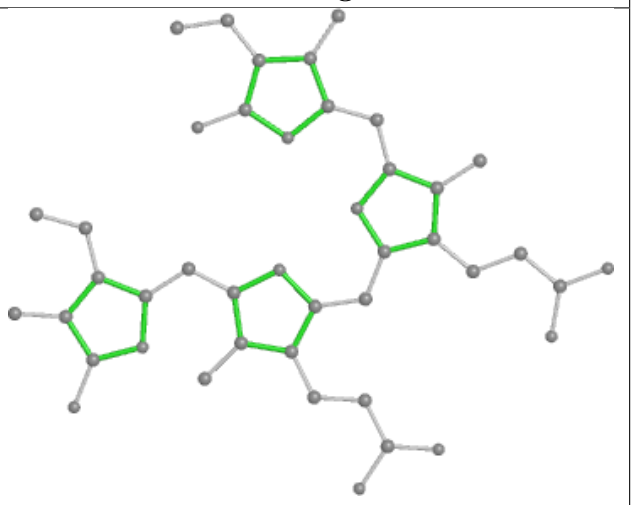
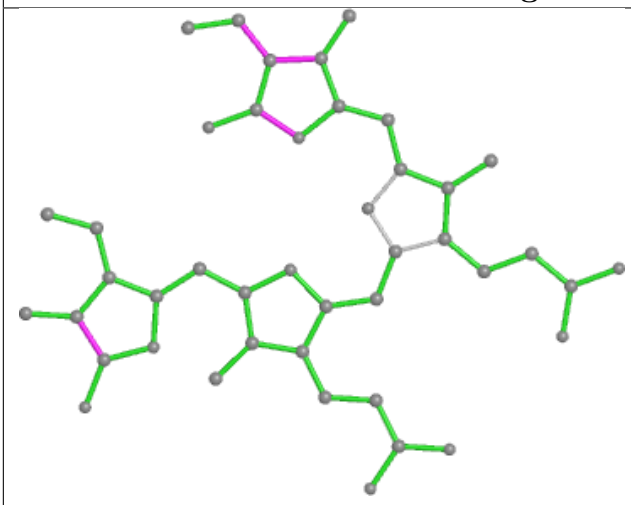


Rings

Ligand PEB z3 201



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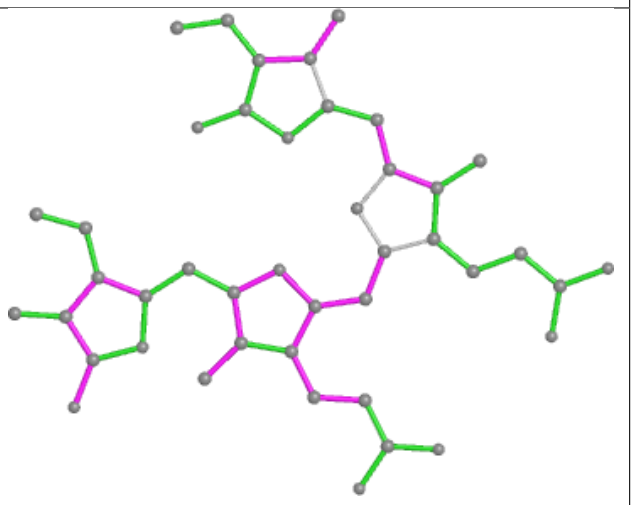

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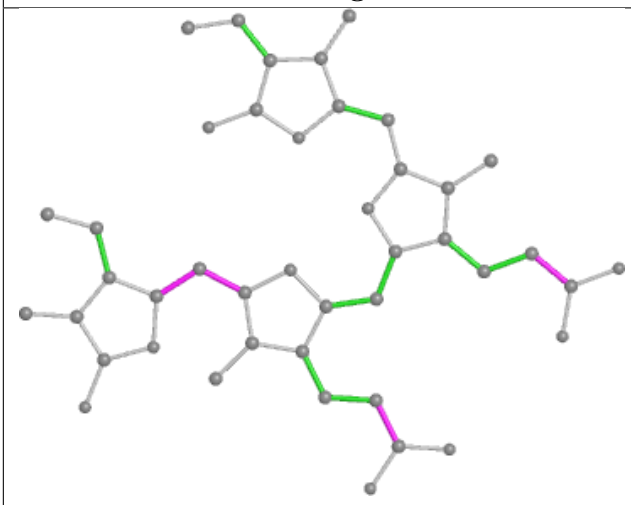

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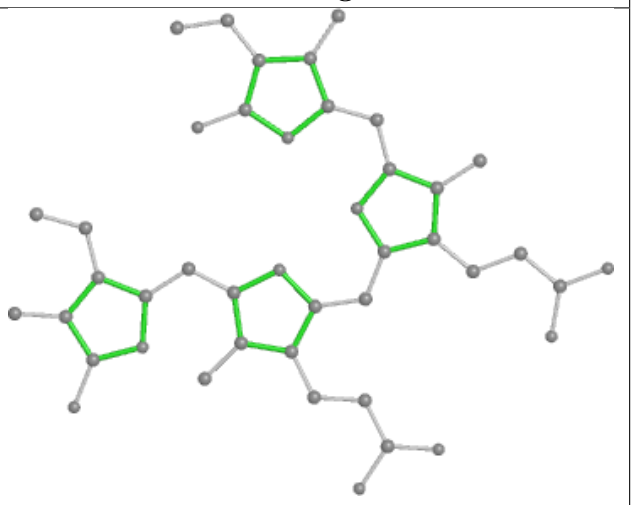
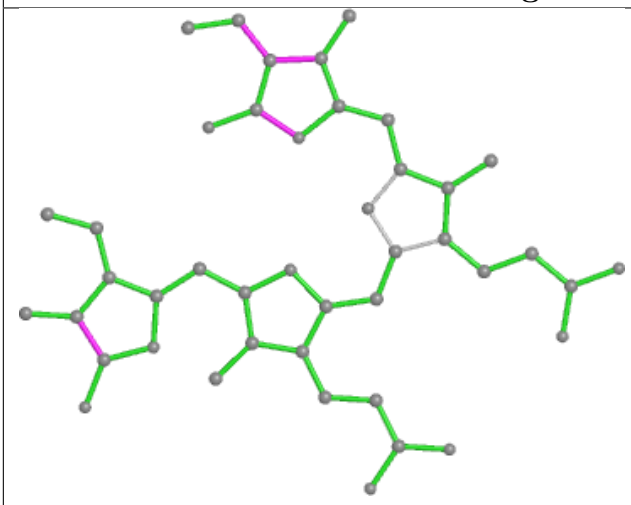


Rings

Ligand PEB t4 201



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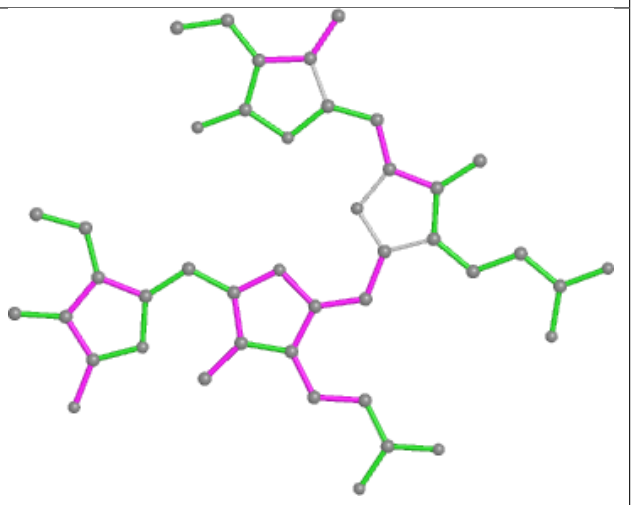

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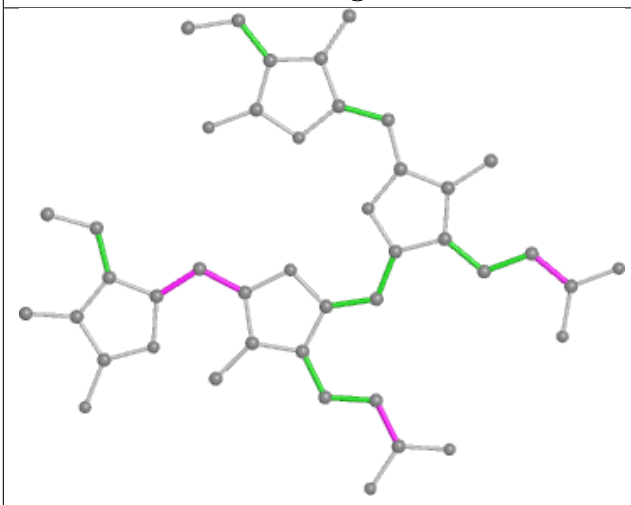

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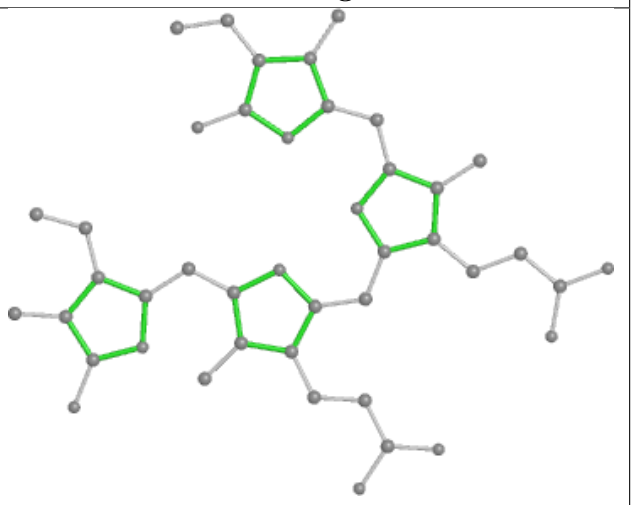

Rings

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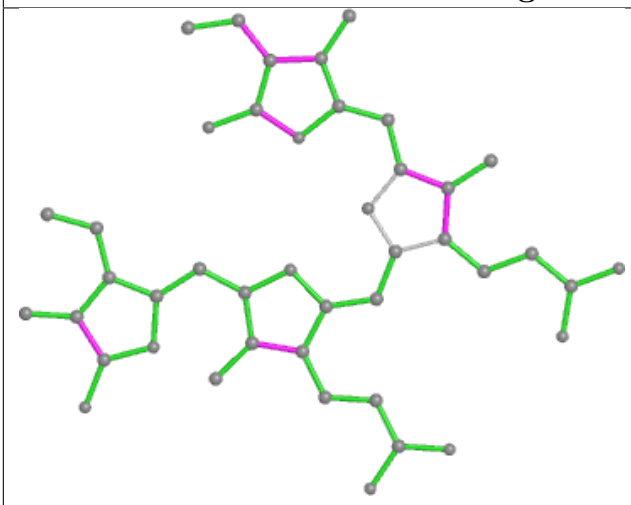

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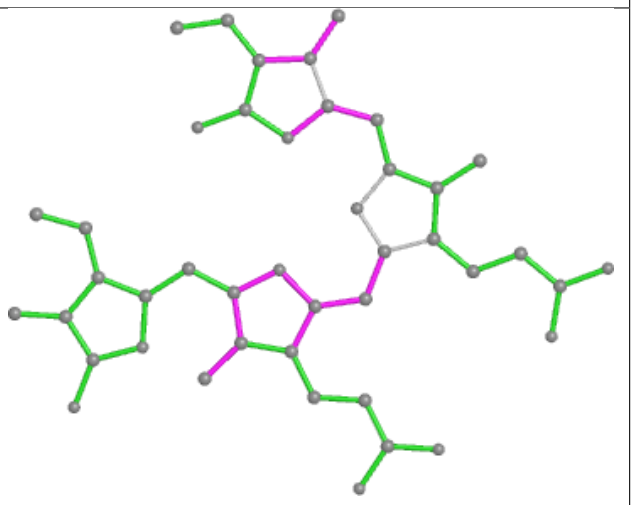

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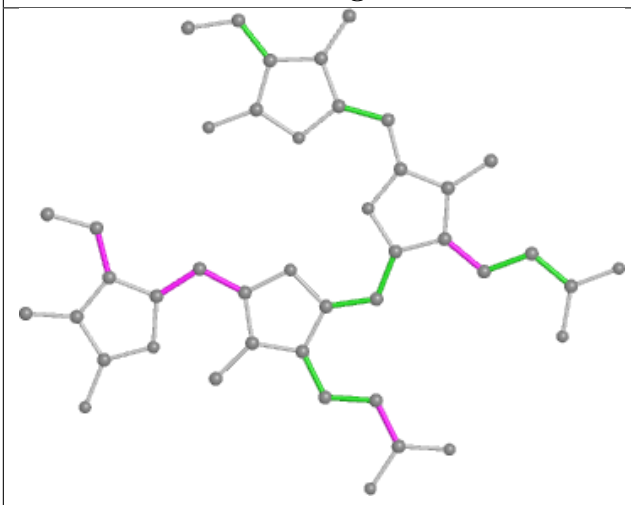

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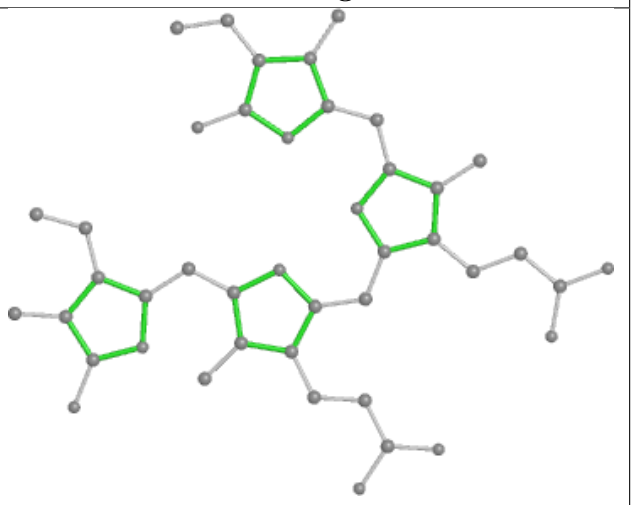

Rings

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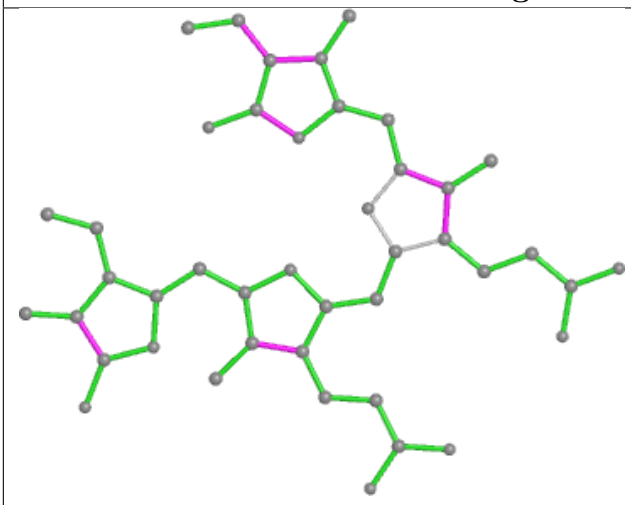

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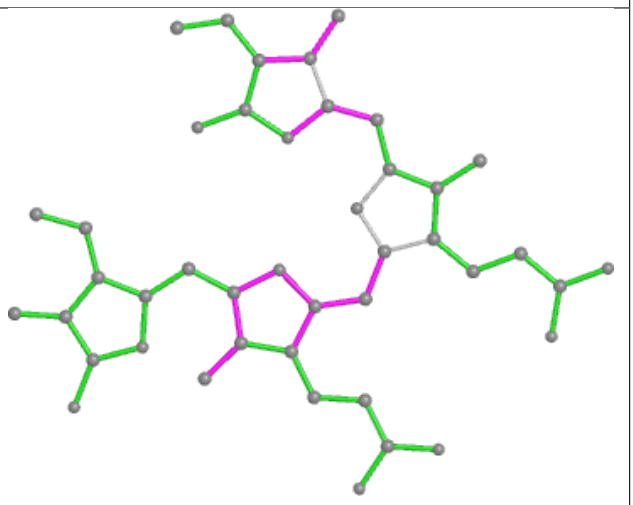

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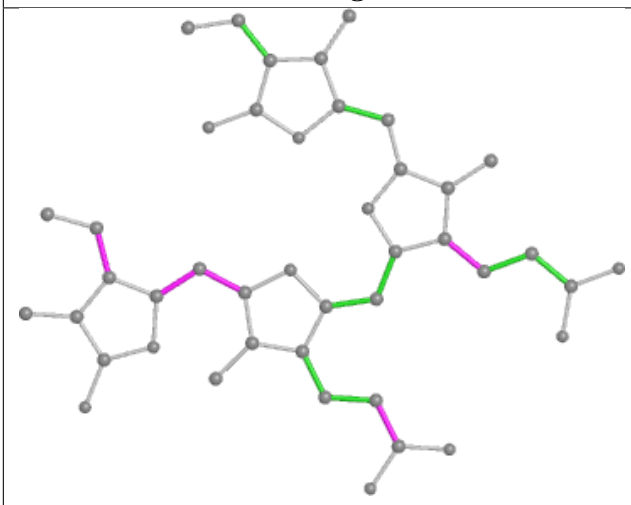

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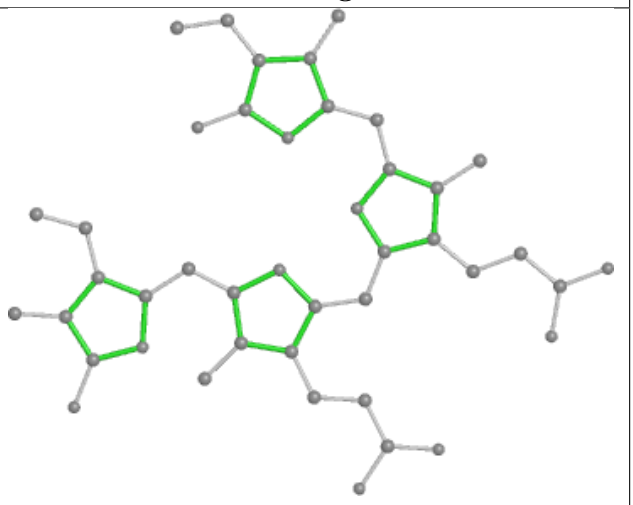

Rings

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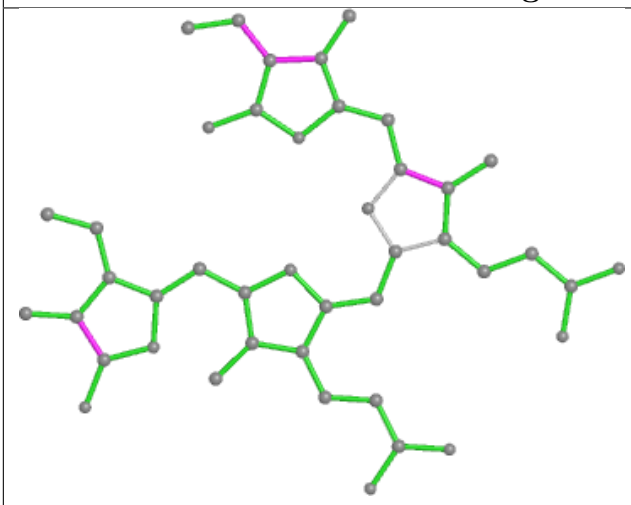

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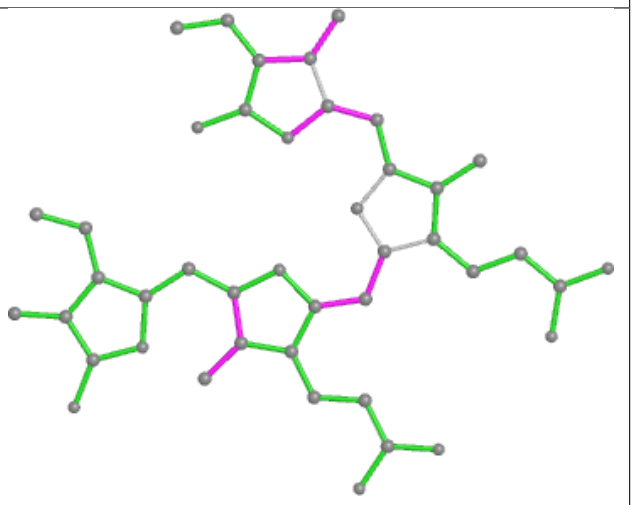

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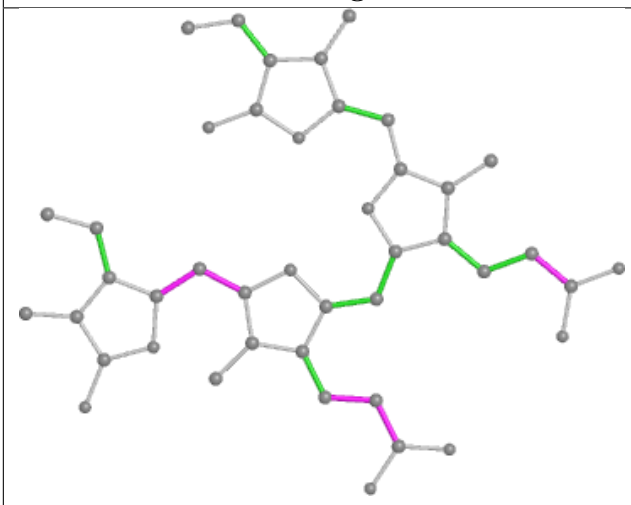

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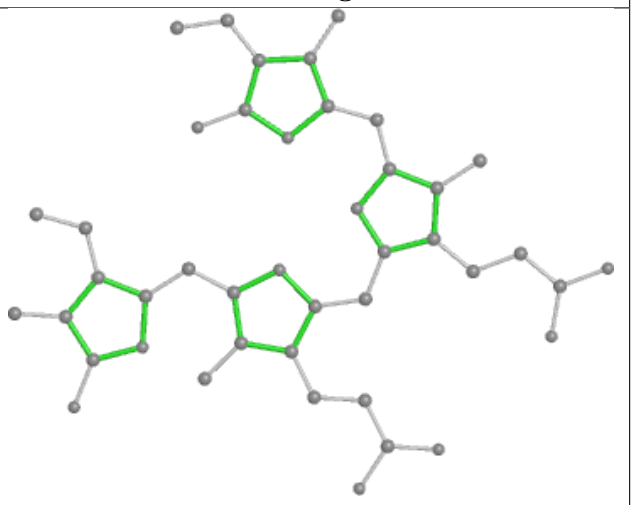
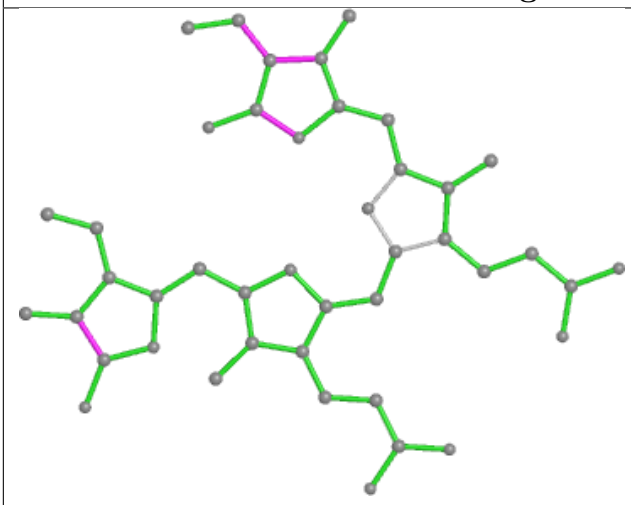


Rings

Ligand PEB ed 201



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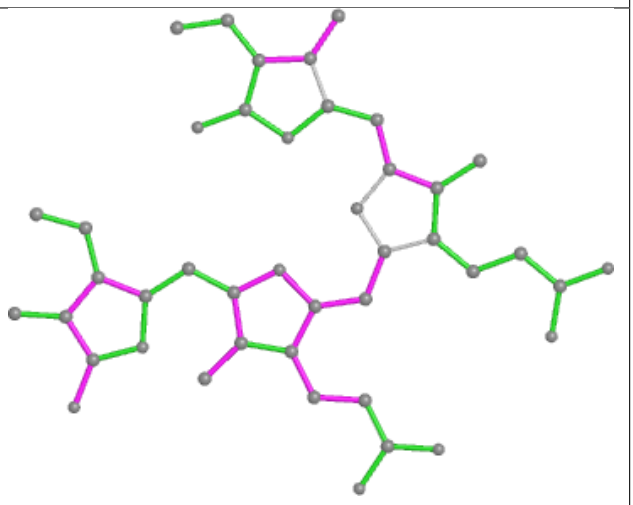

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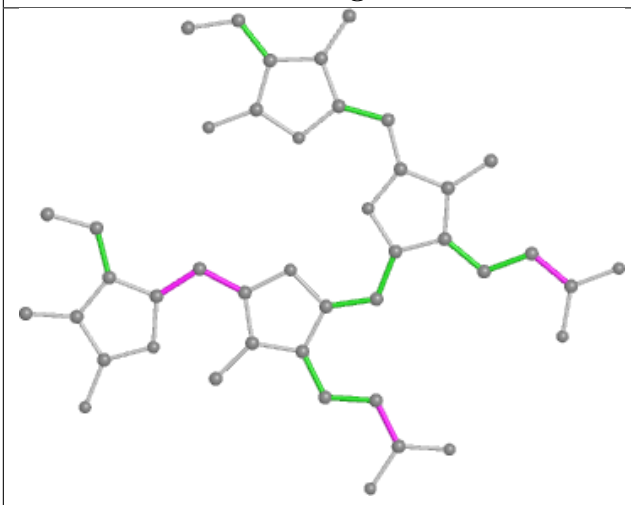

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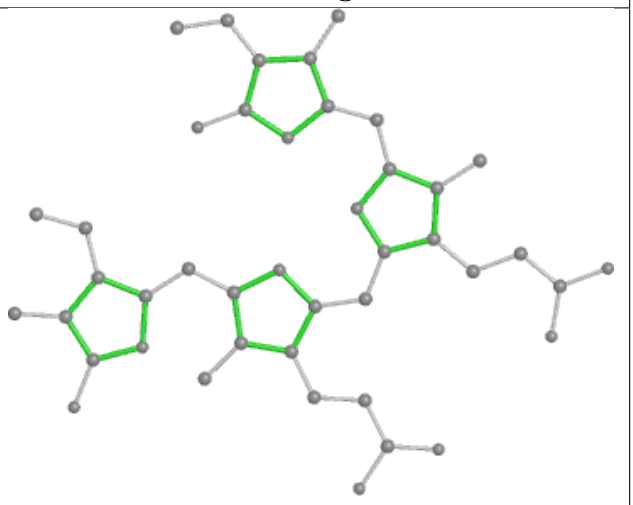

Rings

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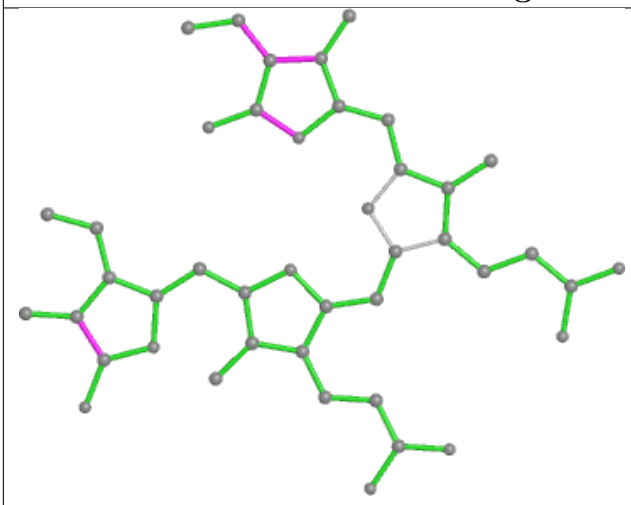

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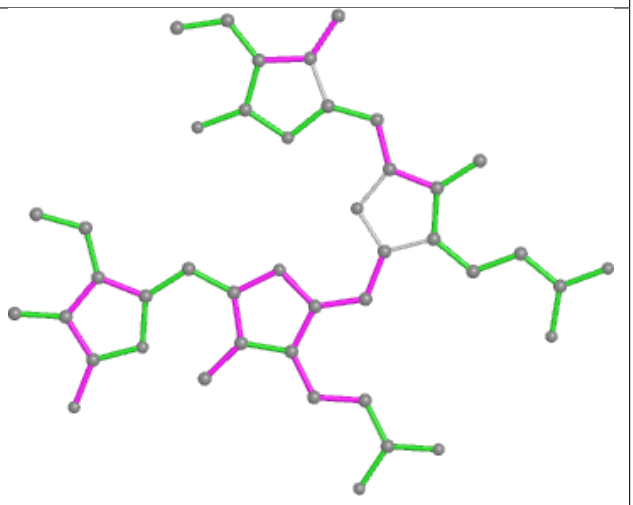

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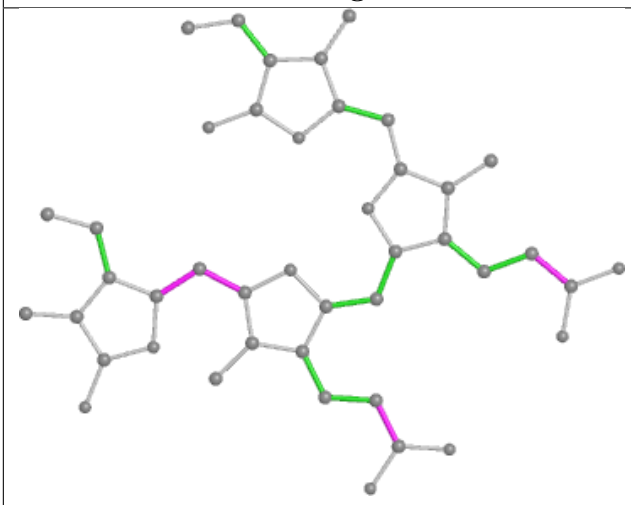

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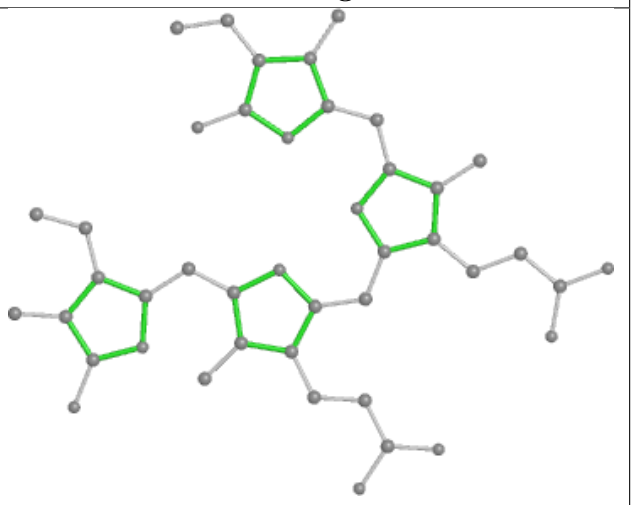

Rings

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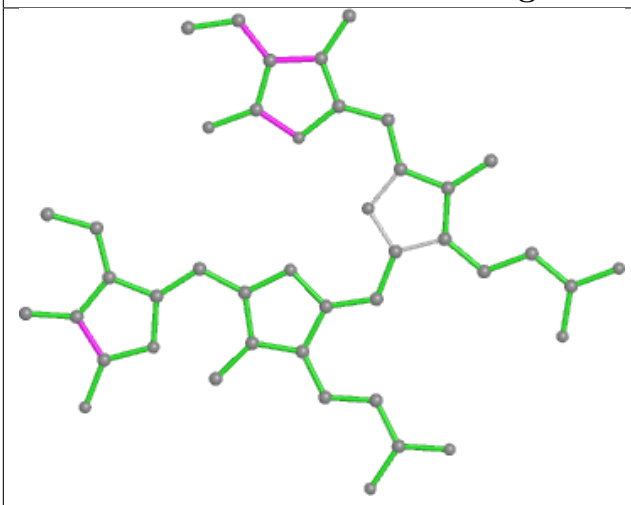

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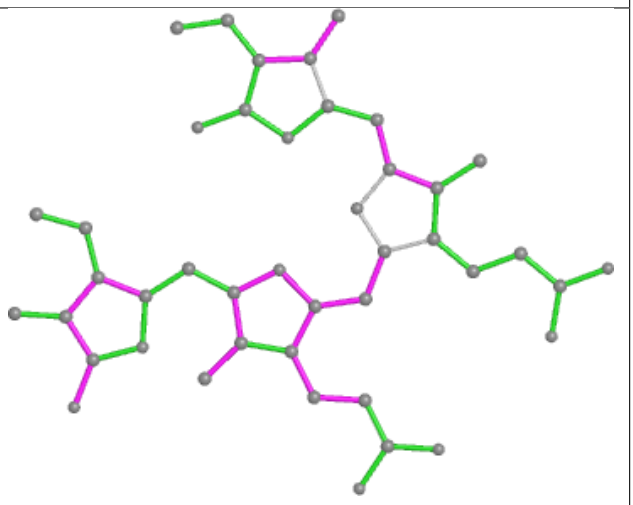

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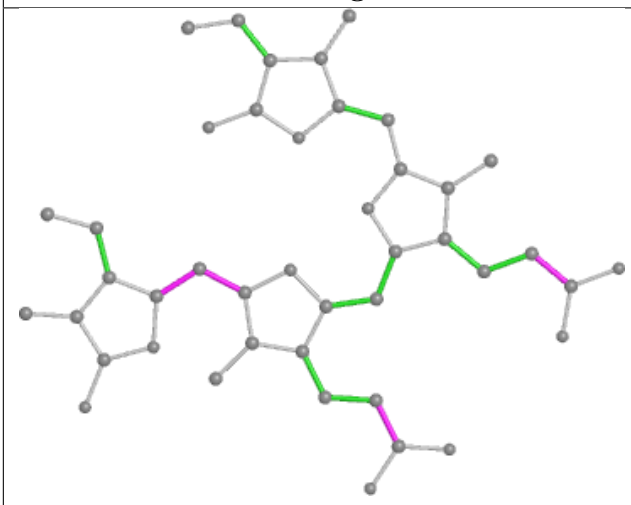

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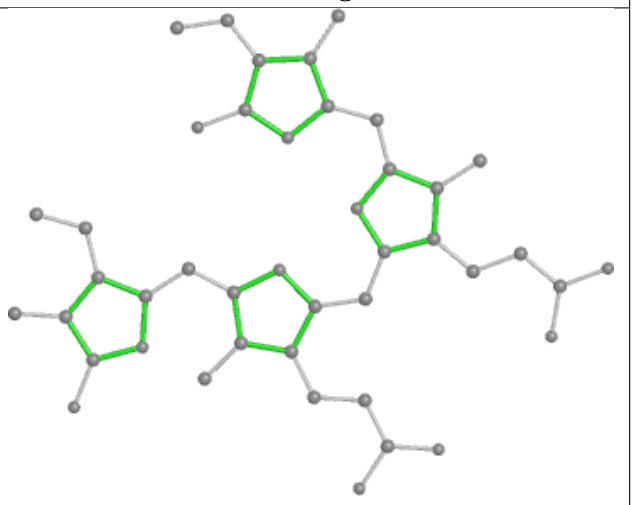

Rings

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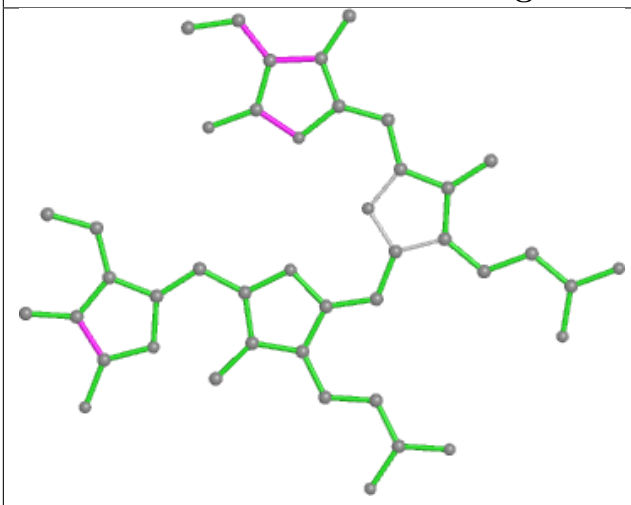

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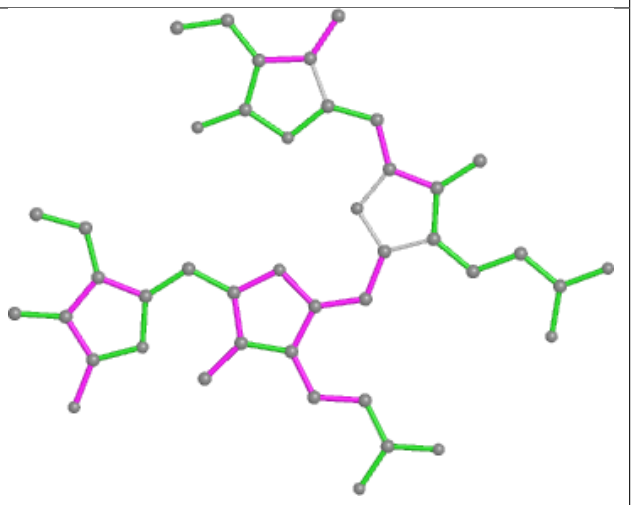

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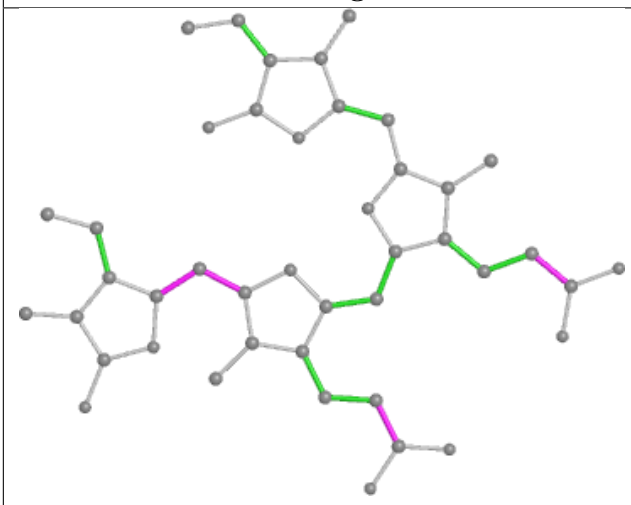

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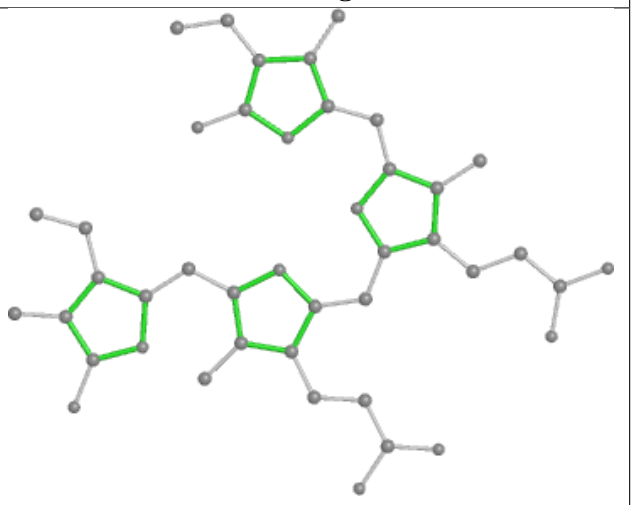

Rings

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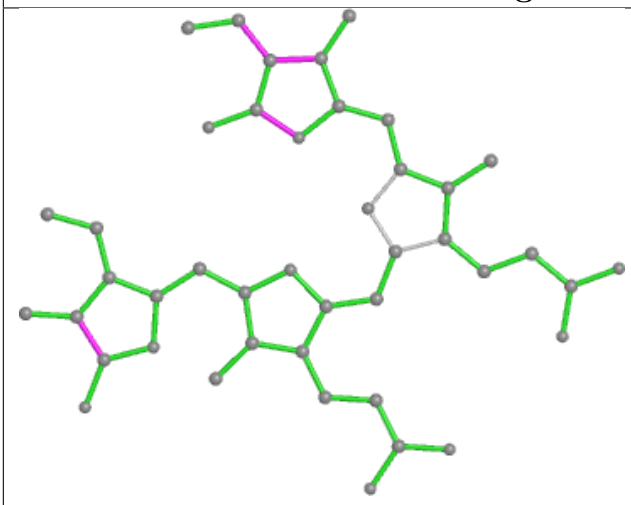

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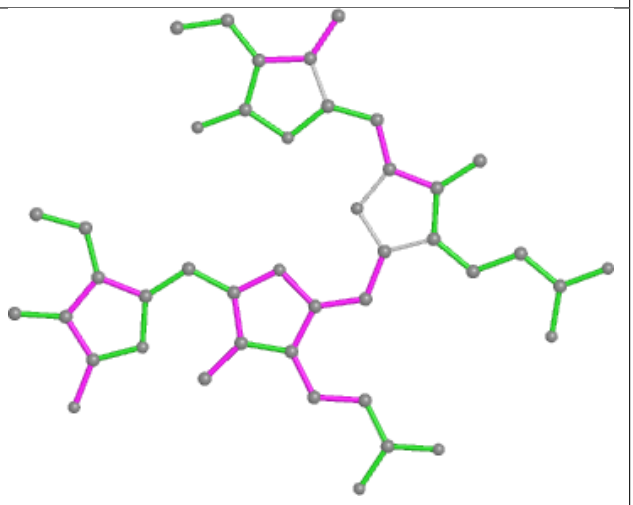

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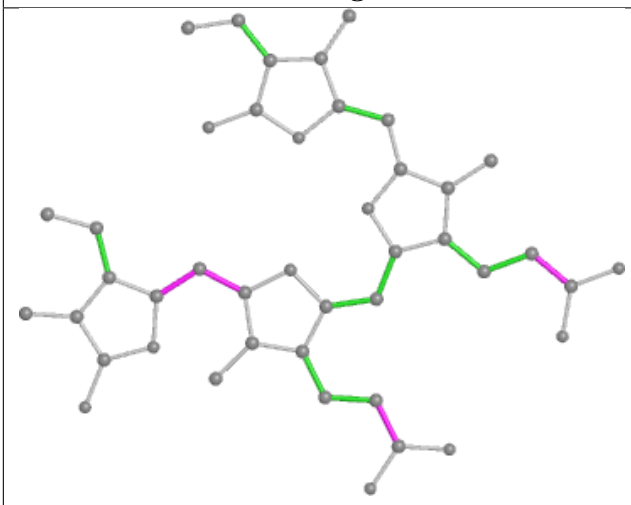

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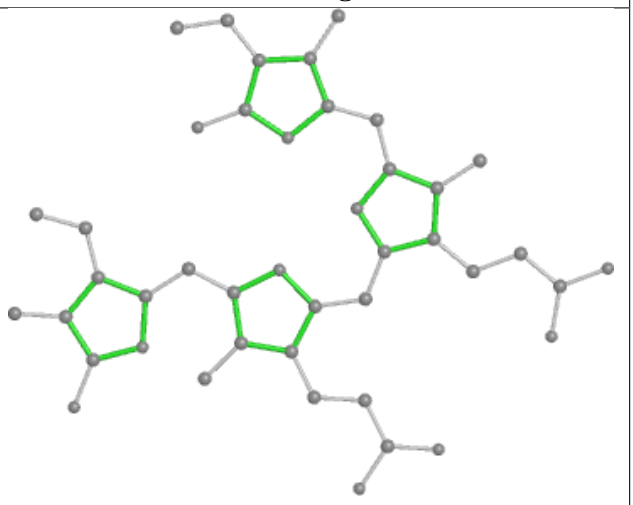
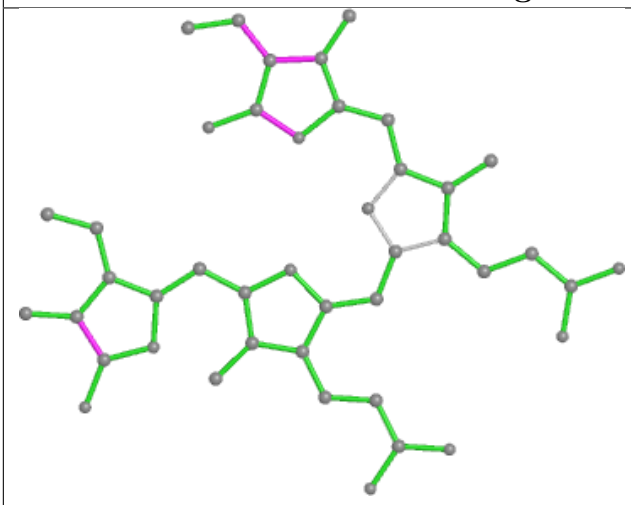


Rings

Ligand PEB dO 202



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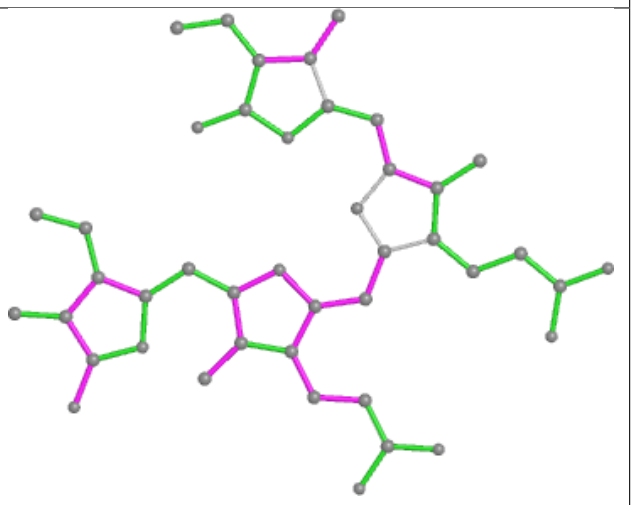

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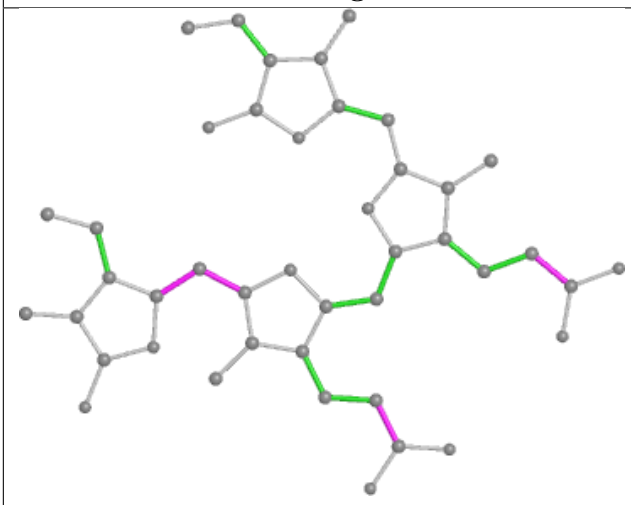

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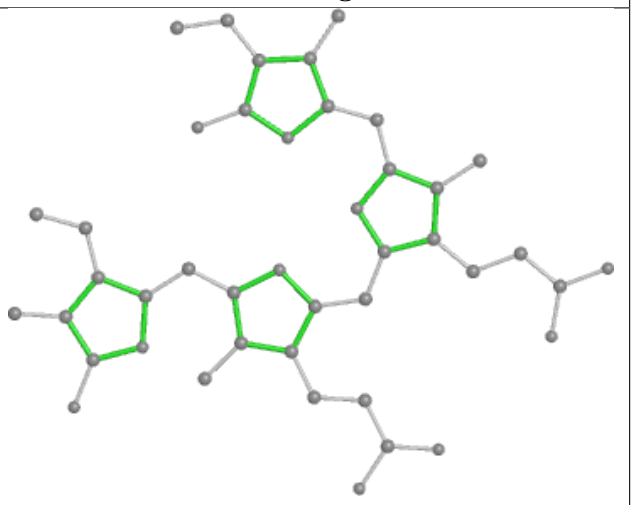

Rings

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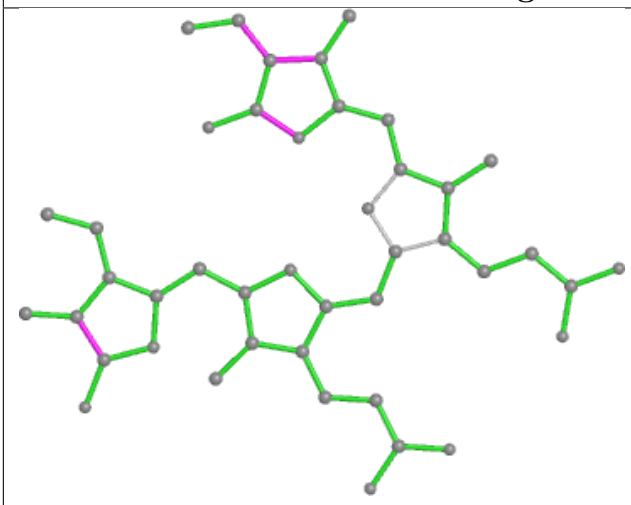

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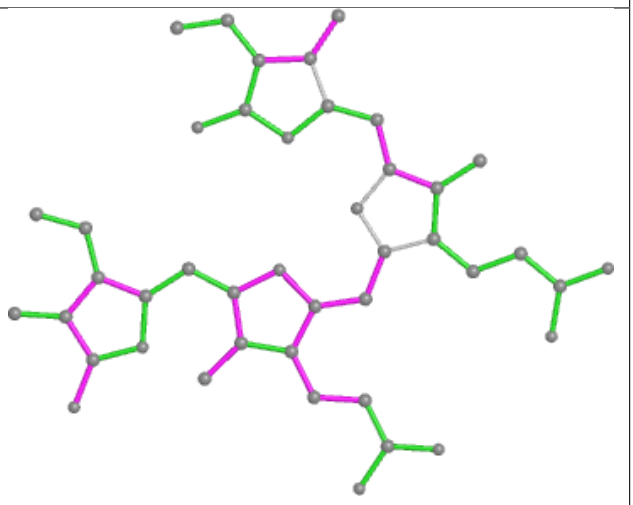
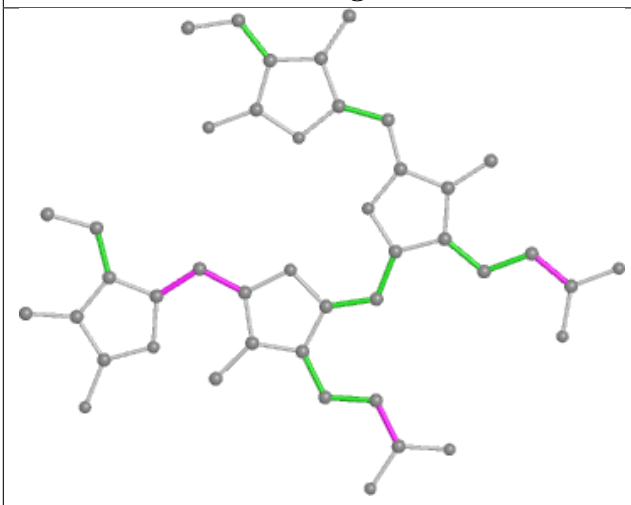
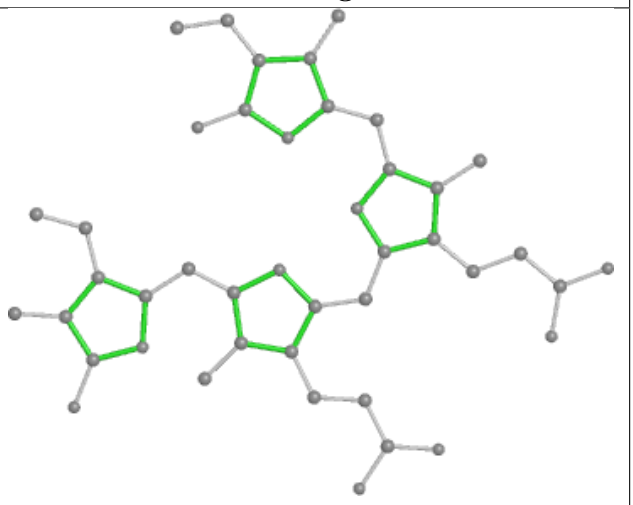


Bond angles

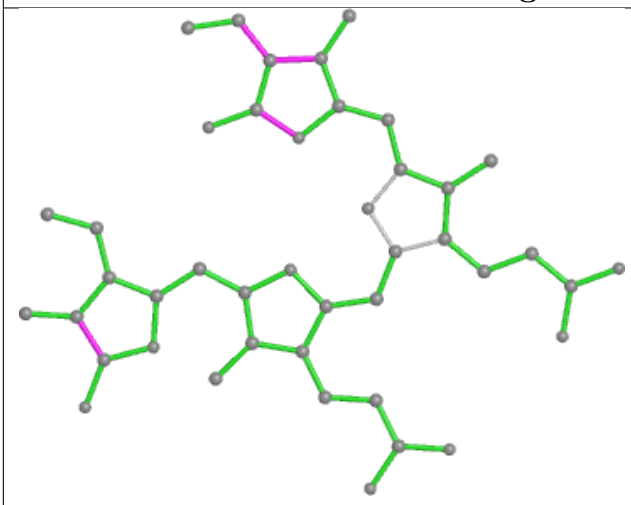


Torsions



Rings

Ligand PEB x4 201



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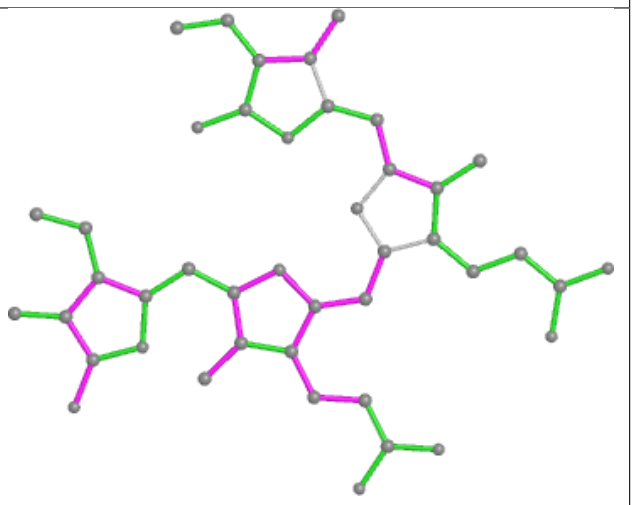

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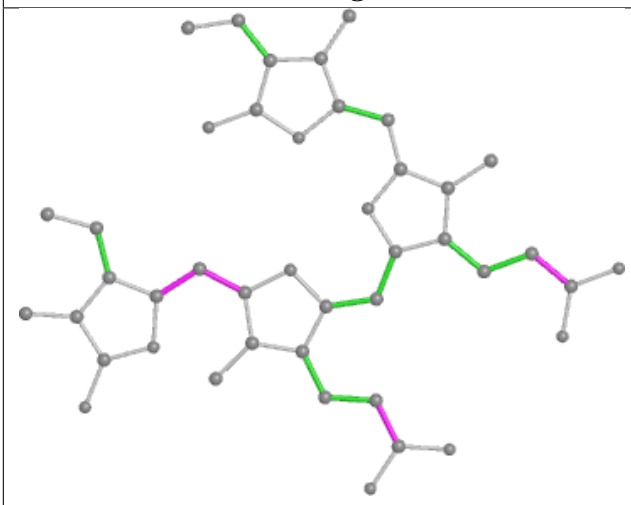

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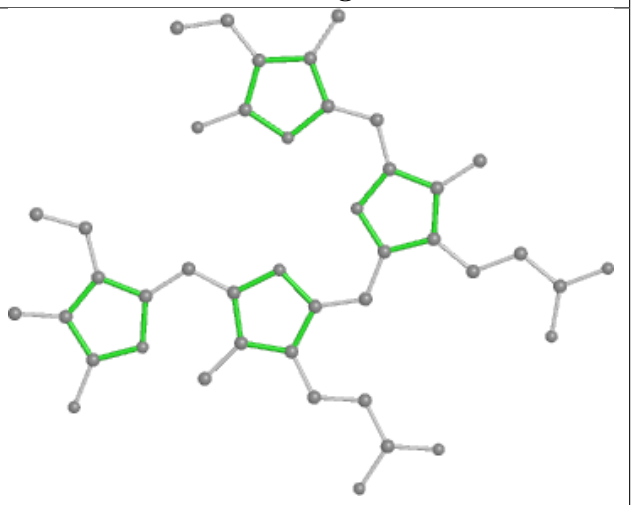
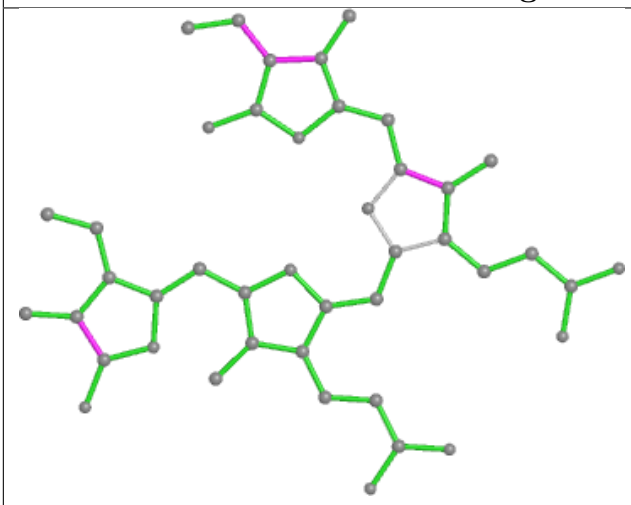


Rings

Ligand PEB o5 202



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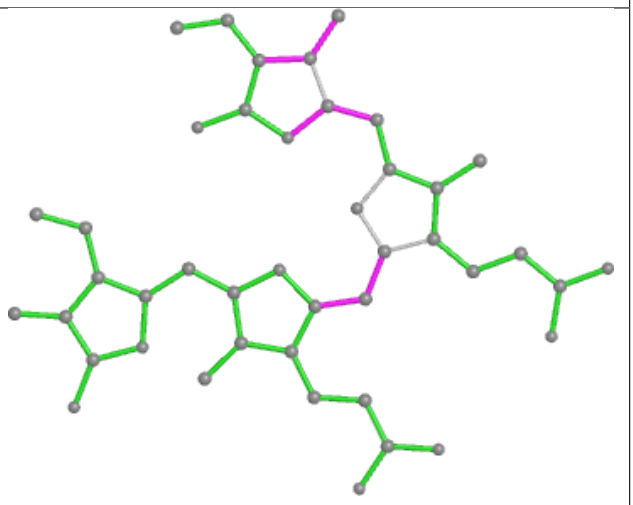

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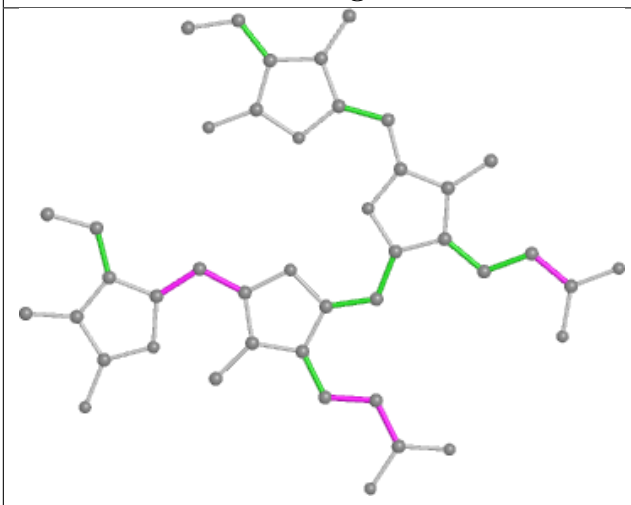

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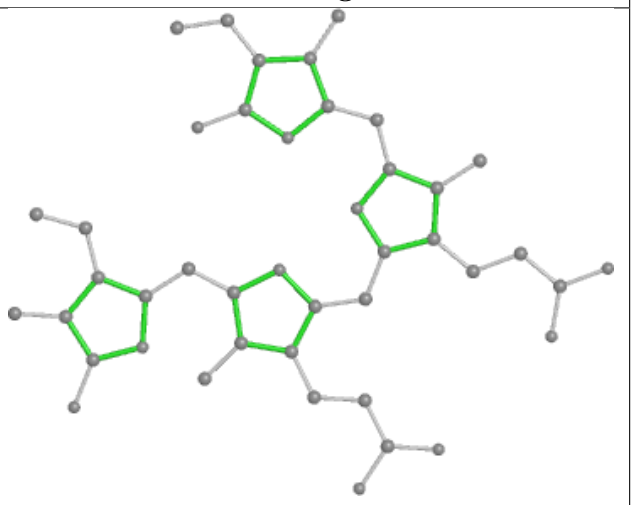
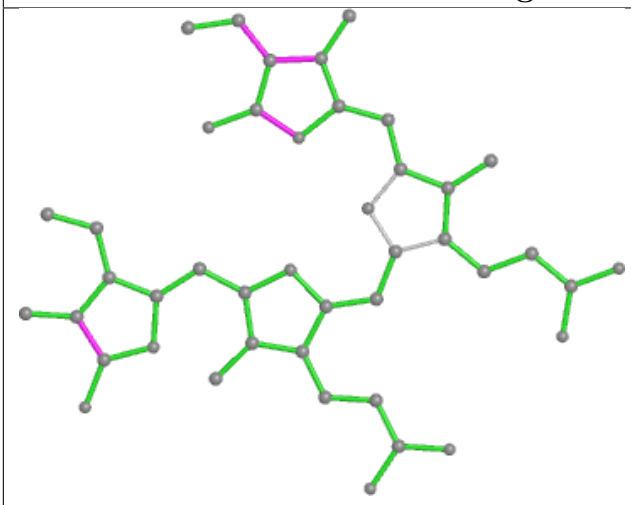


Rings

Ligand PEB T2 201



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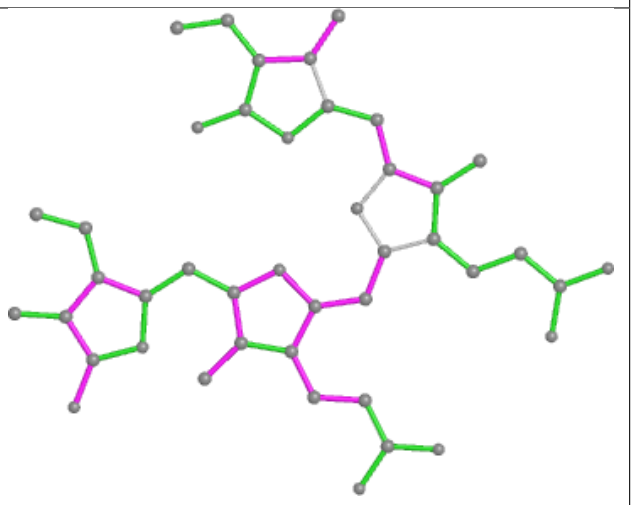
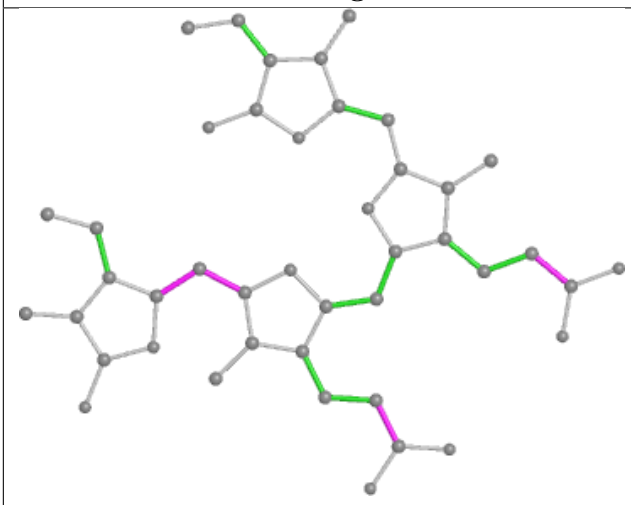


Bond angles



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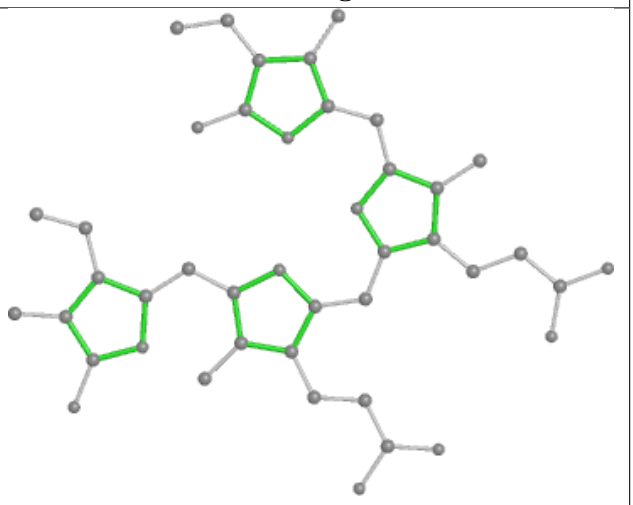
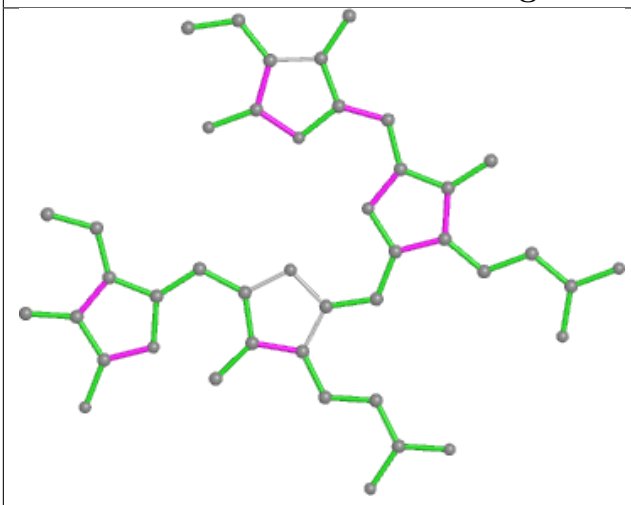


Rings

Ligand PUB r4 202



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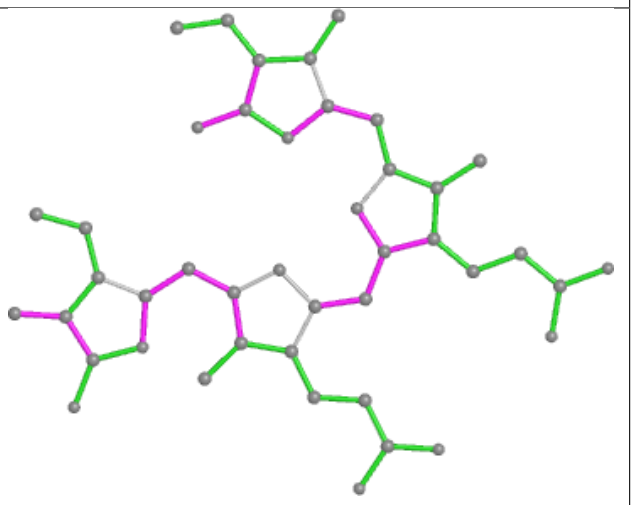

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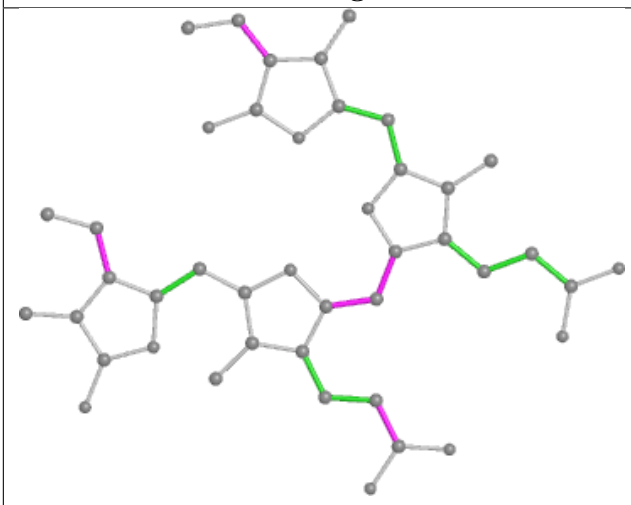

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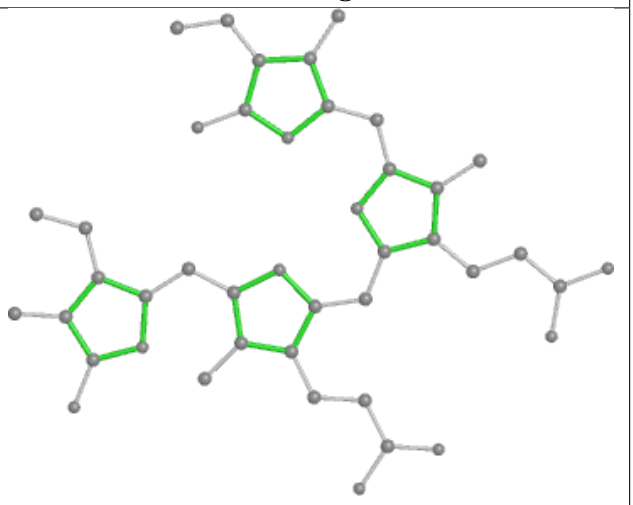
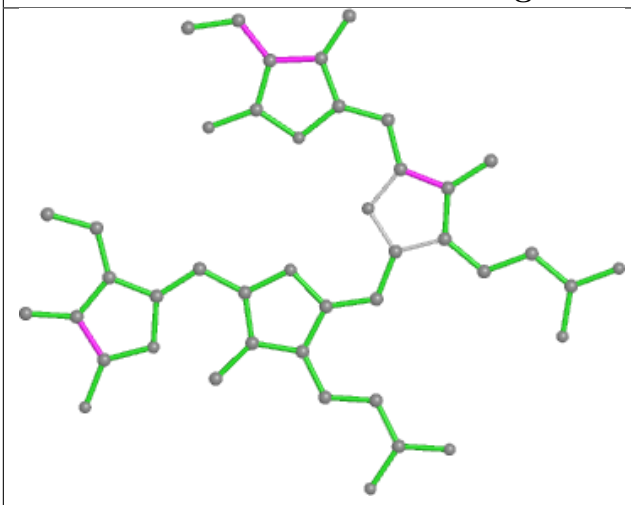


Rings

Ligand PEB hC 202



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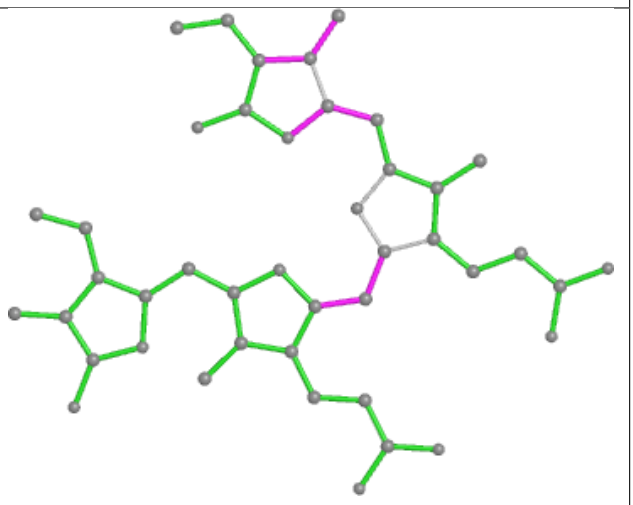

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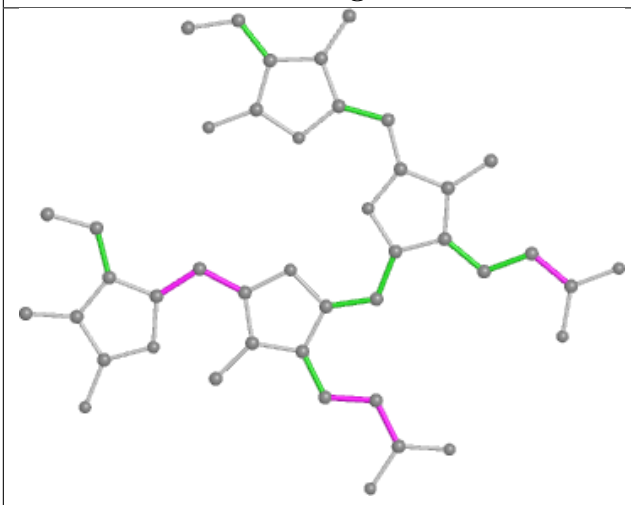

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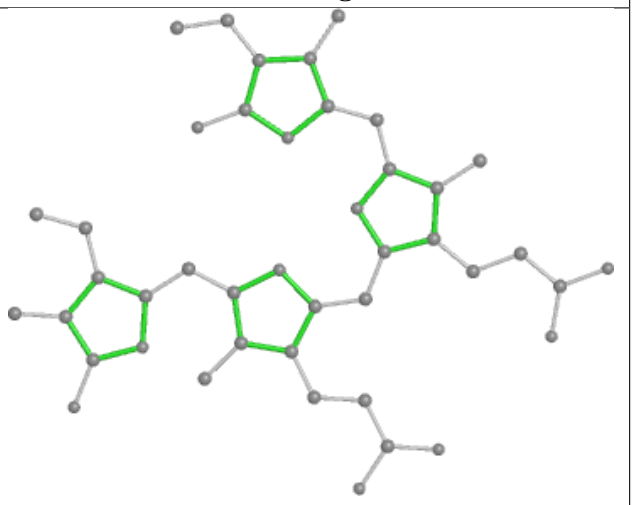
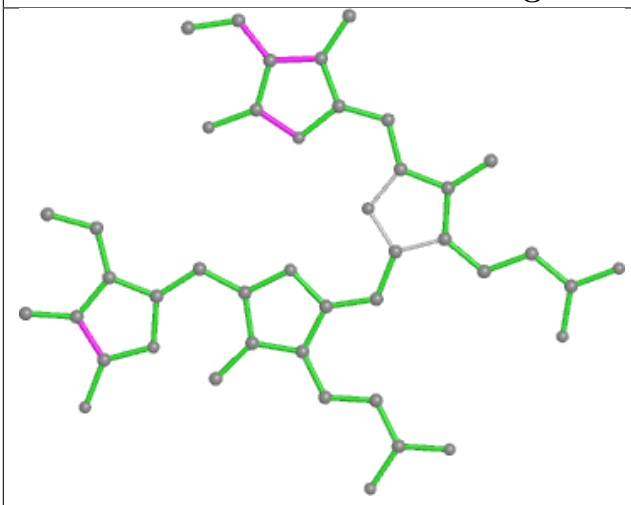


Rings

Ligand PEB i2 201



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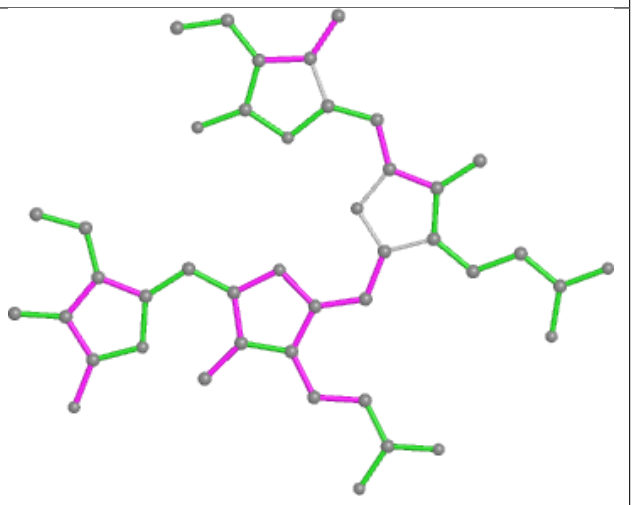

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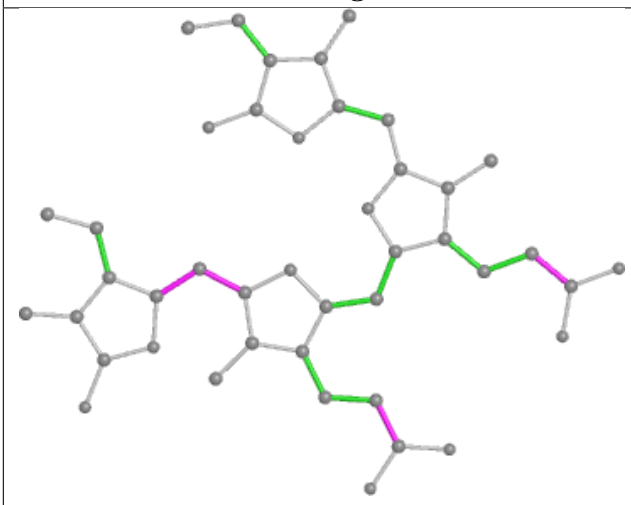

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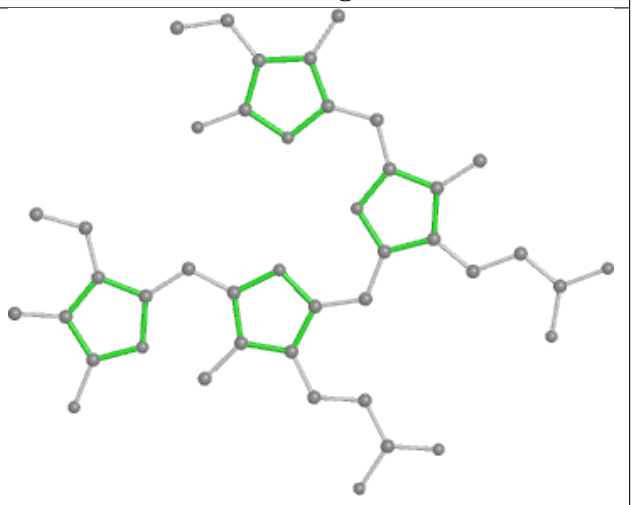

Rings

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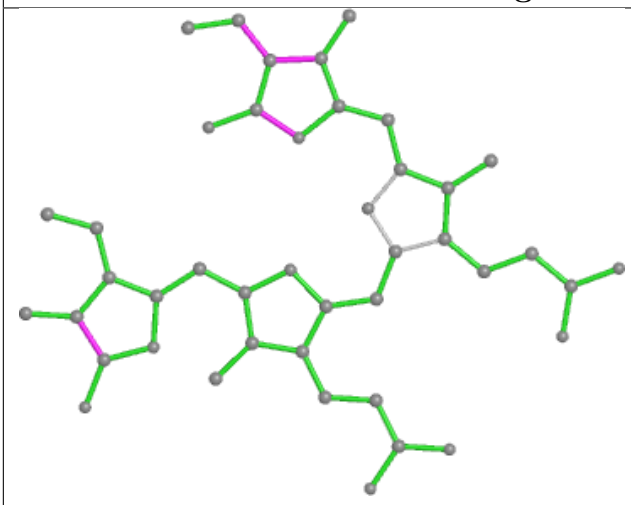

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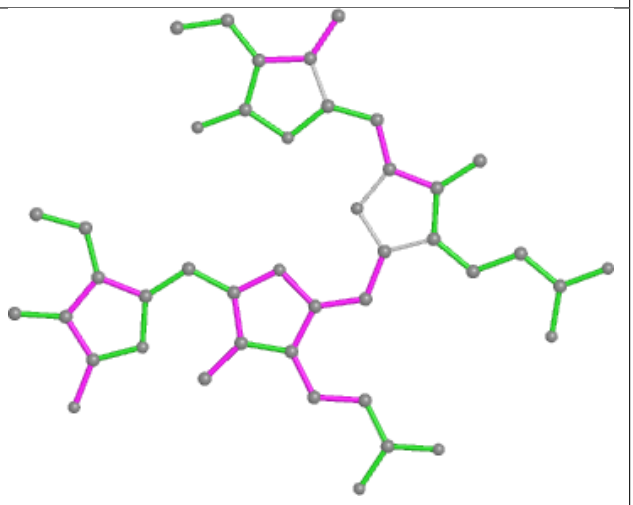

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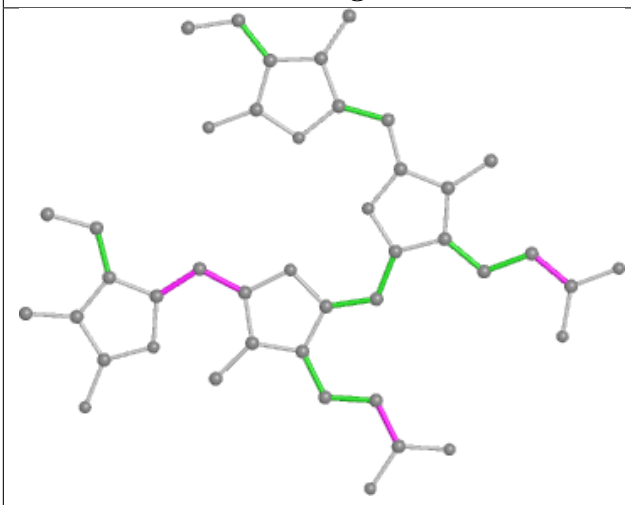

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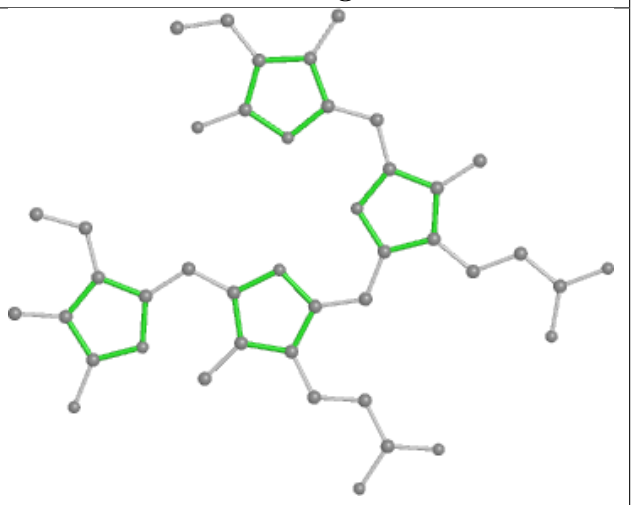
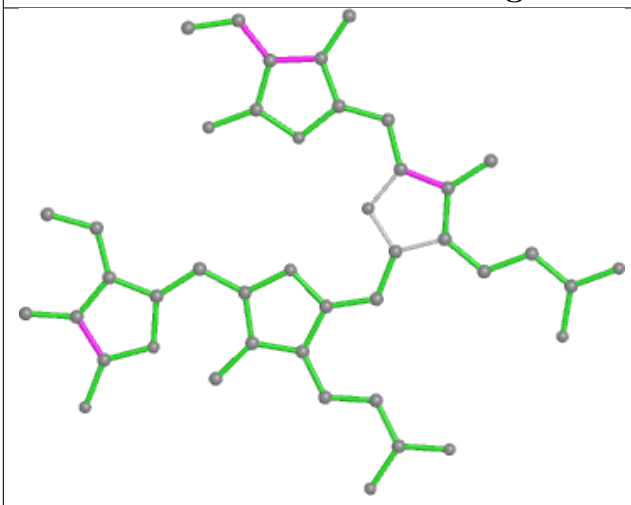


Rings

Ligand PEB cm 1002



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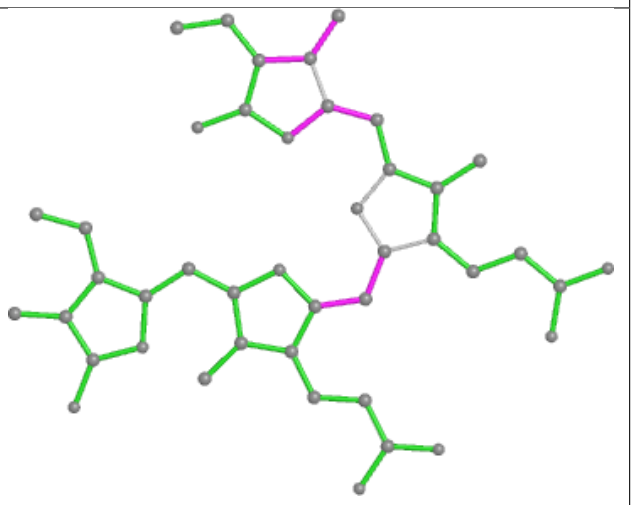

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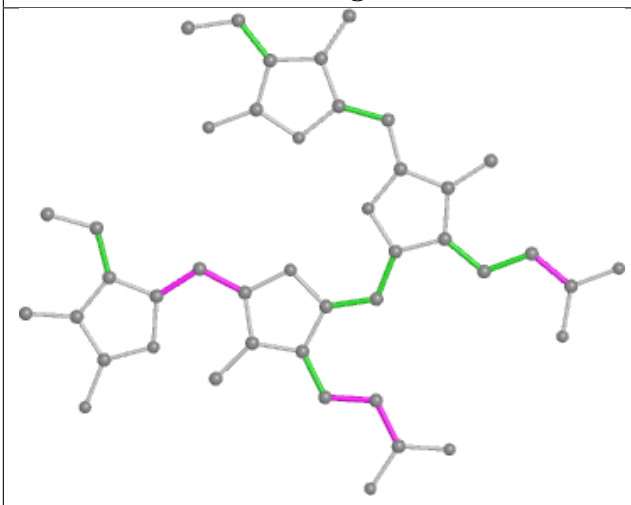

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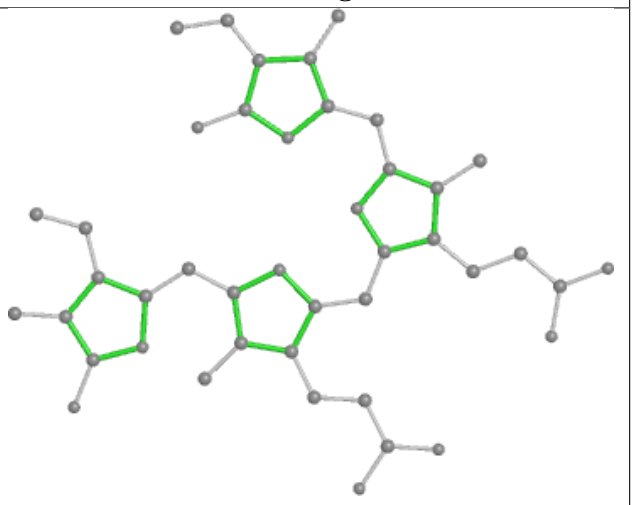
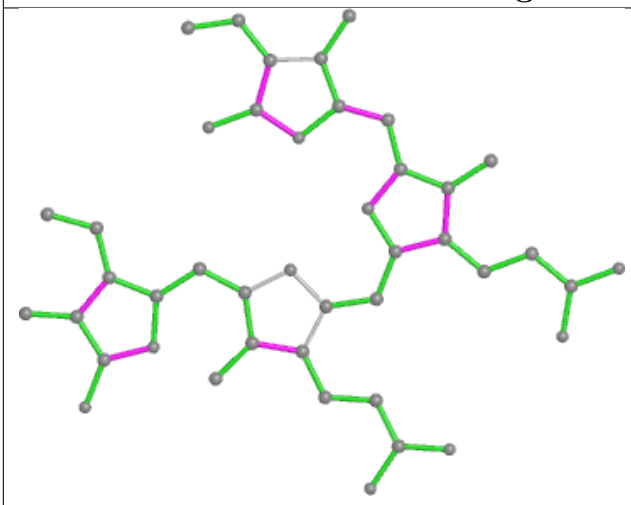


Rings

Ligand PUB dh 203



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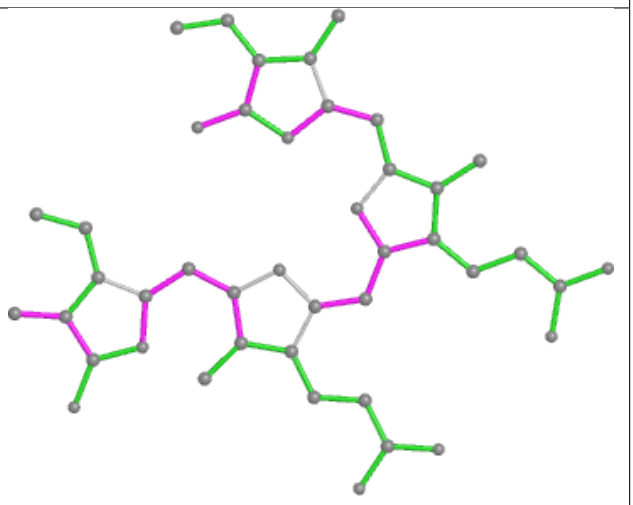

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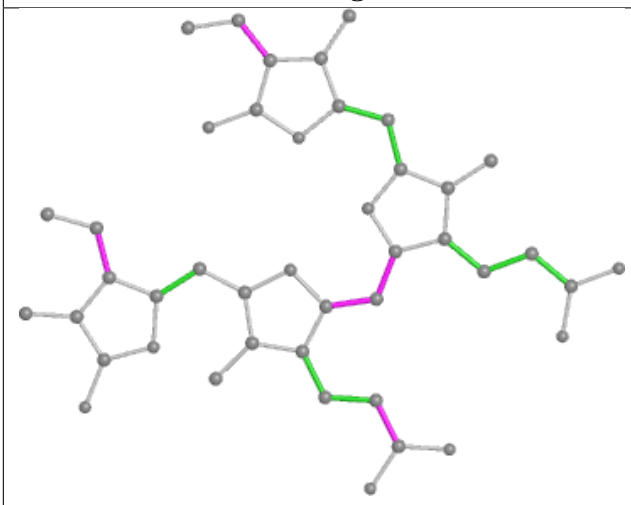

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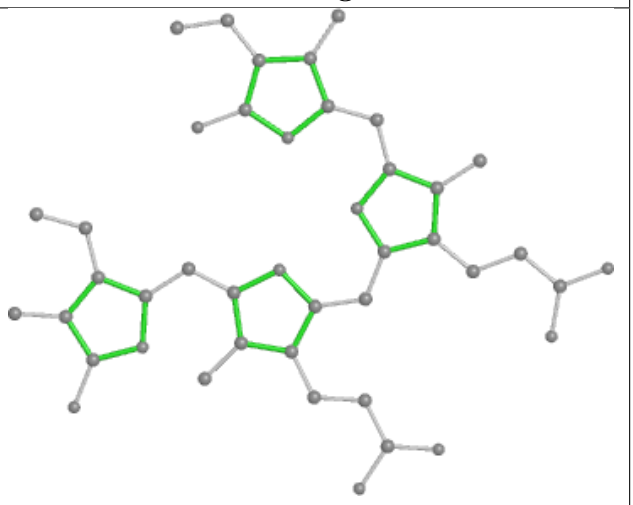
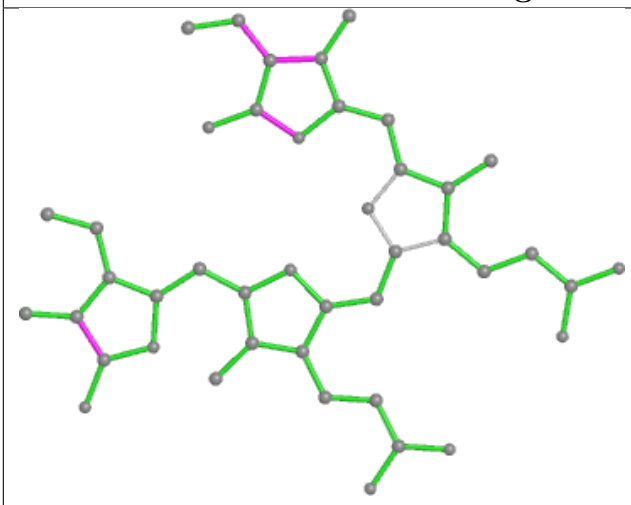


Rings

Ligand PEB K6 202



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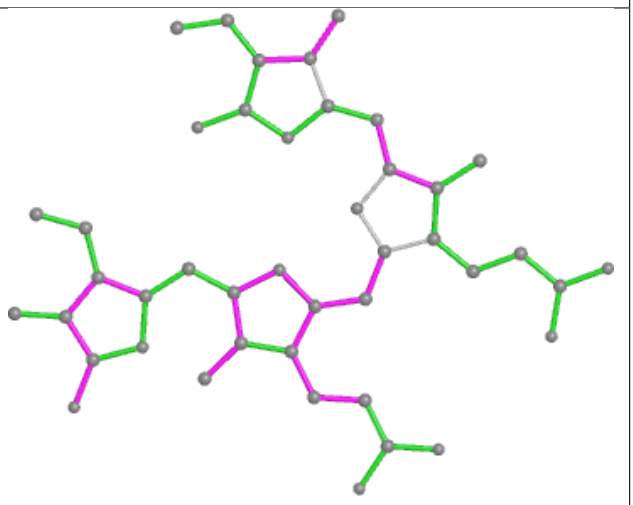

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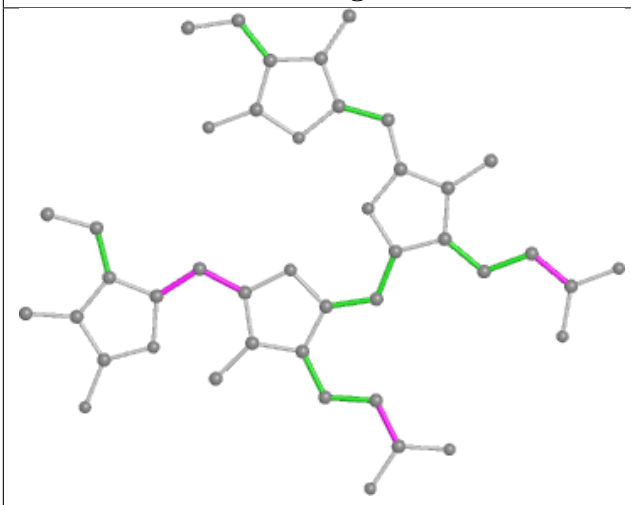

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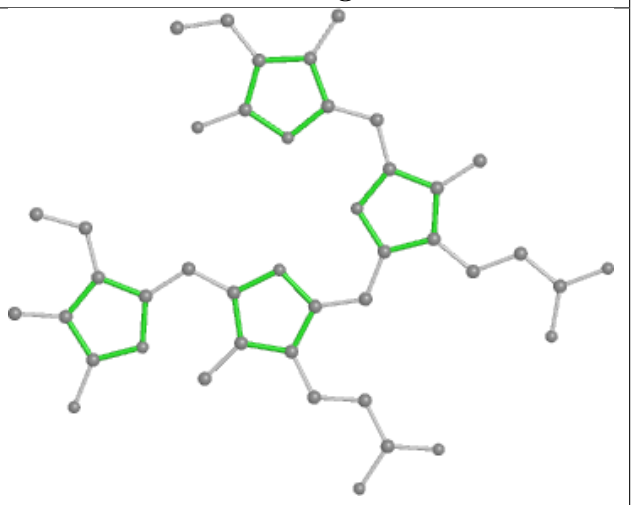

Rings

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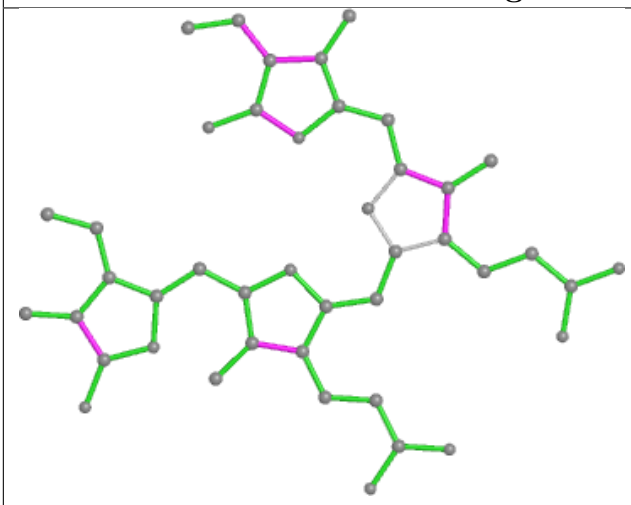

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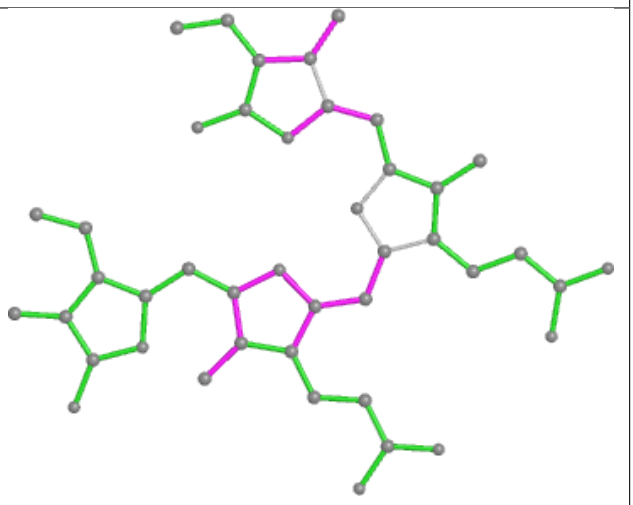

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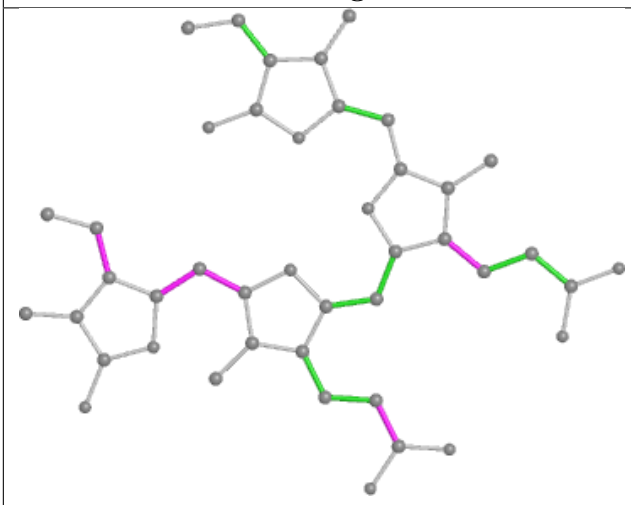

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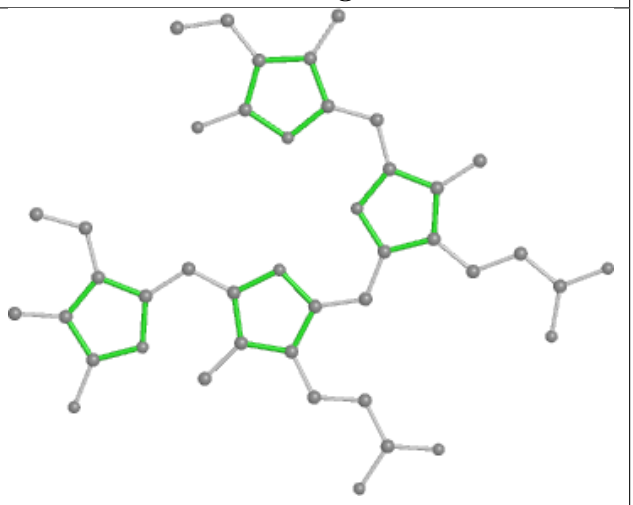
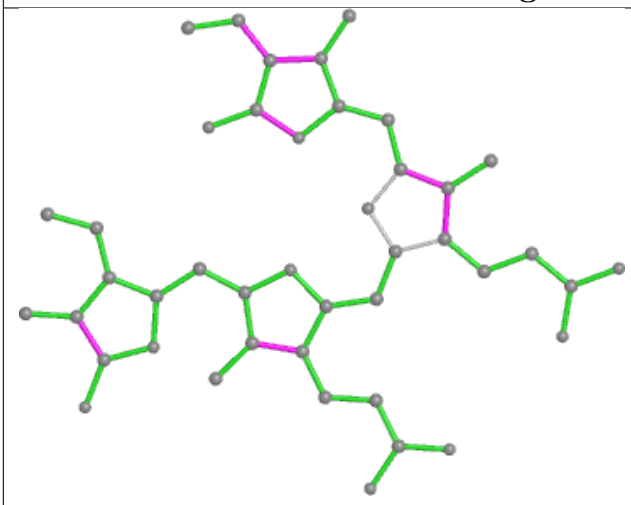


Rings

Ligand PEB v4 202



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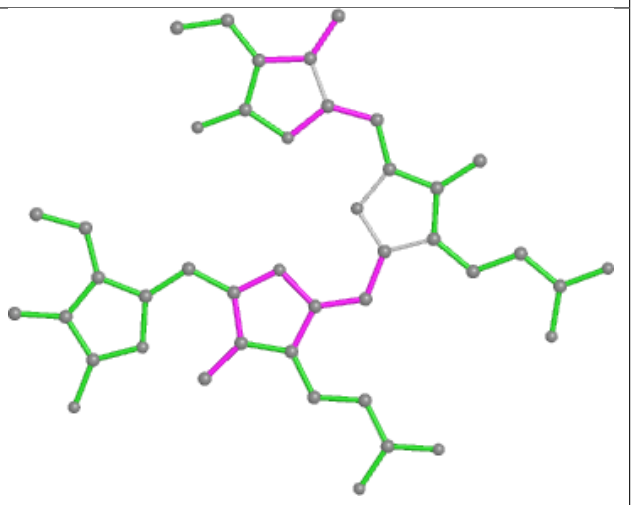

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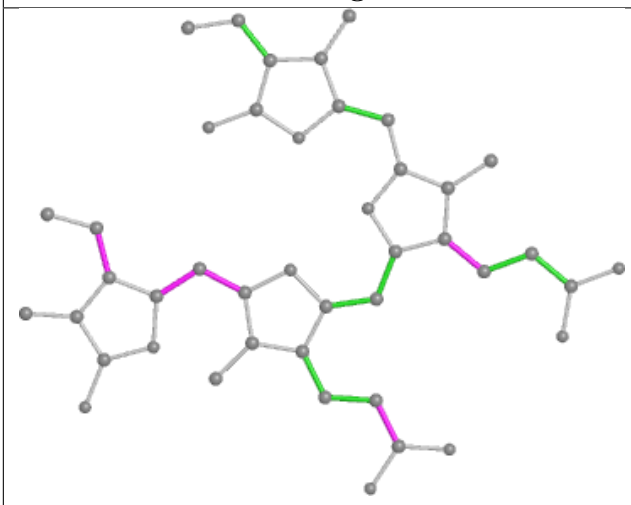

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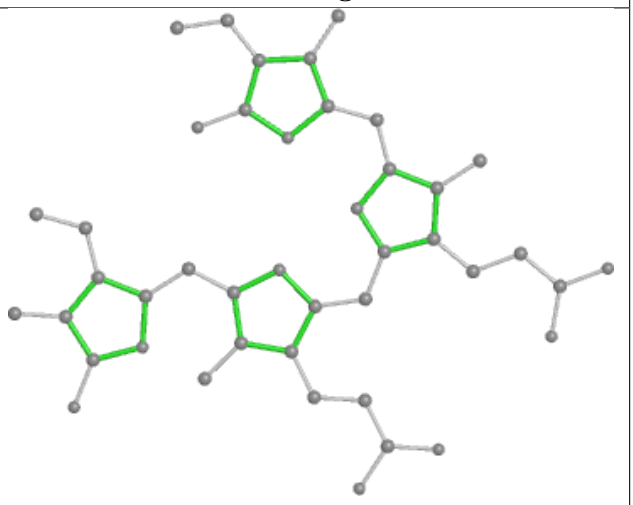
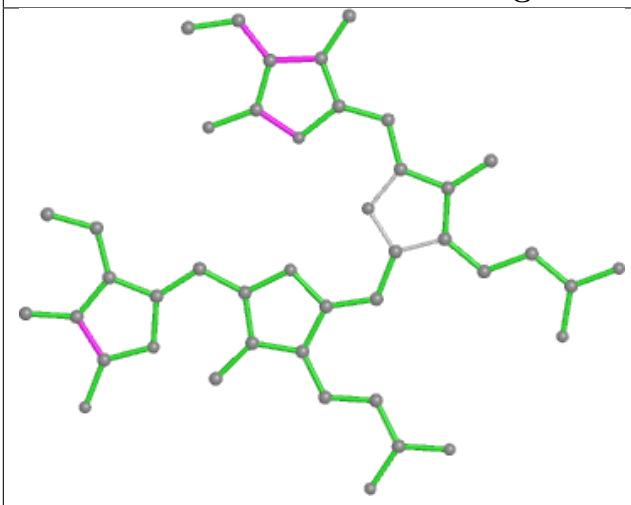


Rings

Ligand PEB dK 202



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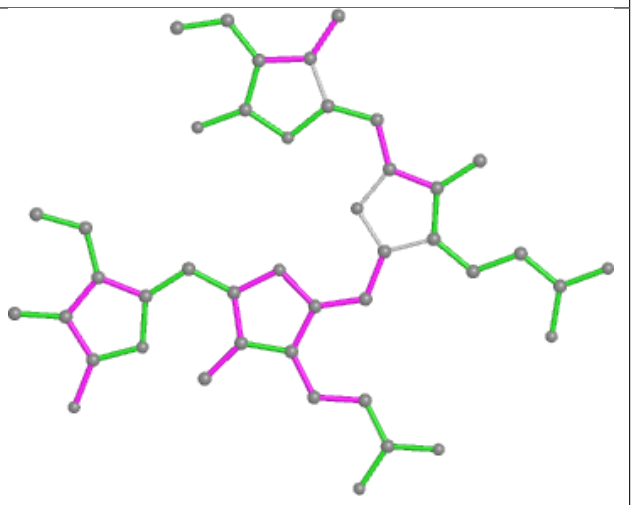

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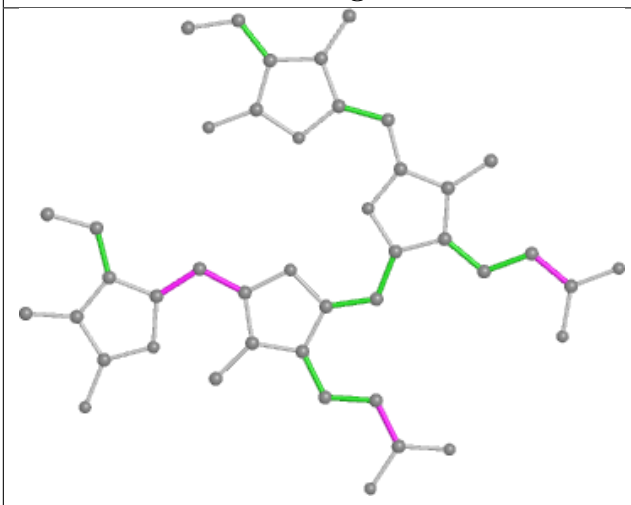
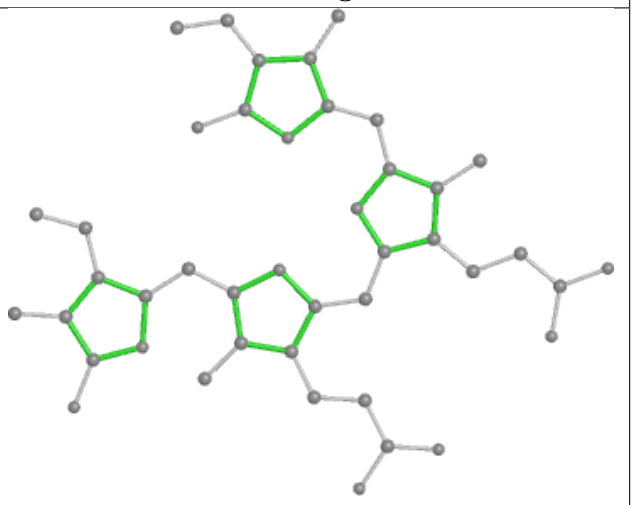
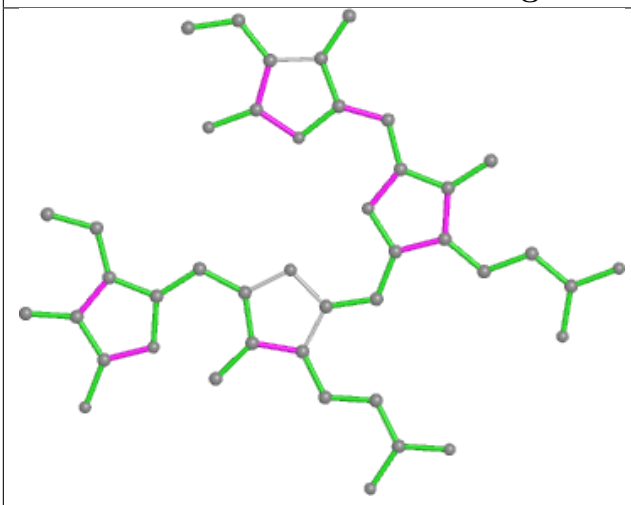


Torsions



Rings

Ligand PUB f2 203



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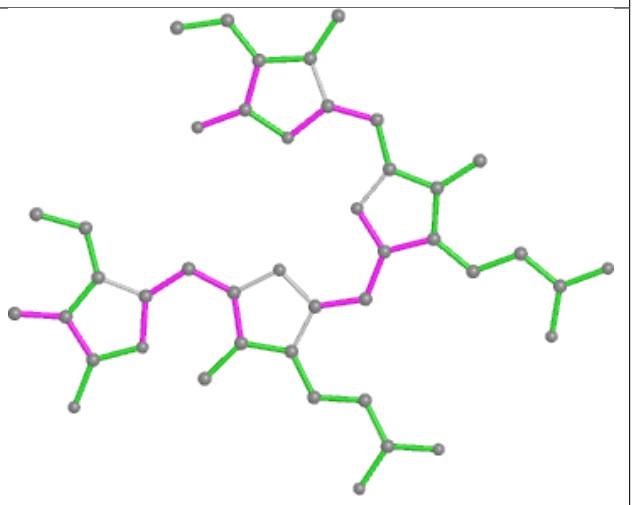

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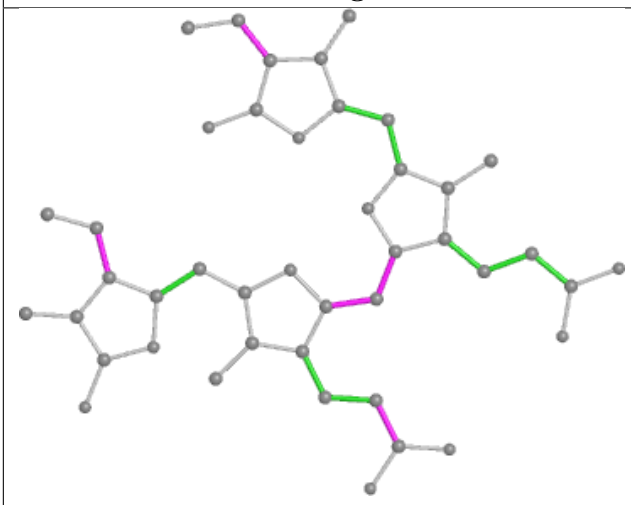

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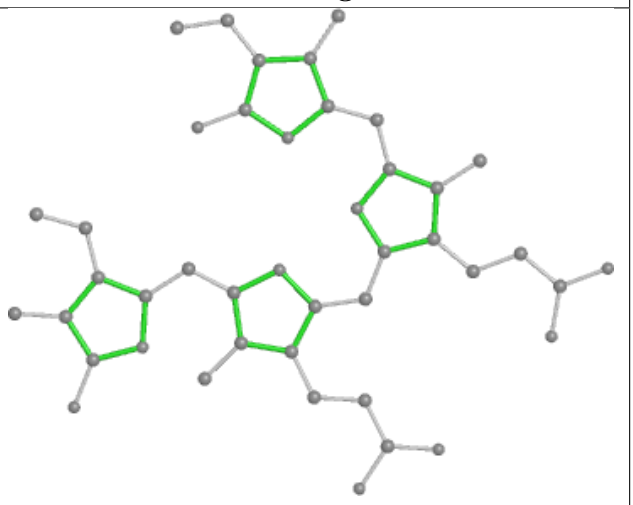
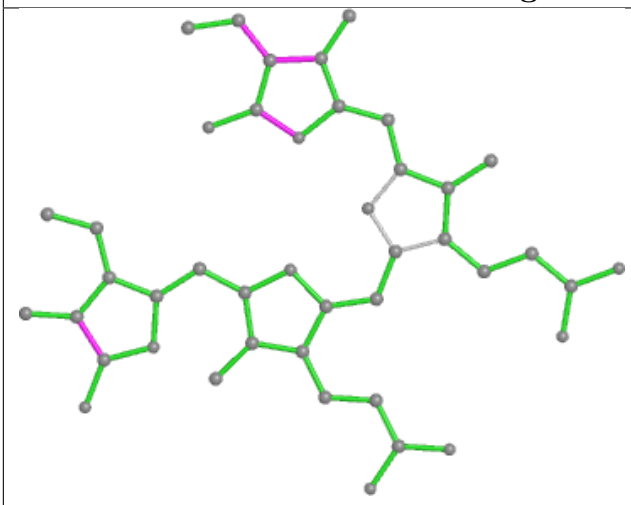


Rings

Ligand PEB ga 201



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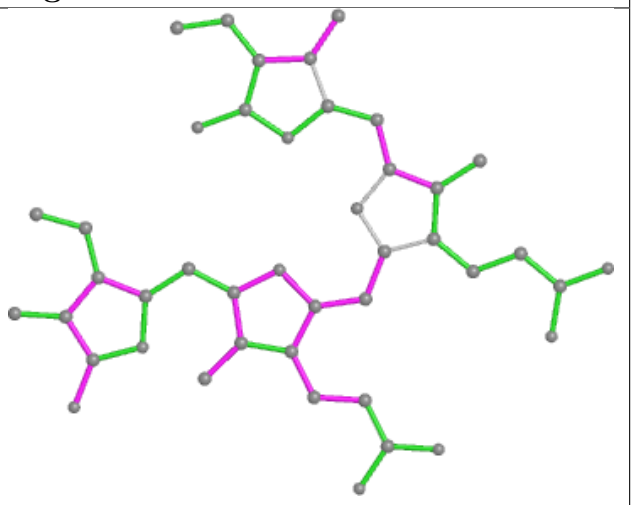

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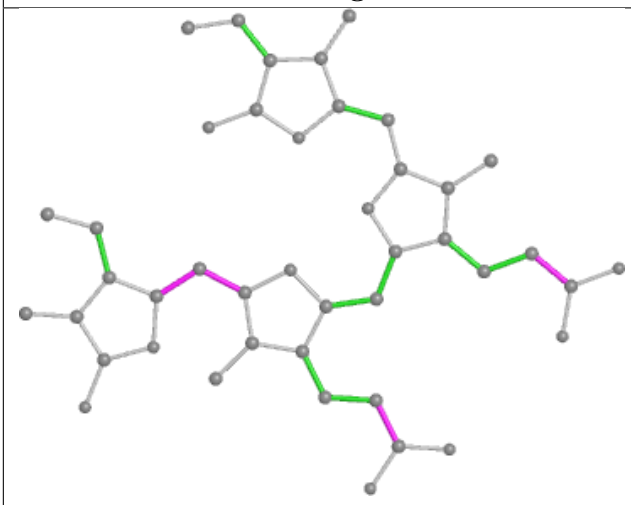

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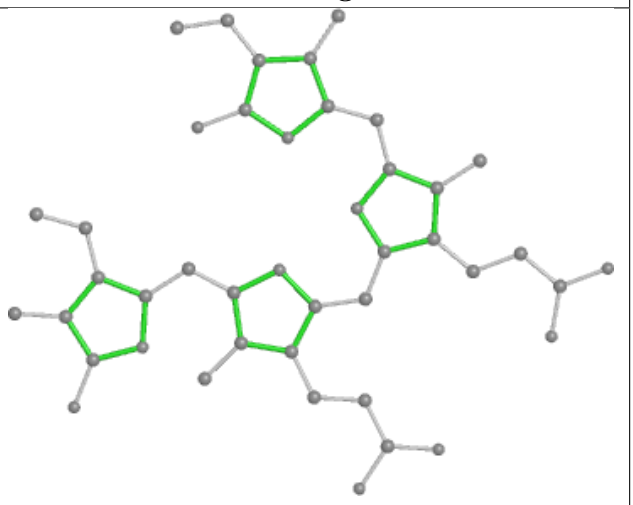
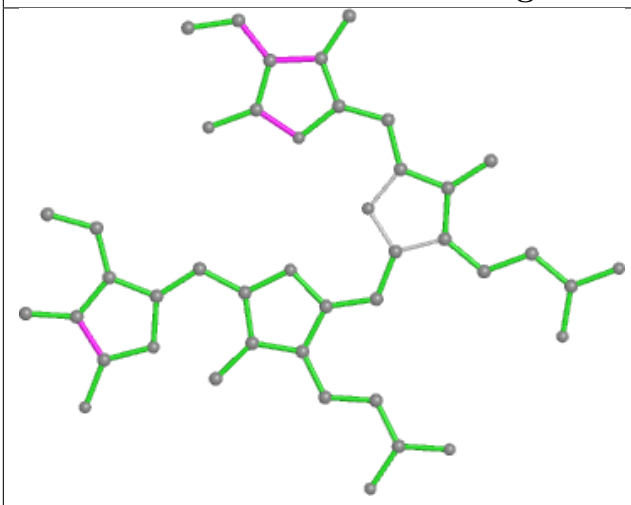


Rings

Ligand PEB hZ 402



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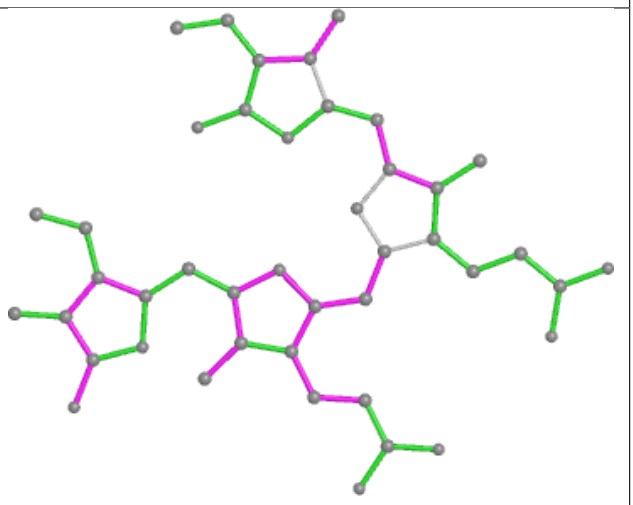

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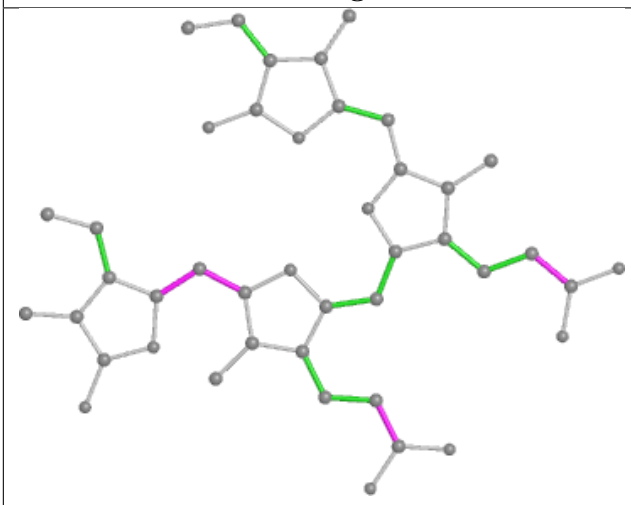

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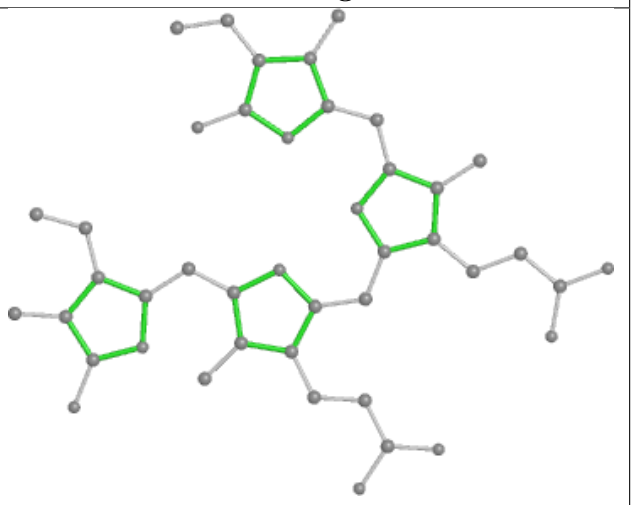
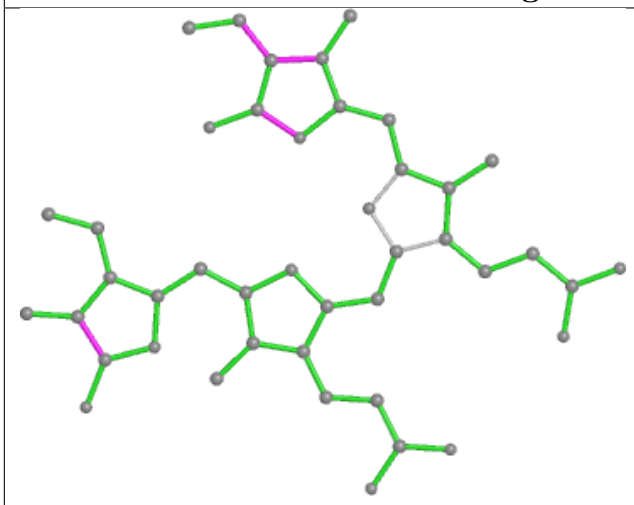


Rings

Ligand PEB c7 201



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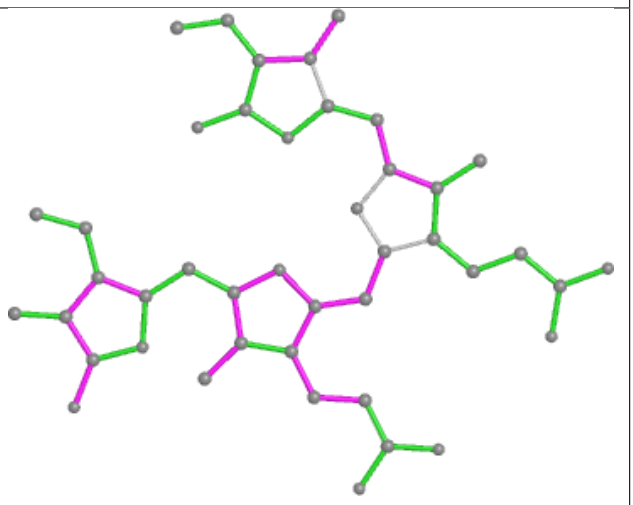
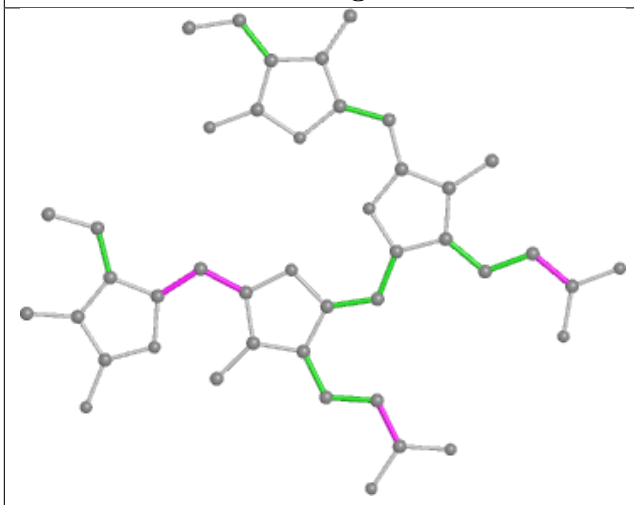


Bond angles



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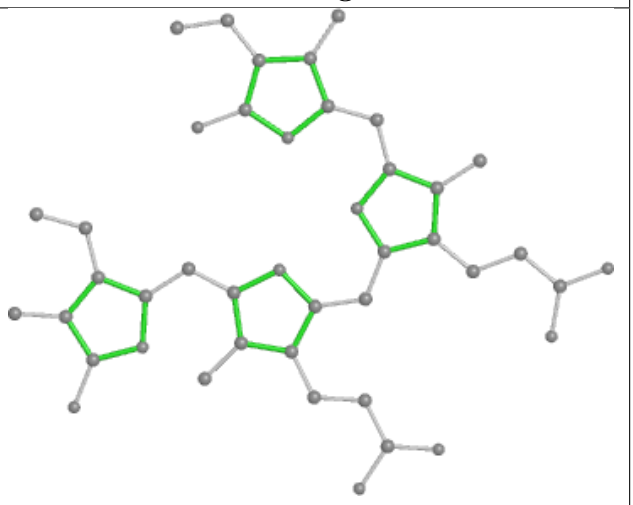
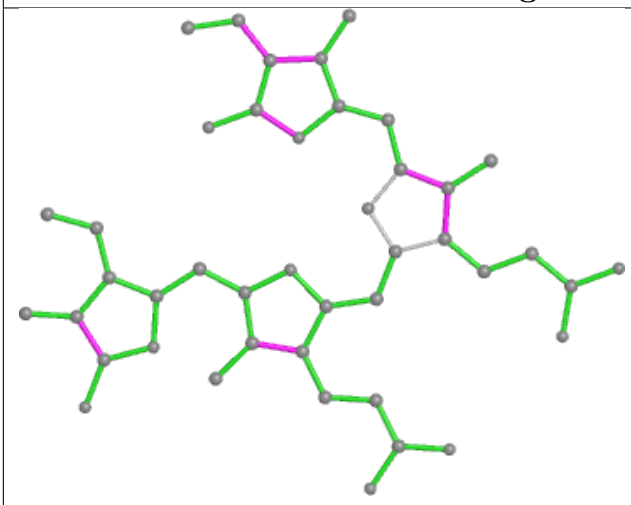


Rings

Ligand PEB J9 202



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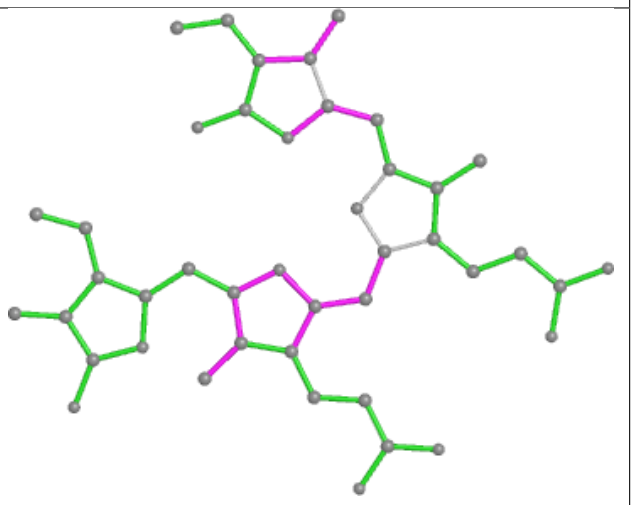

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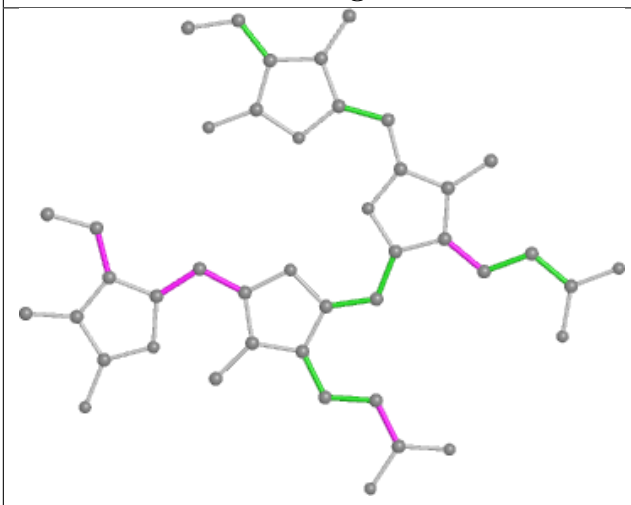

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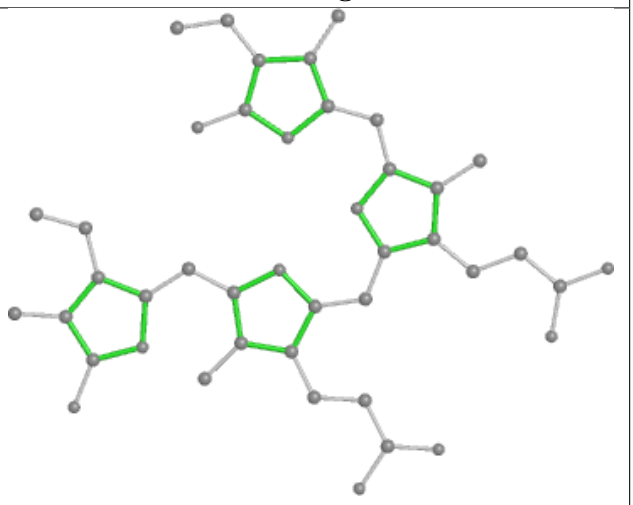

Rings

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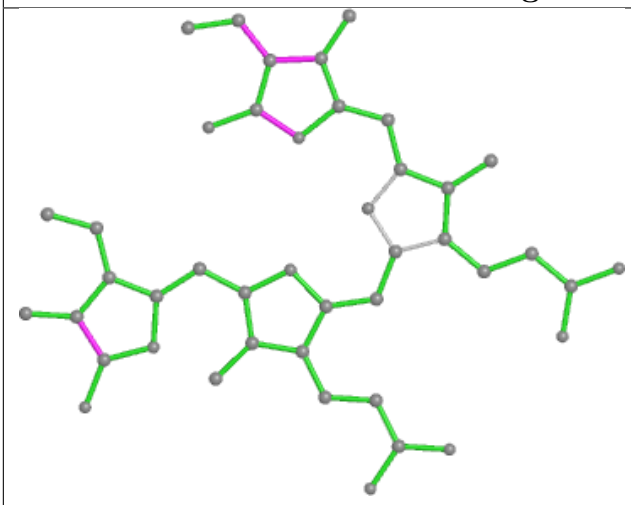

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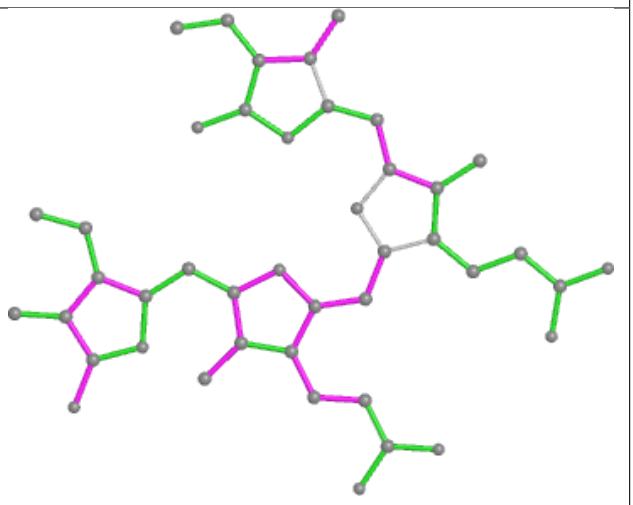

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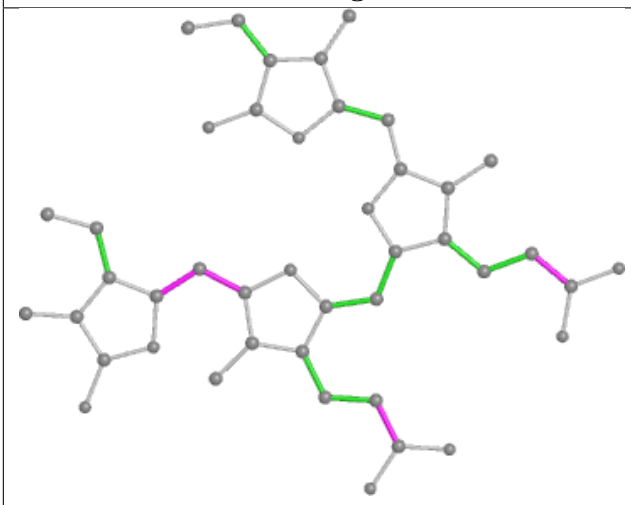

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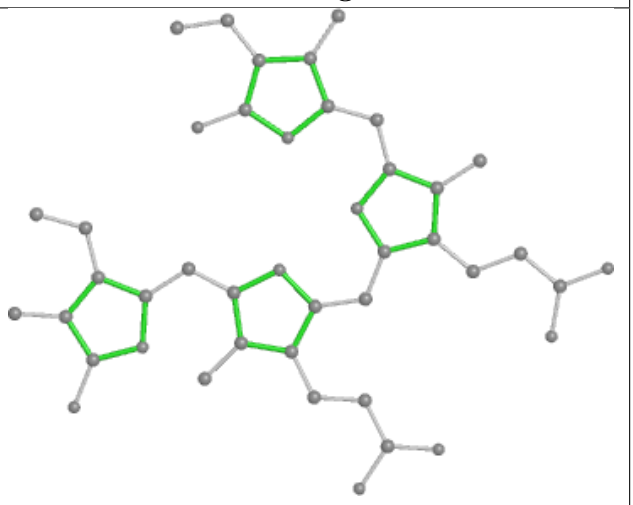
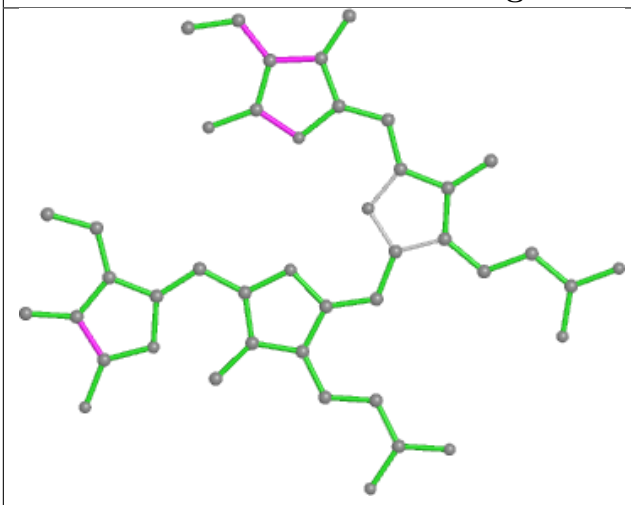


Rings

Ligand PEB Y7 1001



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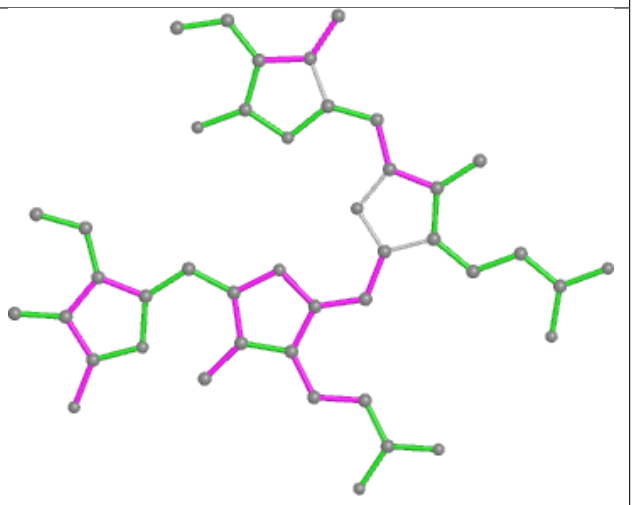

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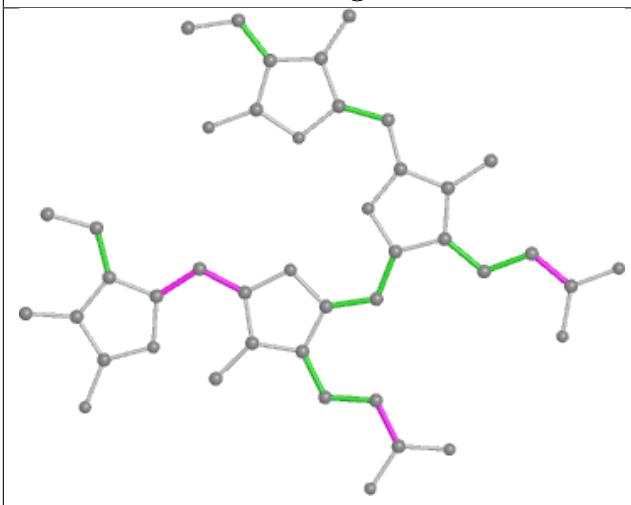

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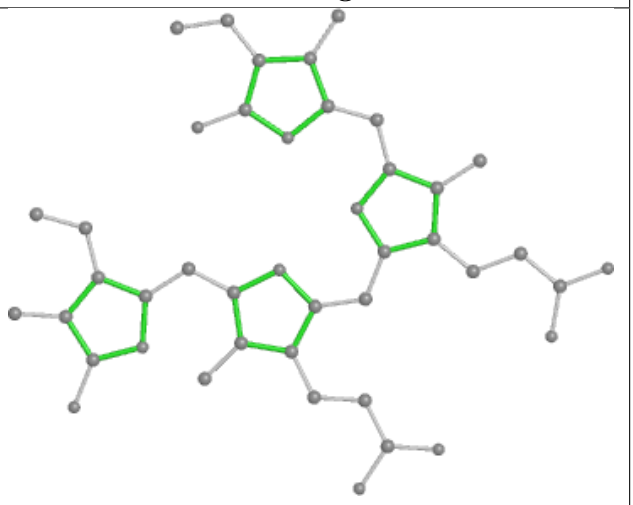
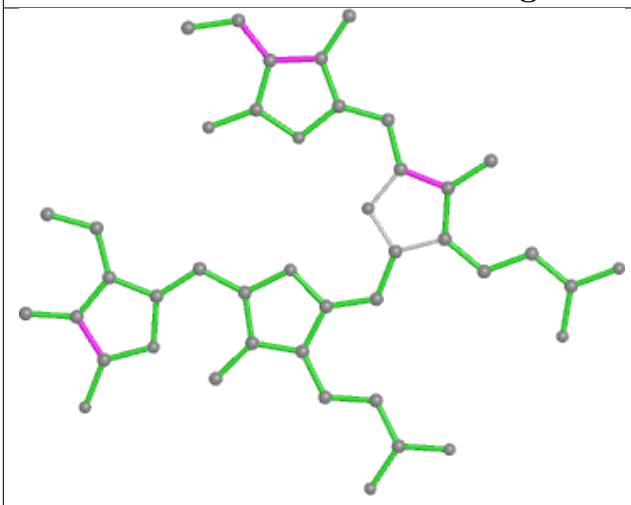


Rings

Ligand PEB eh 202



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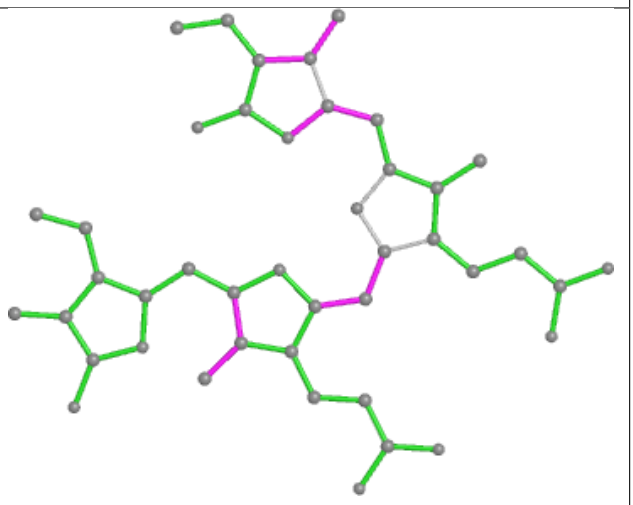

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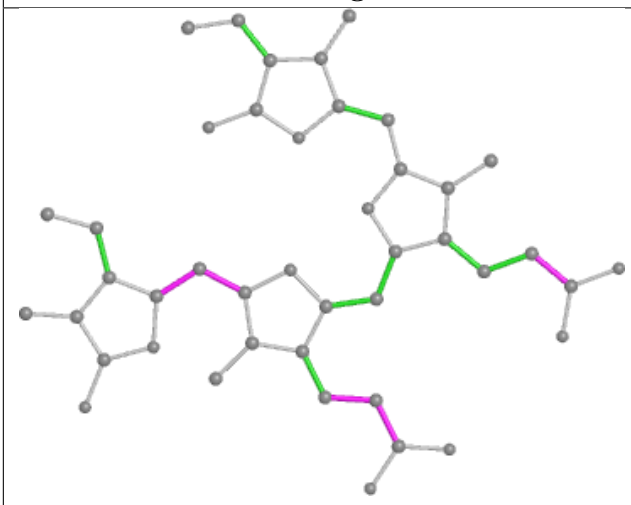

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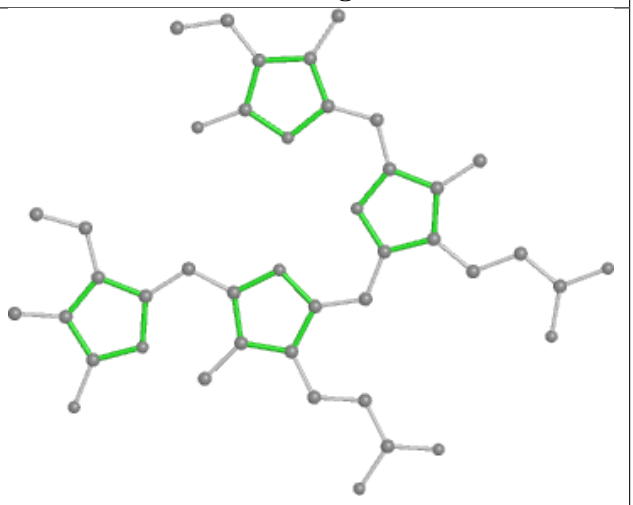
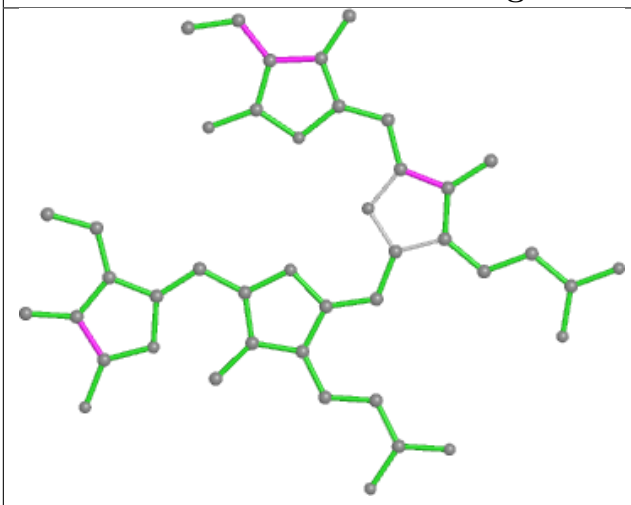


Rings

Ligand PEB hE 1002



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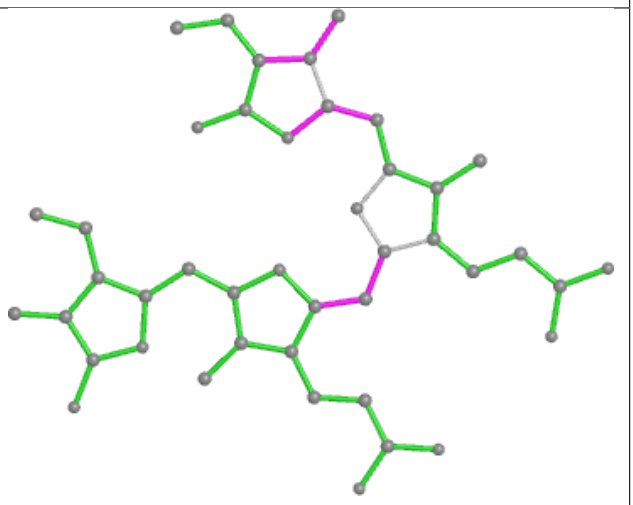

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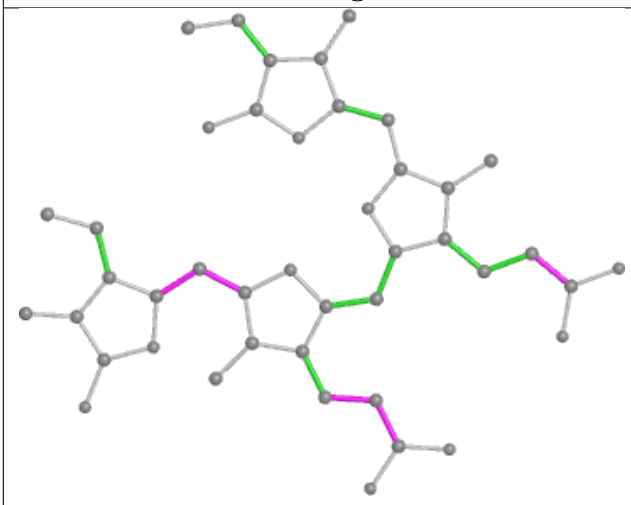

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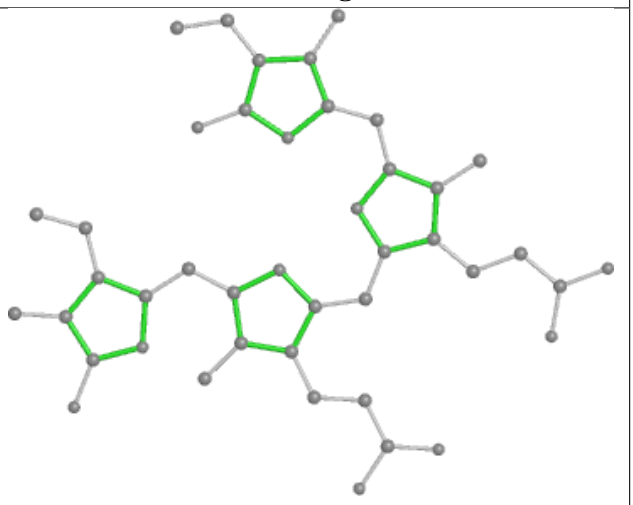
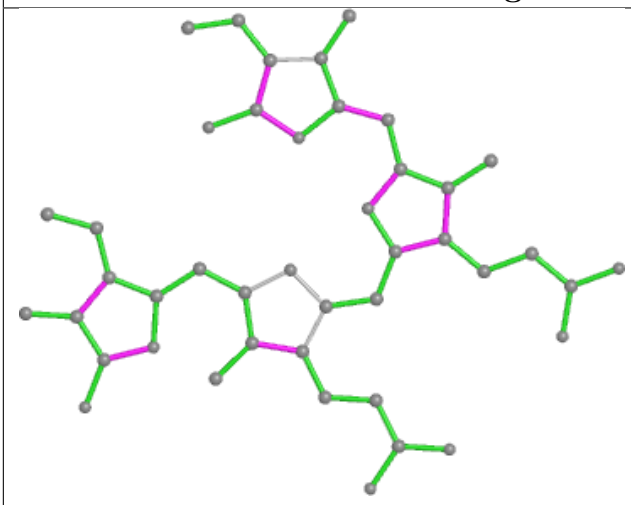


Rings

Ligand PUB A2 1006



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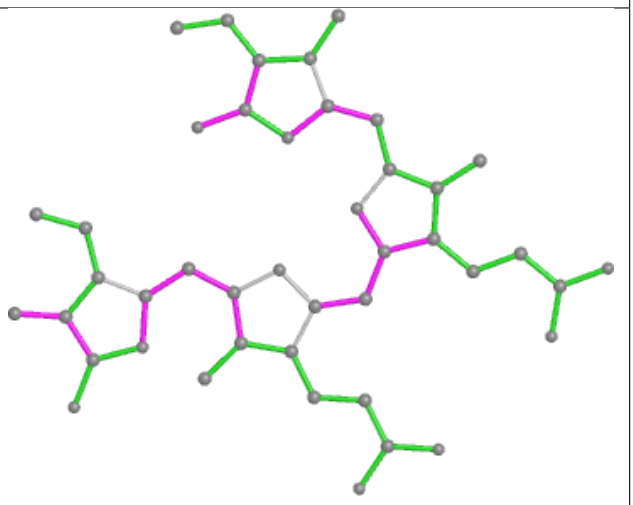

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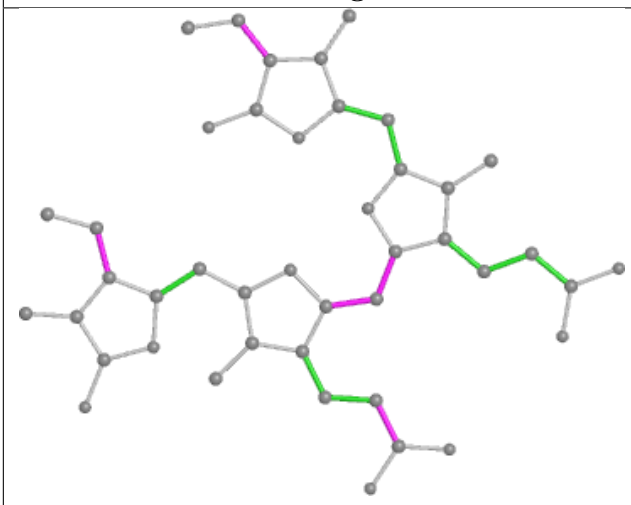

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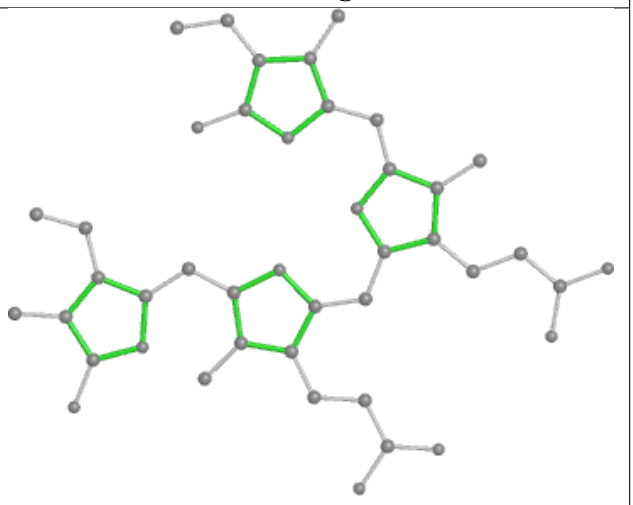
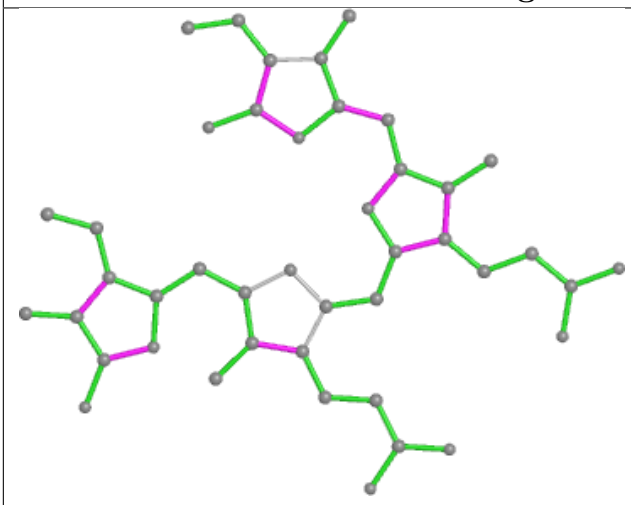


Rings

Ligand PUB eb 202



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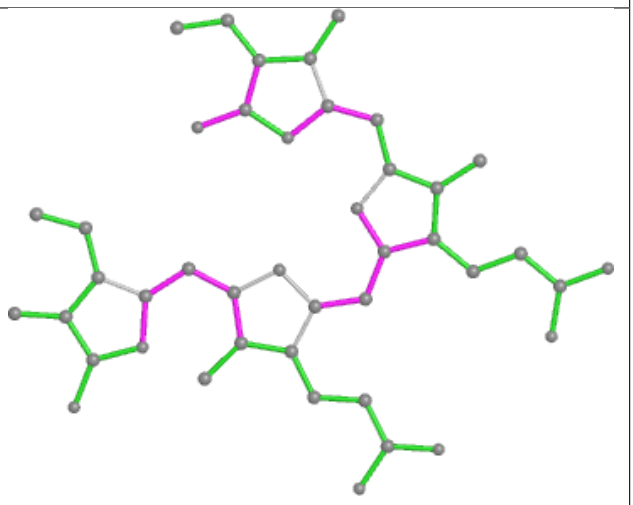

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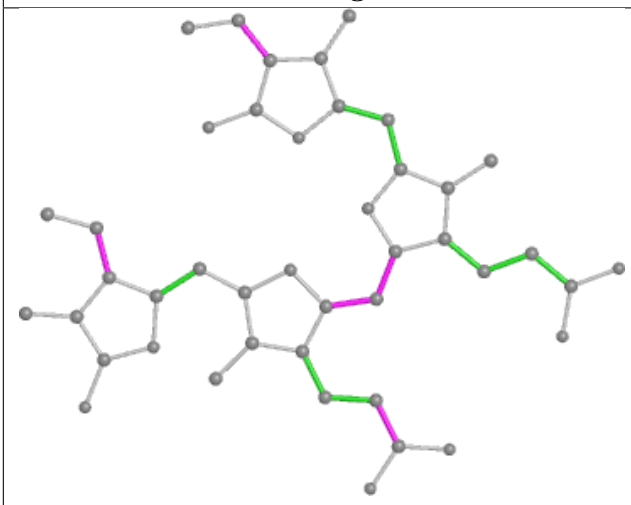

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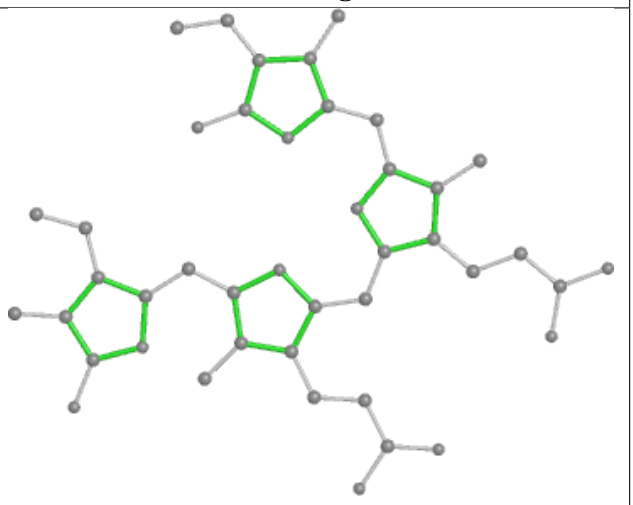
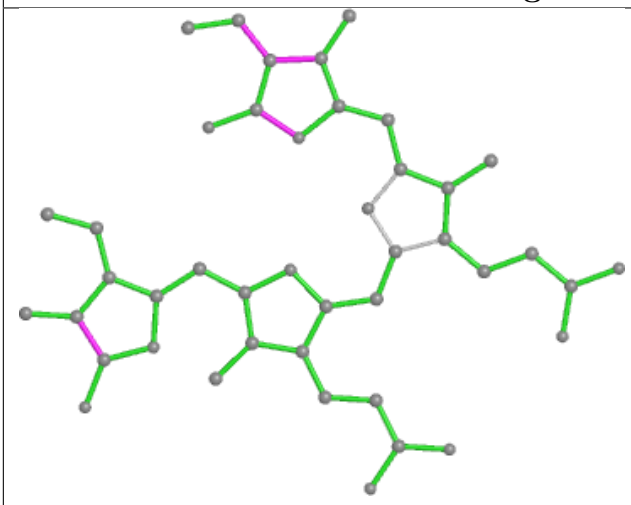


Rings

Ligand PEB l8 202



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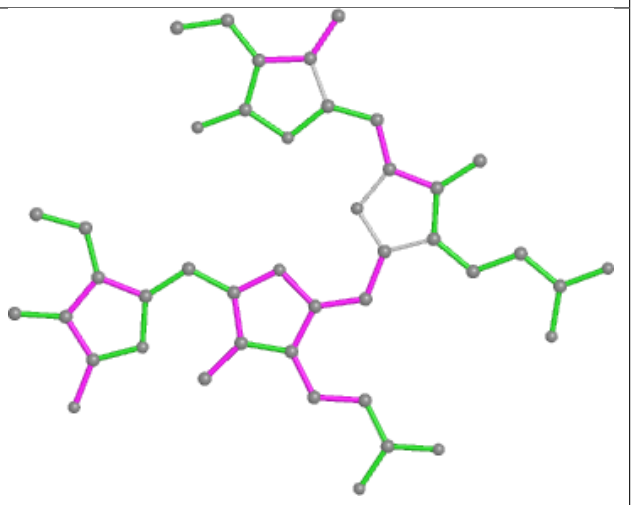
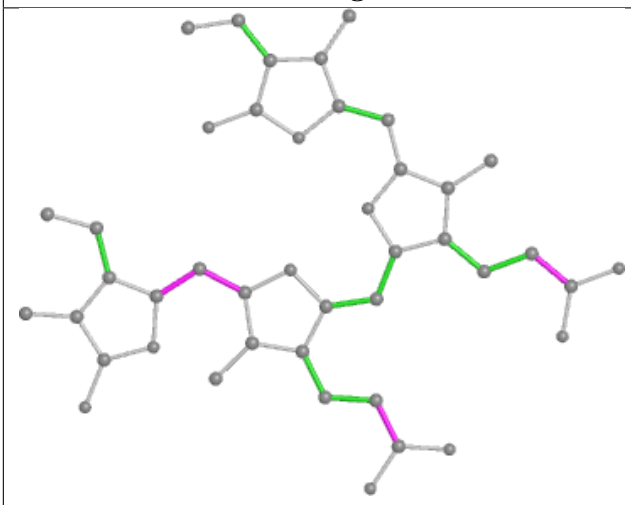


Bond angles



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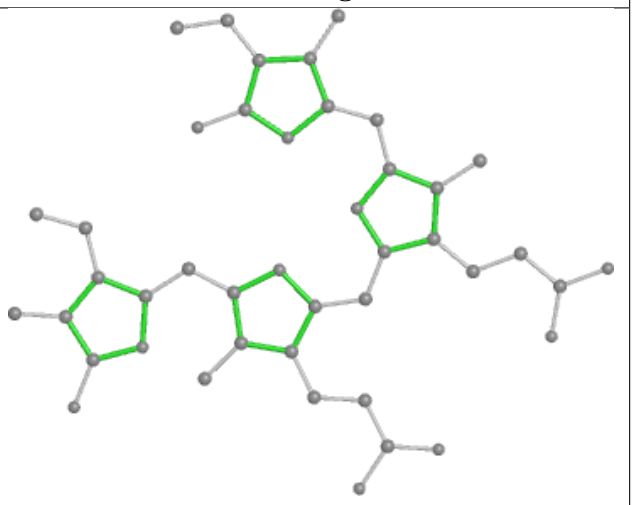
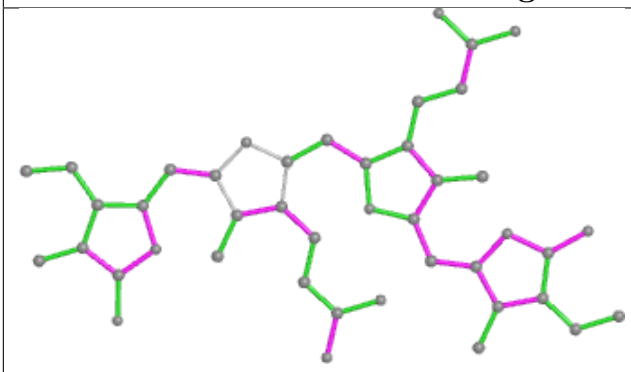


Rings

Ligand CYC z1 201



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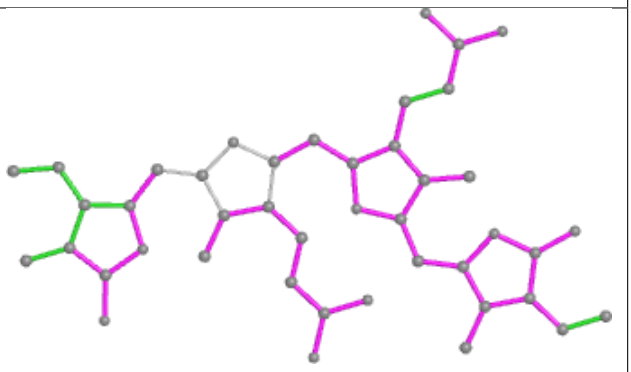
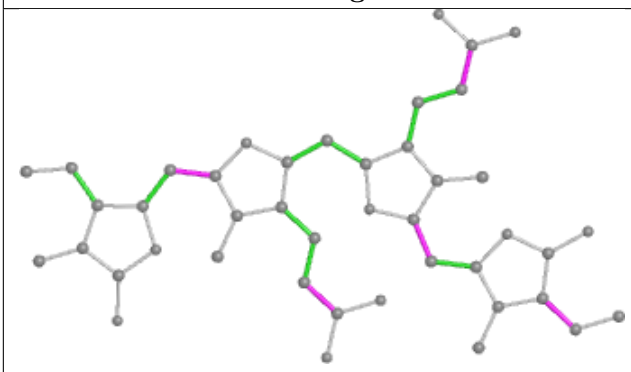


Bond angles



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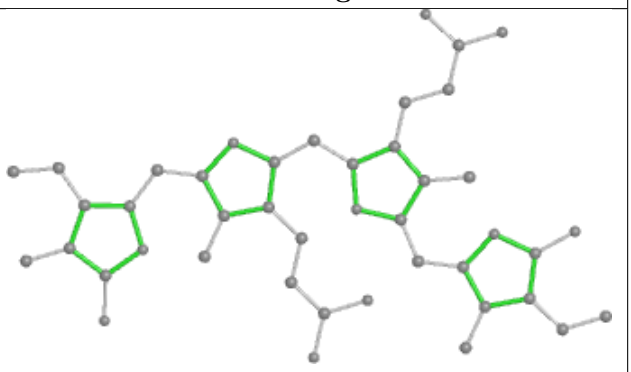
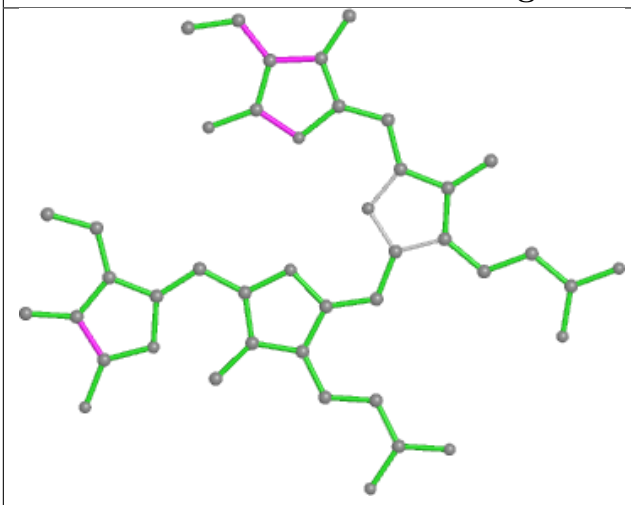
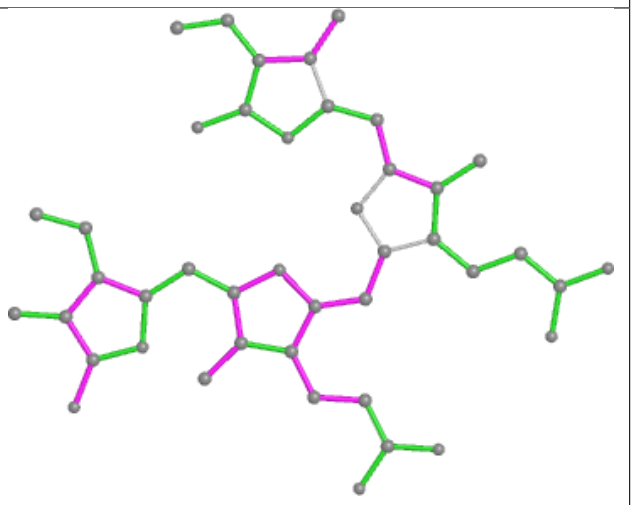


Rings

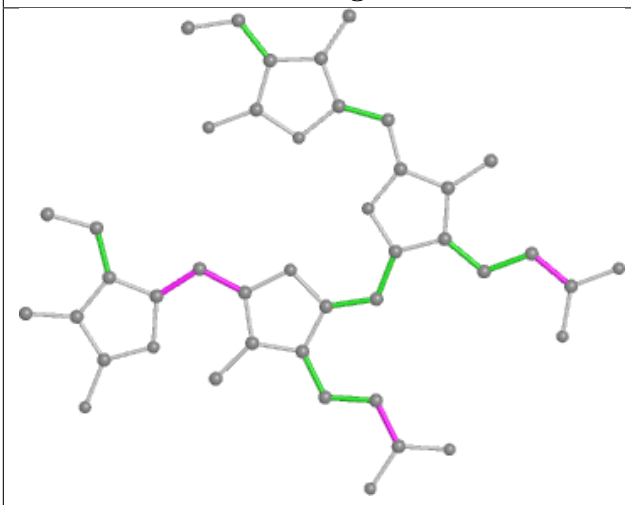
Ligand PEB dn 201



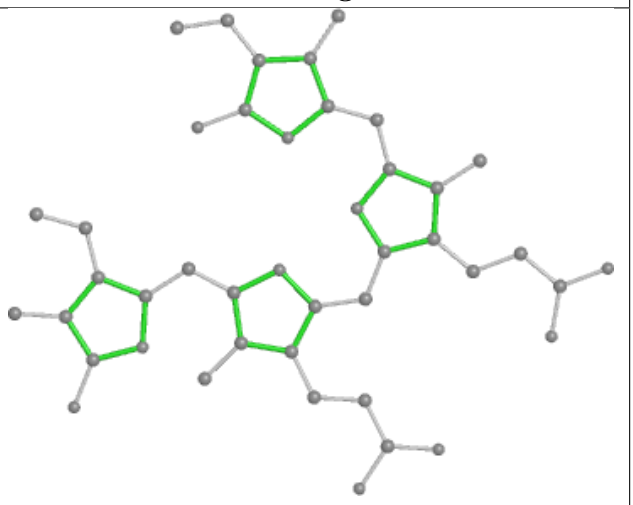
Bond lengths



Bond angles

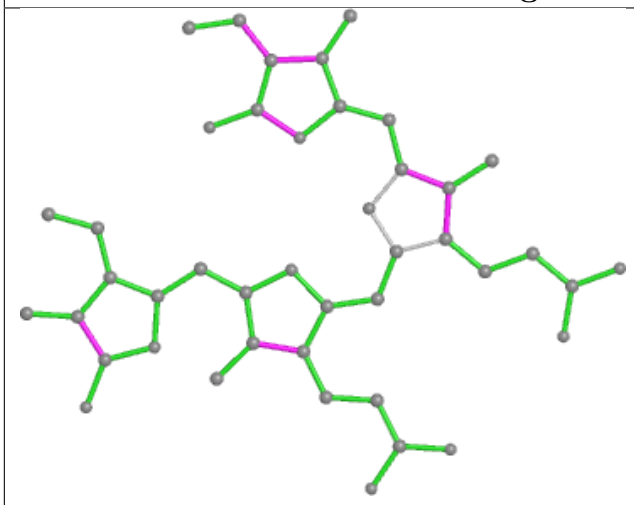


Torsions



Rings

Ligand PEB J5 202



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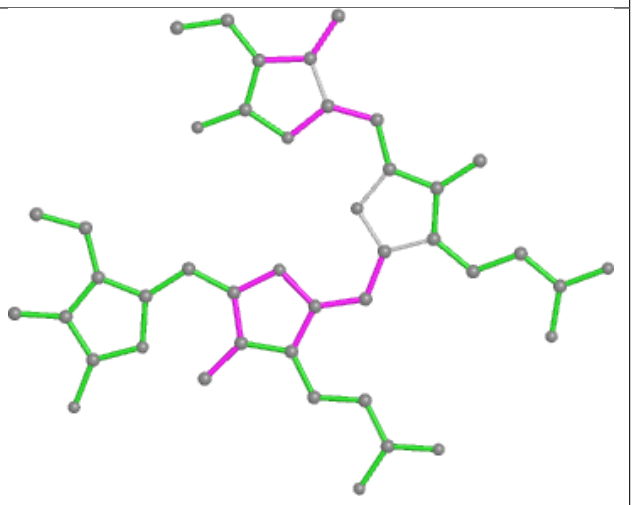

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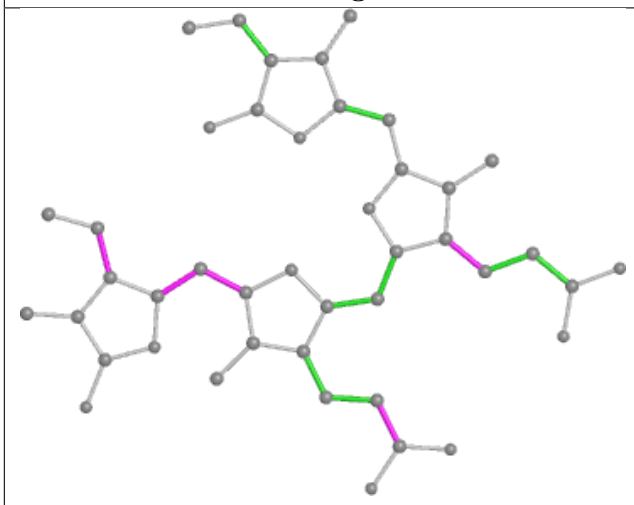

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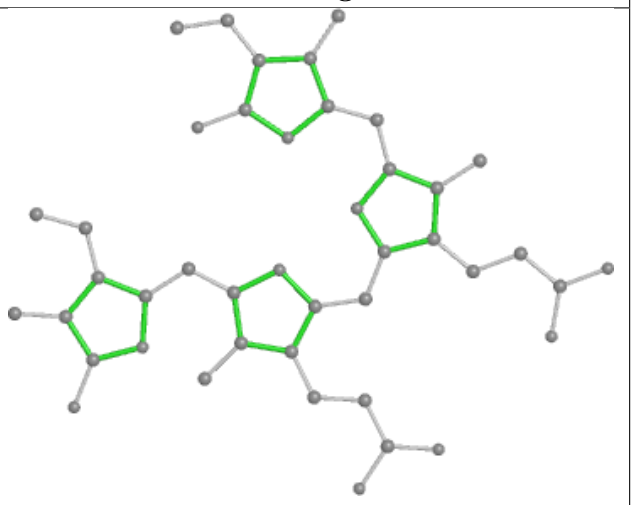
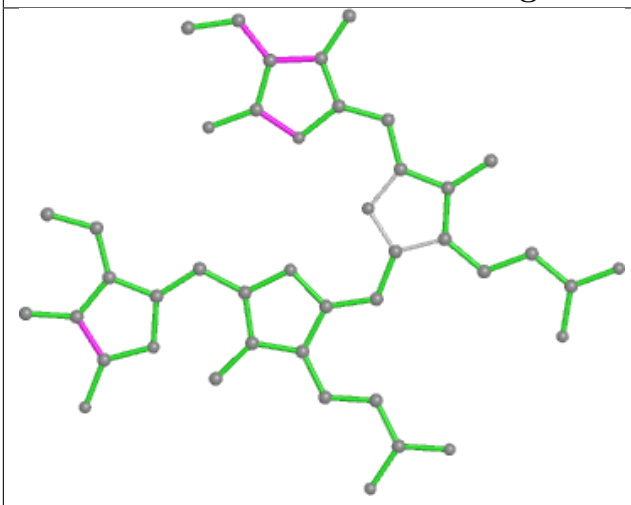


Rings

Ligand PEB eu 201



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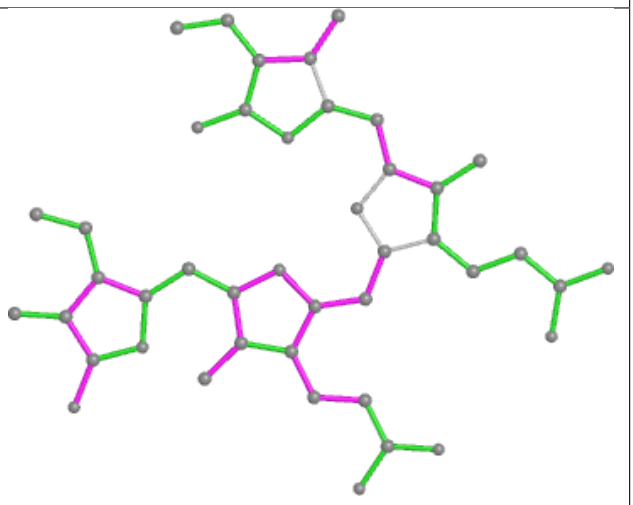

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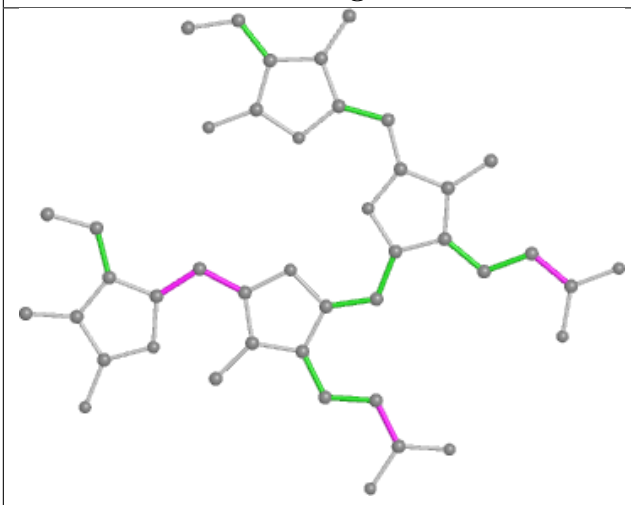

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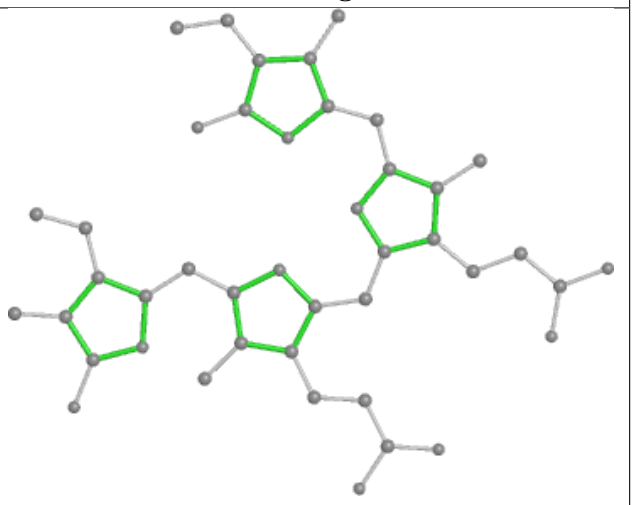

Rings

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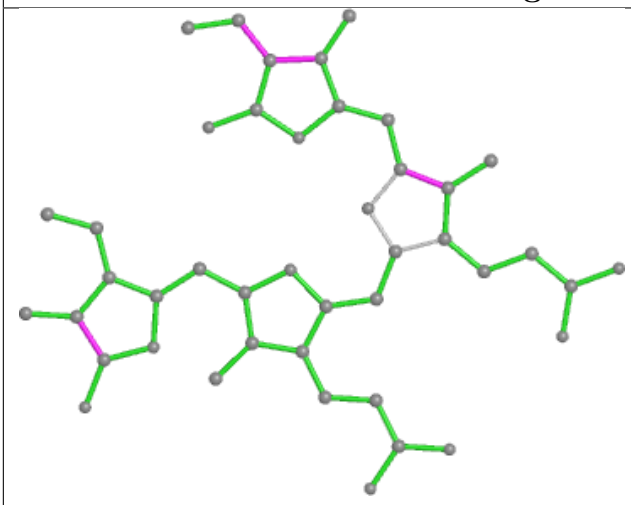

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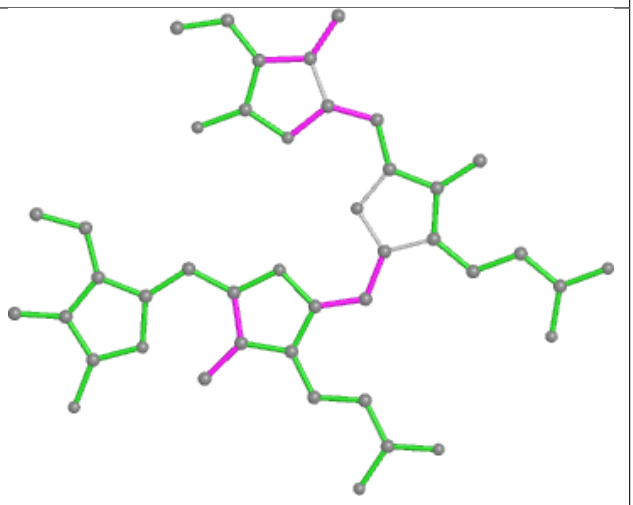

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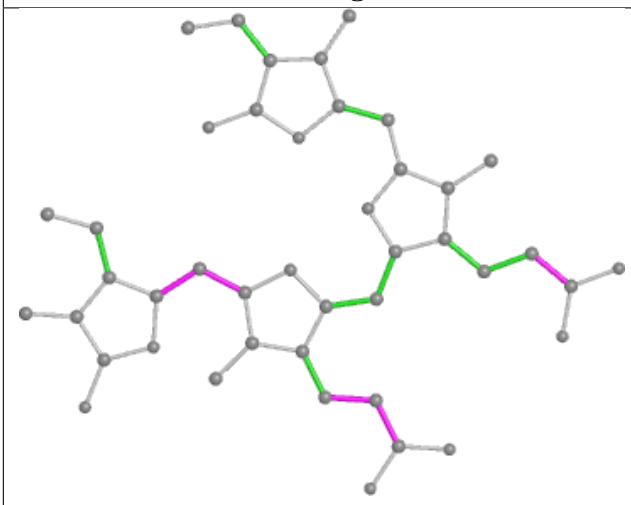

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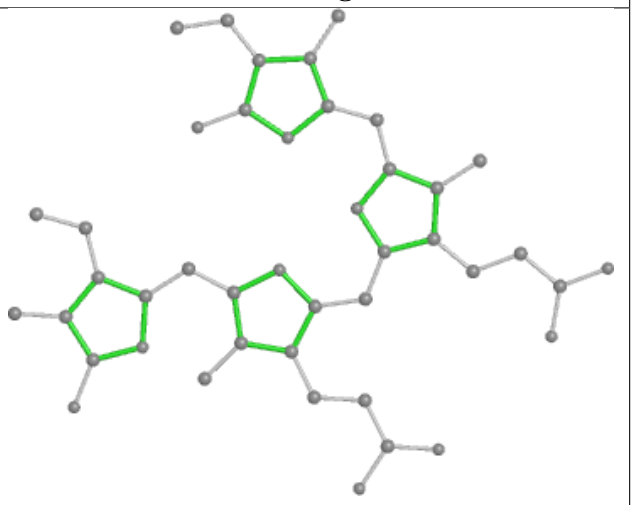

Rings

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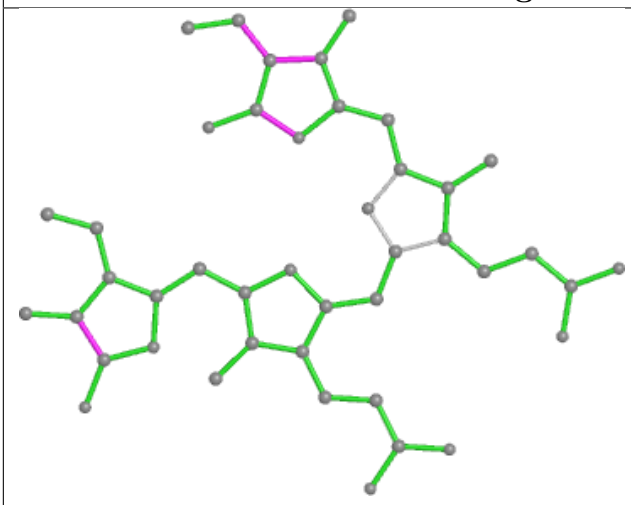

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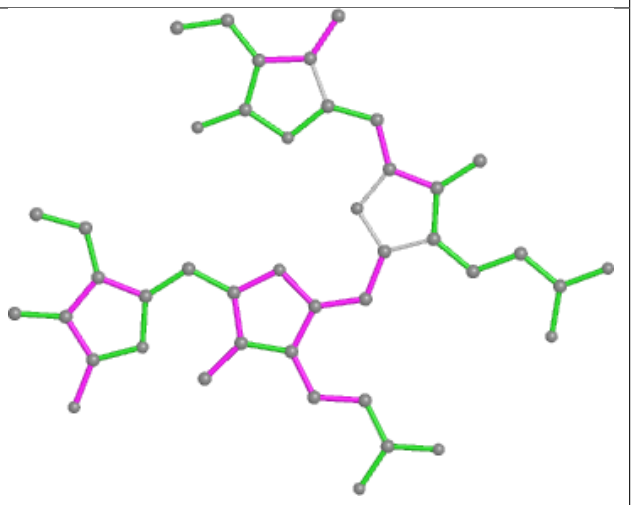

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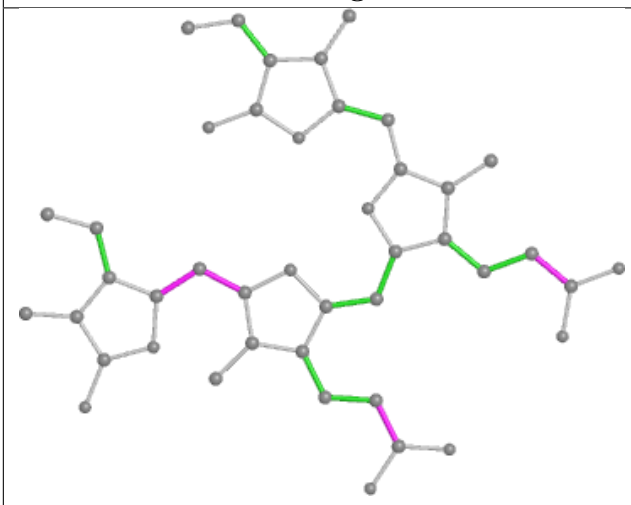

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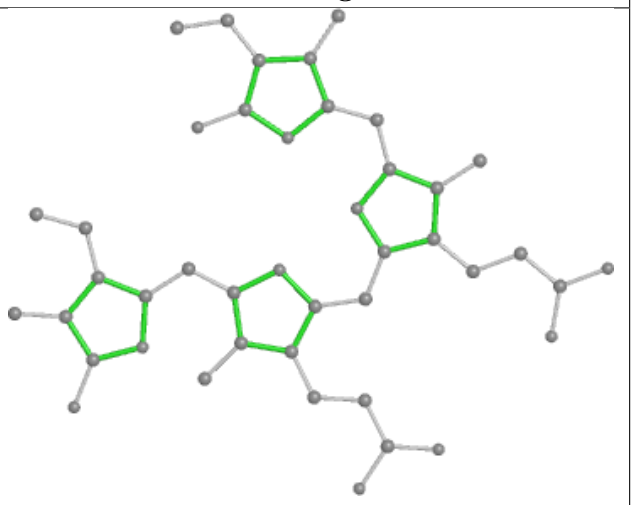

Rings

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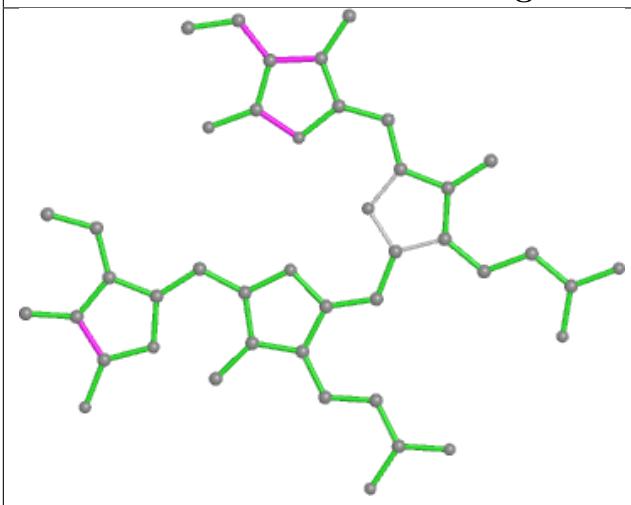

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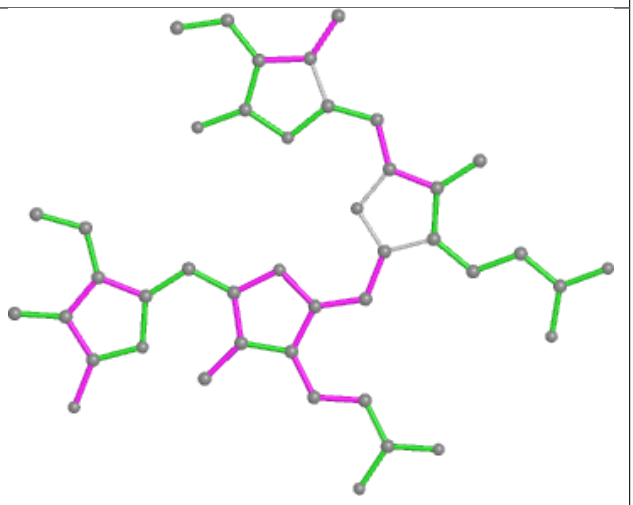

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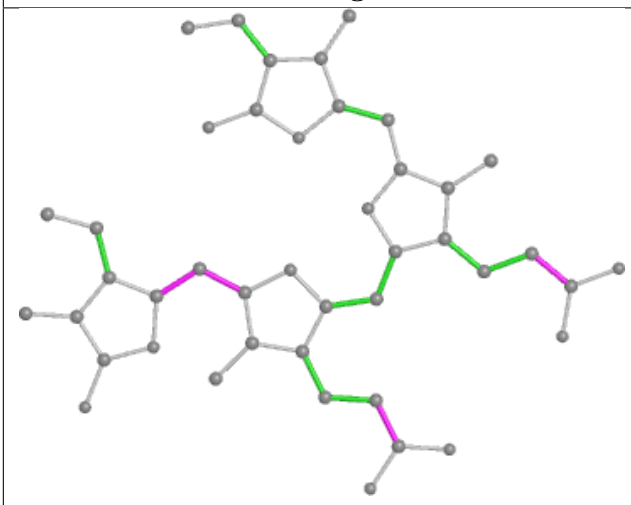

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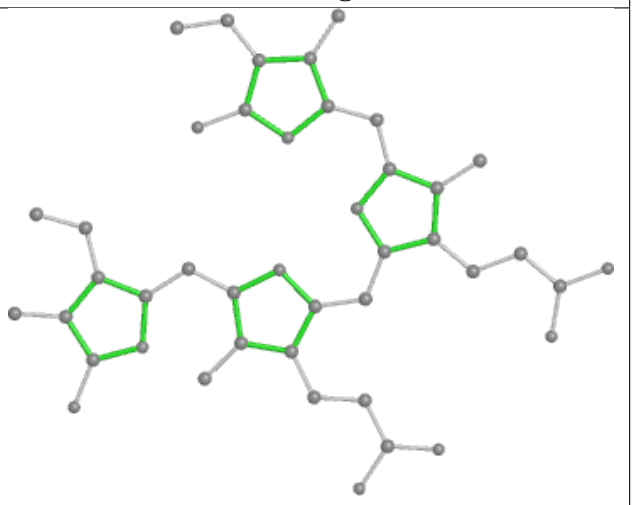

Rings

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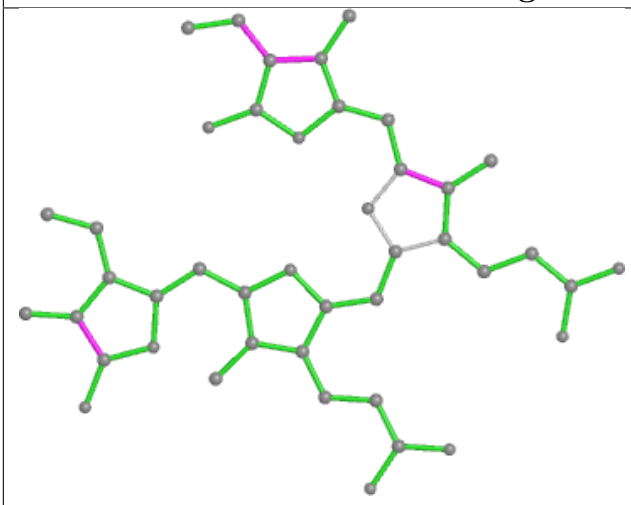

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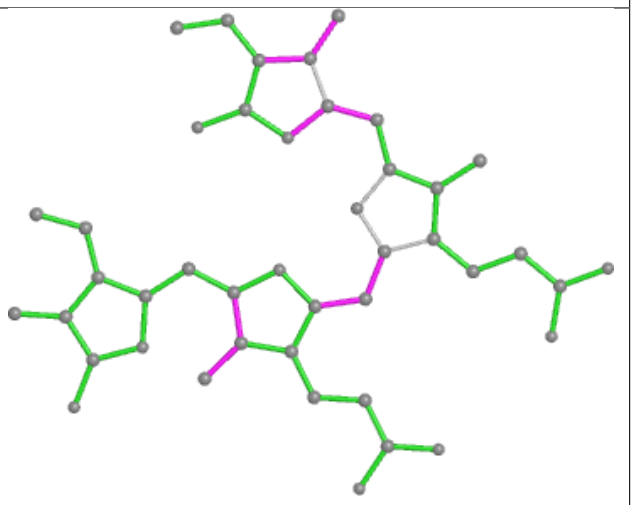

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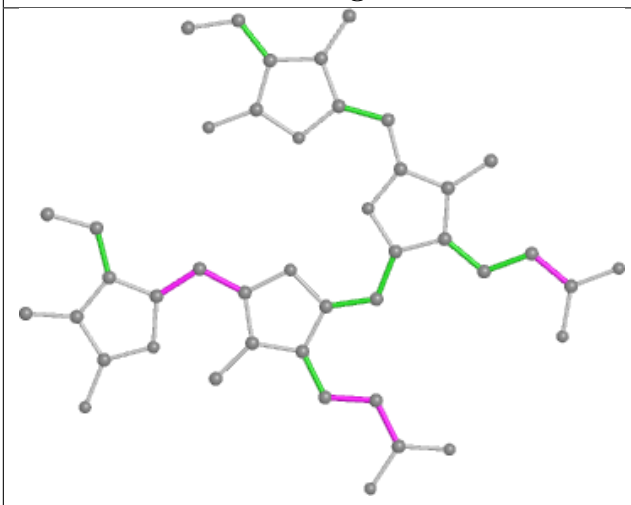

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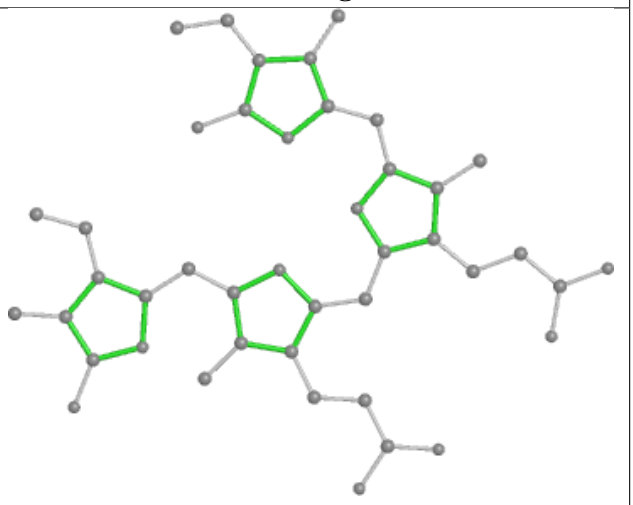

Rings

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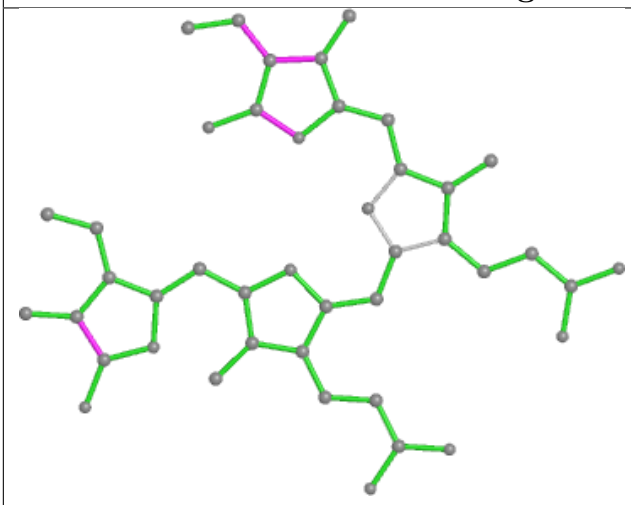

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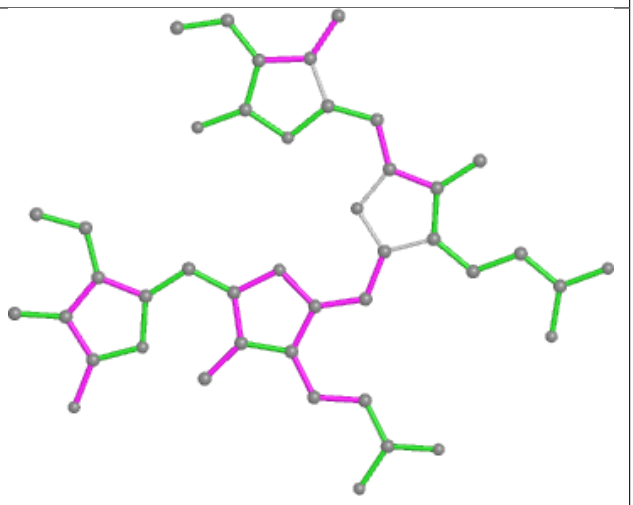

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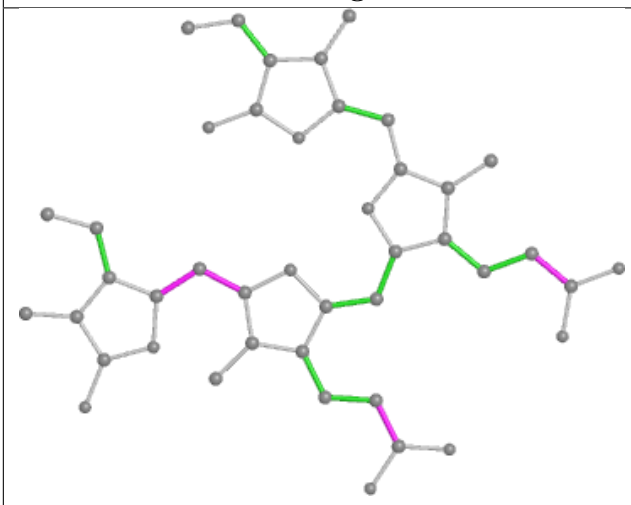

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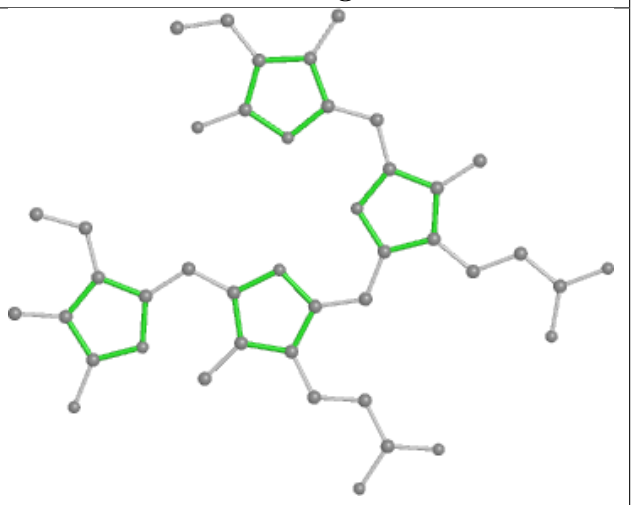

Rings

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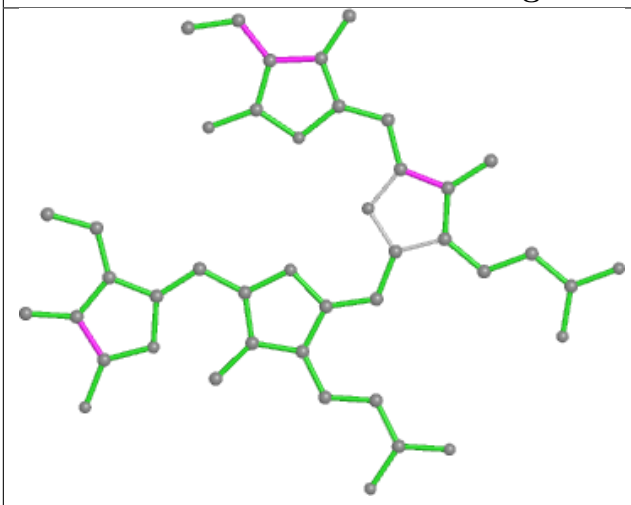

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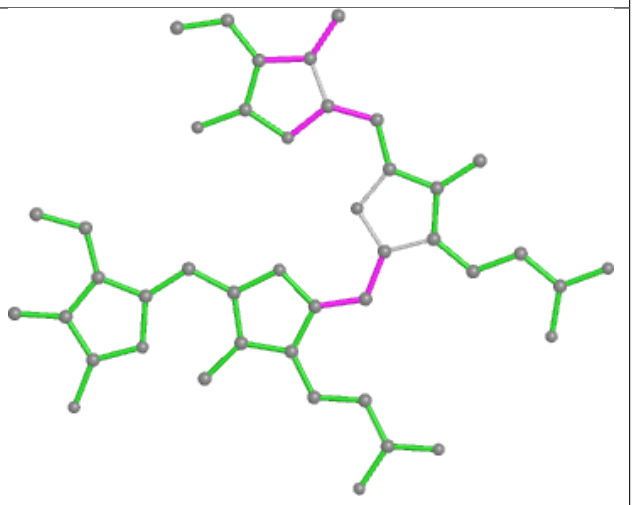

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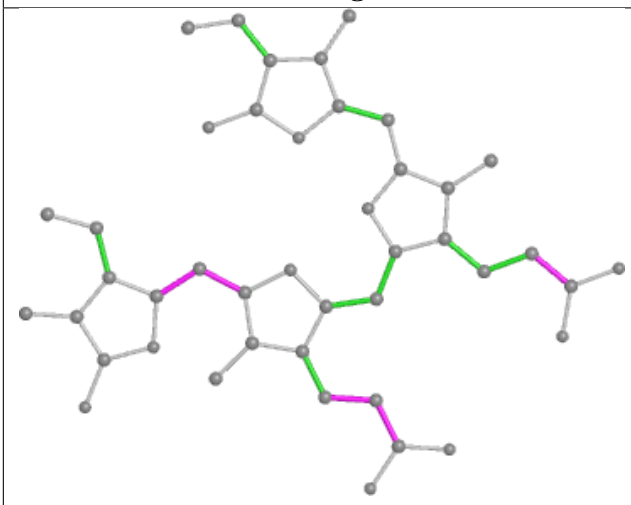

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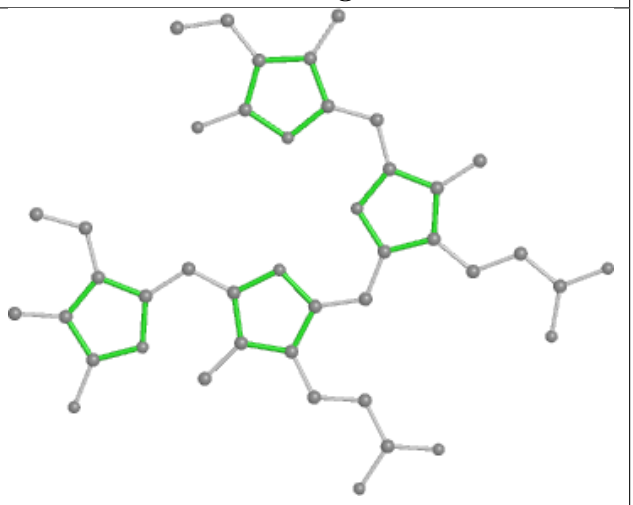

Rings

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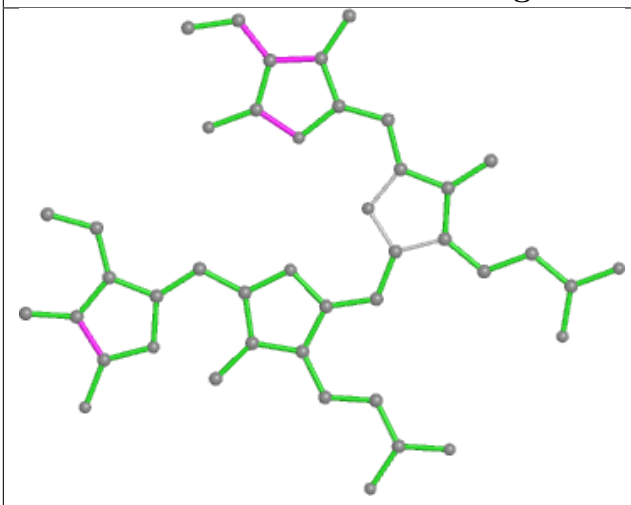

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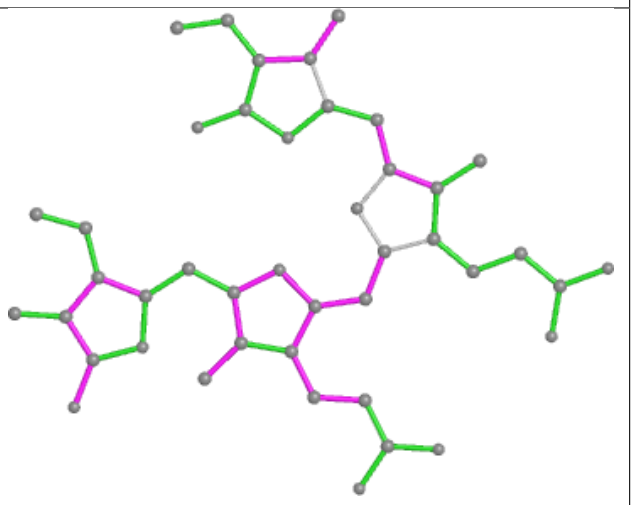

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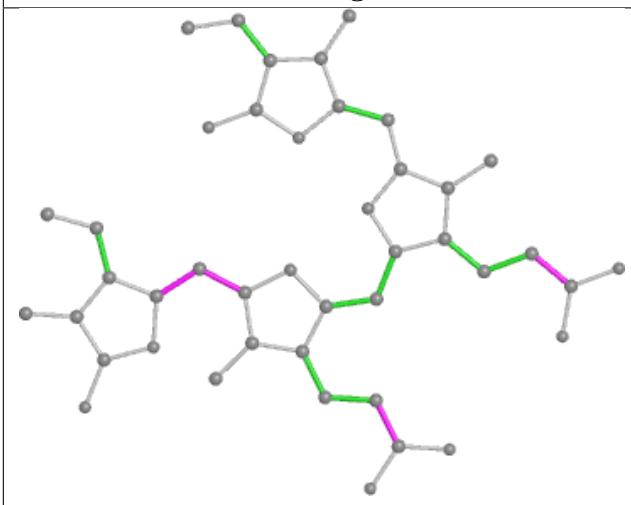

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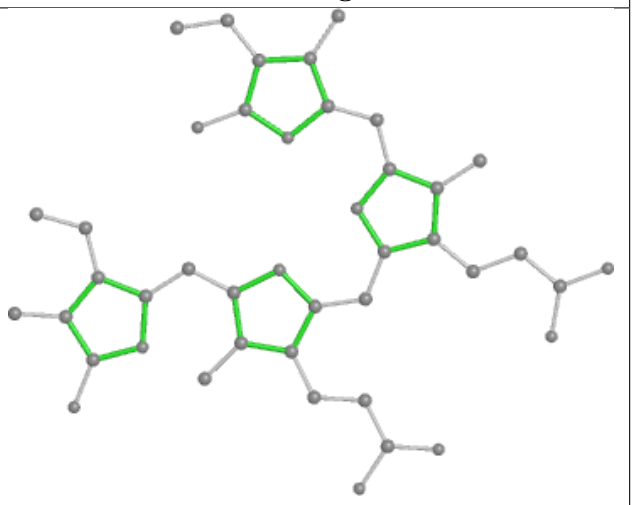

Rings

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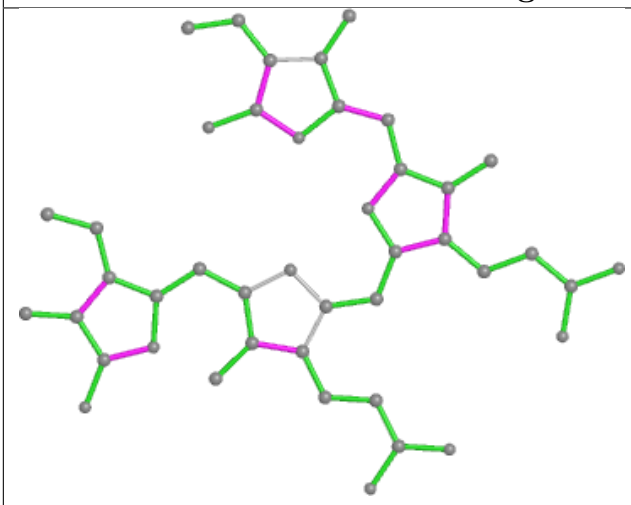

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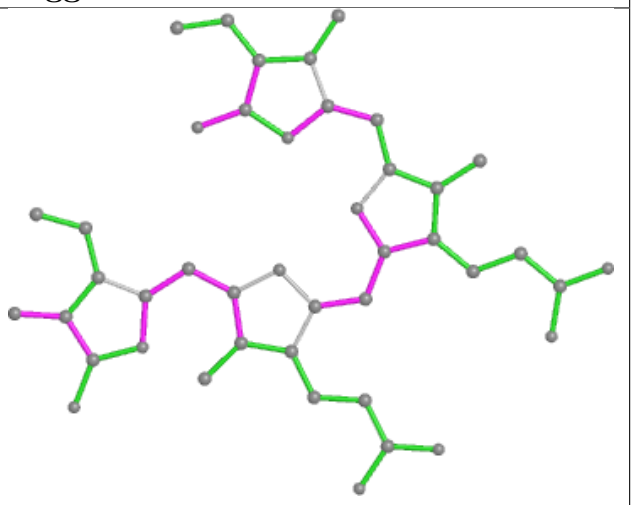

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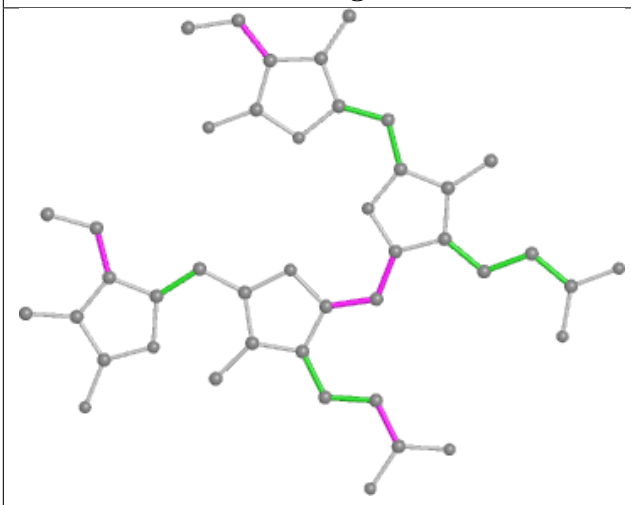

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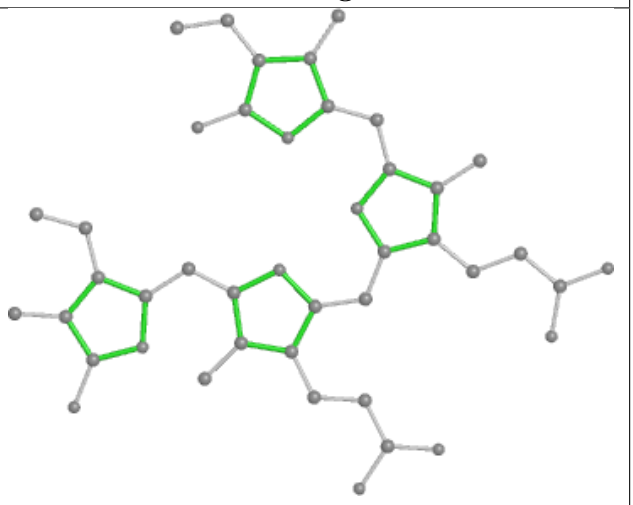
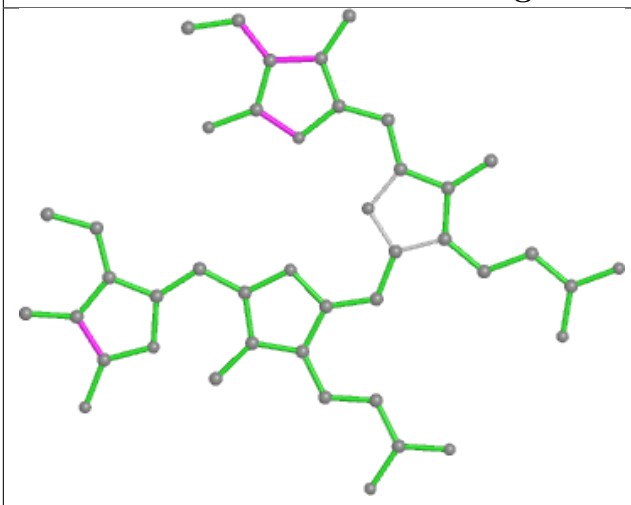


Rings

Ligand PEB dR 201



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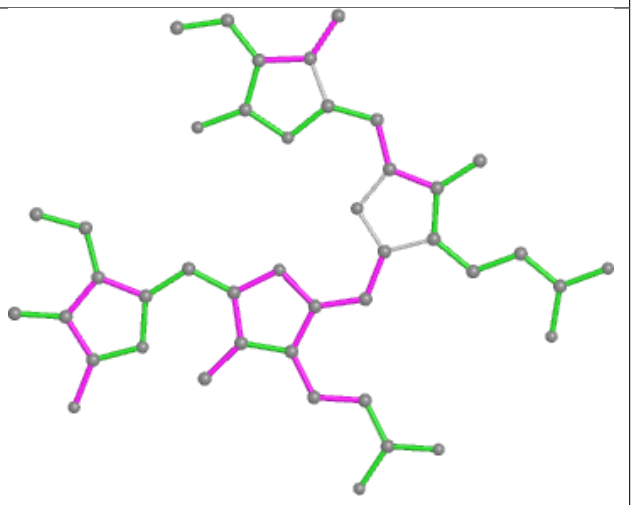

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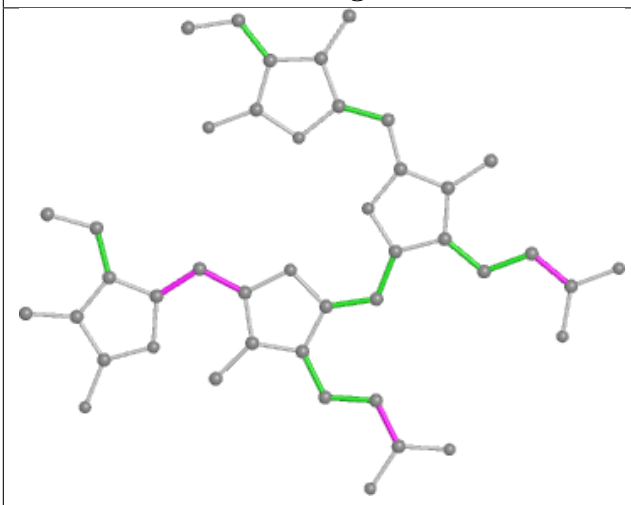

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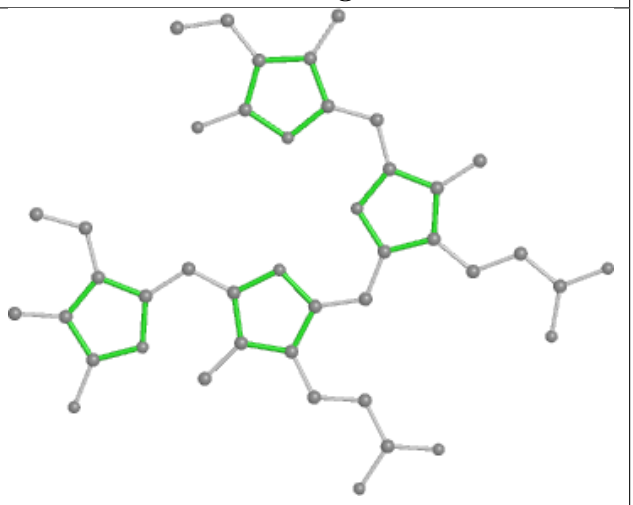

Rings

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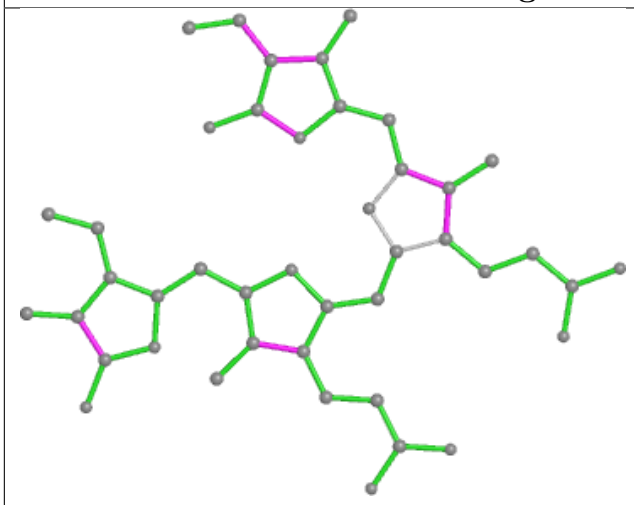

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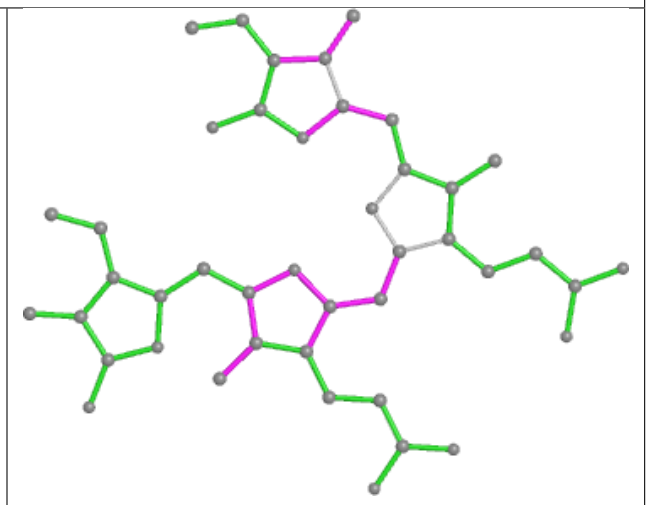

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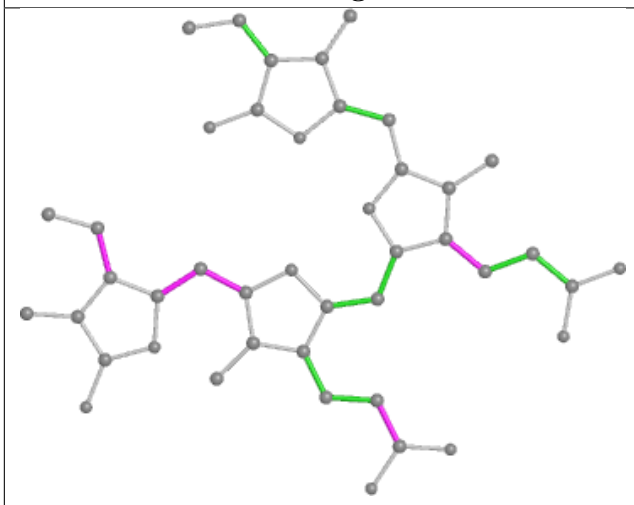

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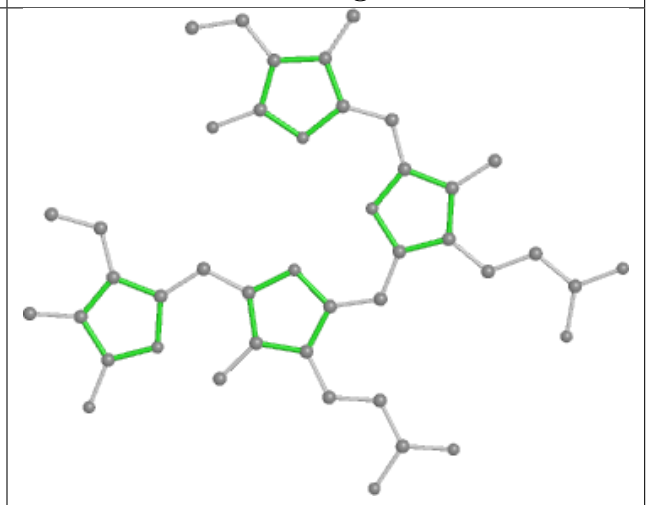
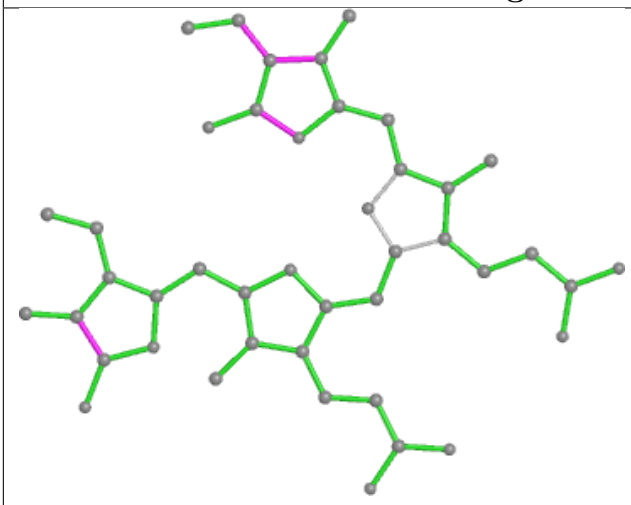


Rings

Ligand PEB w7 1001



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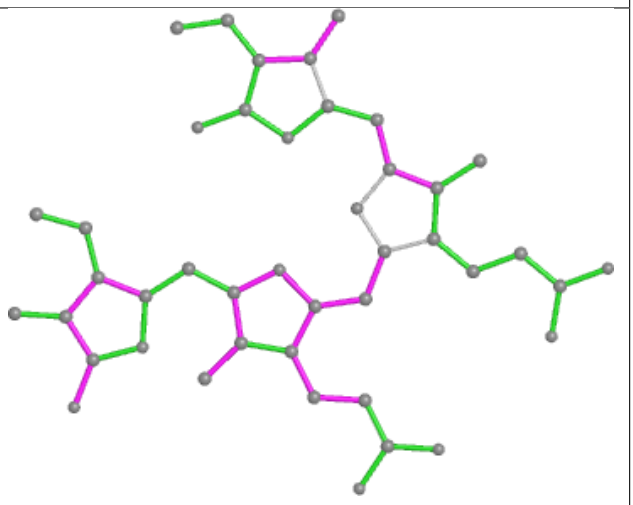
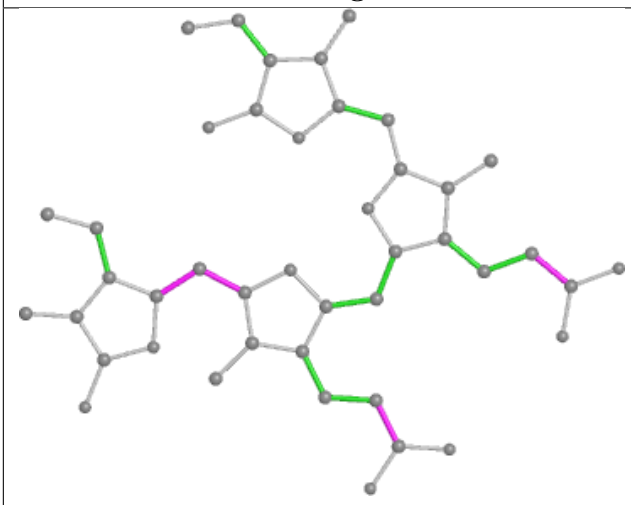
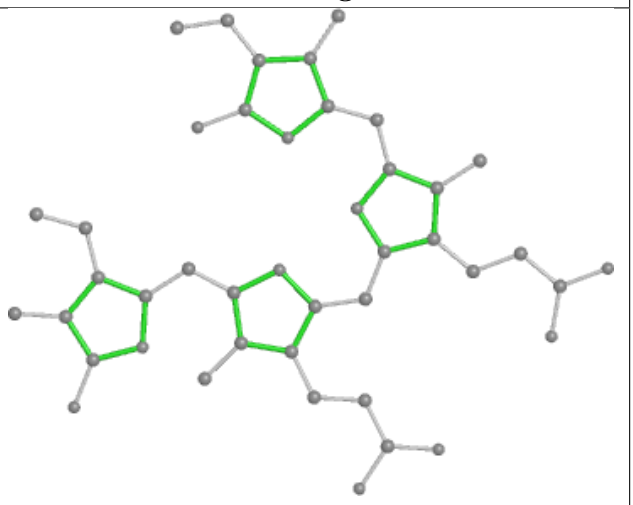


Bond angles

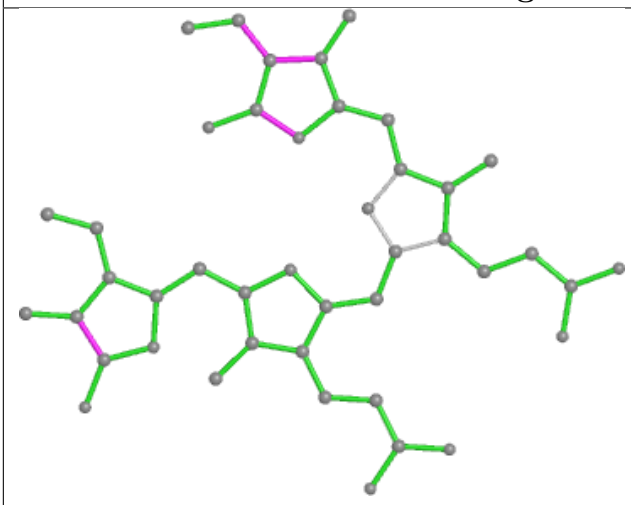


Torsions



Rings

Ligand PEB E9 201



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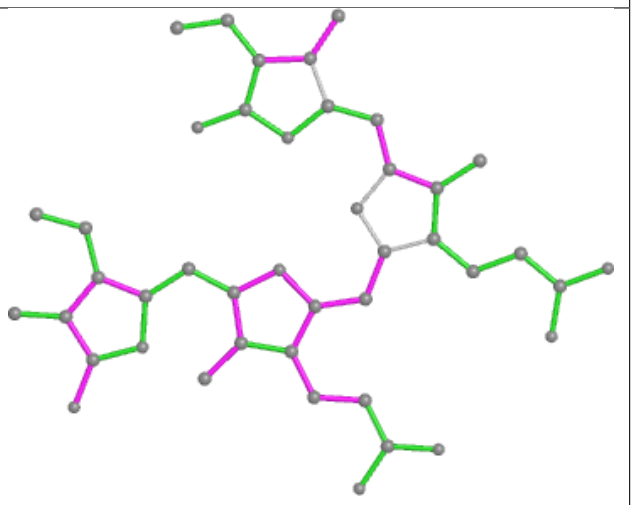

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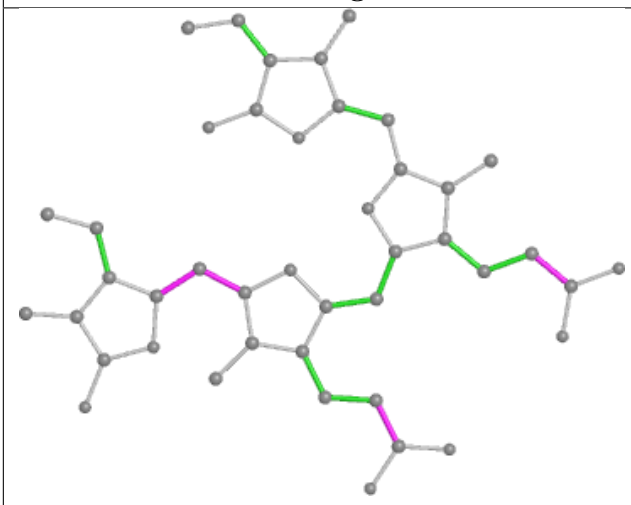

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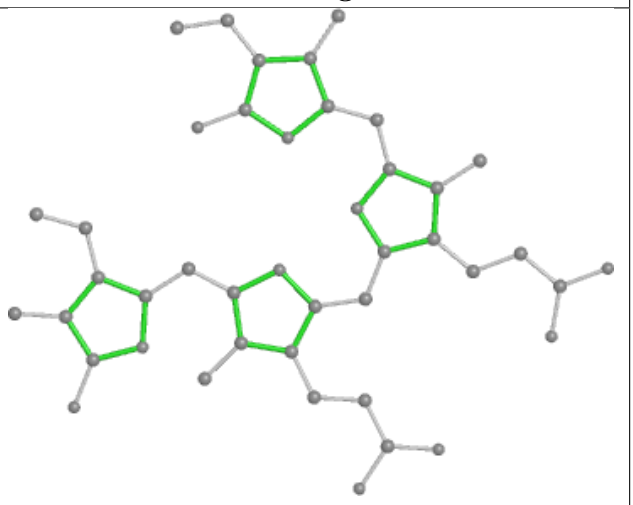
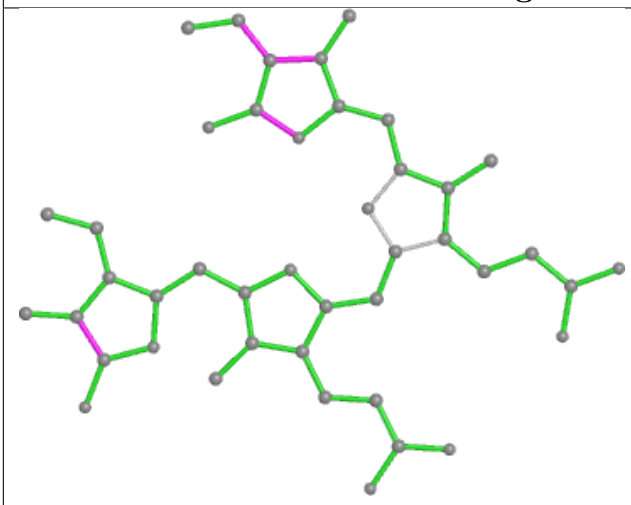


Rings

Ligand PEB bP 201



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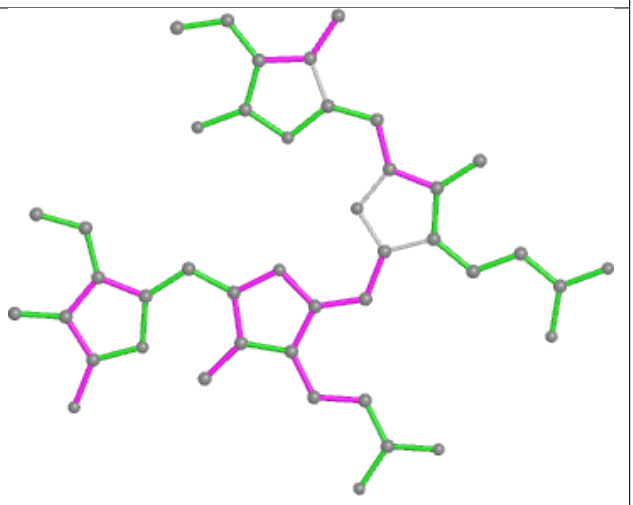
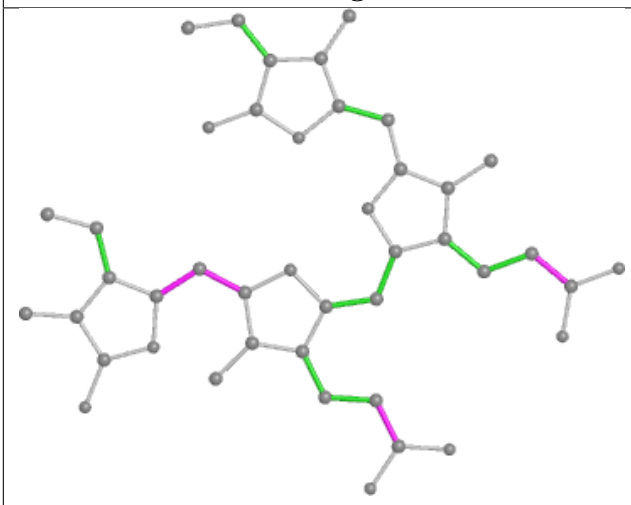


Bond angles



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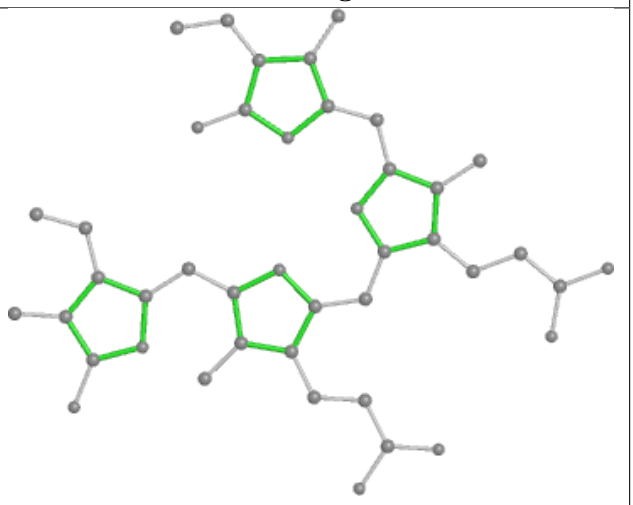
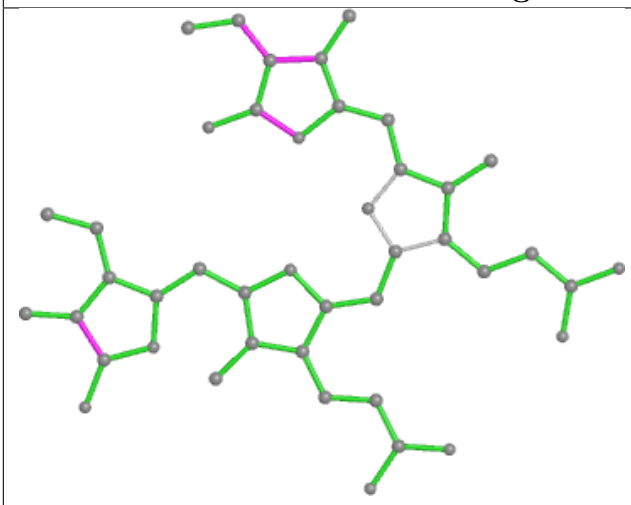


Rings

Ligand PEB ez 1001



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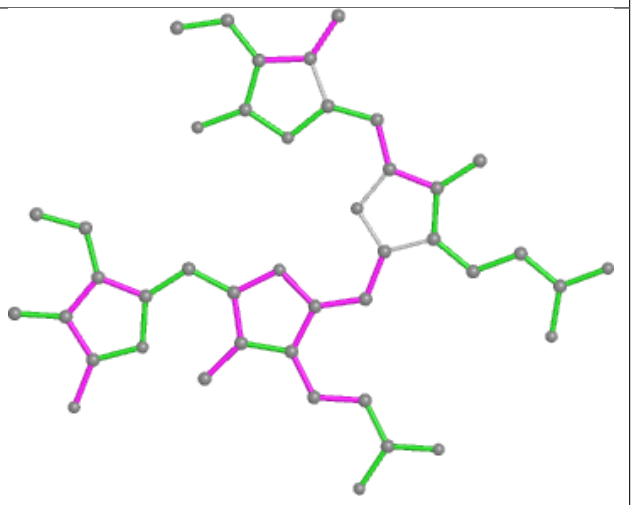
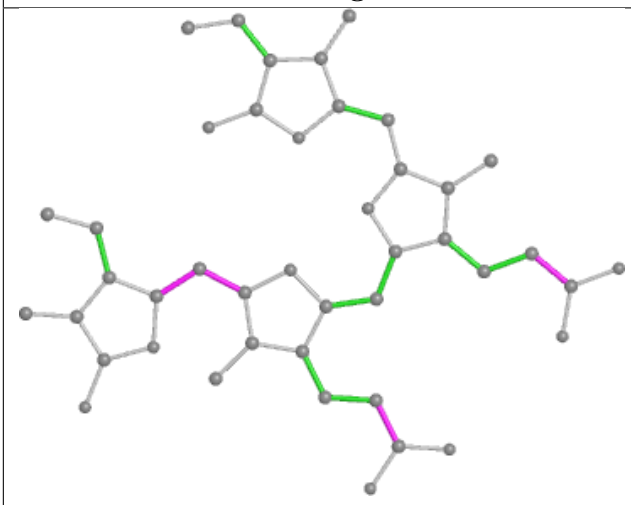


Bond angles



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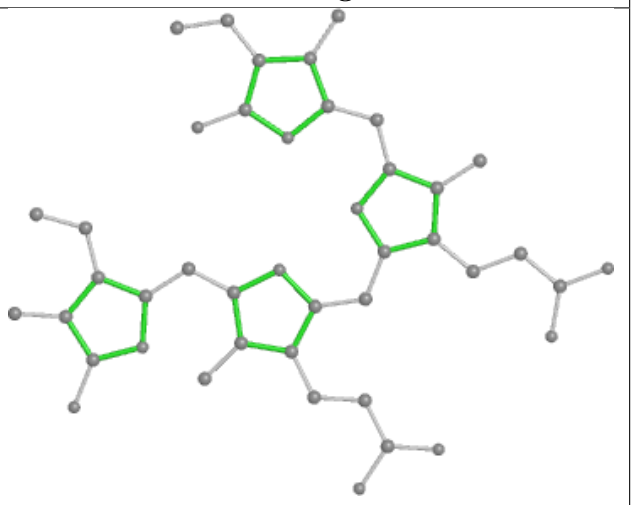
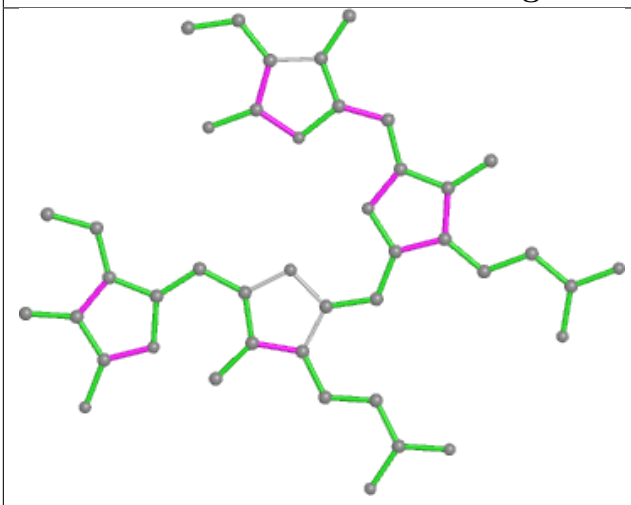


Rings

Ligand PUB fc 203



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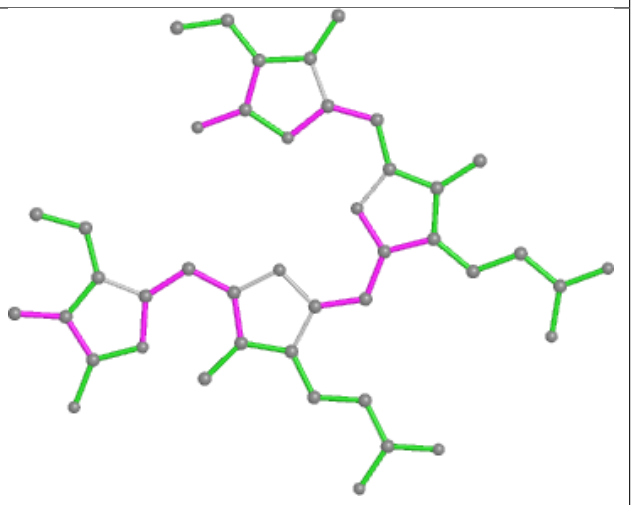

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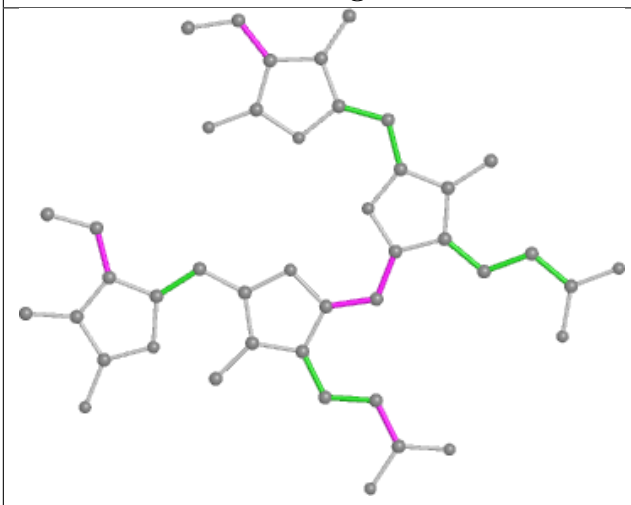

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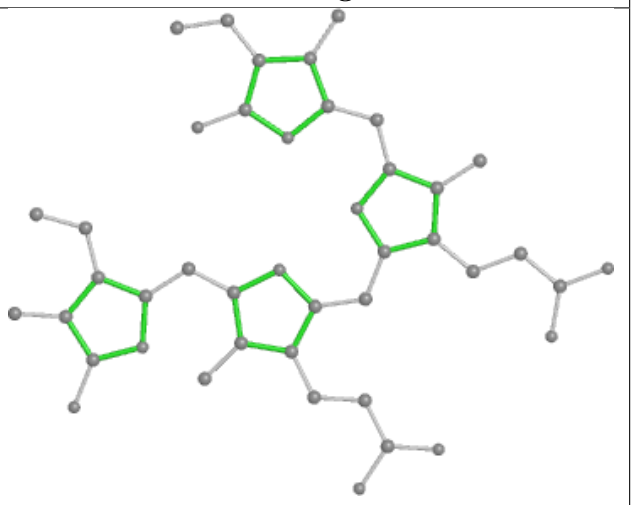

Rings

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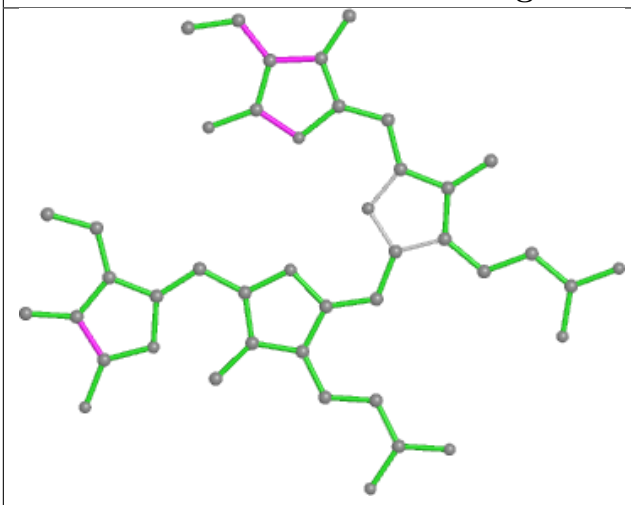

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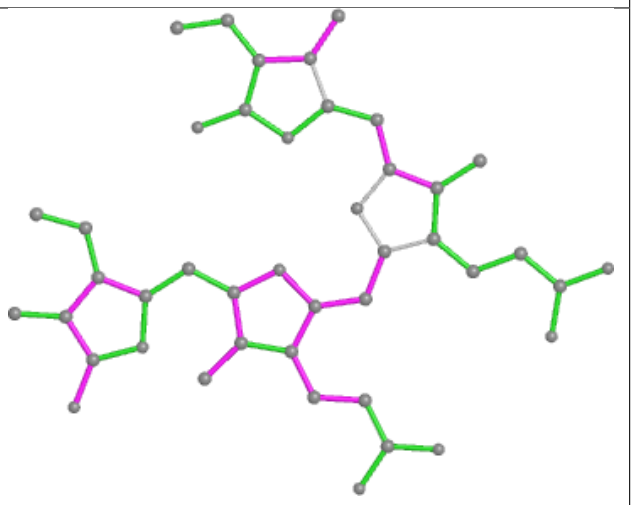

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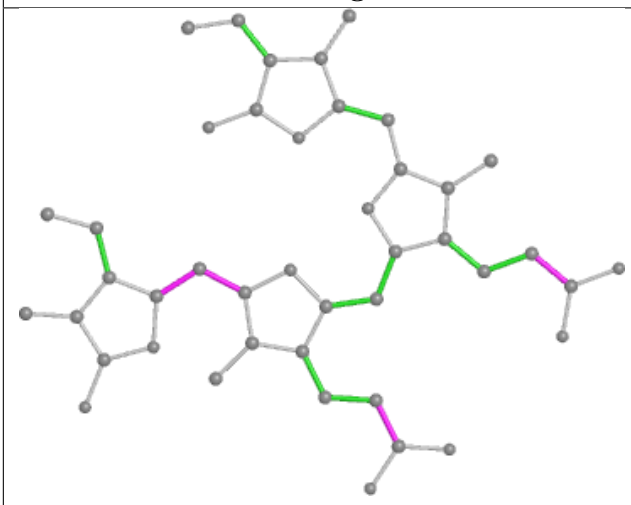

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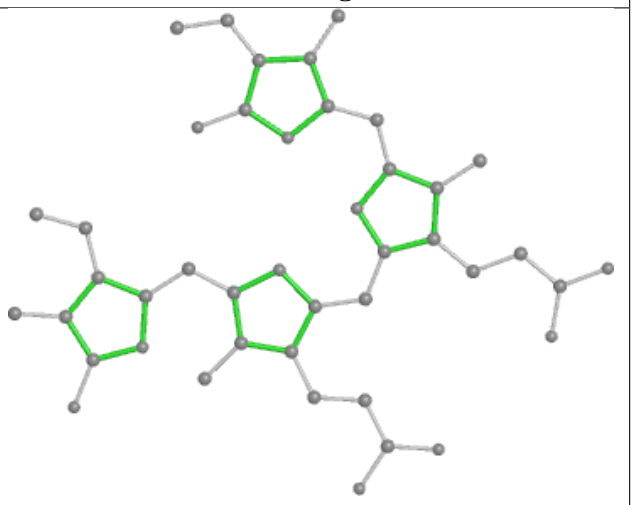

Rings

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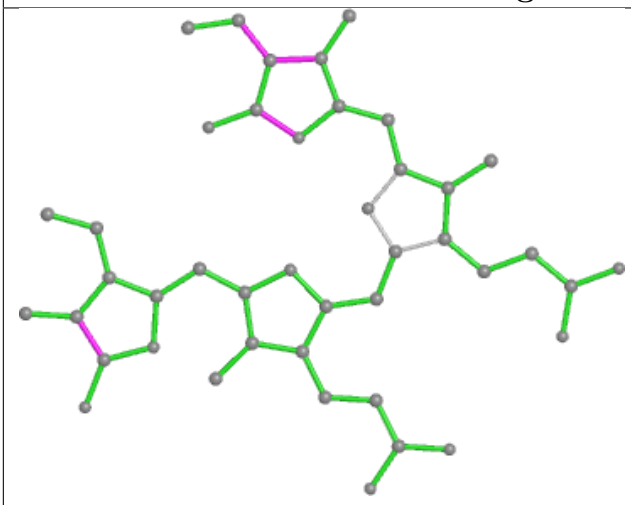

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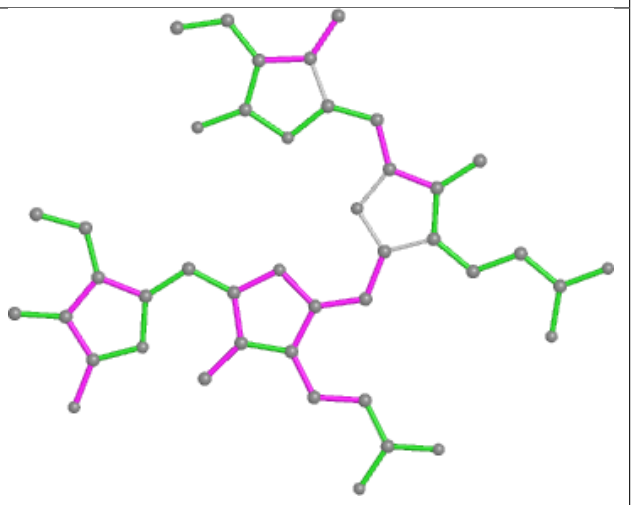

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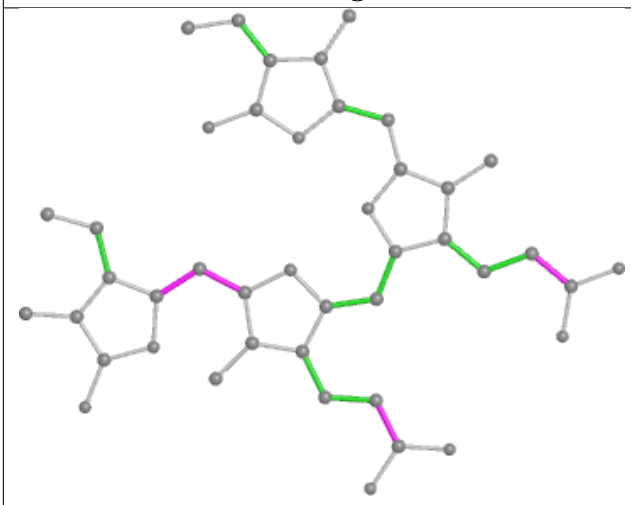

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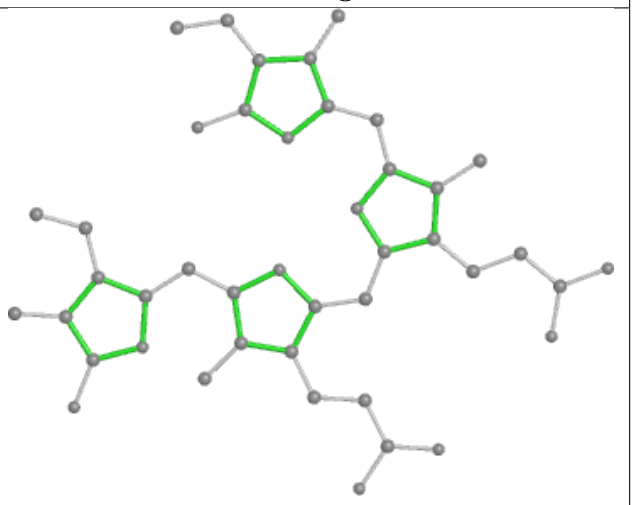

Rings

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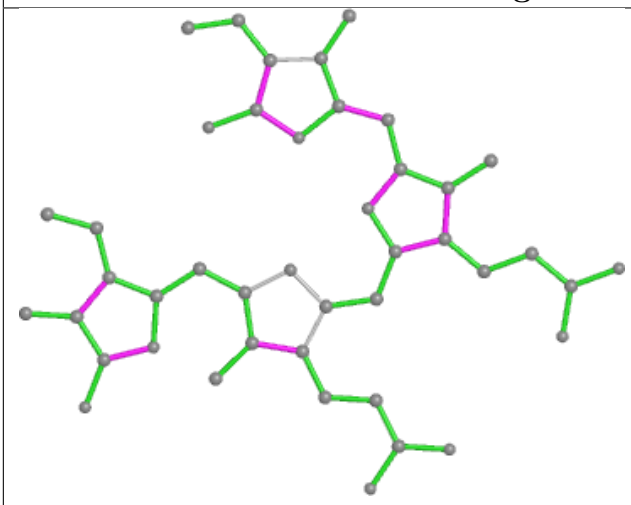

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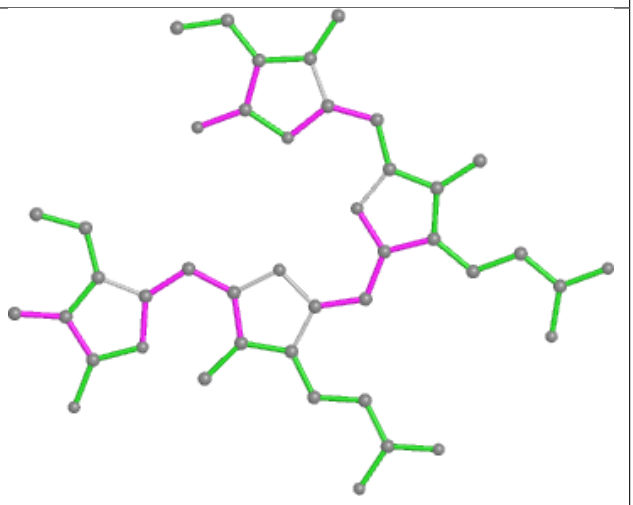

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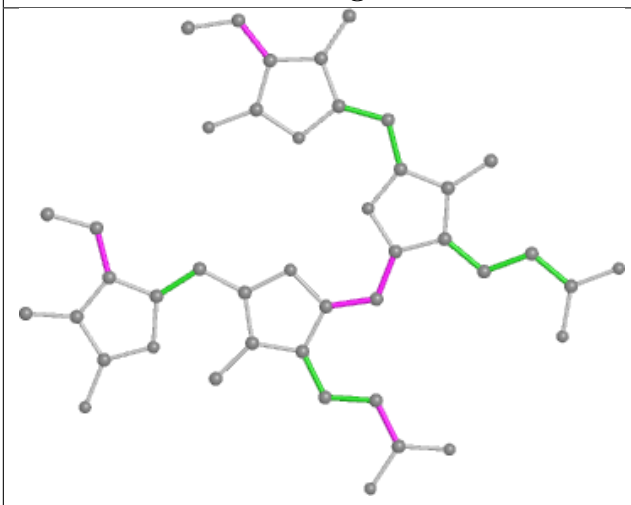

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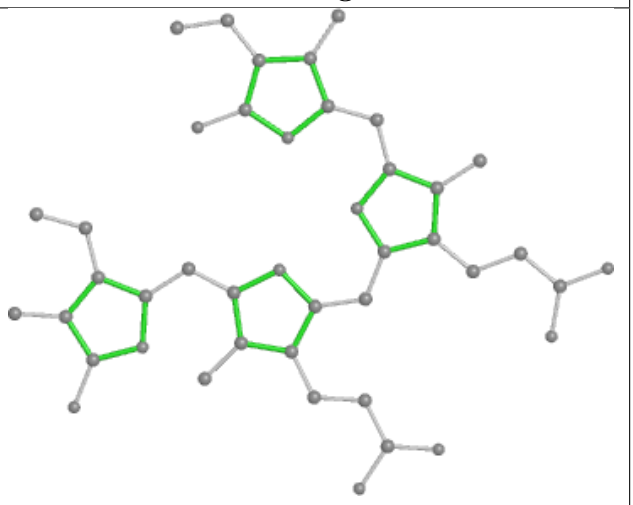

Rings

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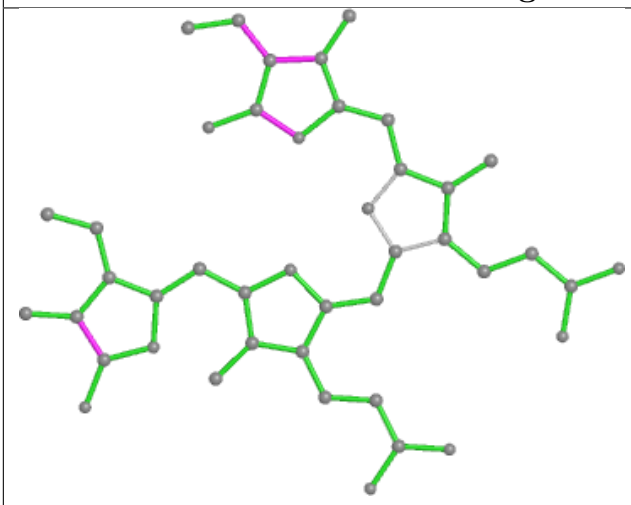

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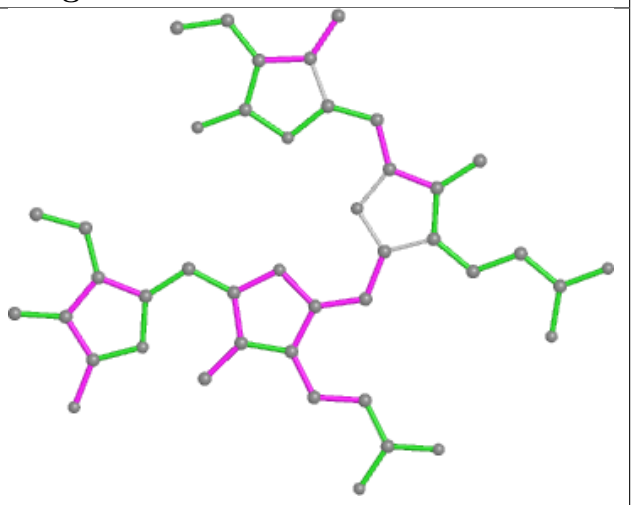

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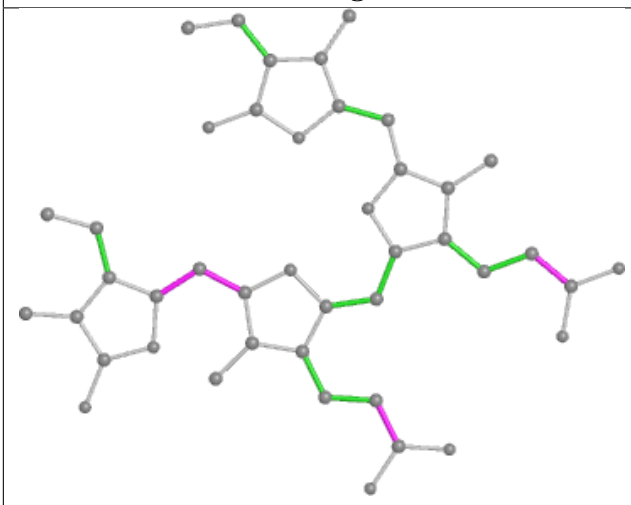

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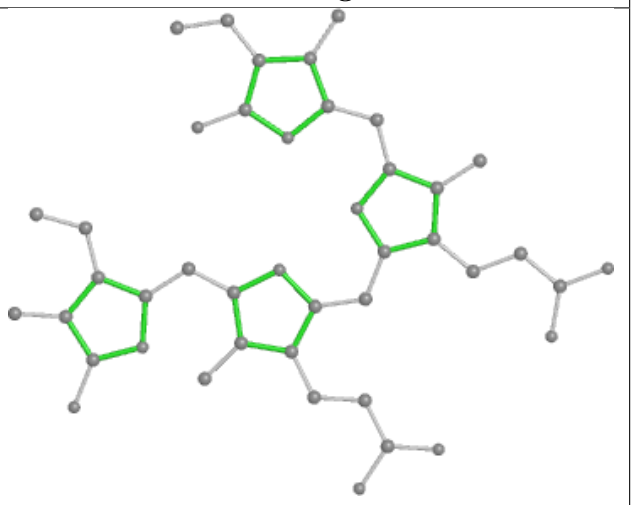
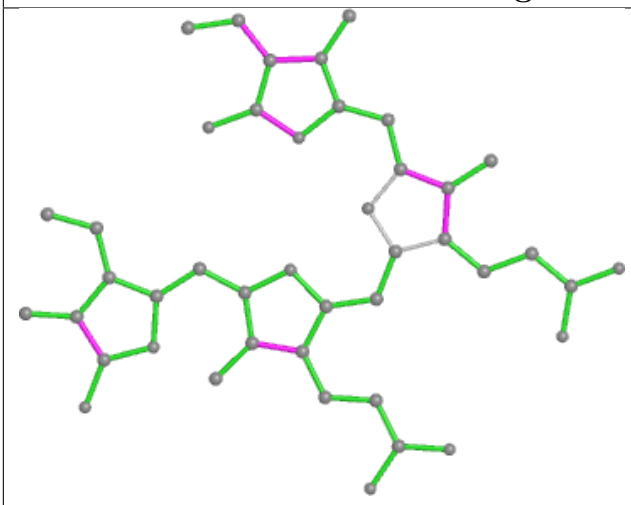


Rings

Ligand PEB H3 202



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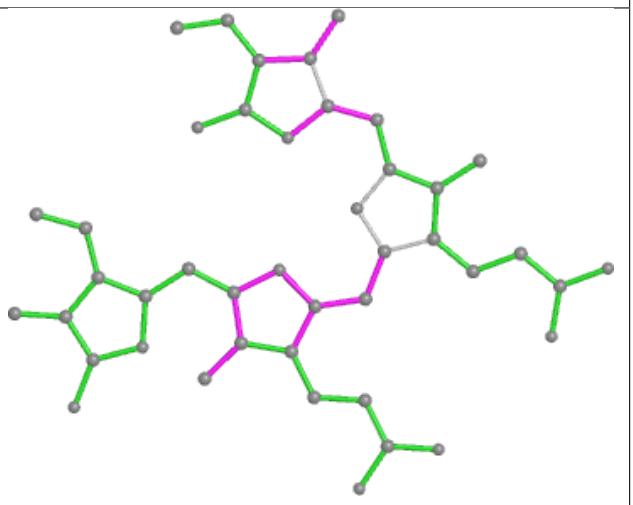

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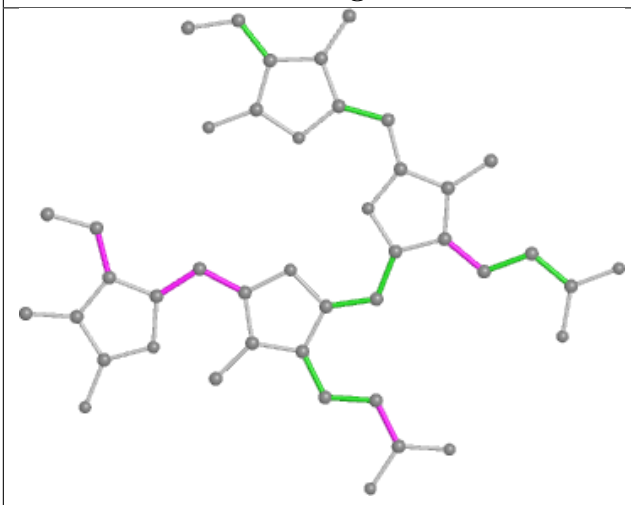

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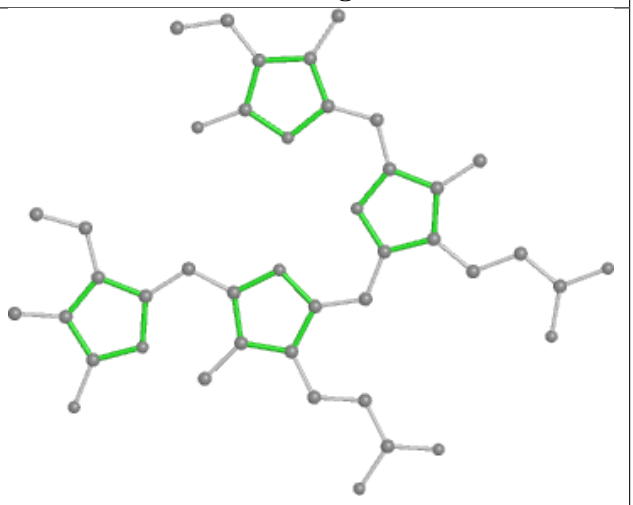

Rings

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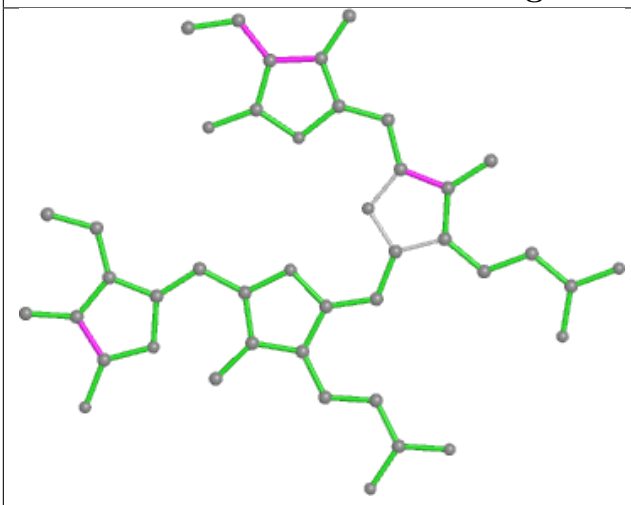

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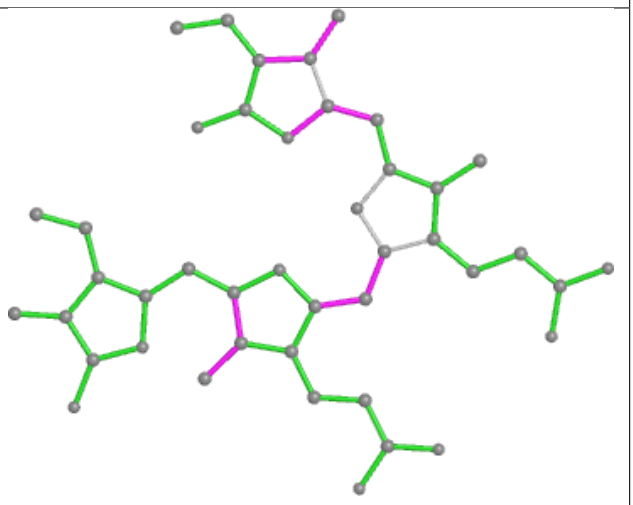

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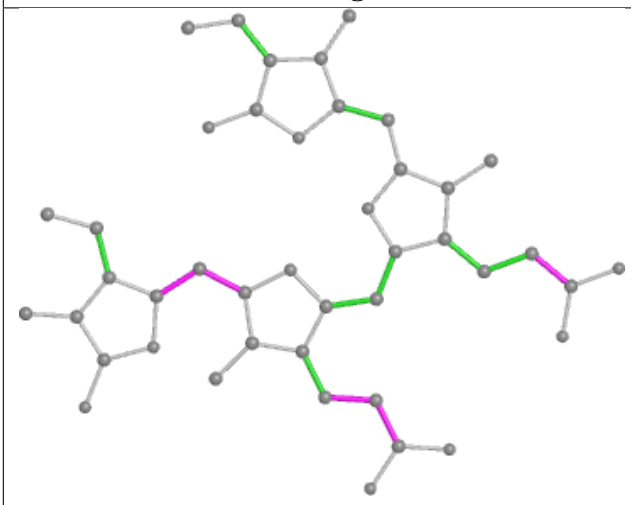

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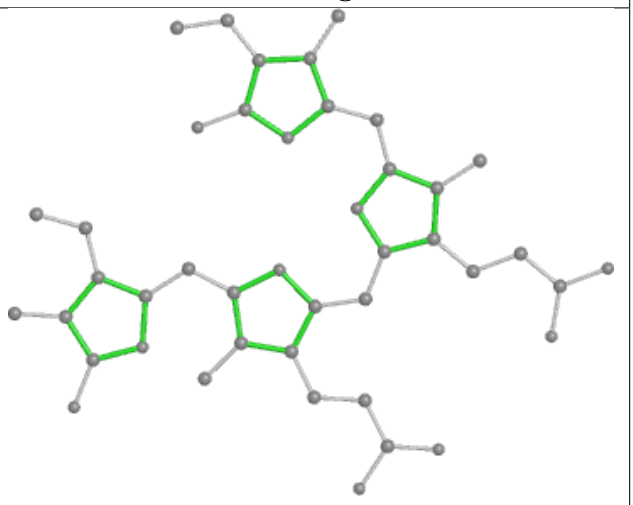

Rings

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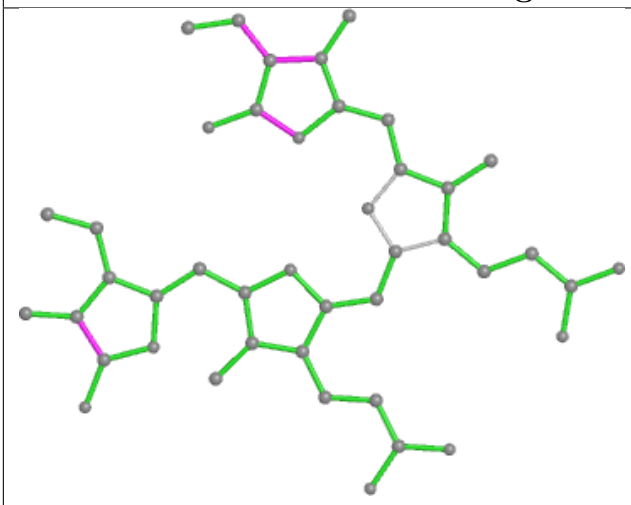

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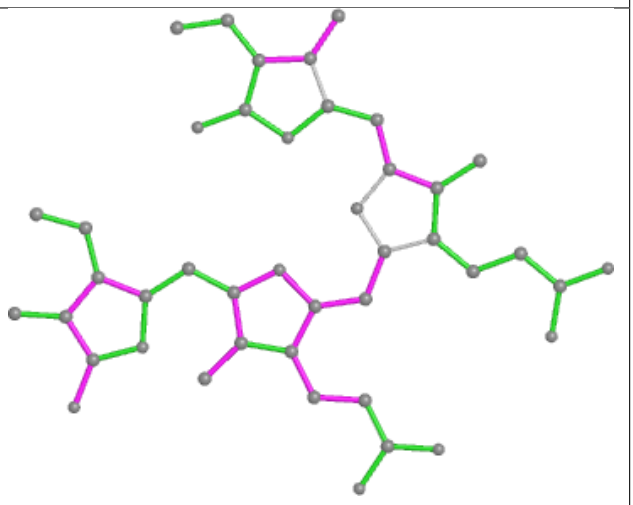

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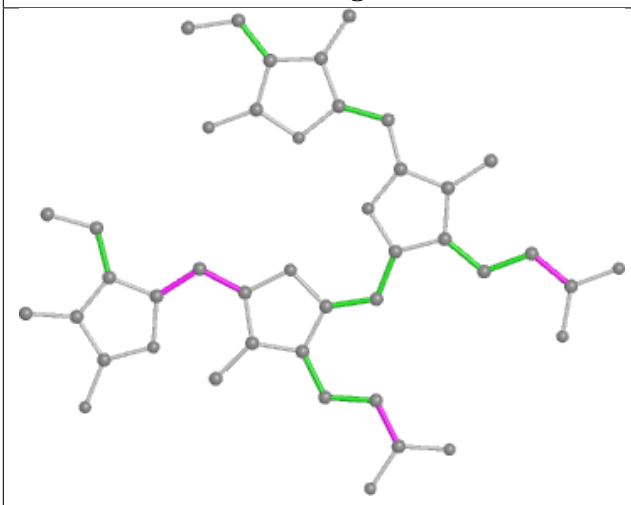

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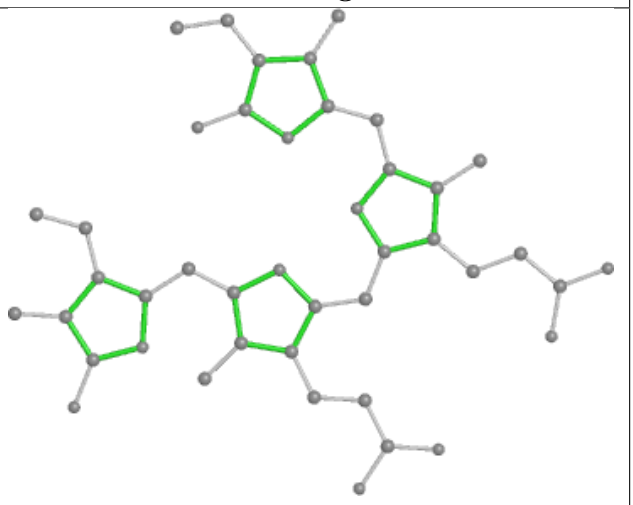

Rings

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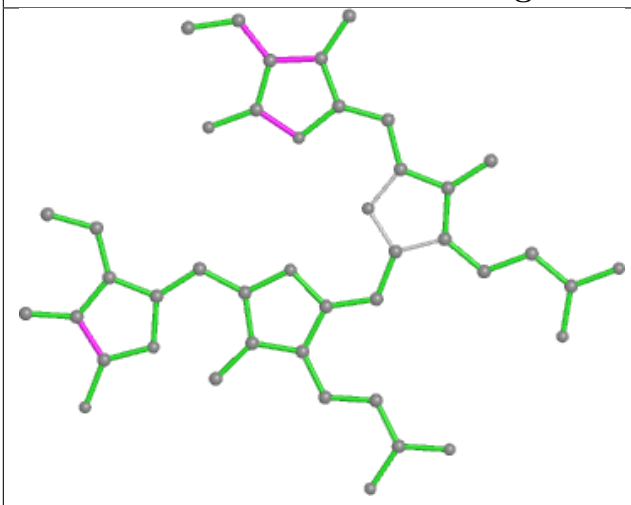

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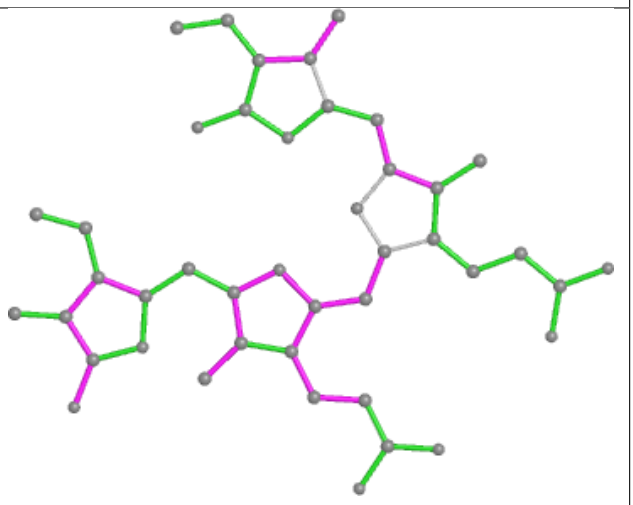

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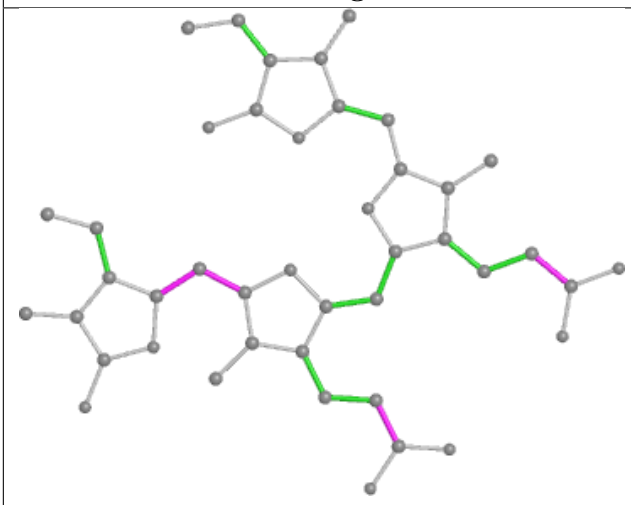

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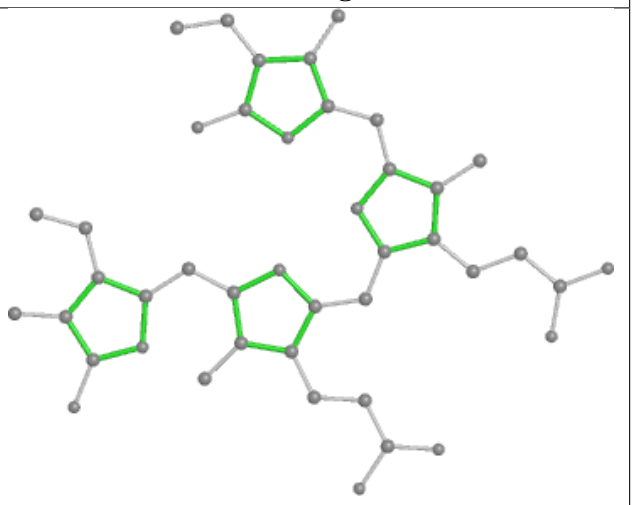
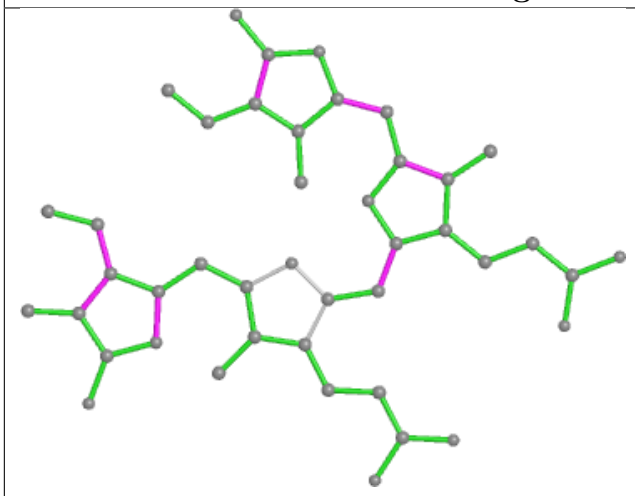


Rings

Ligand PVN D2 303



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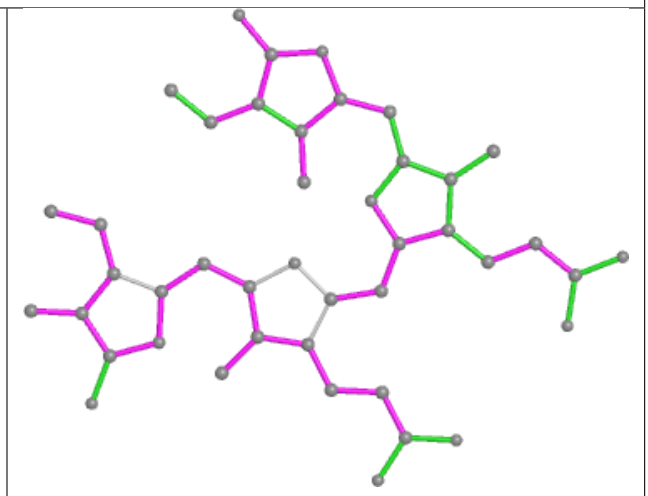
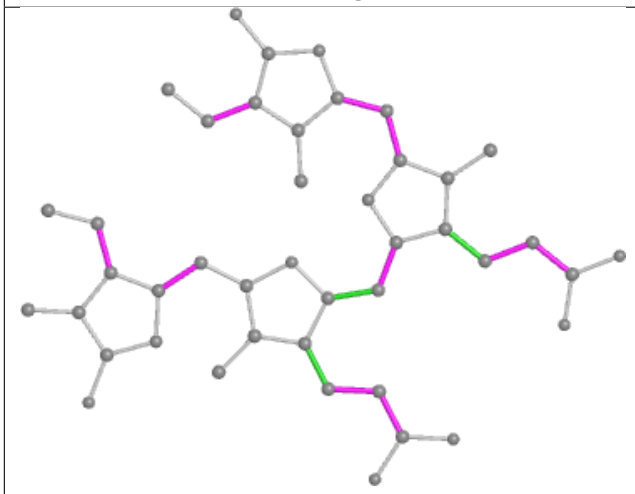
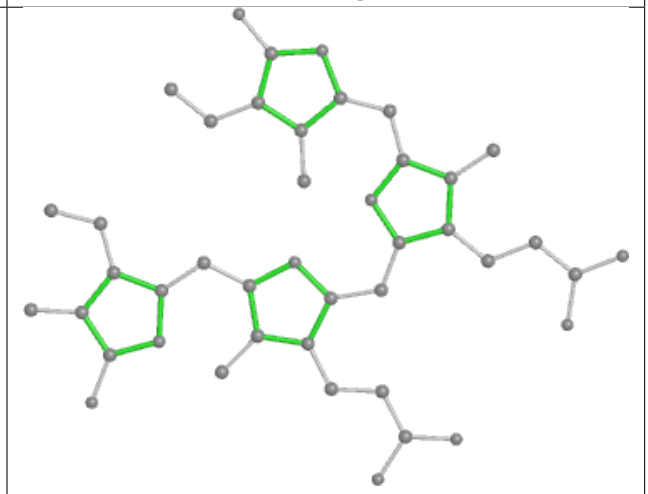


Bond angles

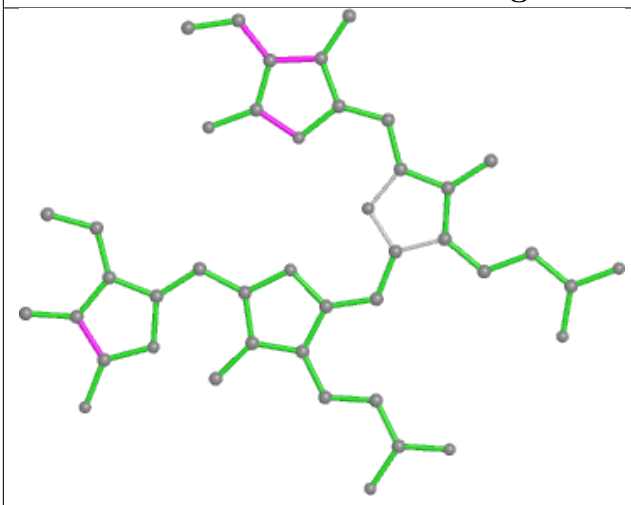


Torsions



Rings

Ligand PEB W6 202



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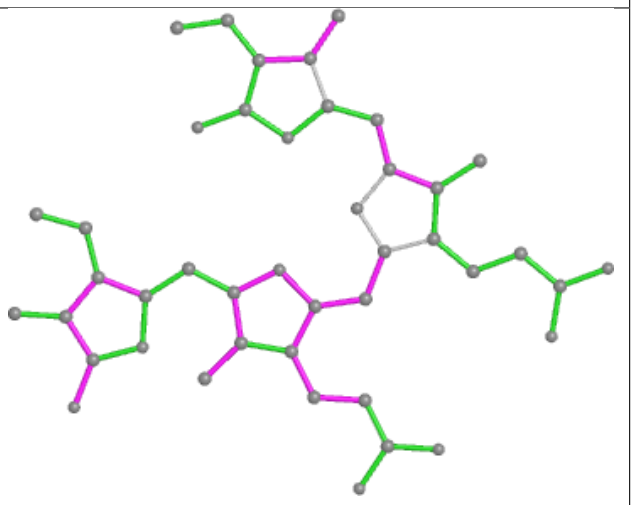
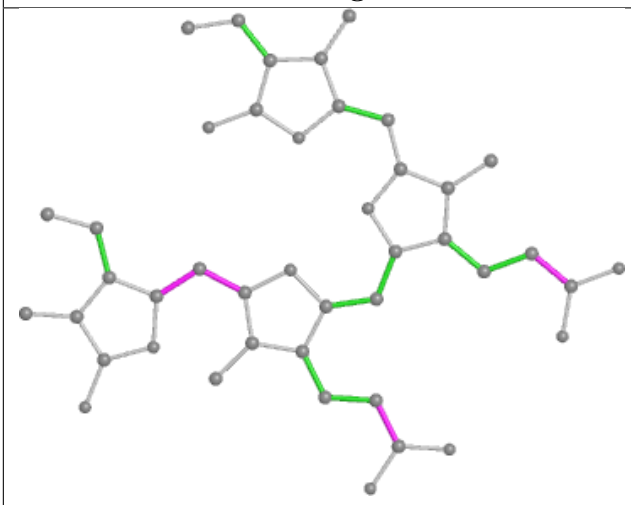


Bond angles



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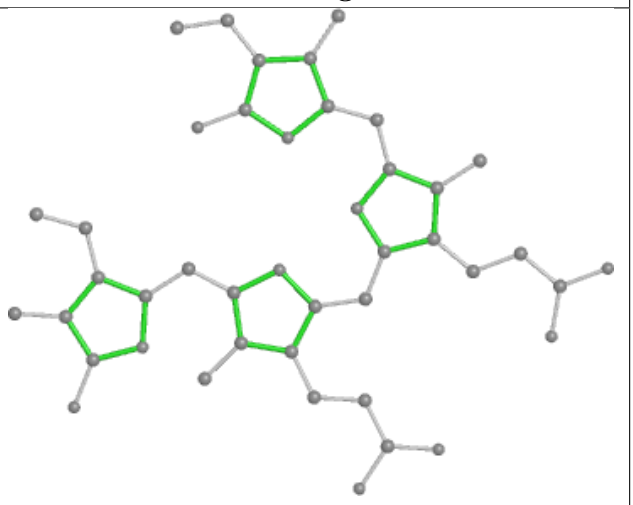
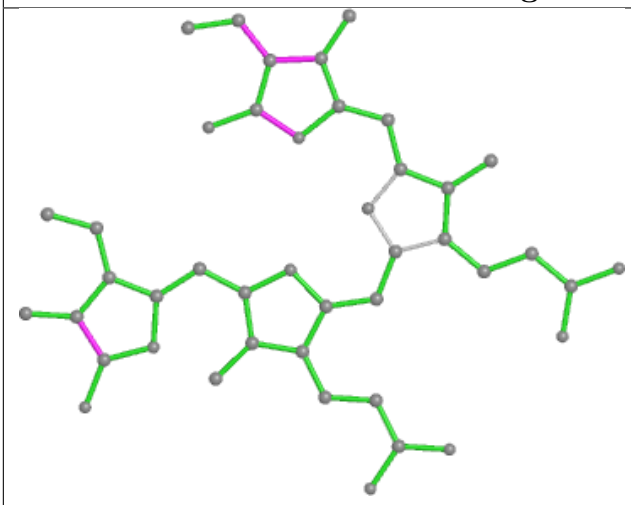


Rings

Ligand PEB c8 302



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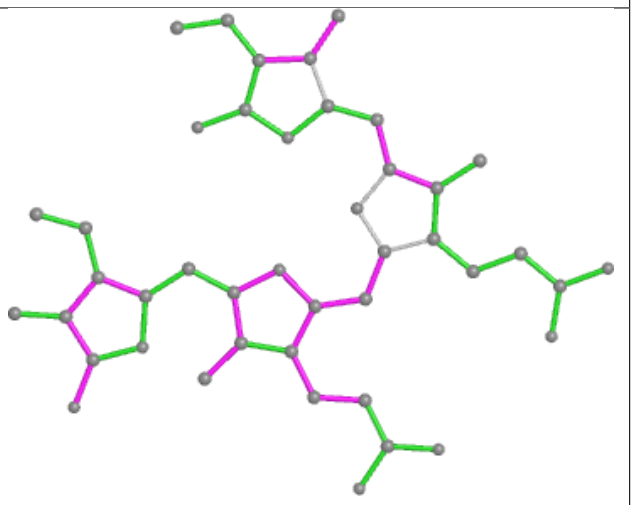

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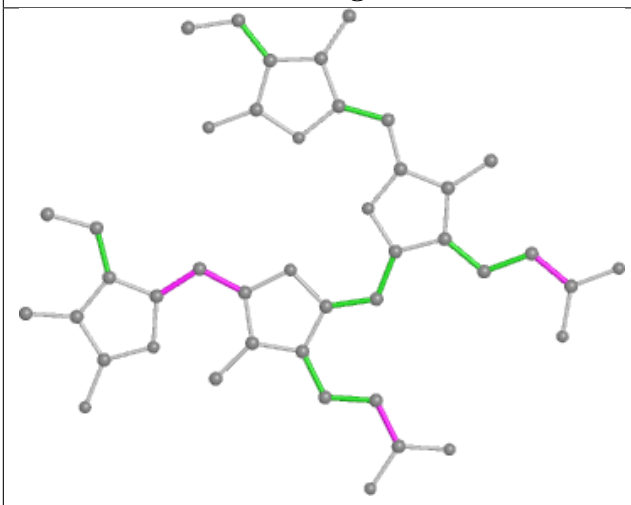

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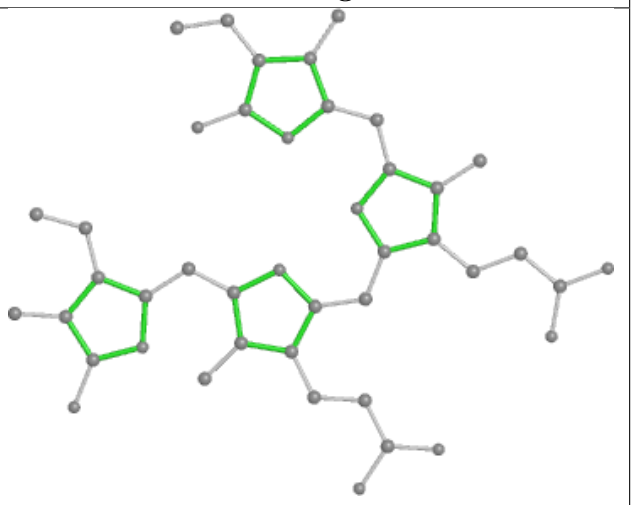
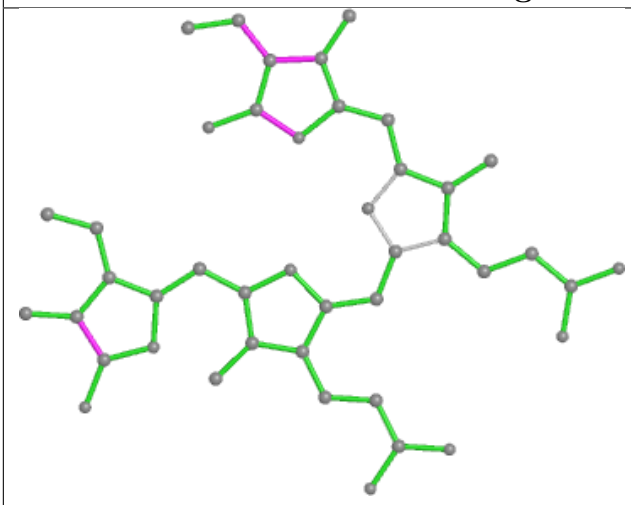


Rings

Ligand PEB G2 202



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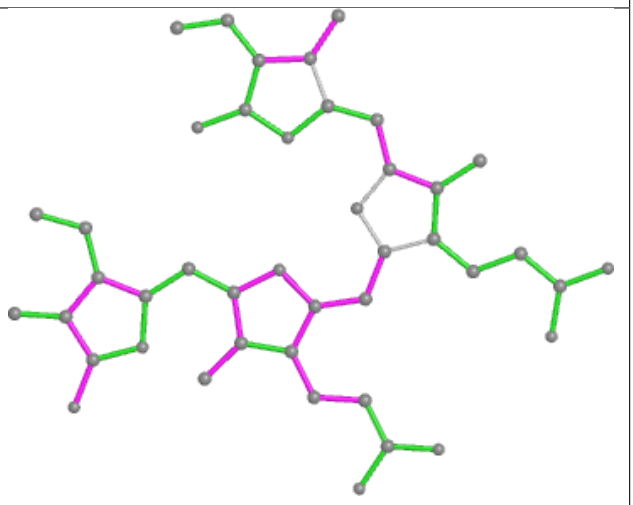
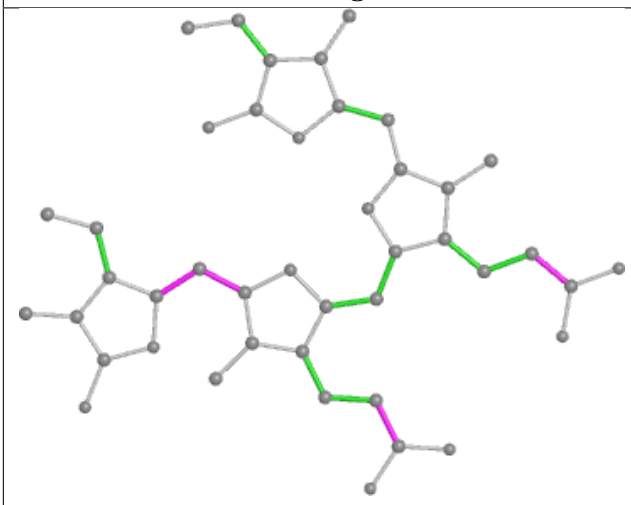


Bond angles



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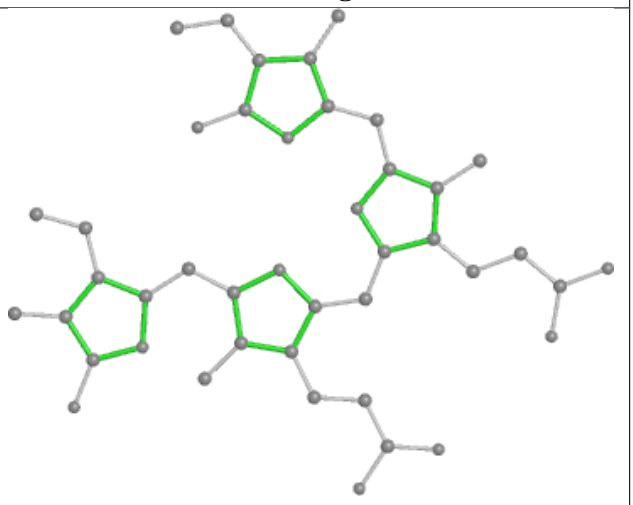
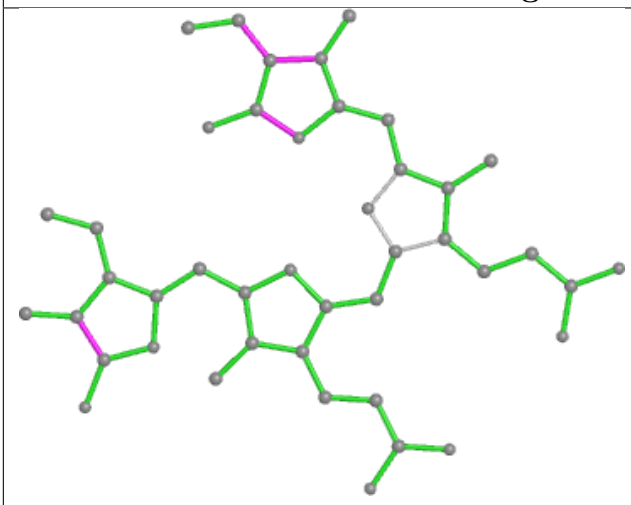


Rings

Ligand PEB t3 201



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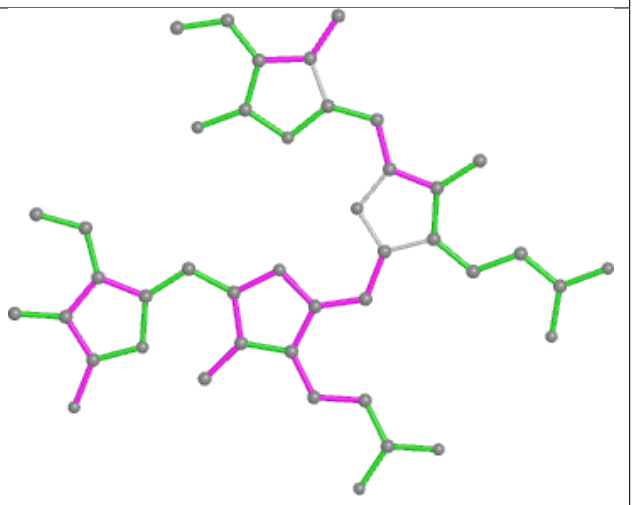
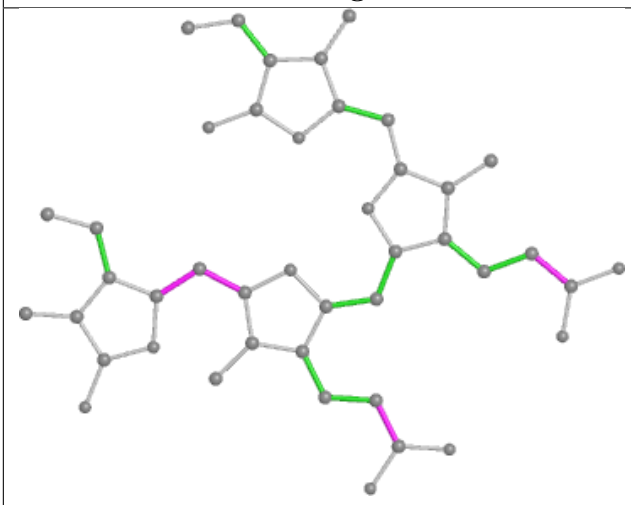


Bond angles



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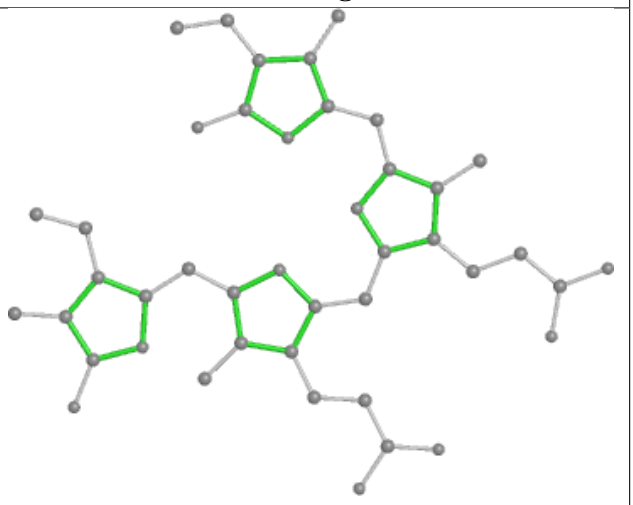
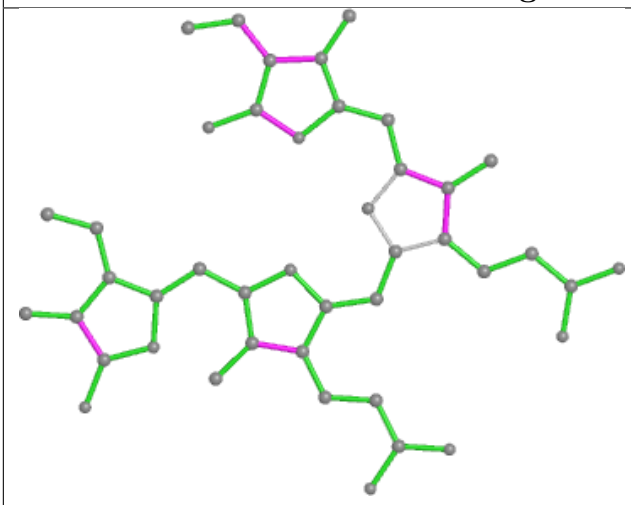


Rings

Ligand PEB v5 202



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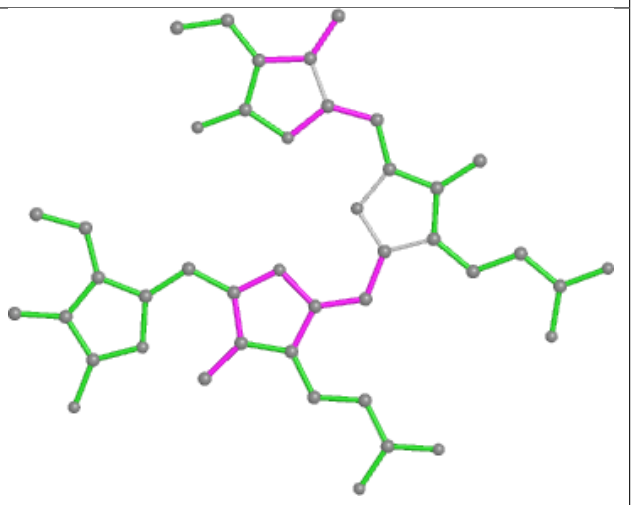

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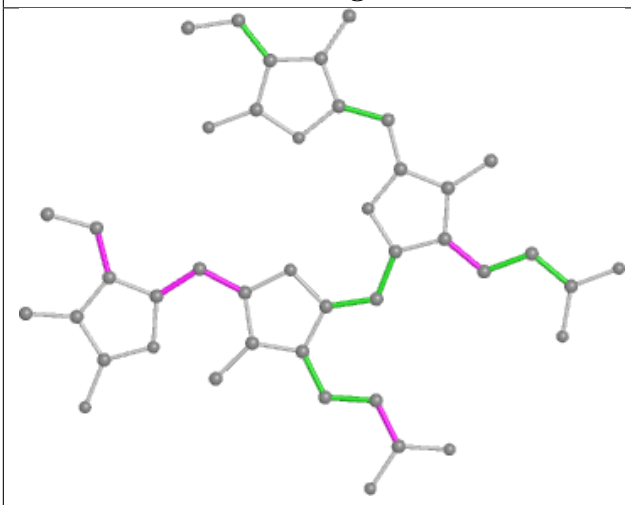

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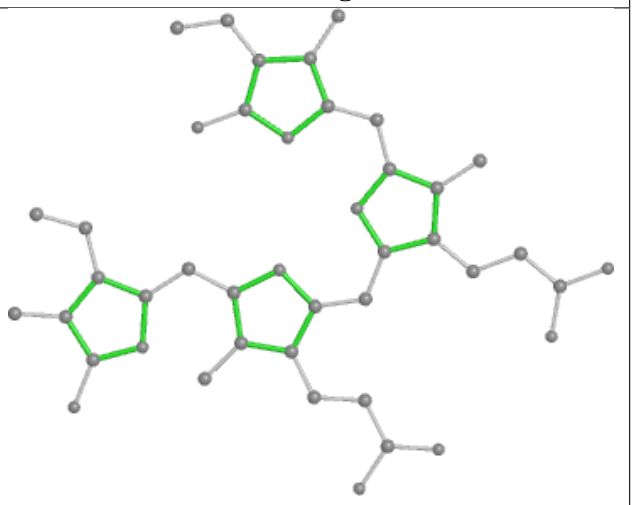

Rings

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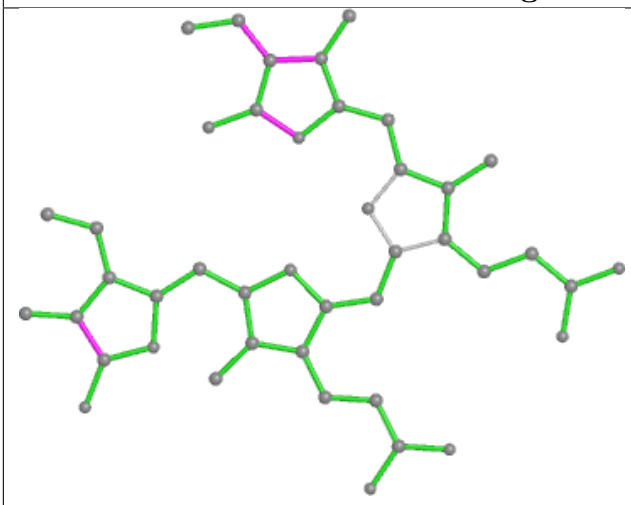

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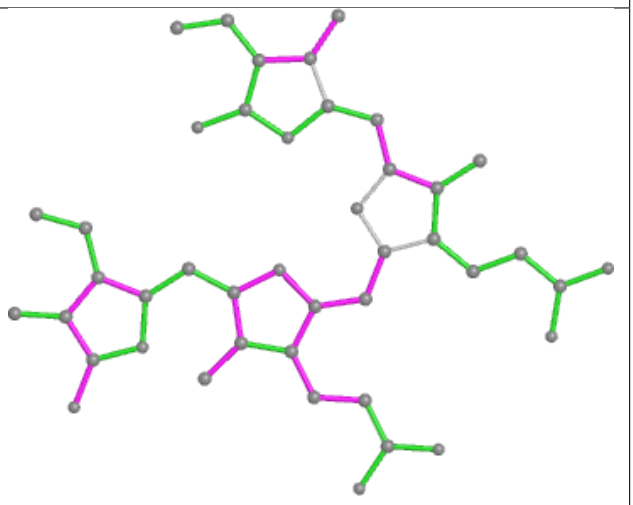

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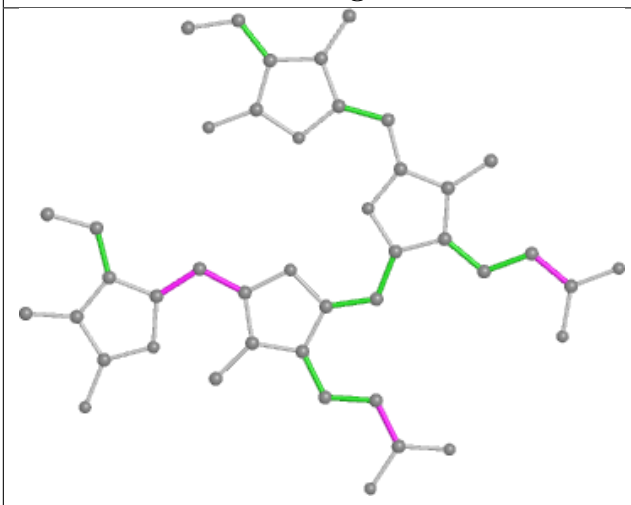

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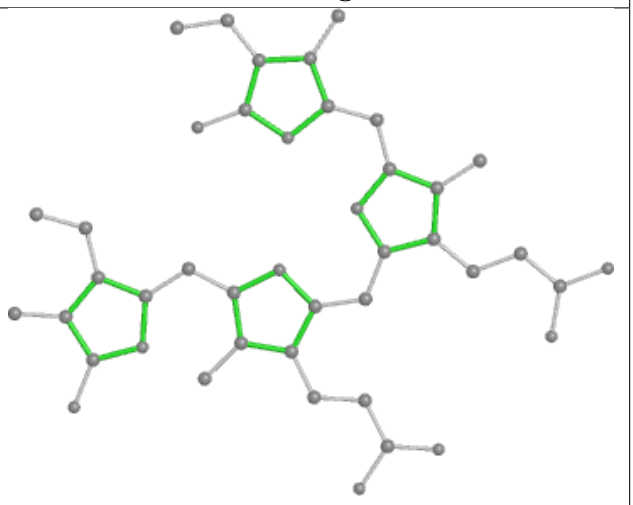
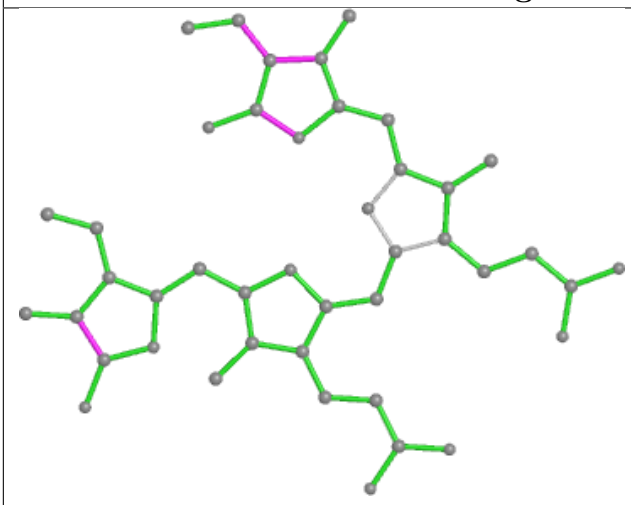


Rings

Ligand PEB hB 201



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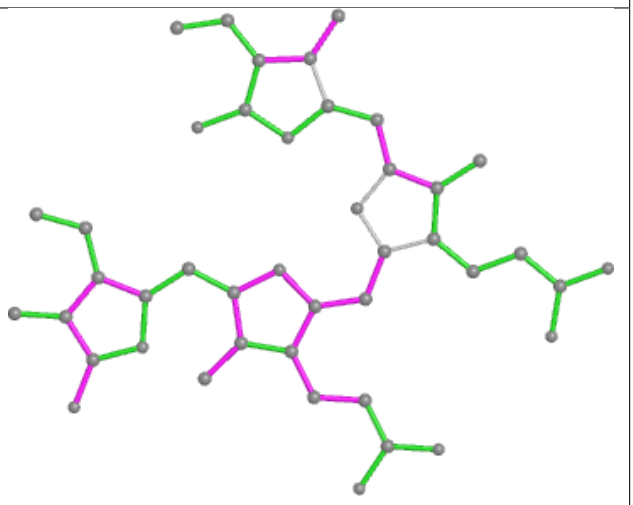

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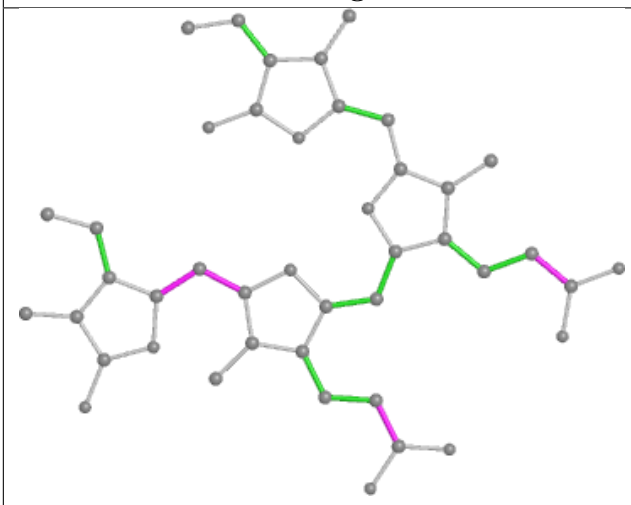

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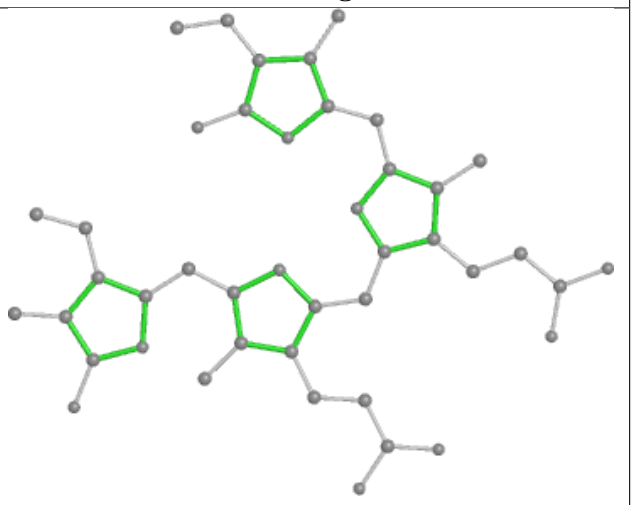
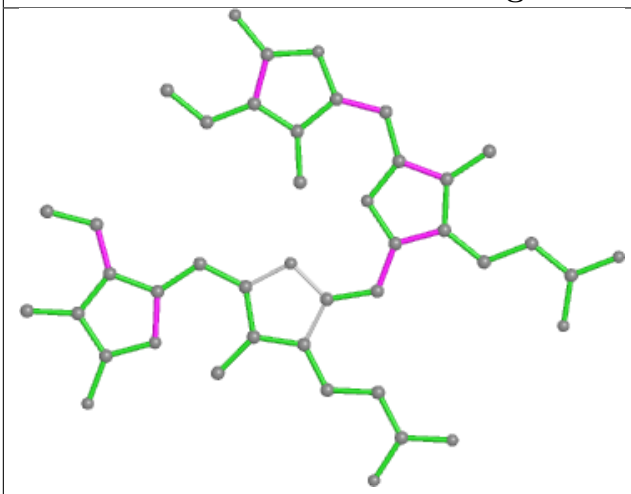


Rings

Ligand PVN b8 1004



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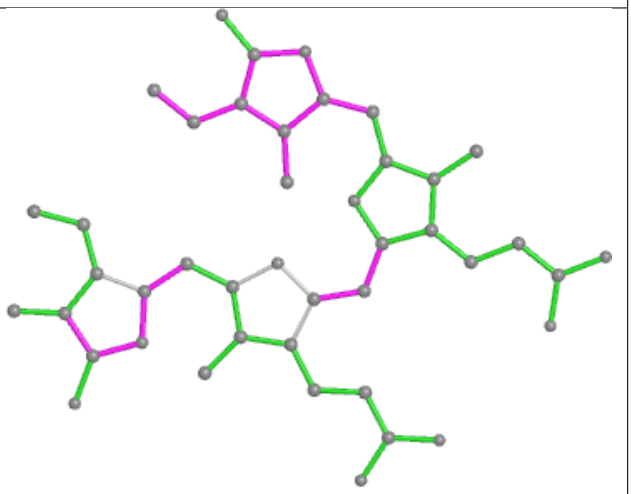
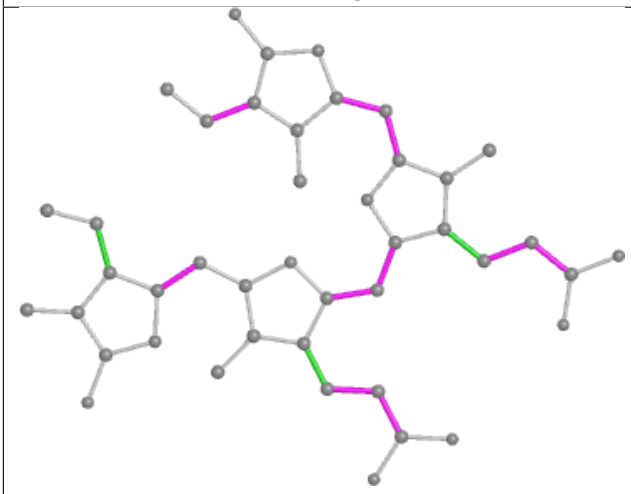


Bond angles



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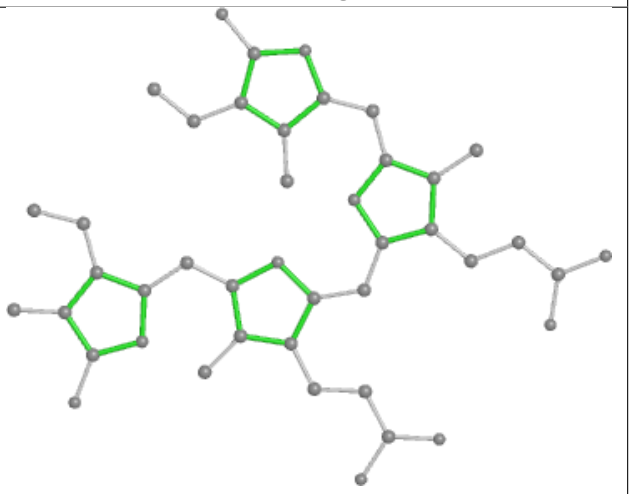
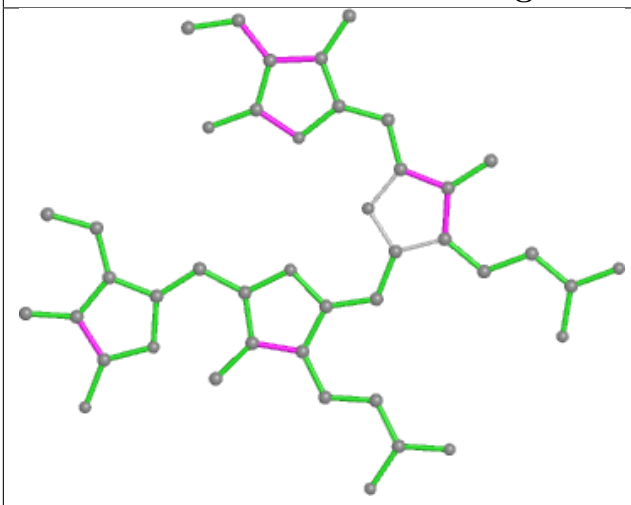


Rings

Ligand PEB bP 202



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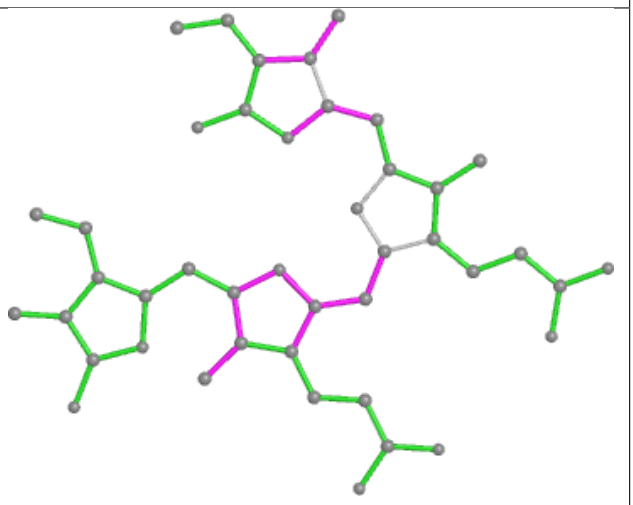

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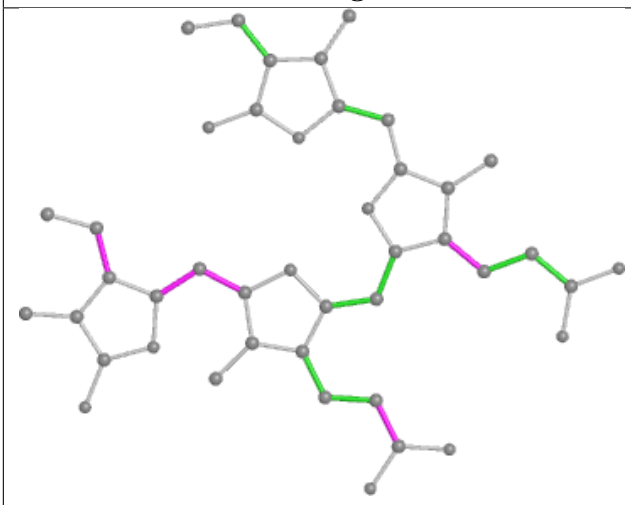

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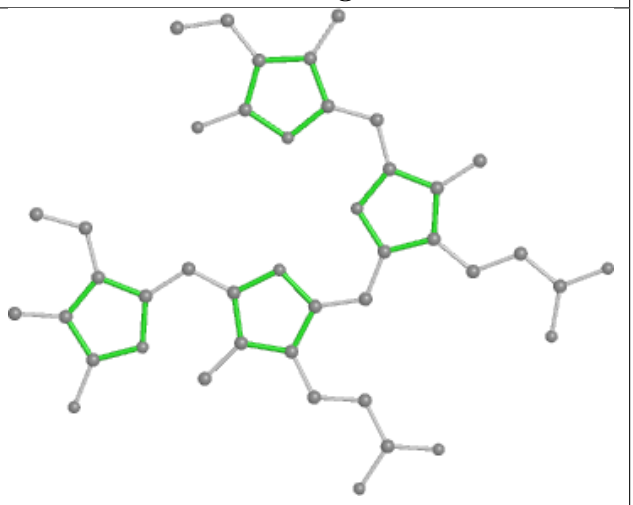
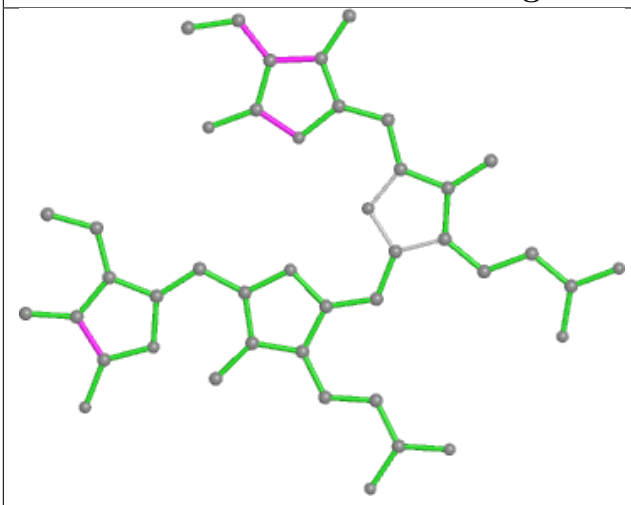


Rings

Ligand PEB lb 202



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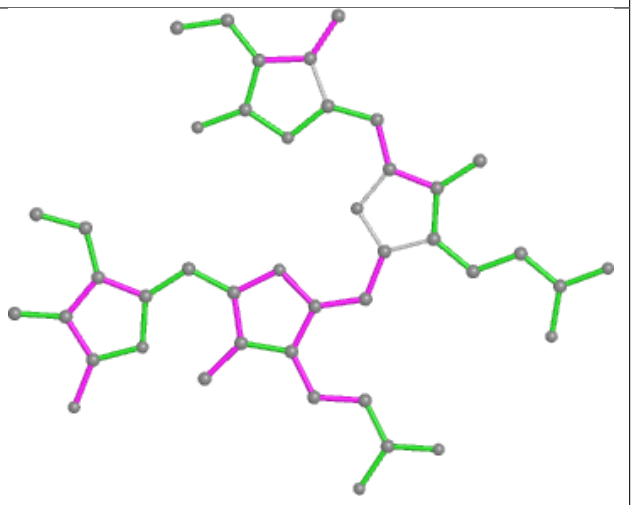

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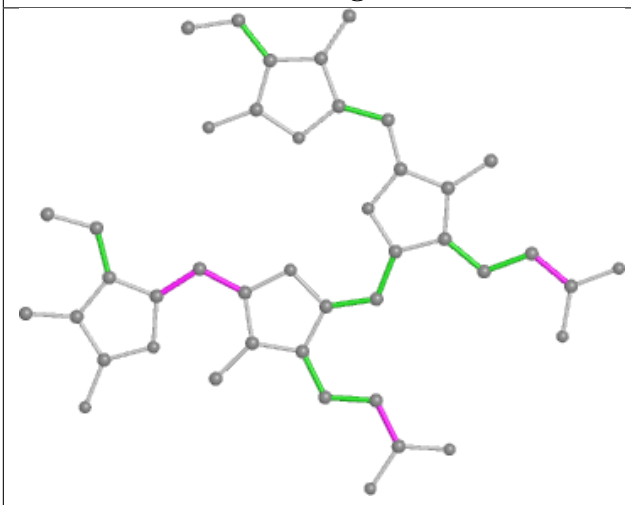

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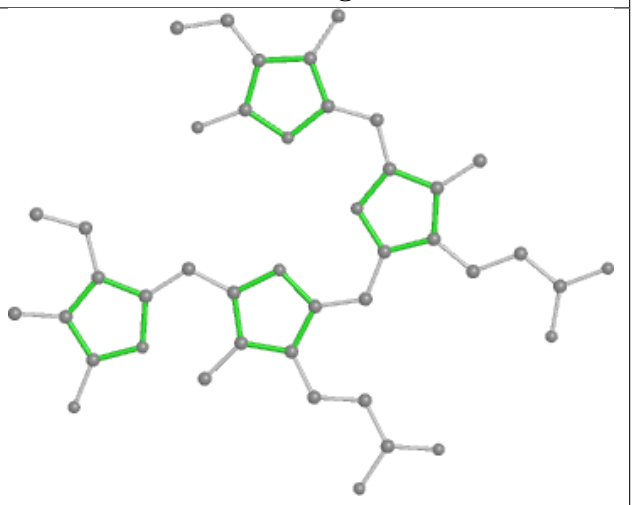
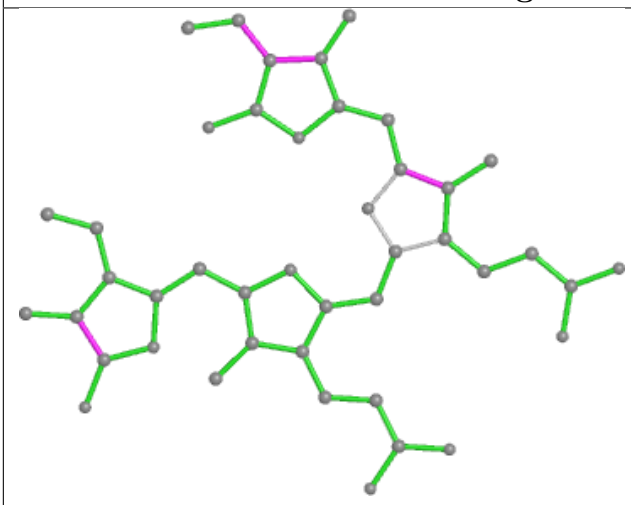


Rings

Ligand PEB cD 202



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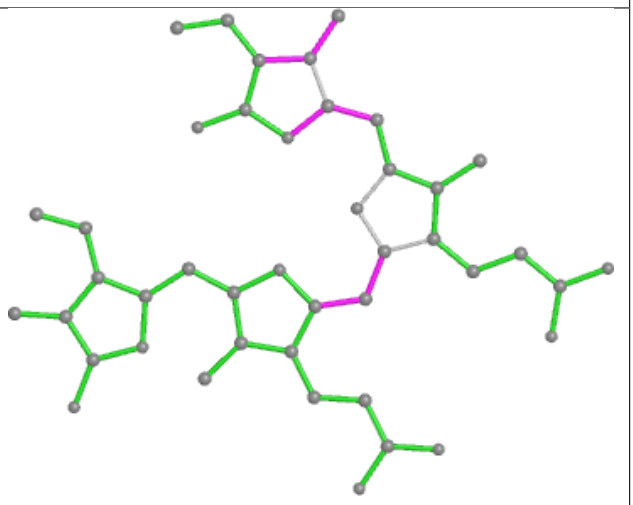

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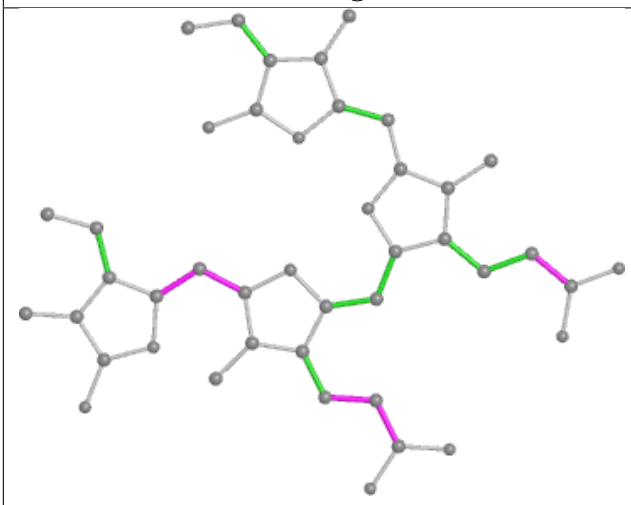

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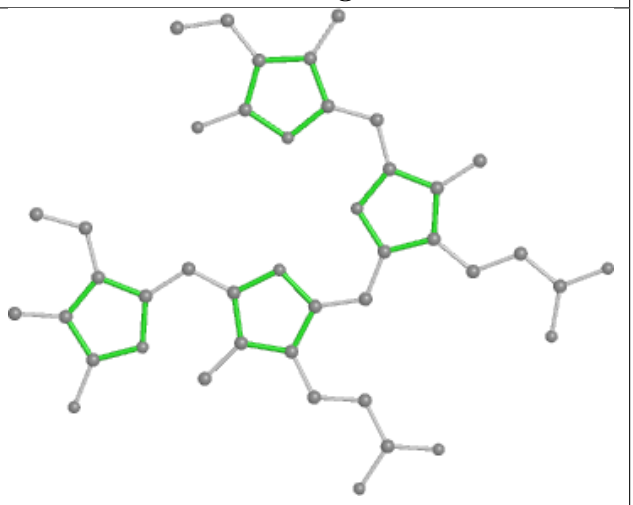
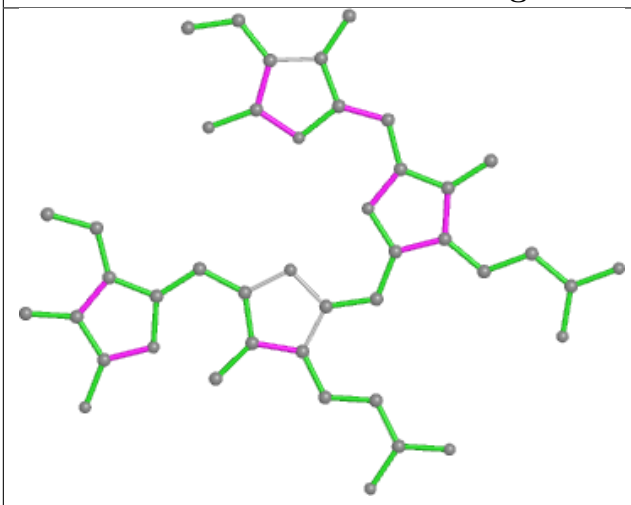


Rings

Ligand PUB bs 1004



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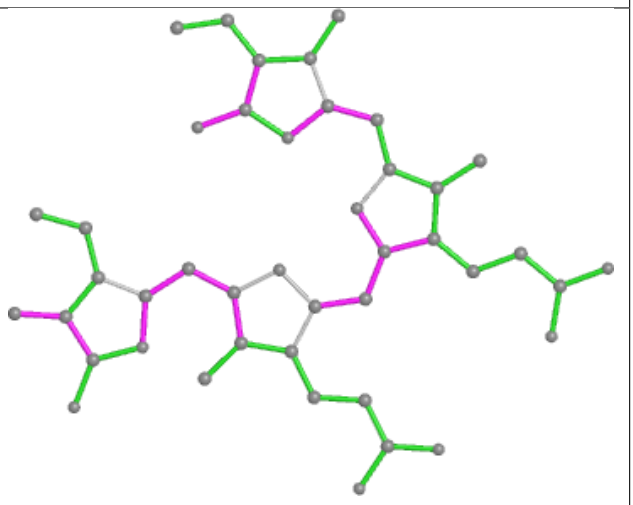
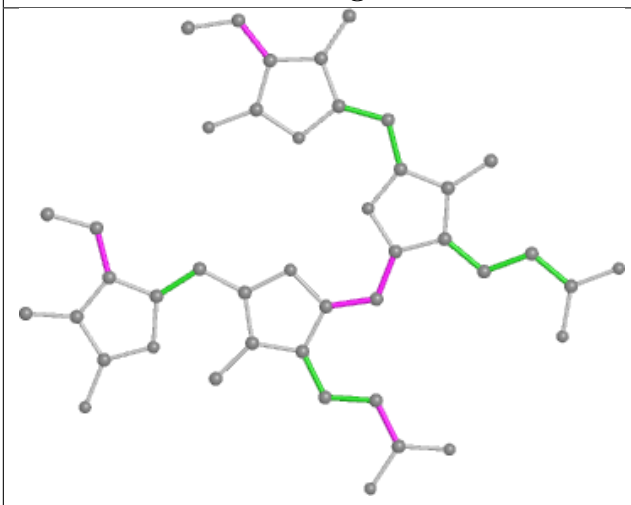


Bond angles



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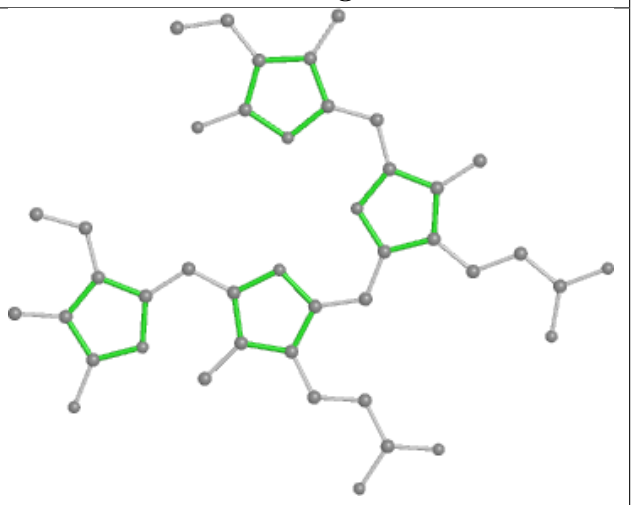
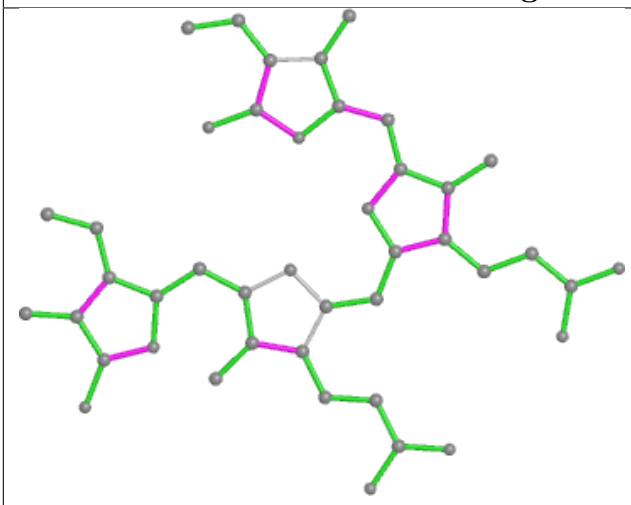


Rings

Ligand PUB ln 203



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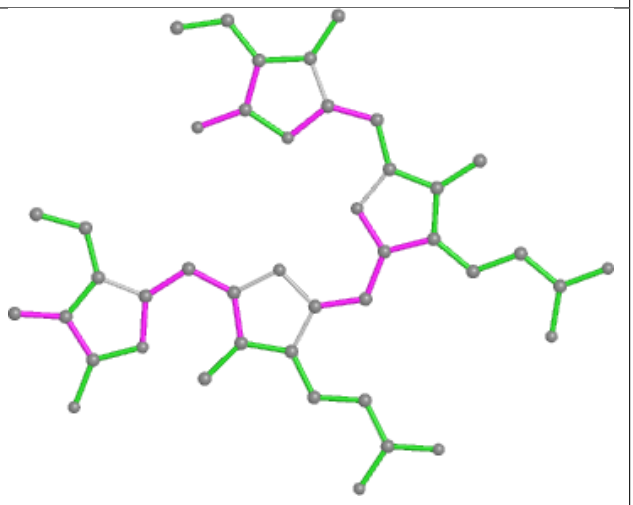
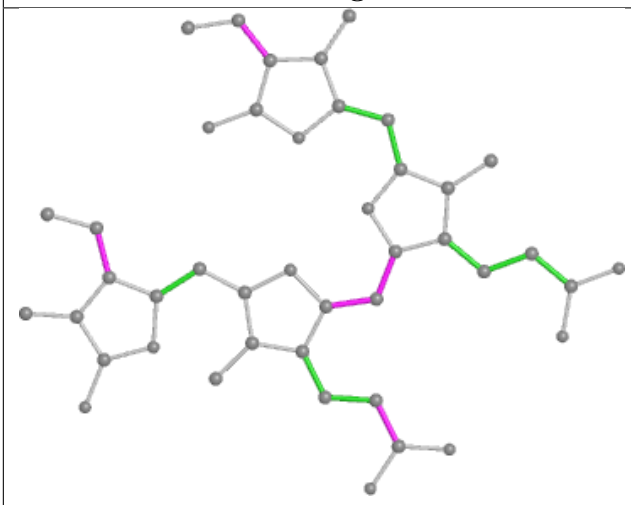


Bond angles



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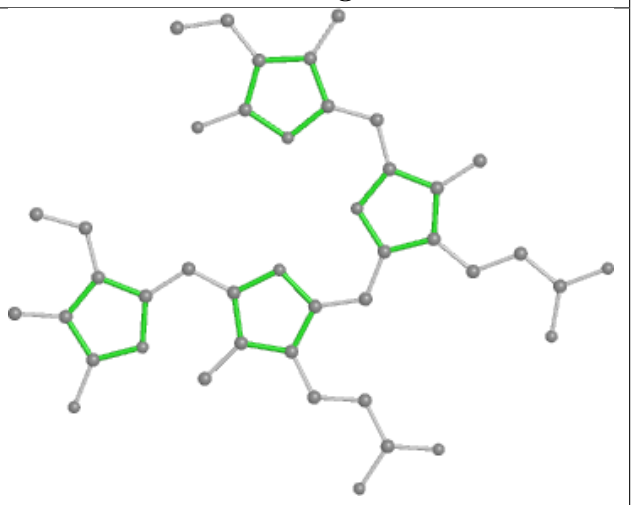
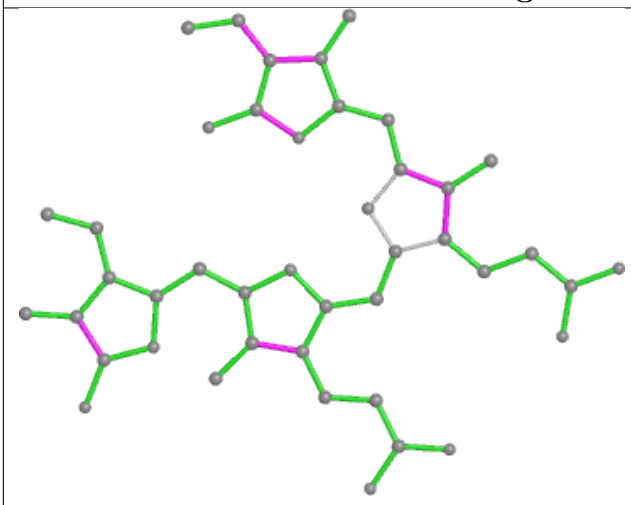
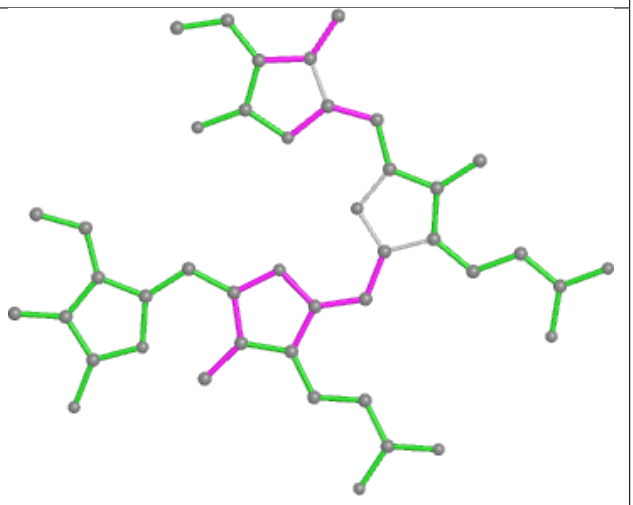


Rings

Ligand PEB B3 202



Bond lengths



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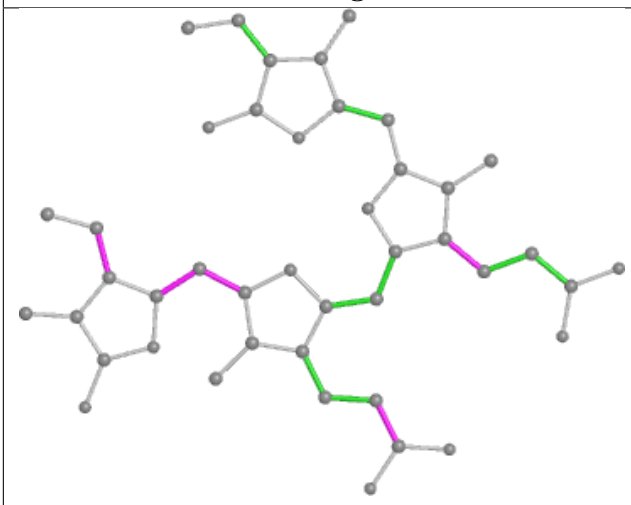
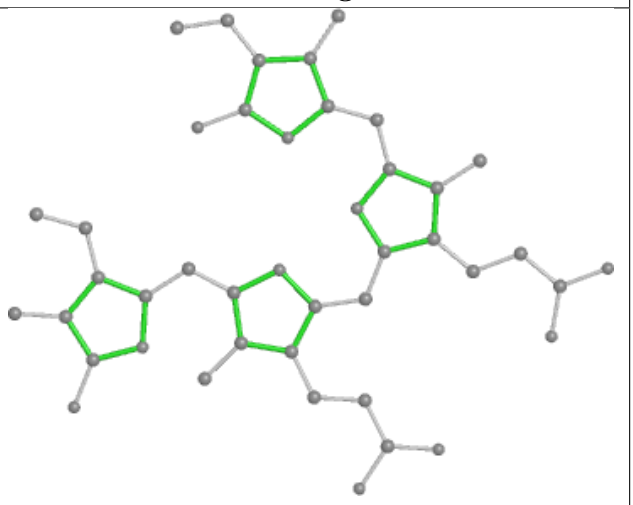
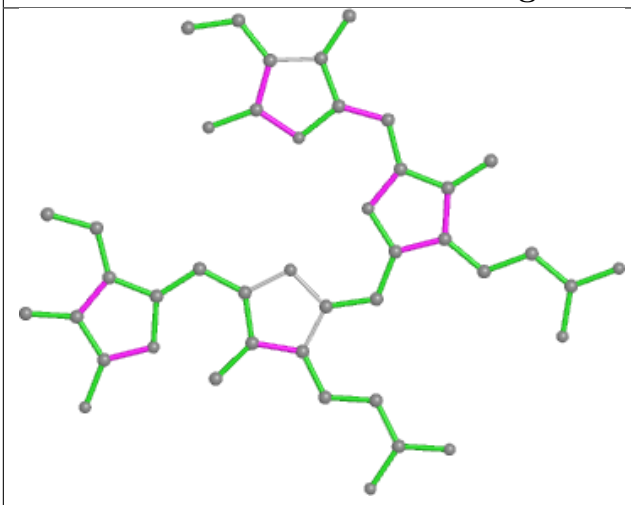


Torsions



Rings

Ligand PUB z2 203



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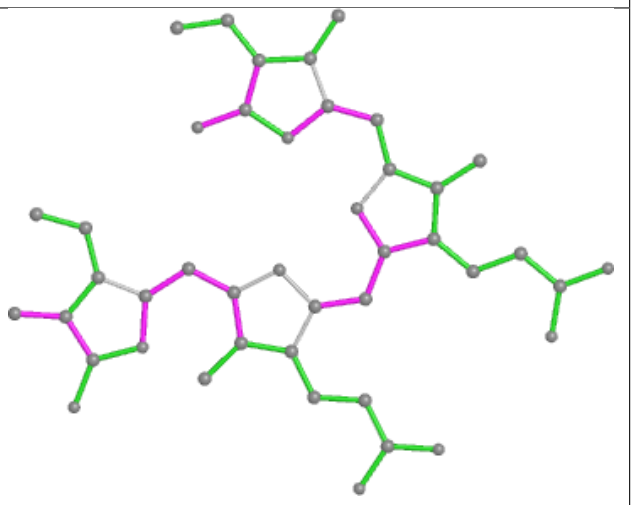

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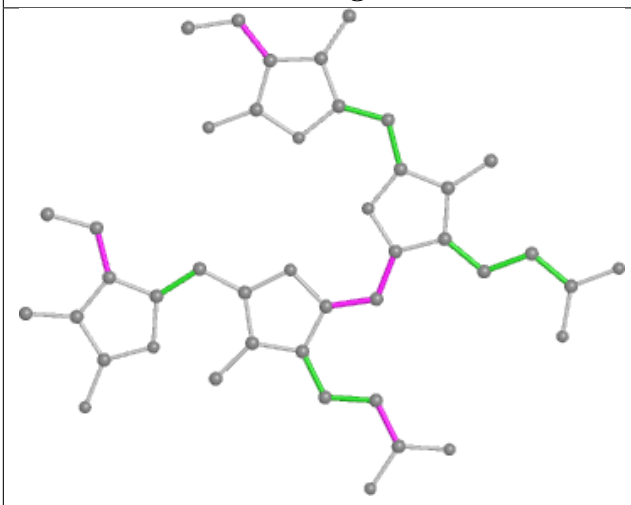

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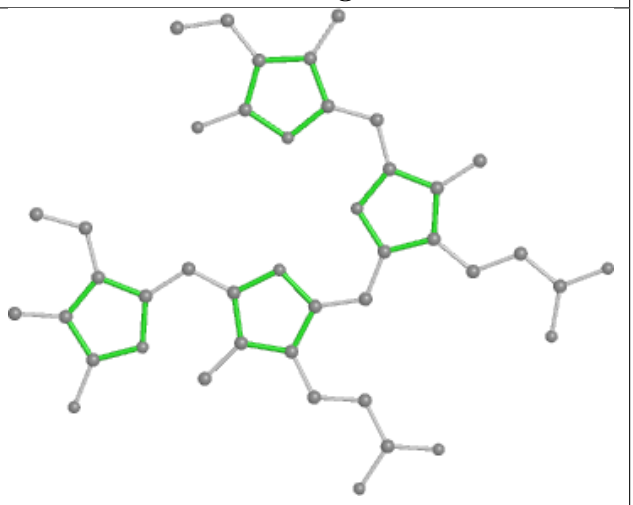

Rings

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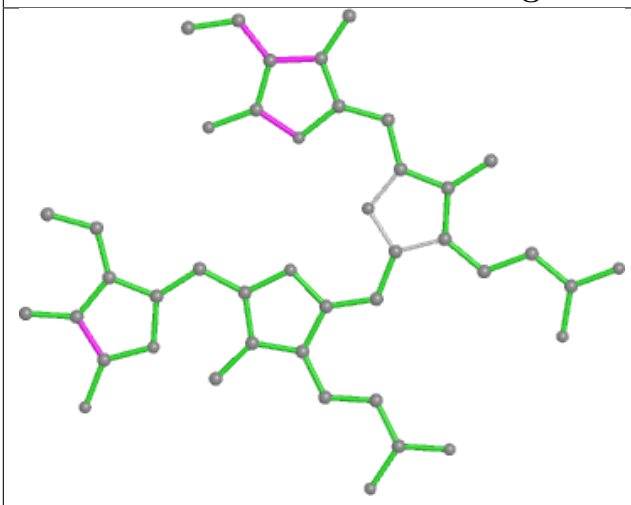

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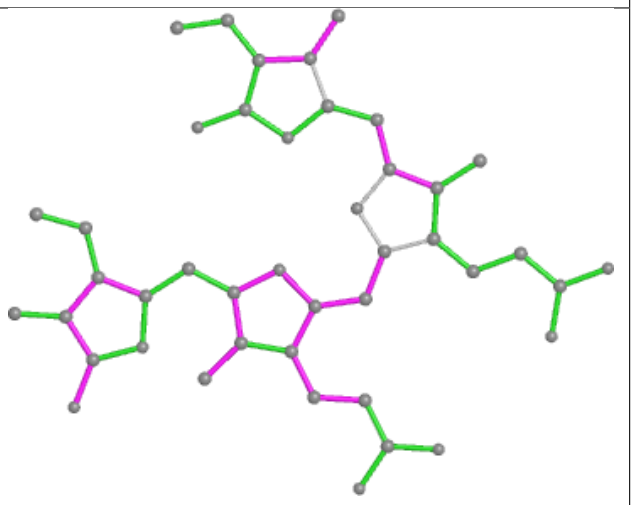

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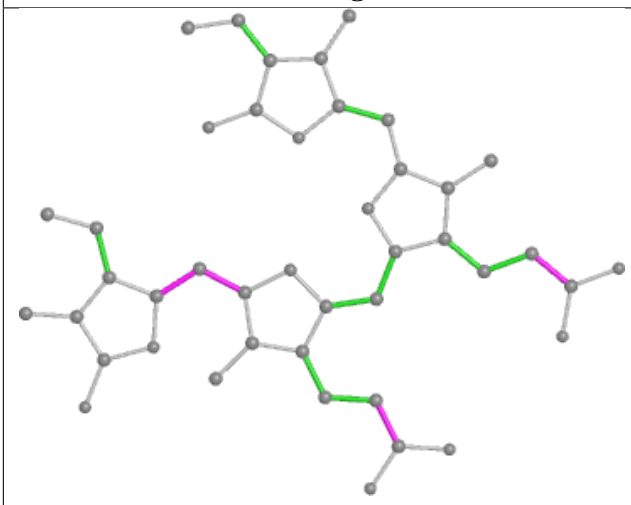

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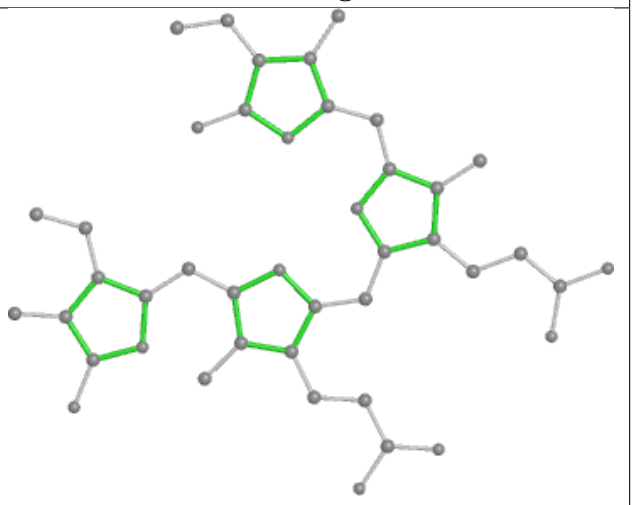

Rings

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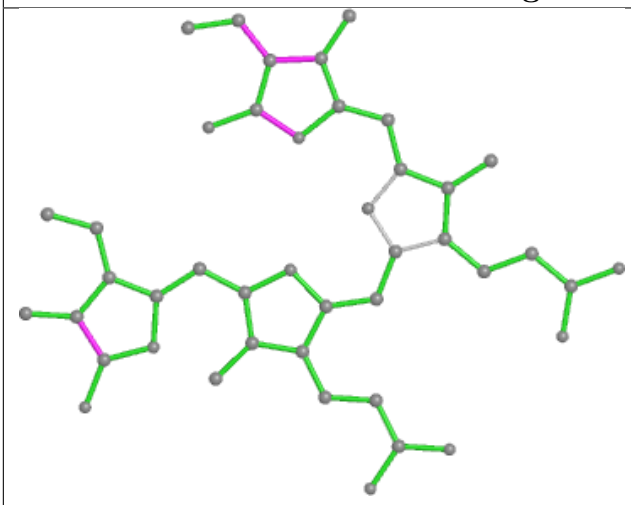

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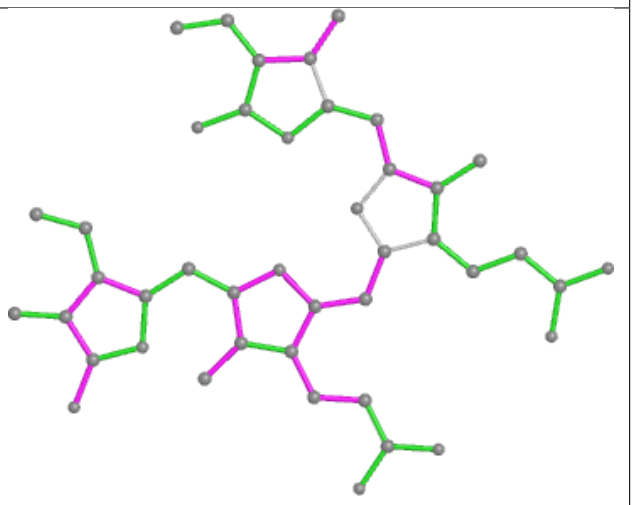

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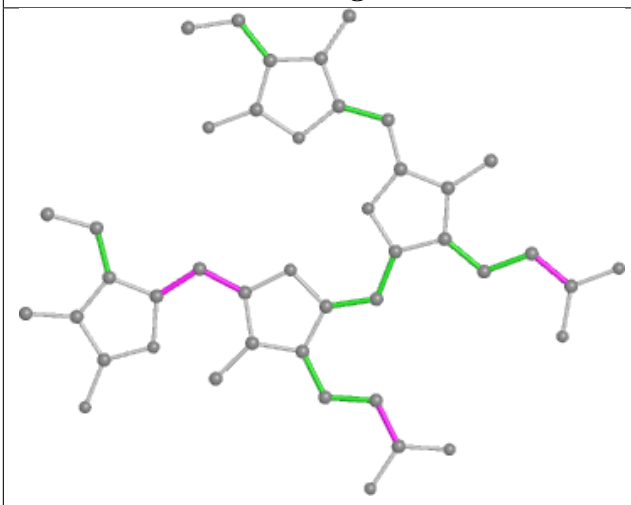

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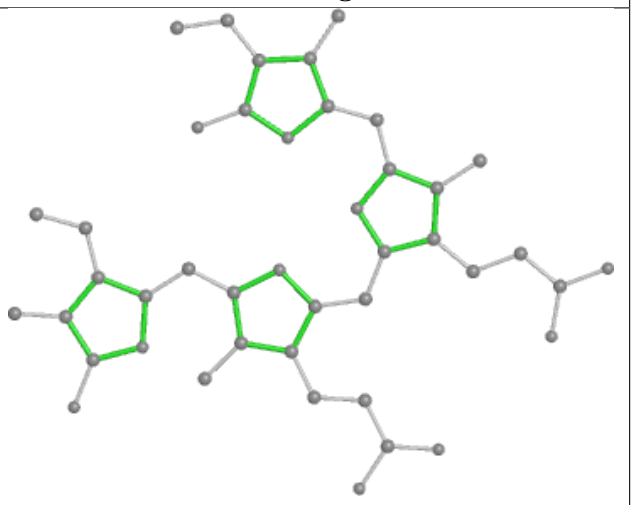
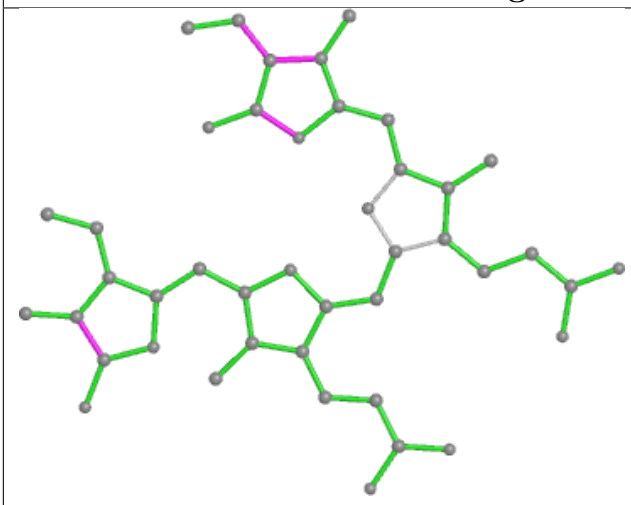


Rings

Ligand PEB cT 1001



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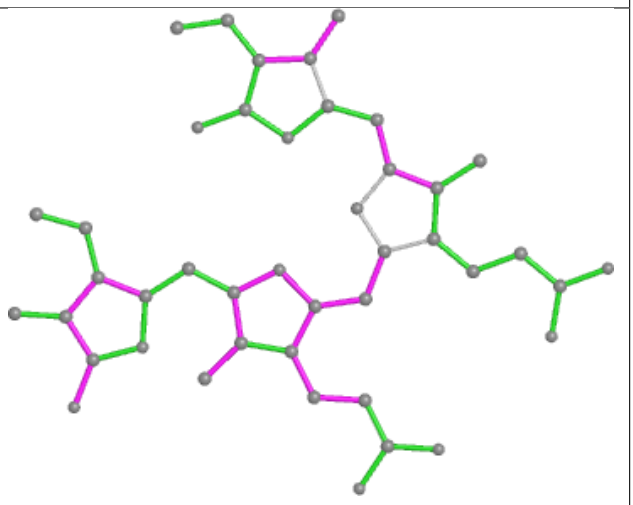

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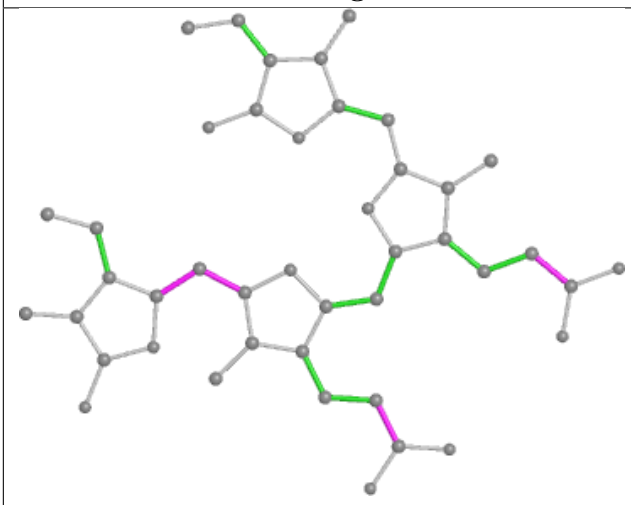

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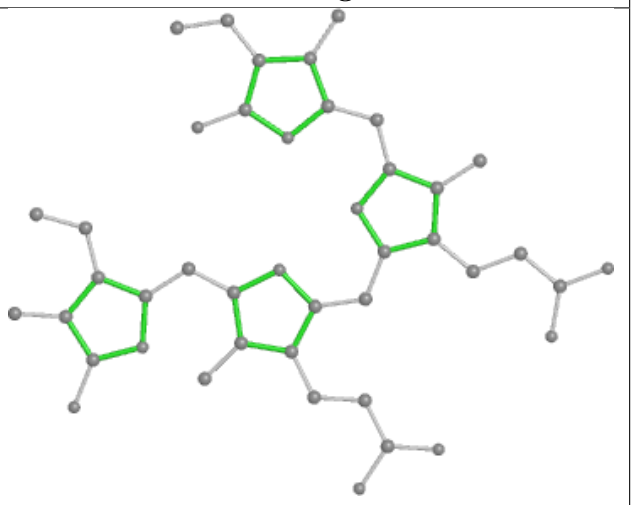

Rings

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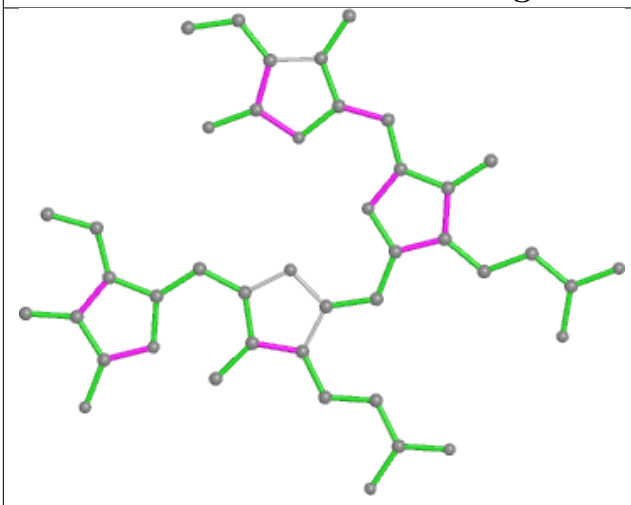

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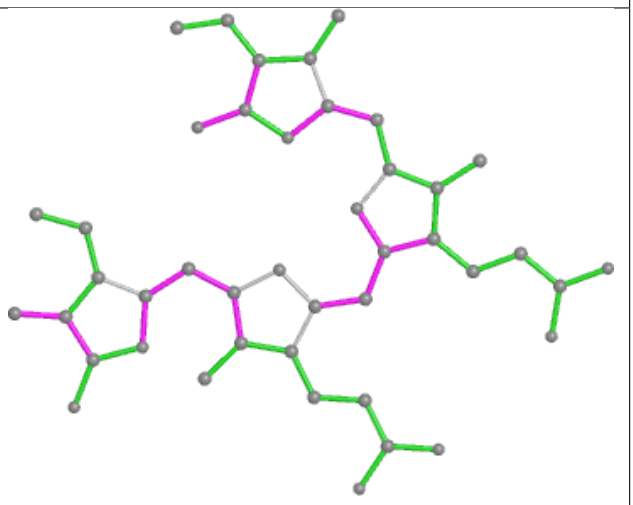

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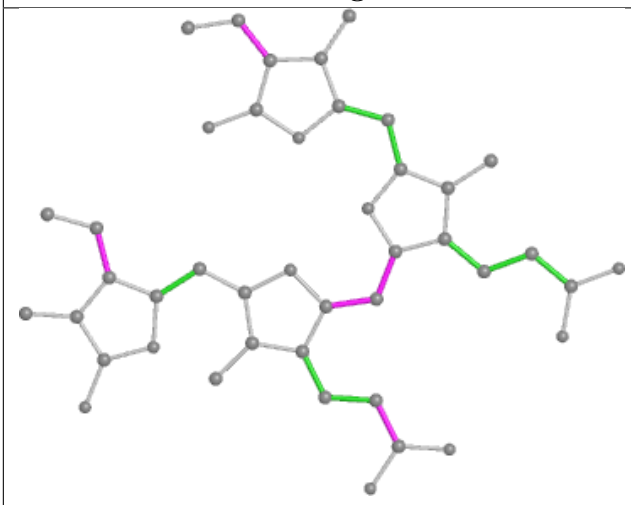

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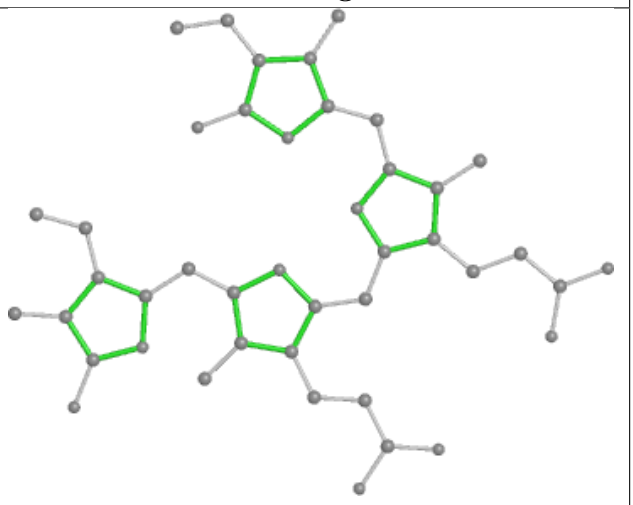

Rings

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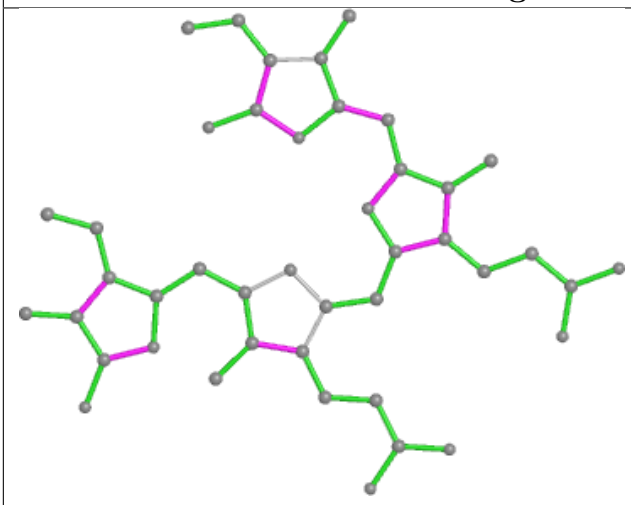

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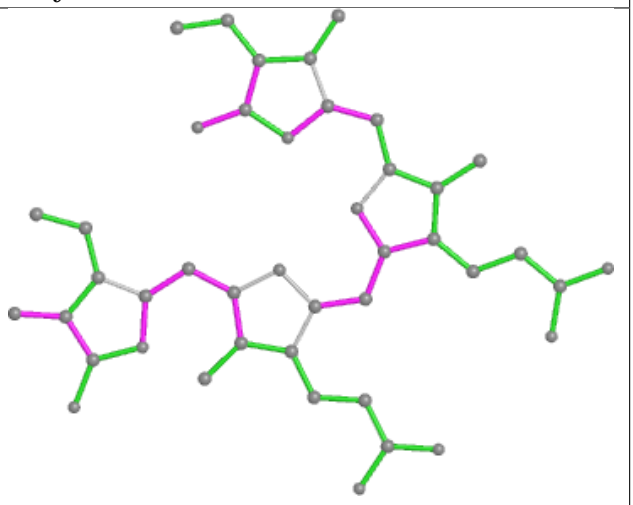

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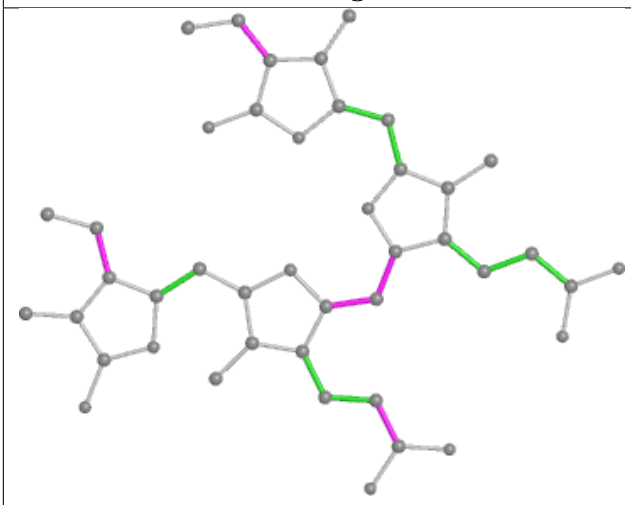

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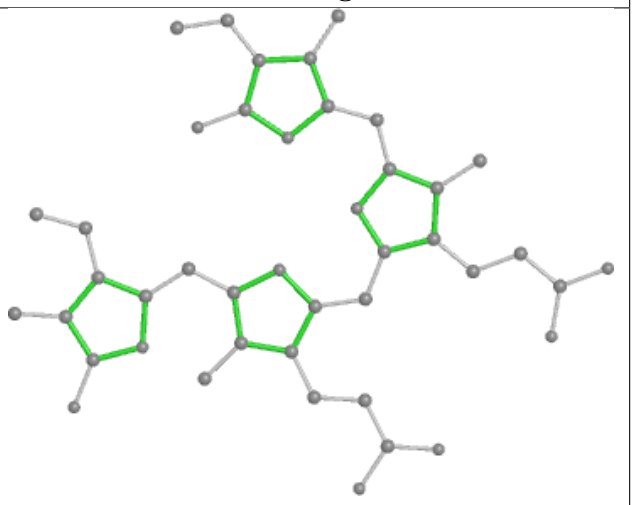
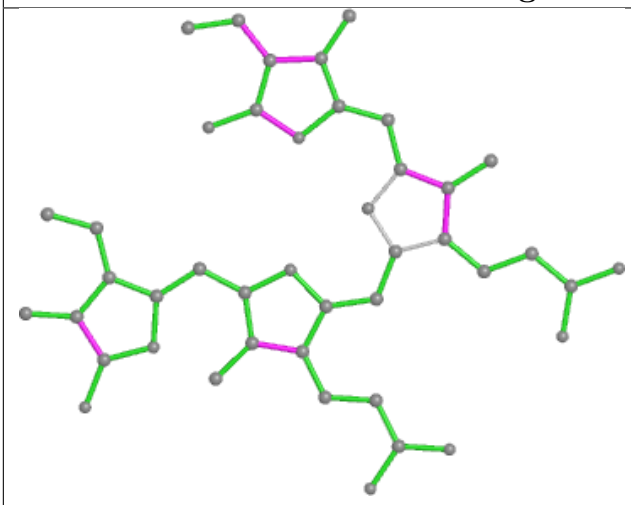


Rings

Ligand PEB n8 201



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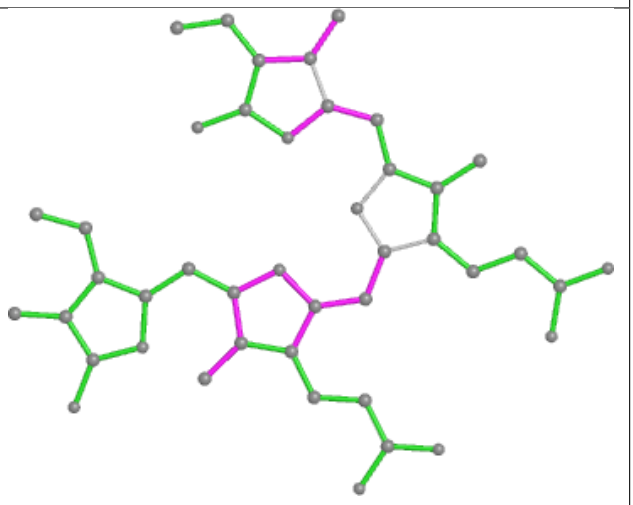

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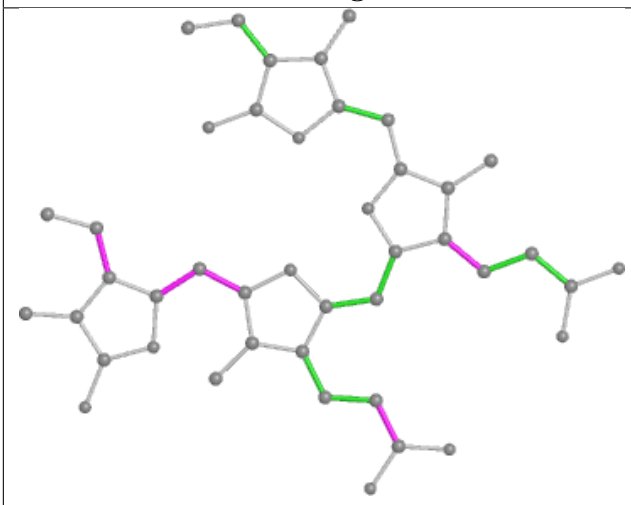

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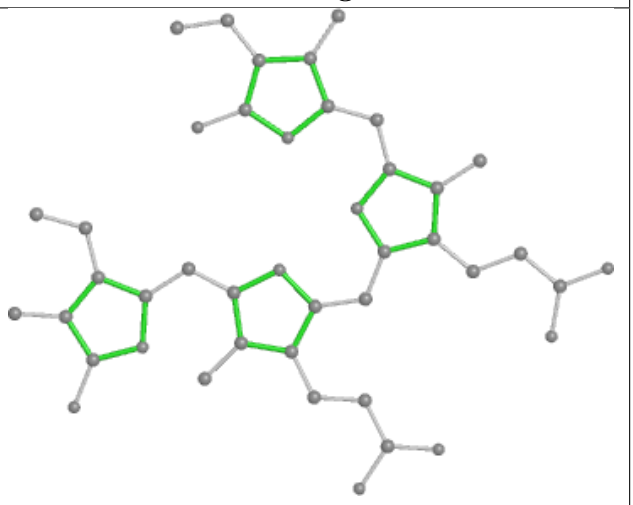
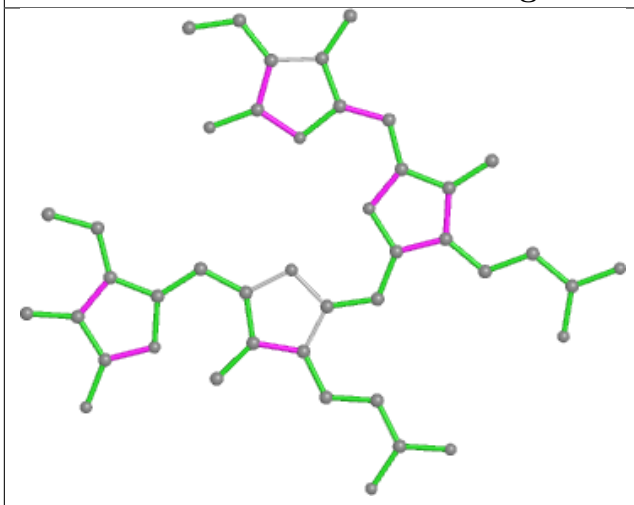


Rings

Ligand PUB z4 203



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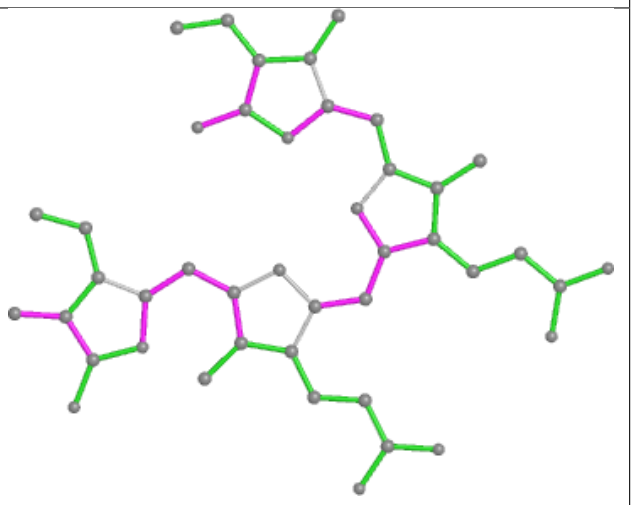

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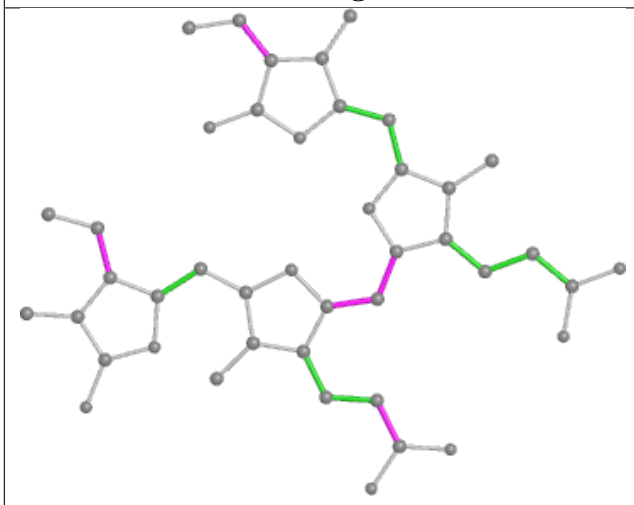

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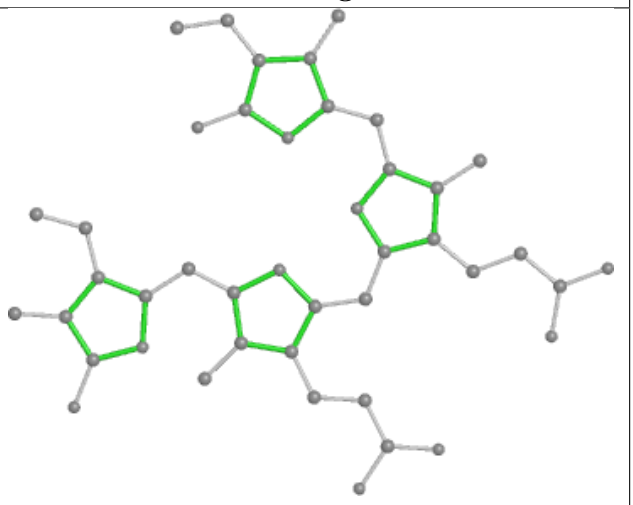

Rings

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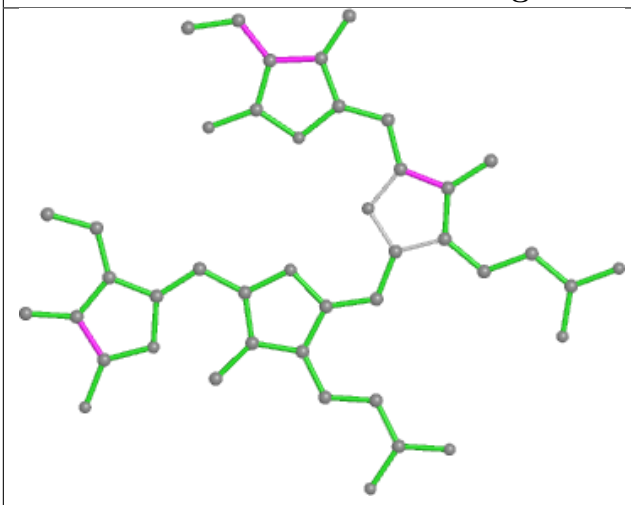

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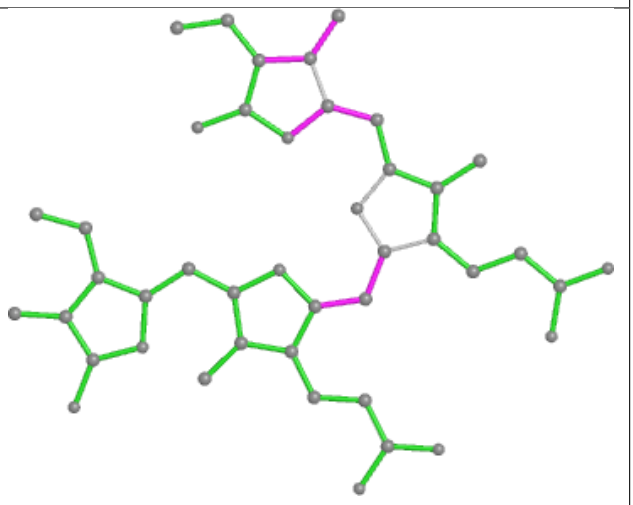

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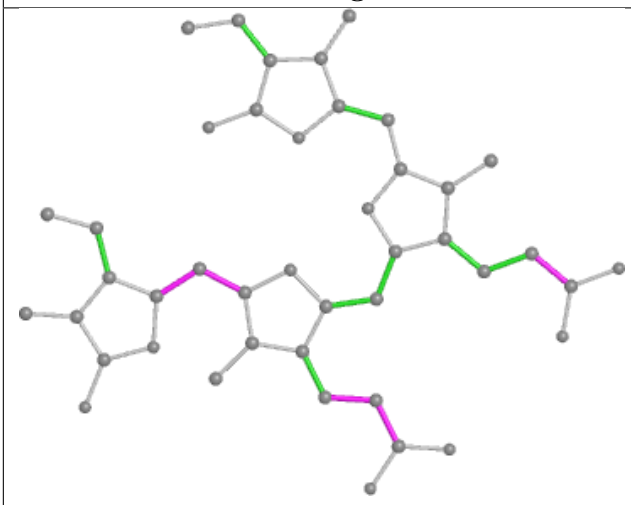

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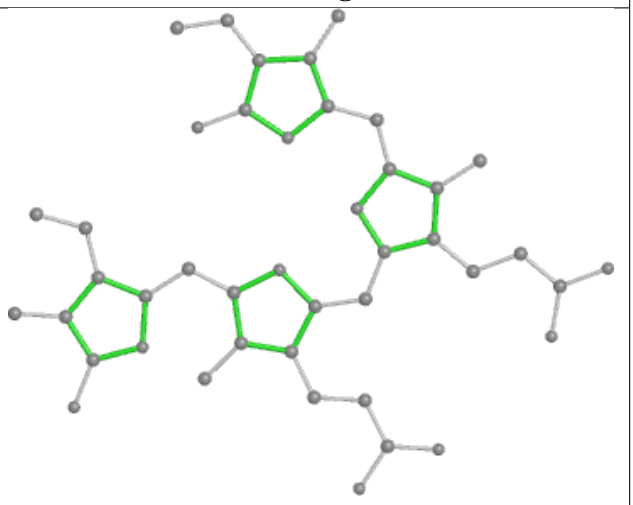
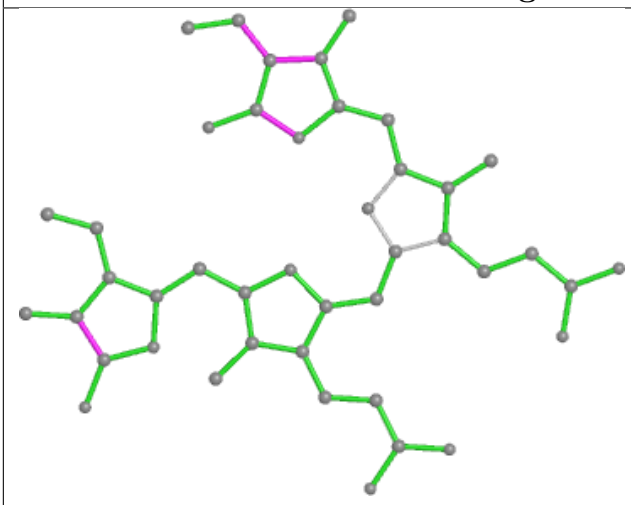


Rings

Ligand PEB n2 201



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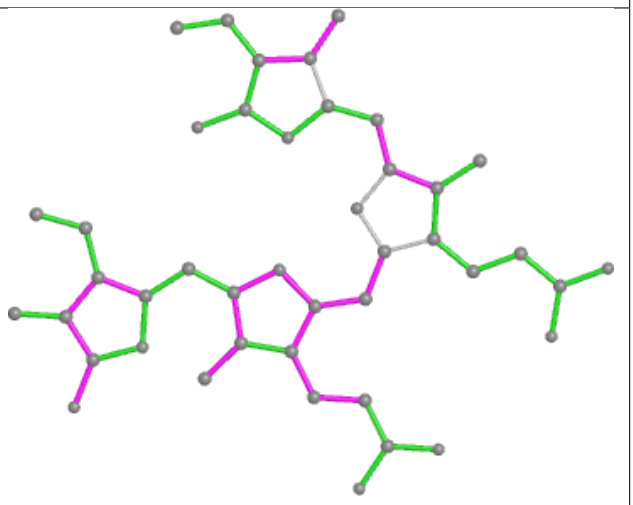

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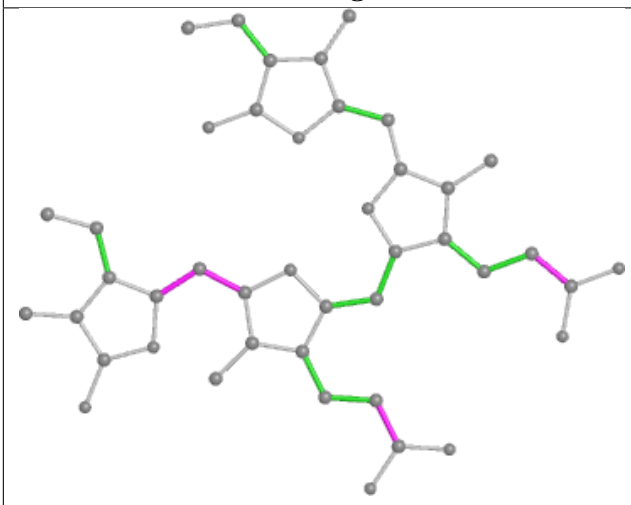

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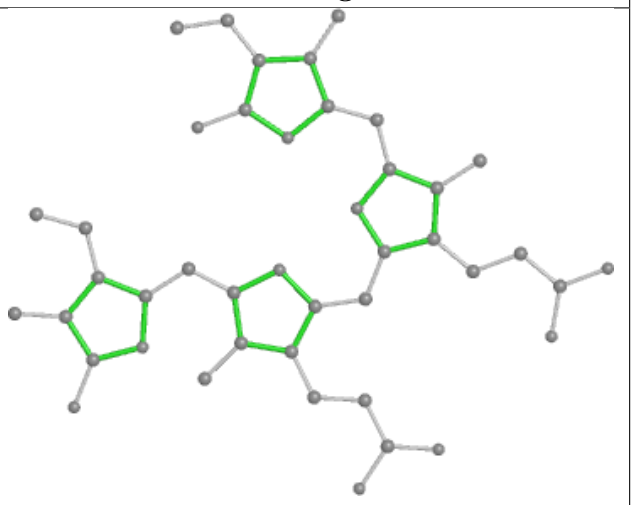
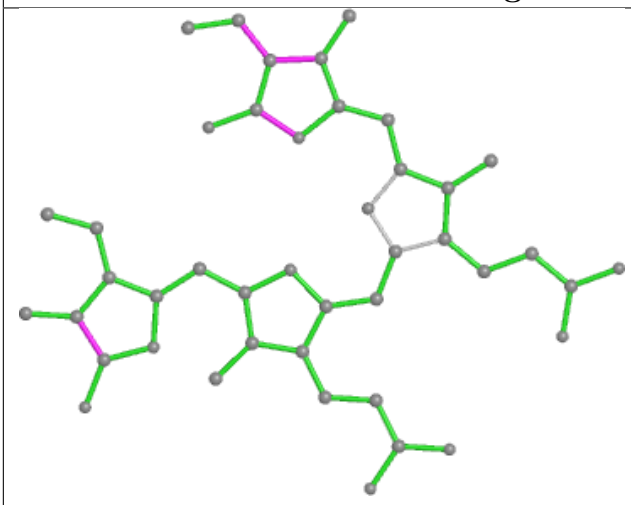


Rings

Ligand PEB bm 1001



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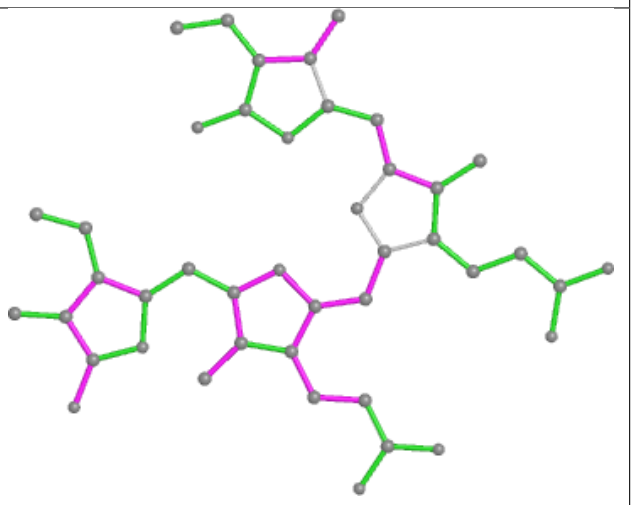

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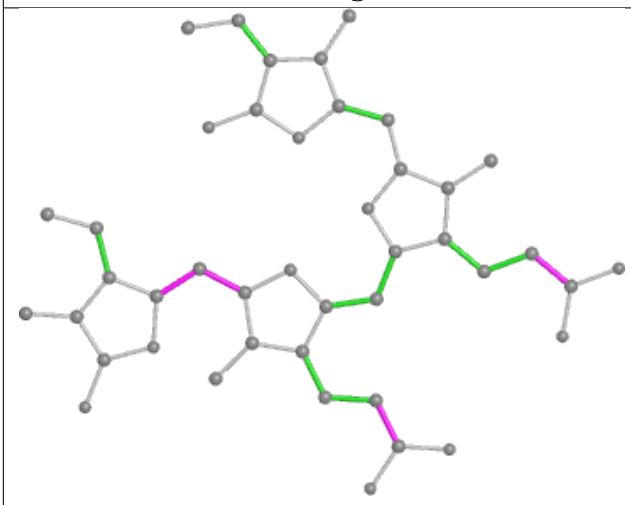

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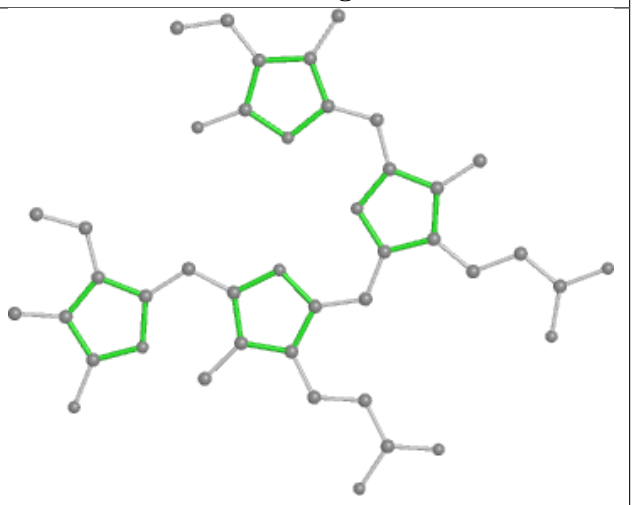

Rings

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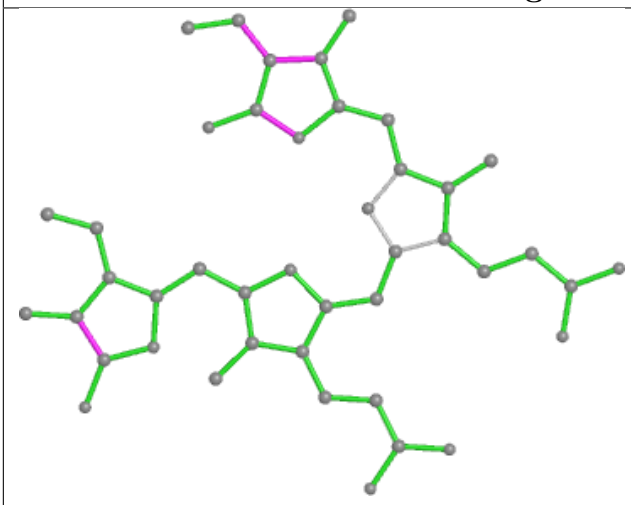

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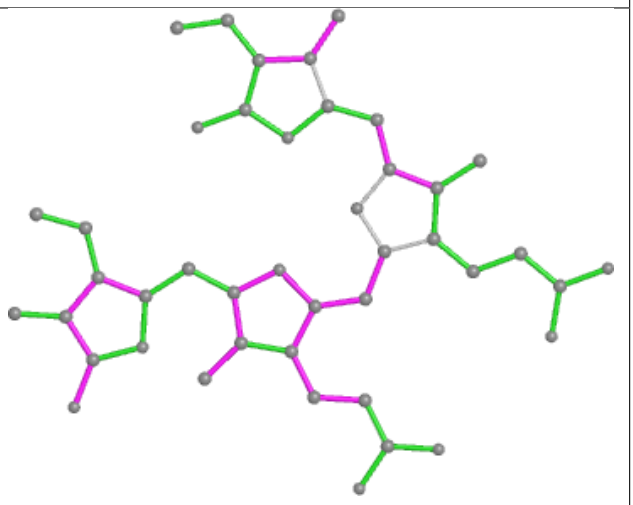

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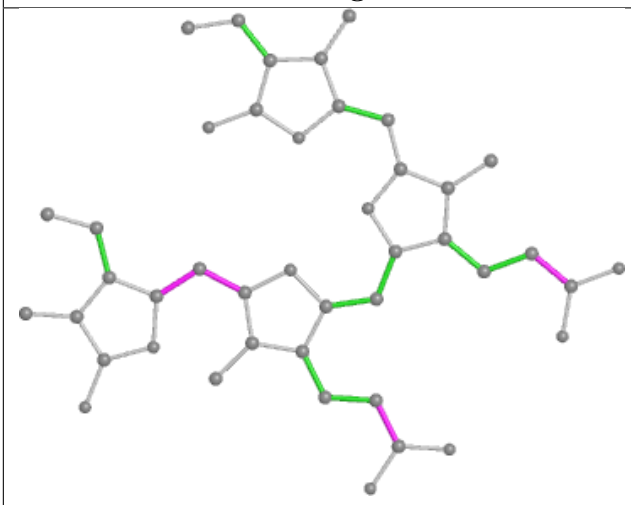

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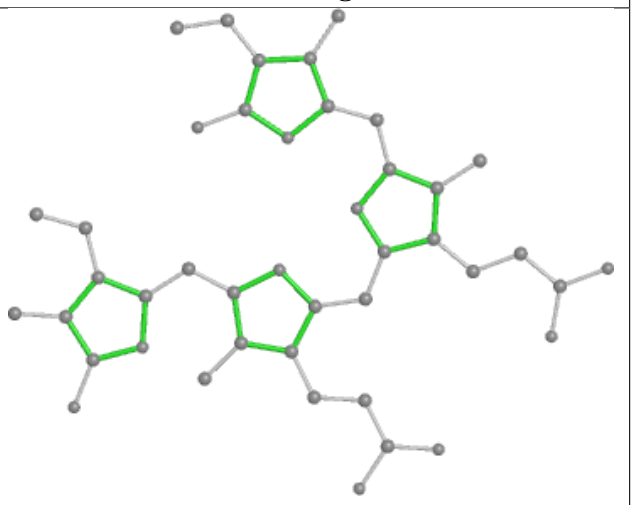
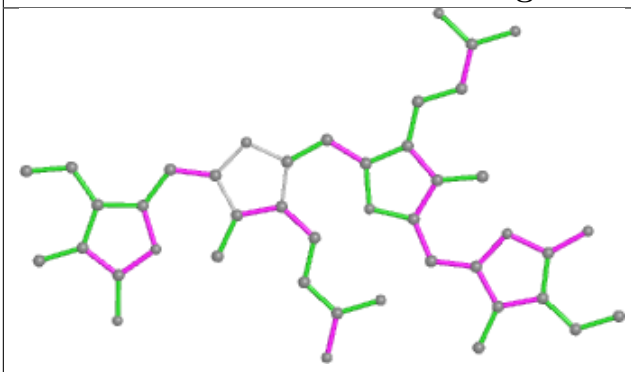


Rings

Ligand CYC h1 201



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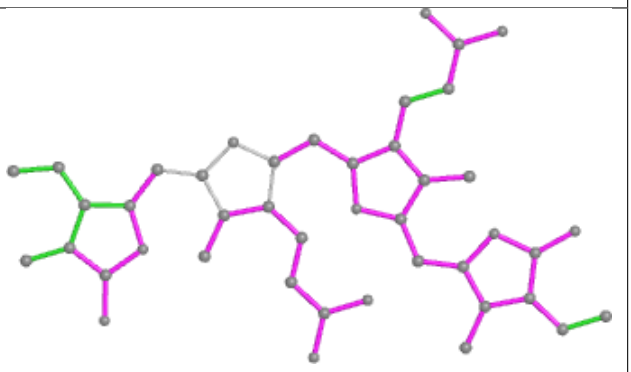
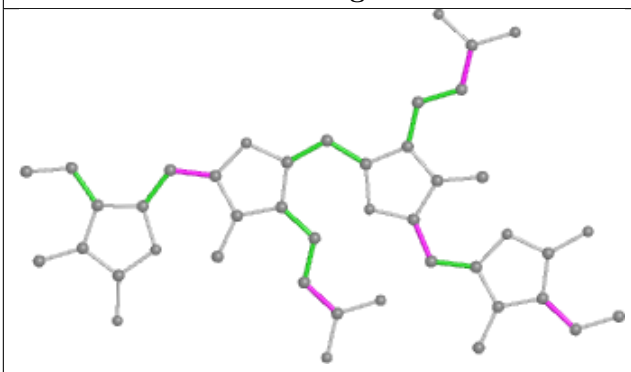
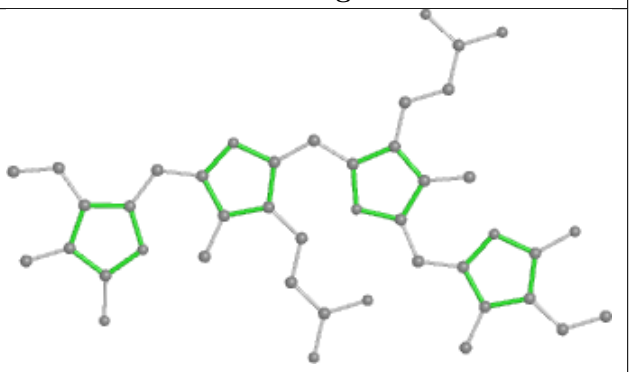


Bond angles

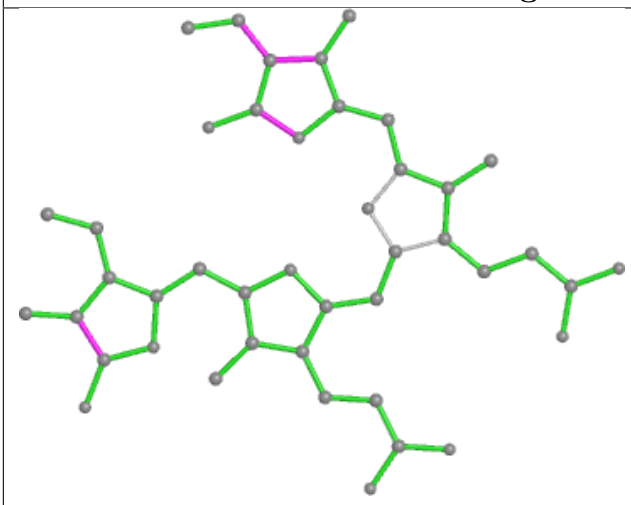


Torsions



Rings

Ligand PEB a8 602



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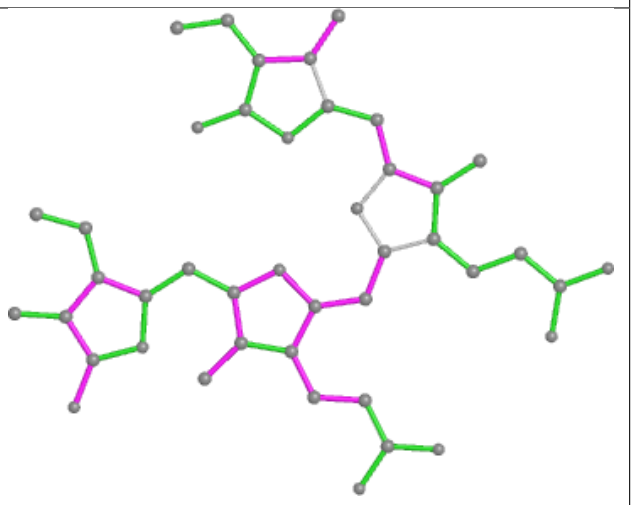

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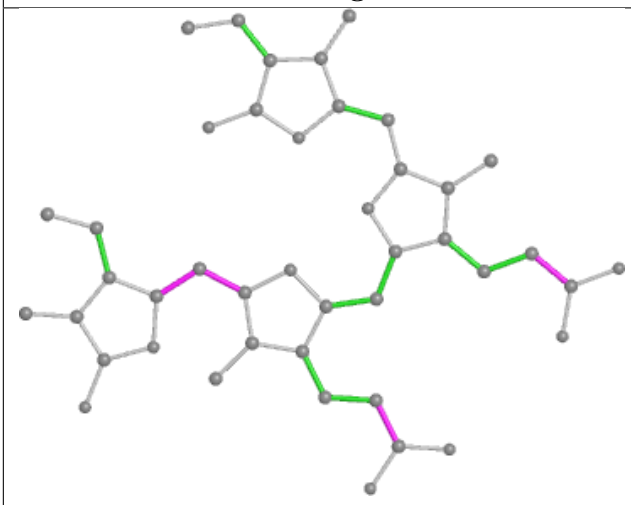

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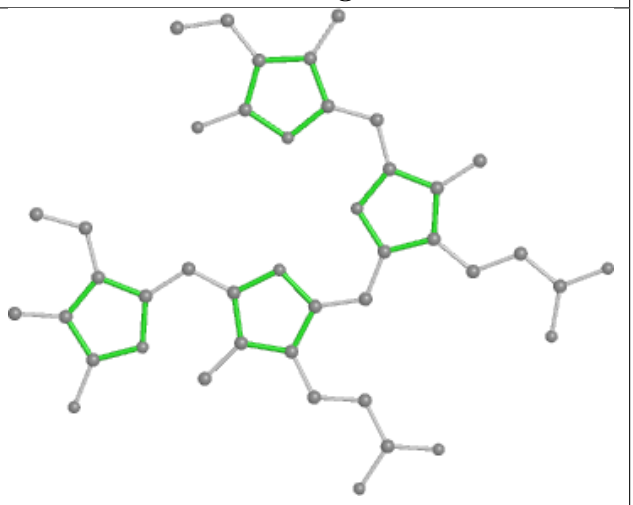
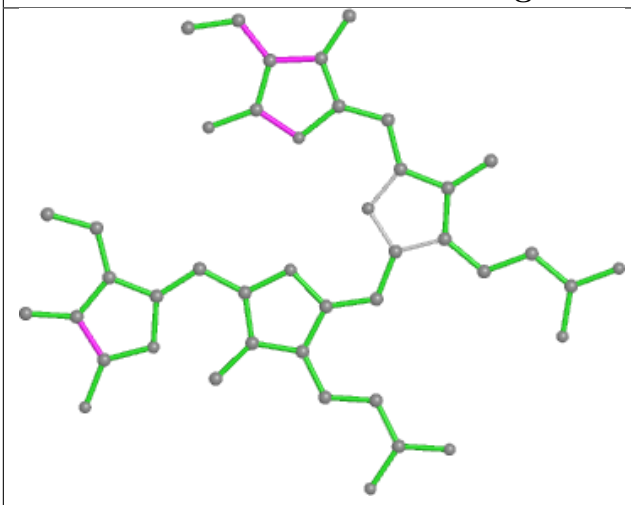


Rings

Ligand PEB H8 202



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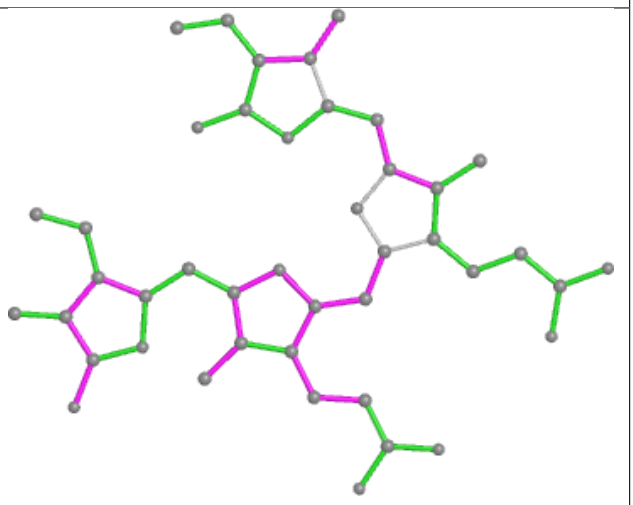

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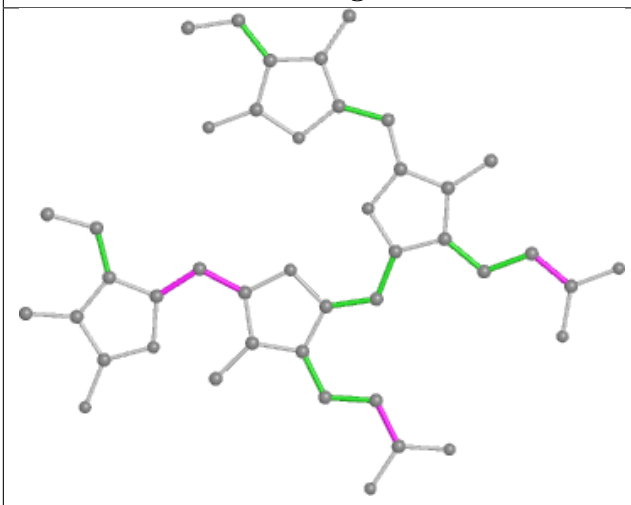

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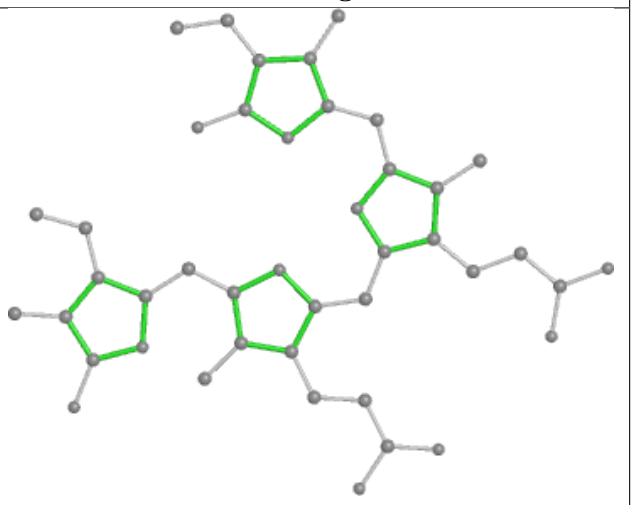
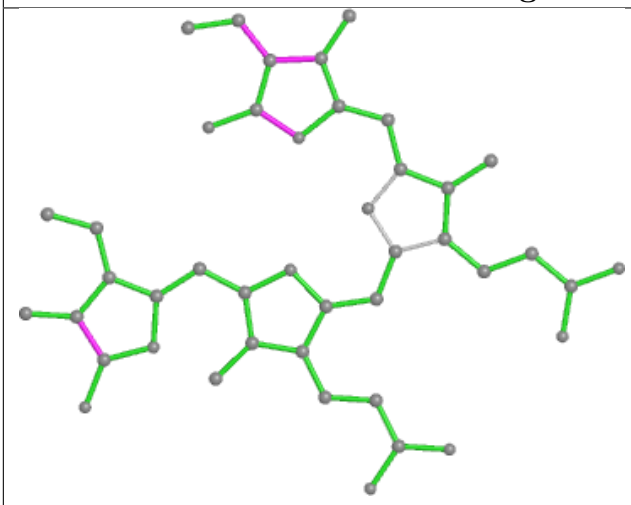


Rings

Ligand PEB y6 201



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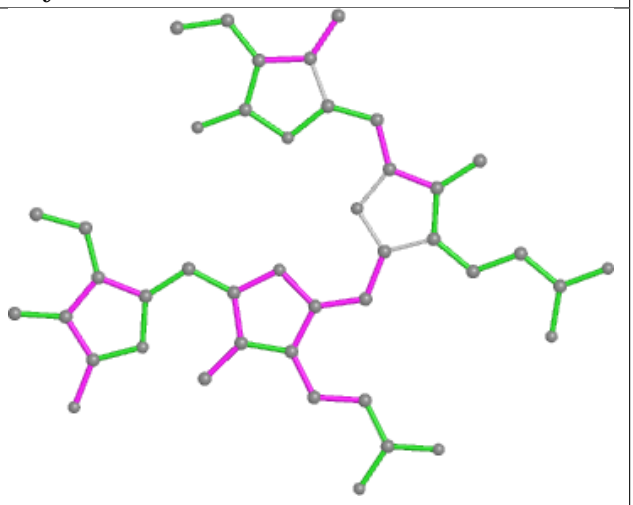

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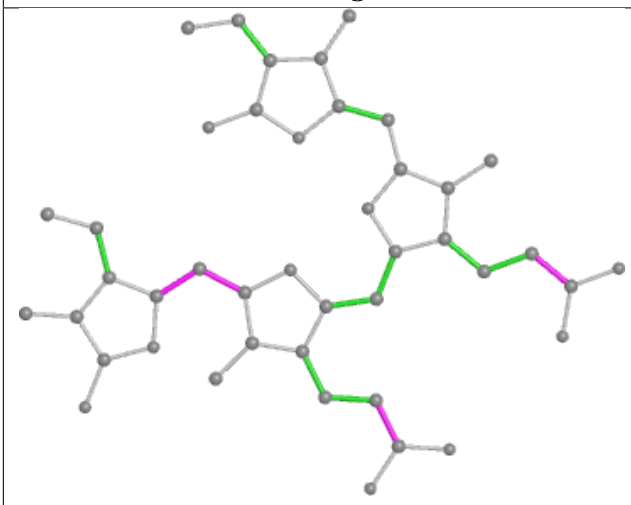

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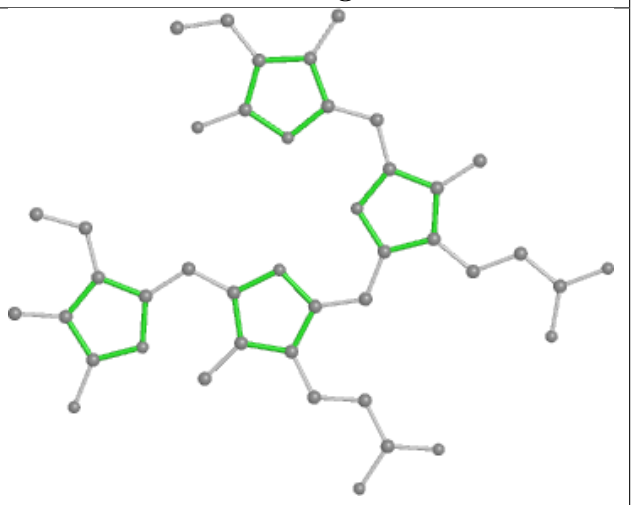
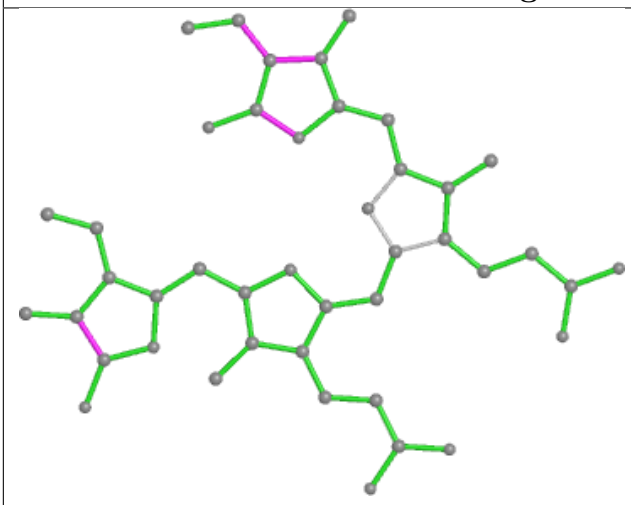


Rings

Ligand PEB a9 603



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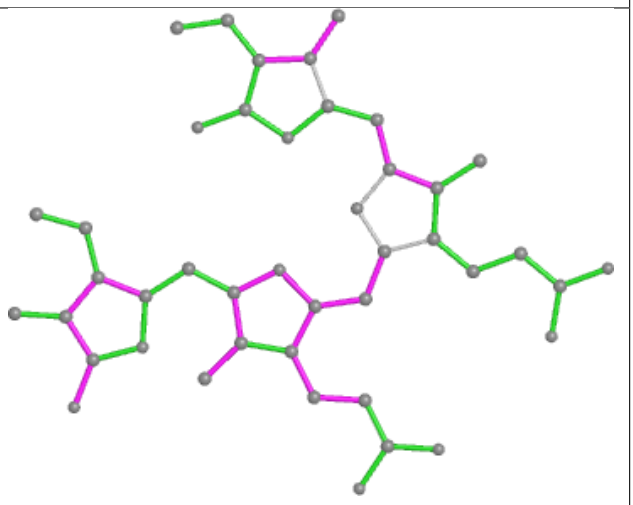

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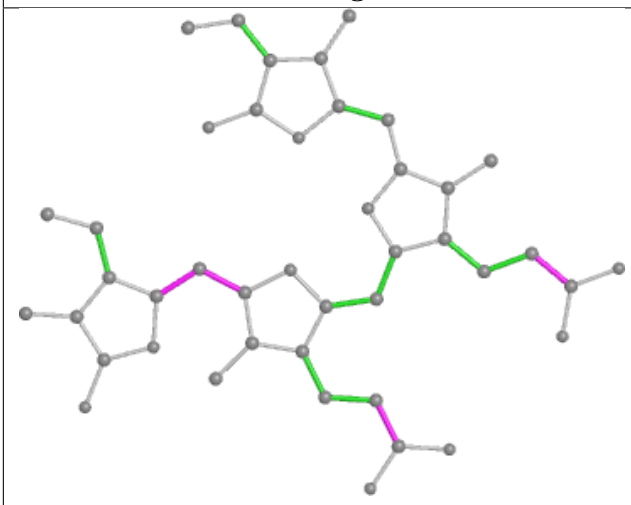

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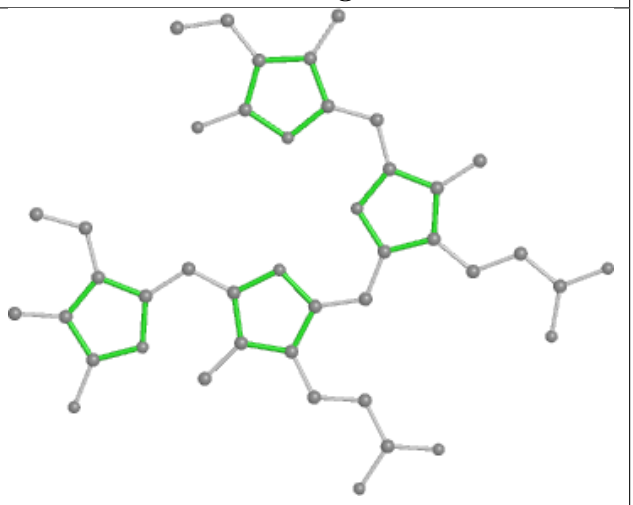
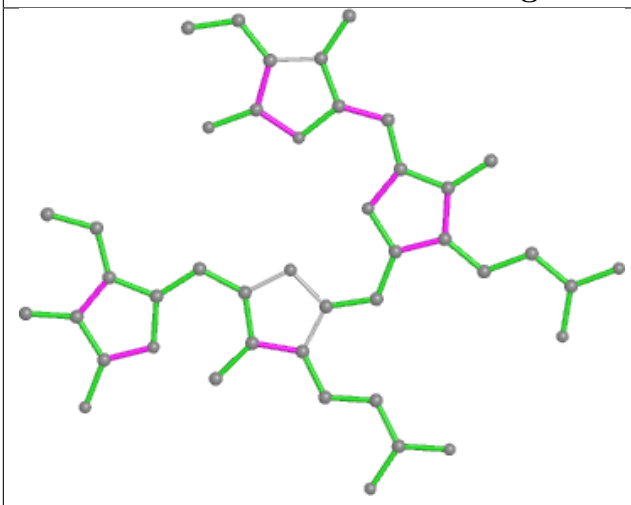


Rings

Ligand PUB fy 202



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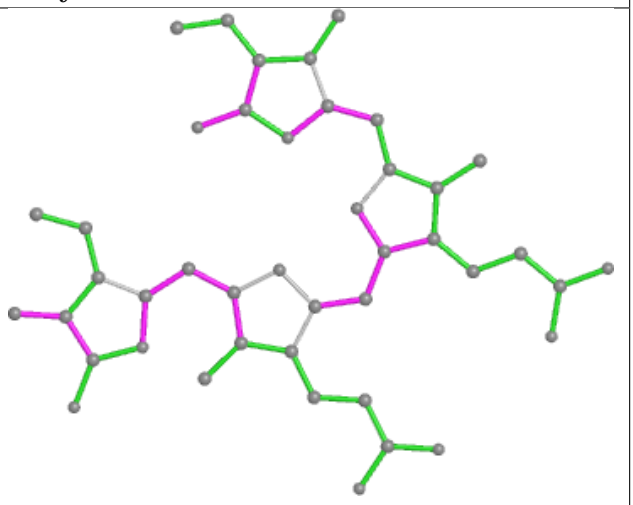

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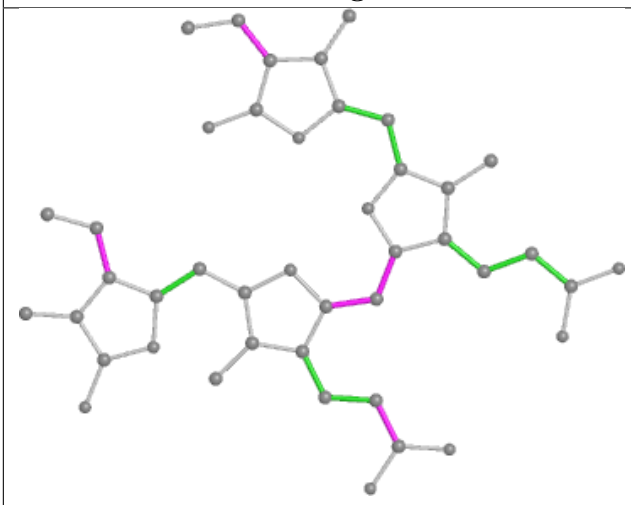

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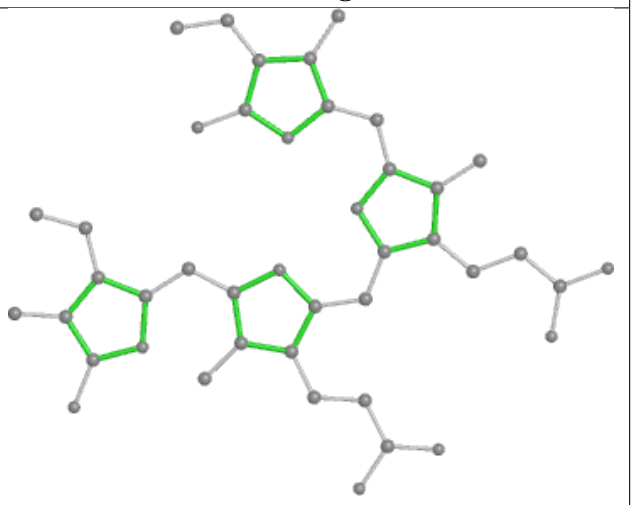
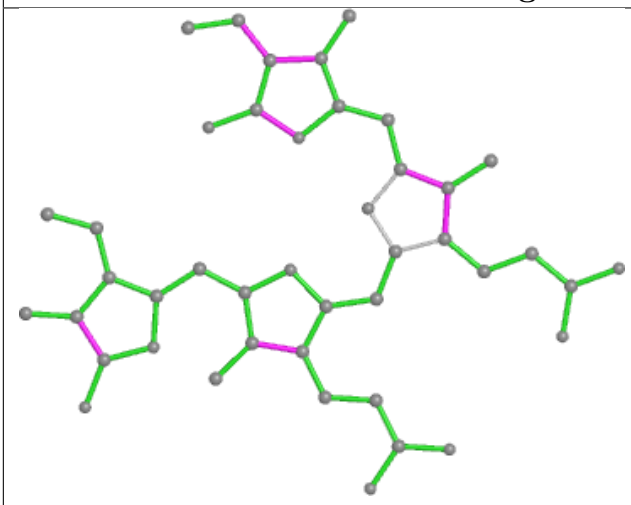


Rings

Ligand PEB p7 201



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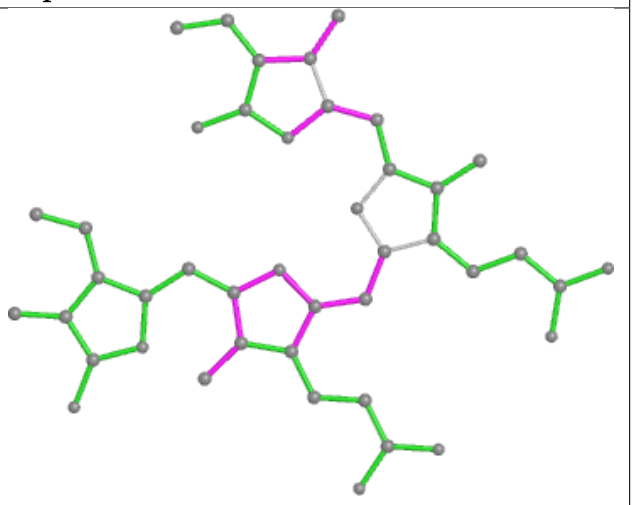

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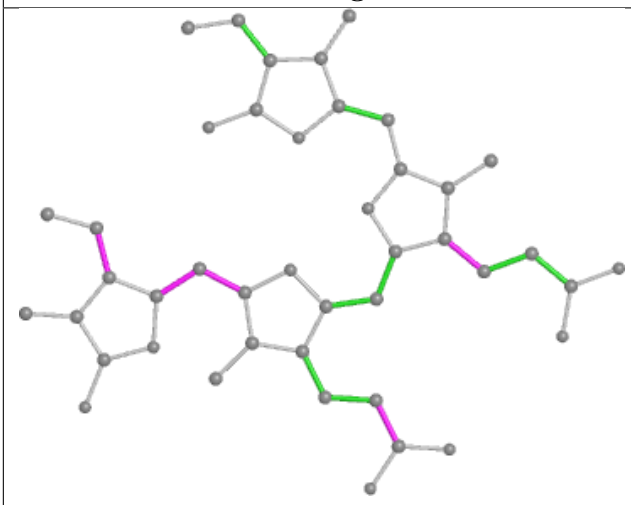

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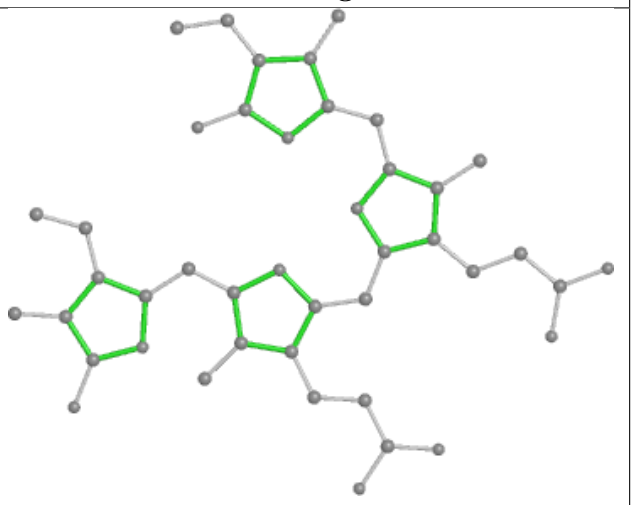
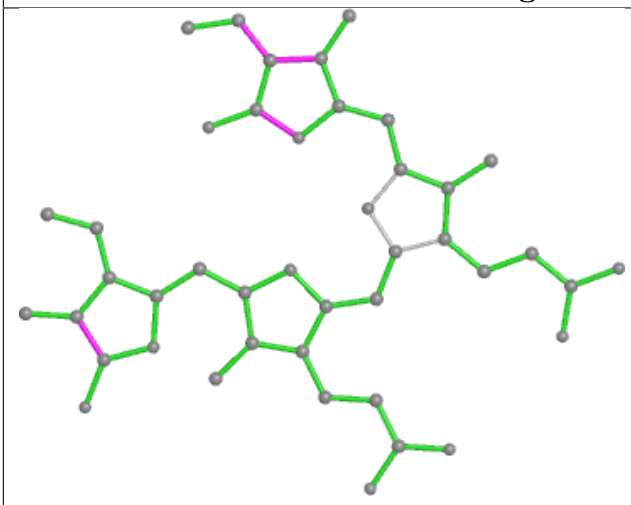


Rings

Ligand PEB u2 201



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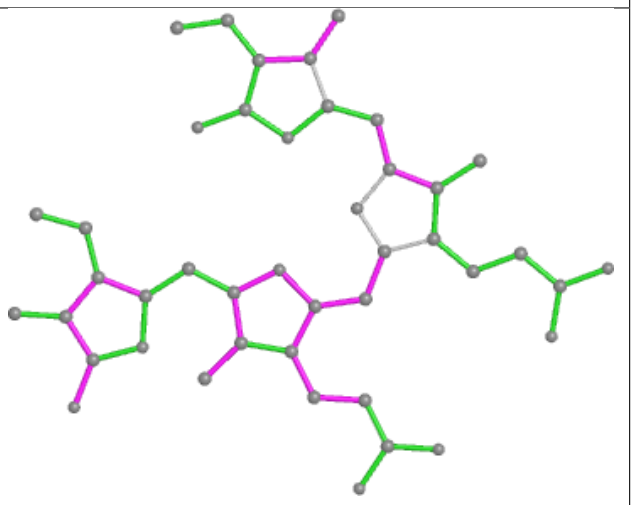

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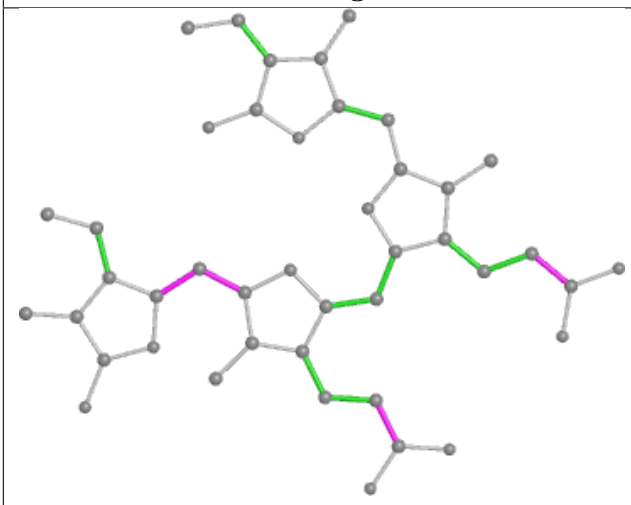

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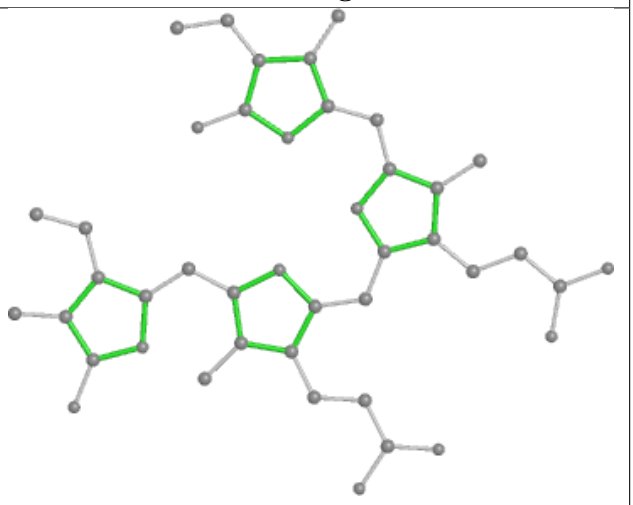
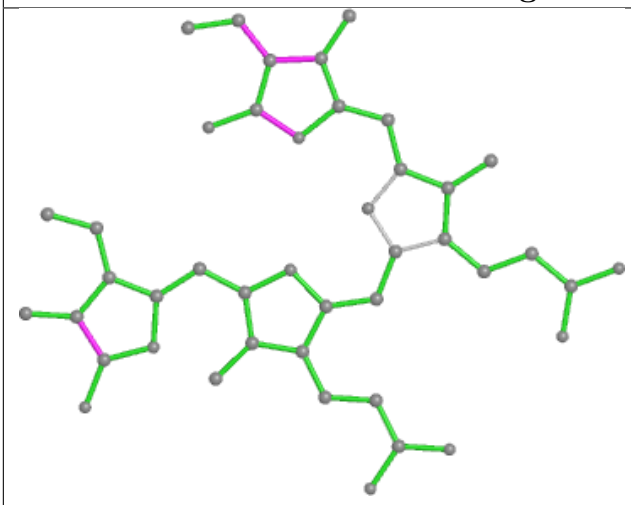


Rings

Ligand PEB q4 202



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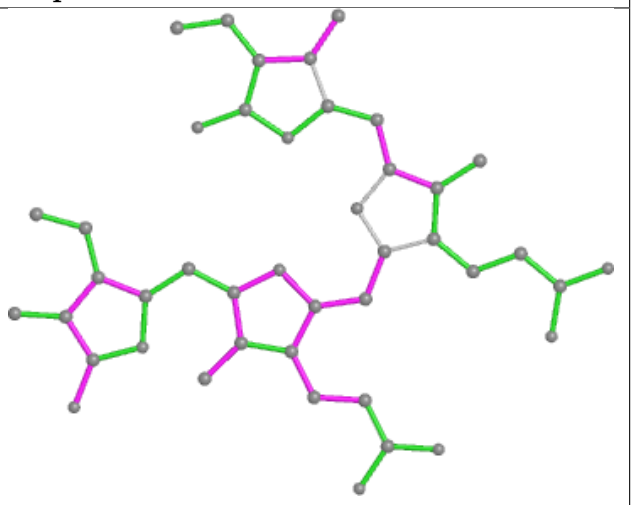
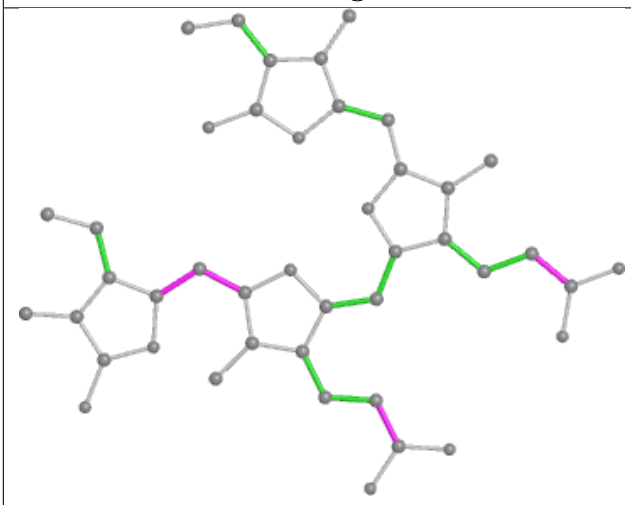


Bond angles



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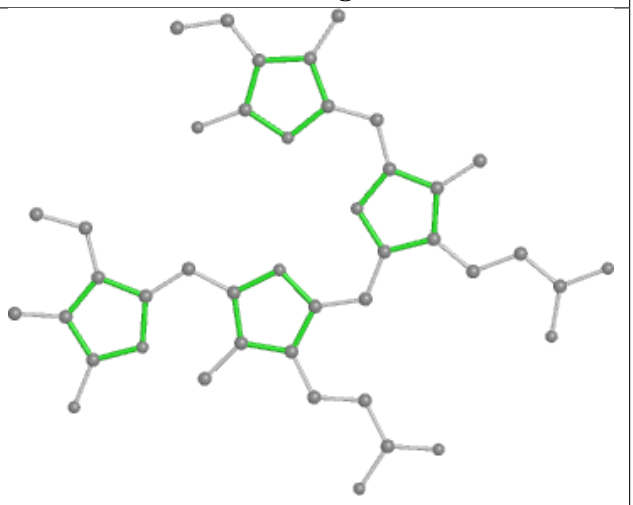
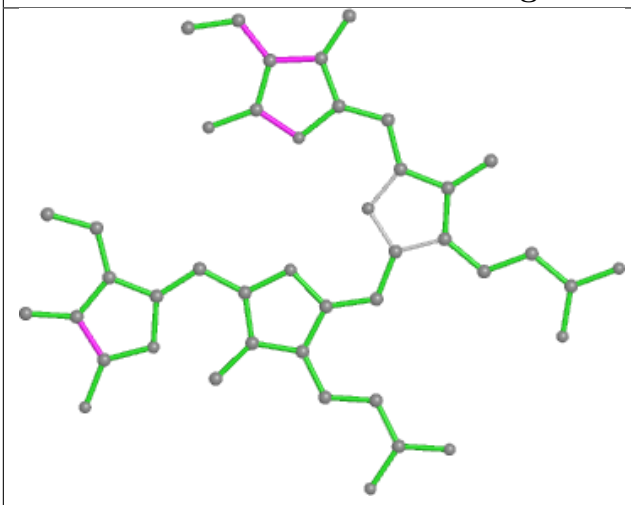


Rings

Ligand PEB eq 201



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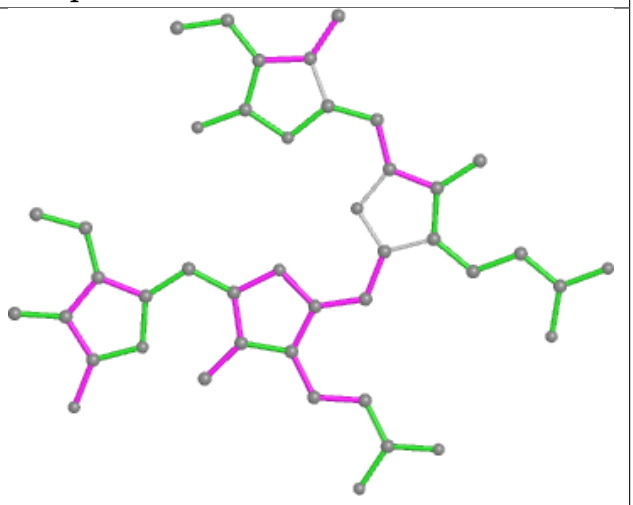

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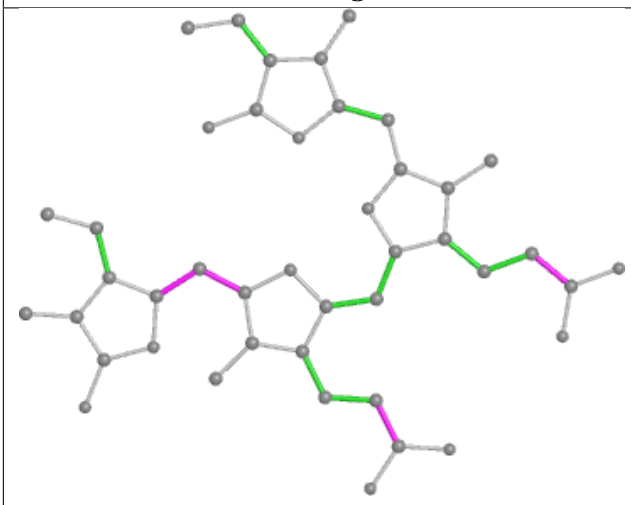

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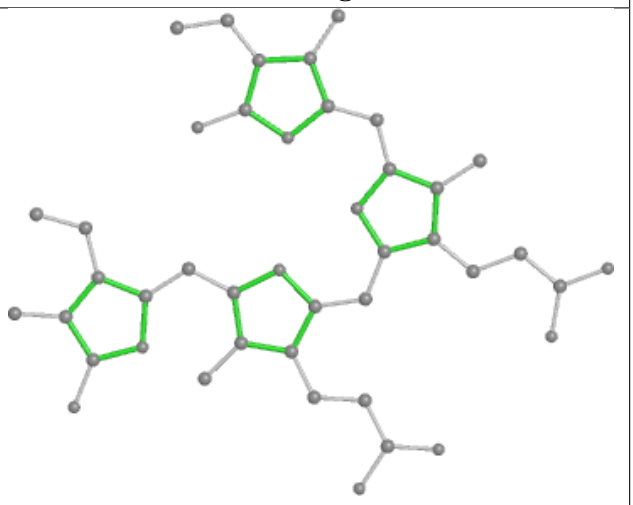
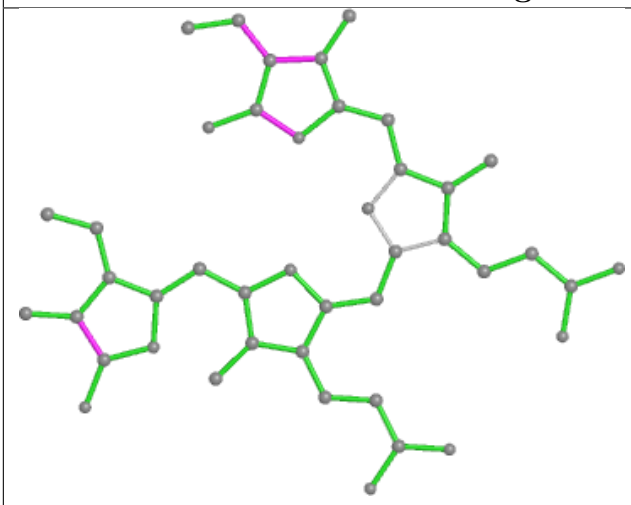


Rings

Ligand PEB bV 201



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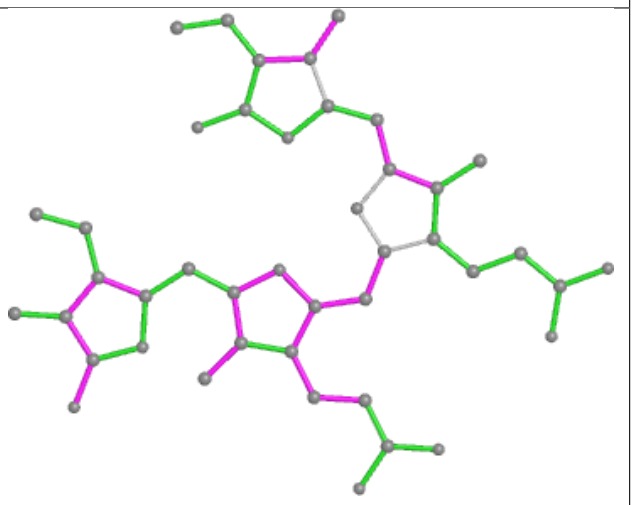

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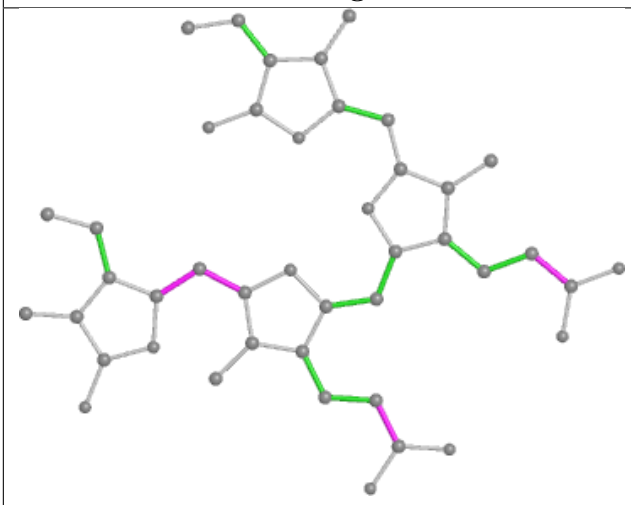

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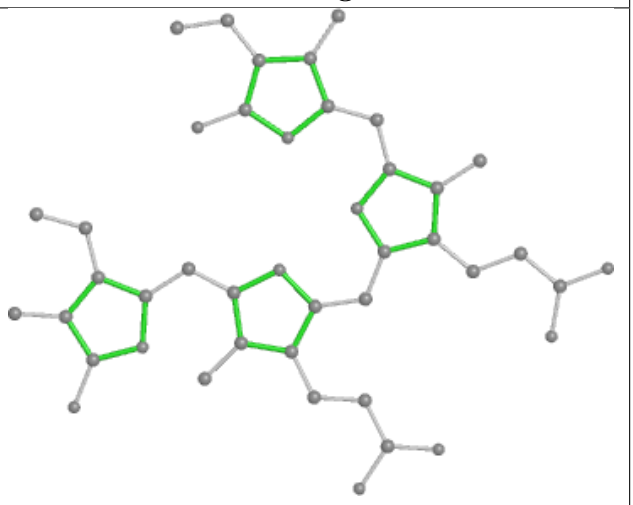
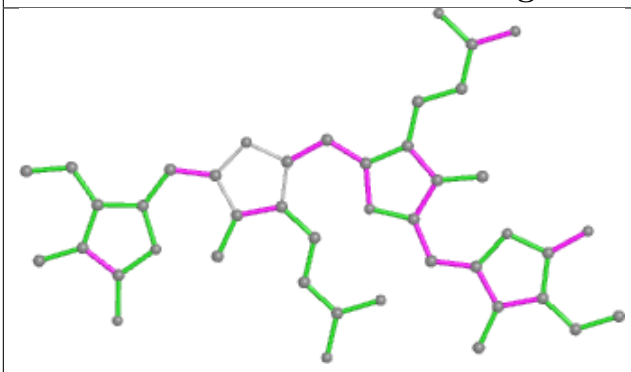


Rings

Ligand CYC a1 201



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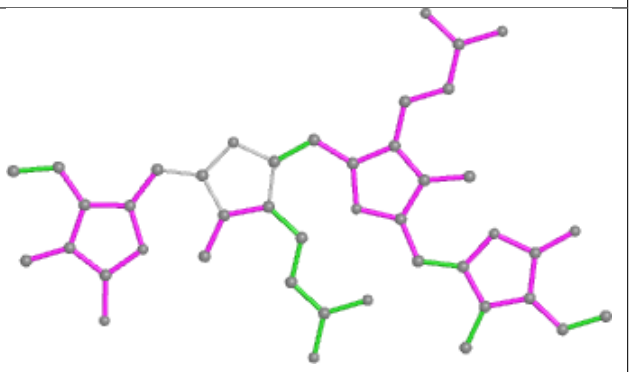

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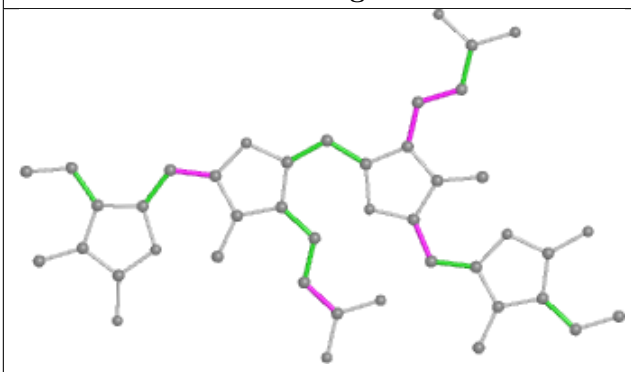

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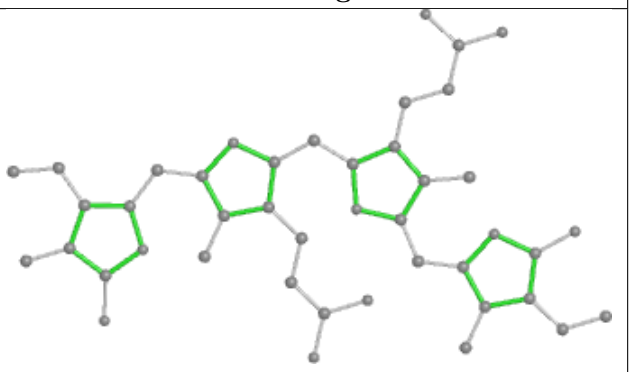
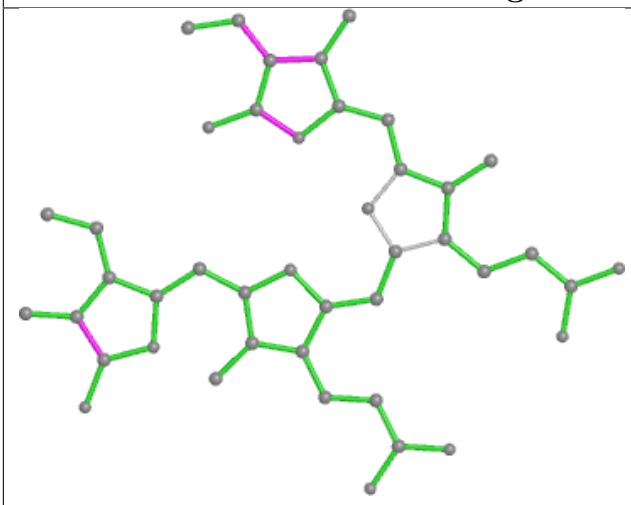


Rings

Ligand PEB kT 1001



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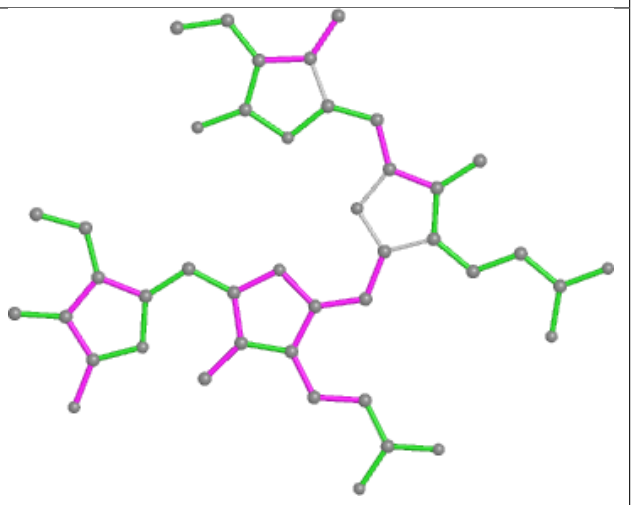

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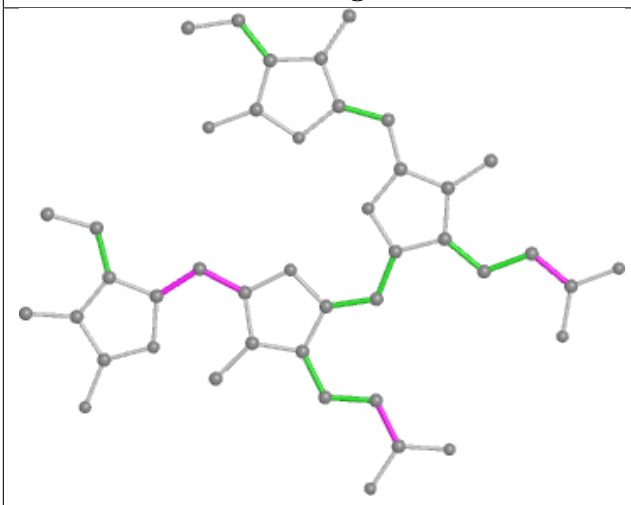

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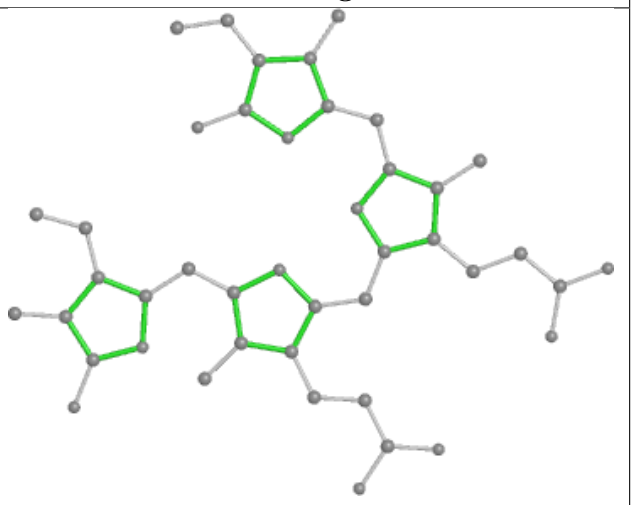
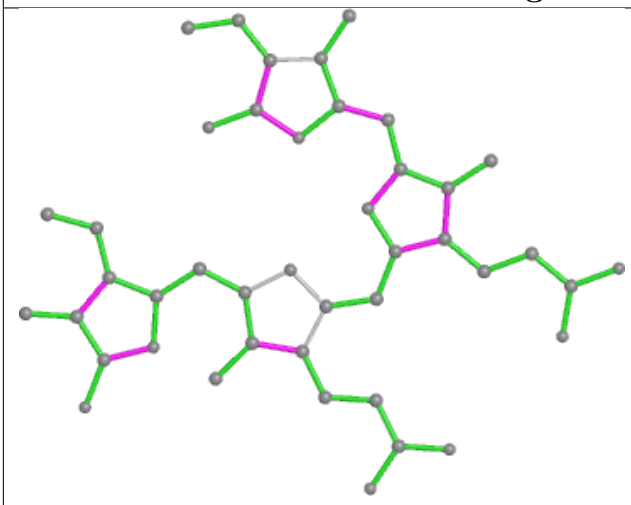


Rings

Ligand PUB ll 203



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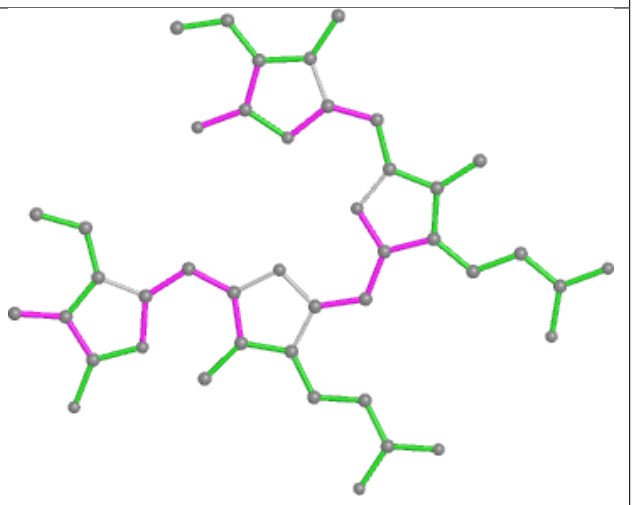
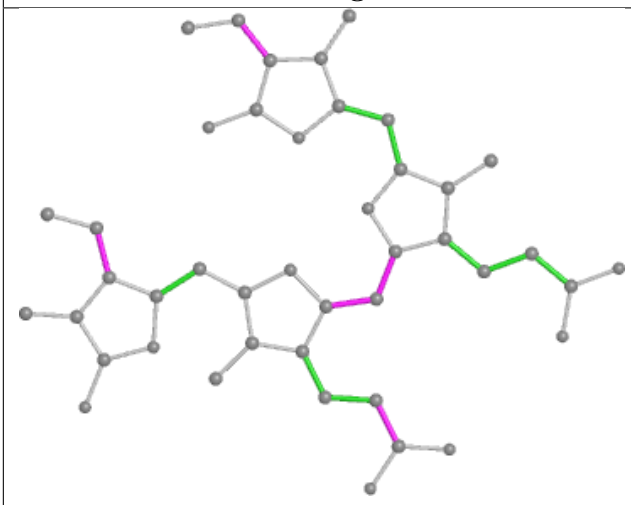
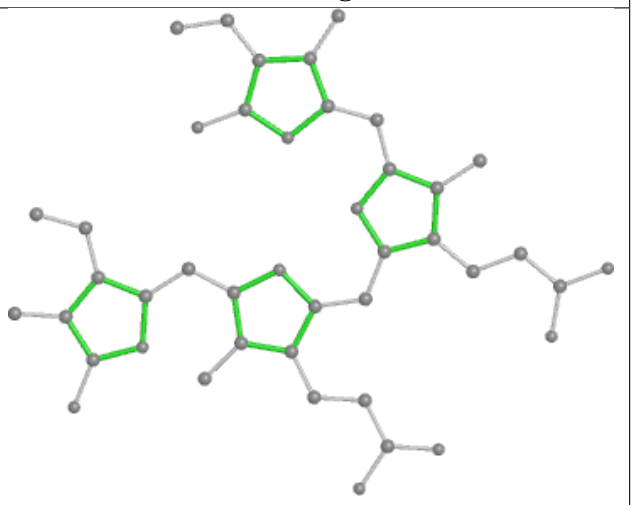


Bond angles

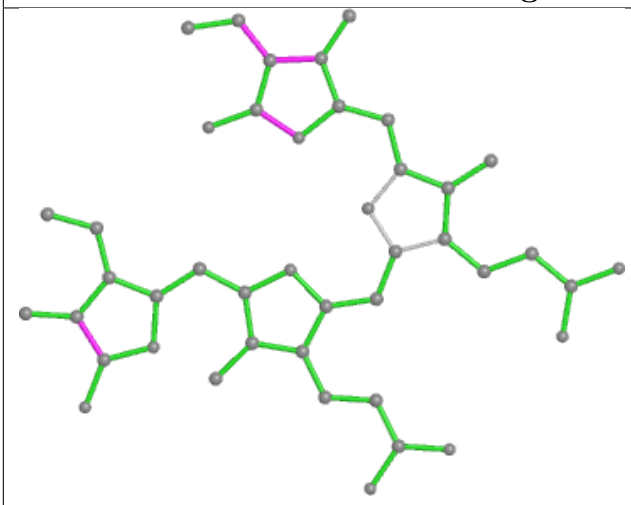


Torsions

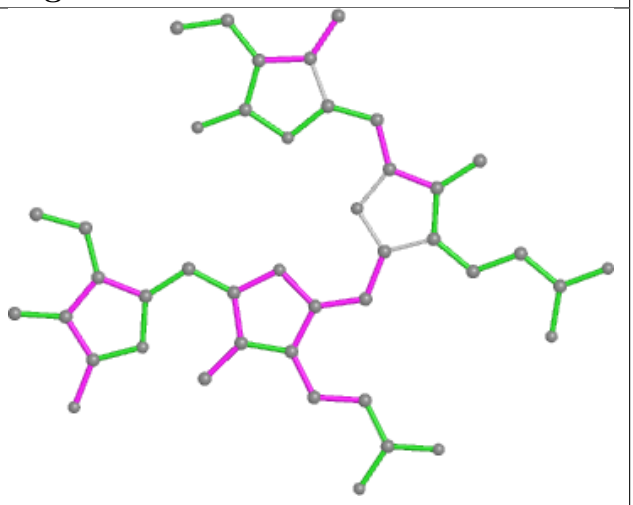


Rings

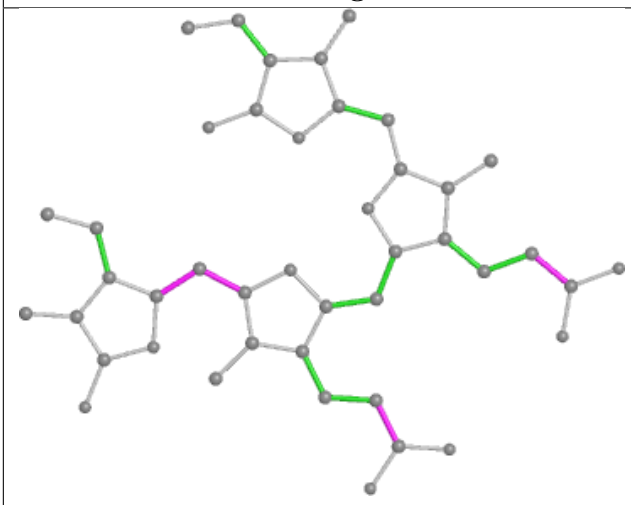
Ligand PEB gc 201



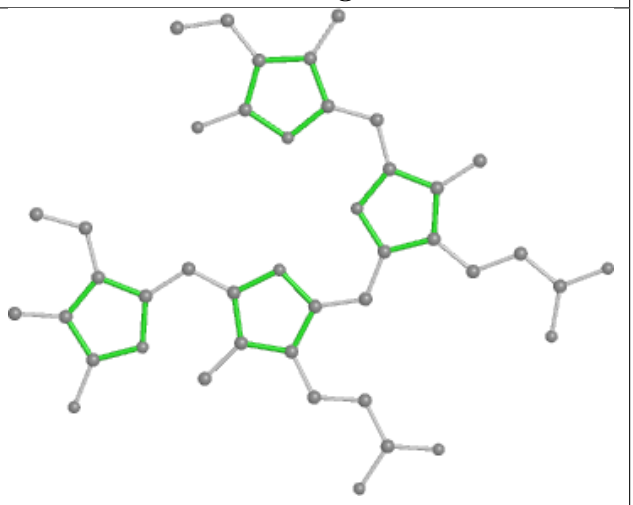
Bond lengths



Bond angles

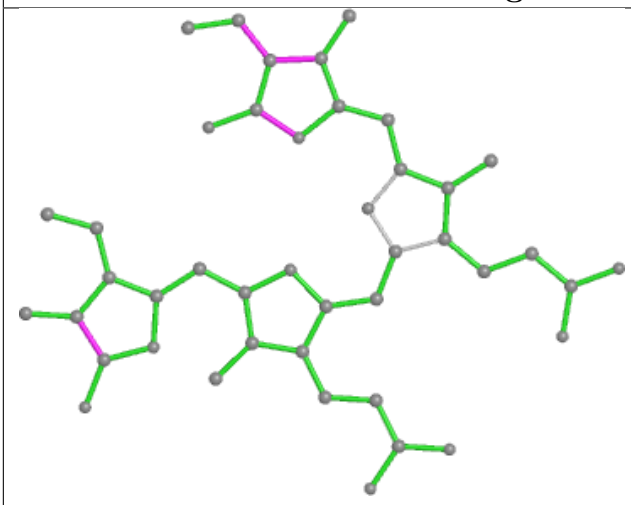


Torsions

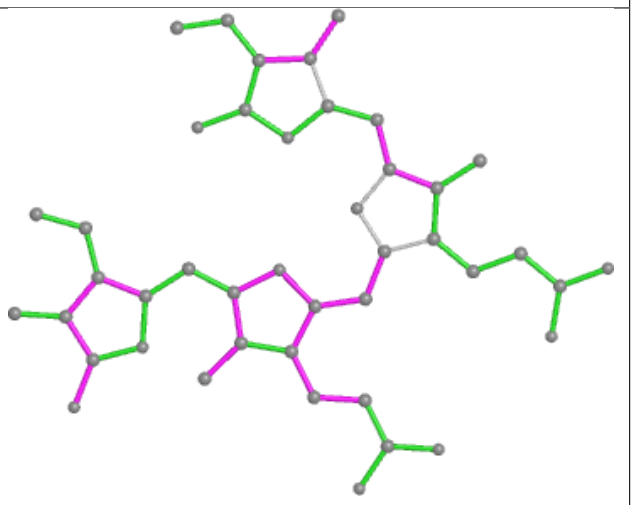


Rings

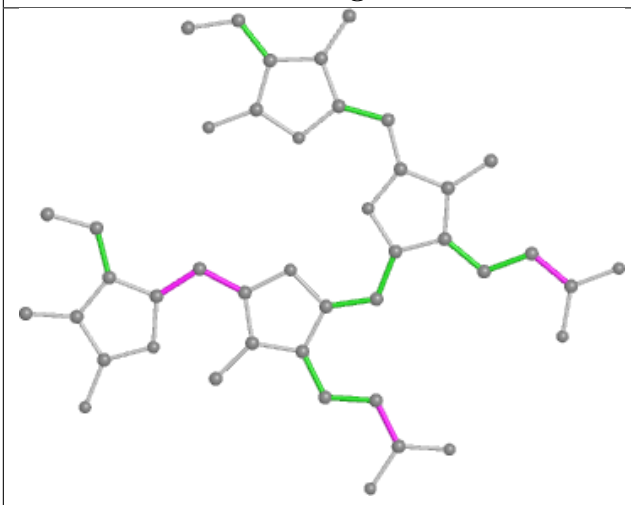
Ligand PEB kX 1001



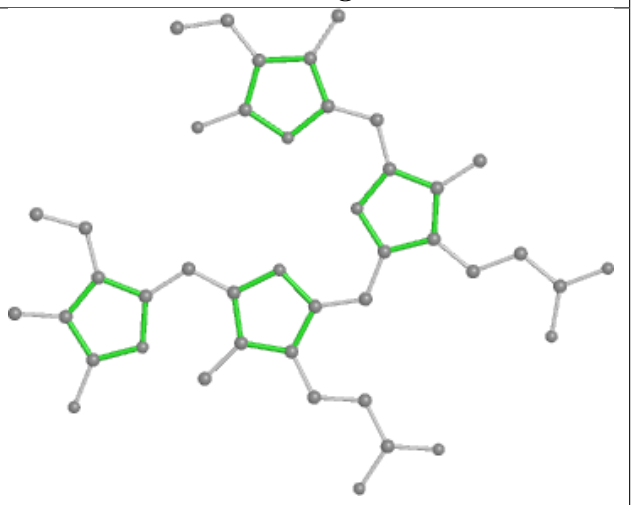
Bond lengths



Bond angles

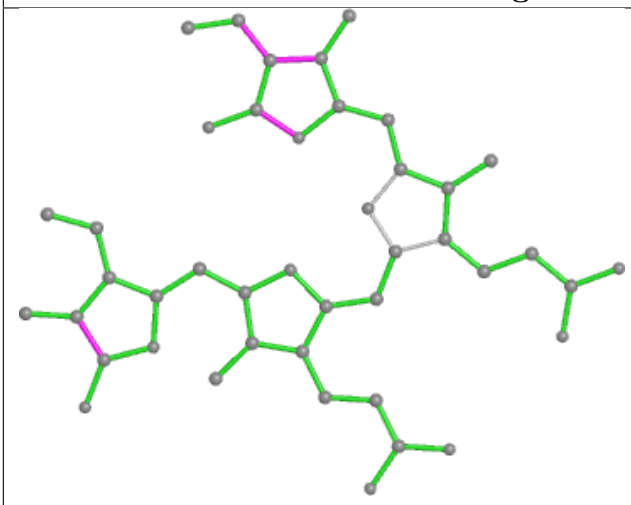


Torsions

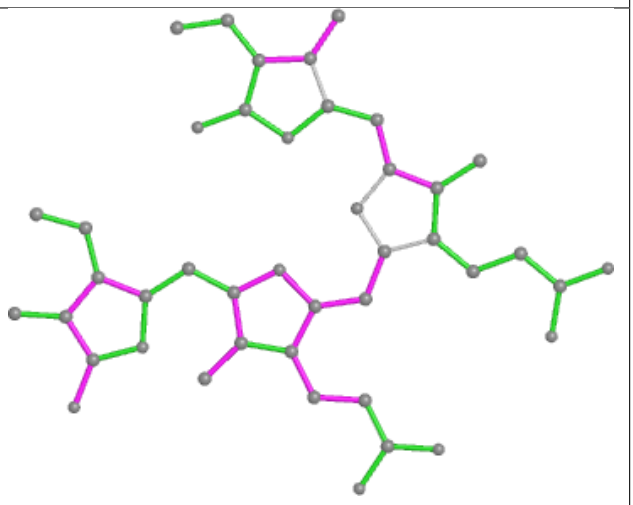


Rings

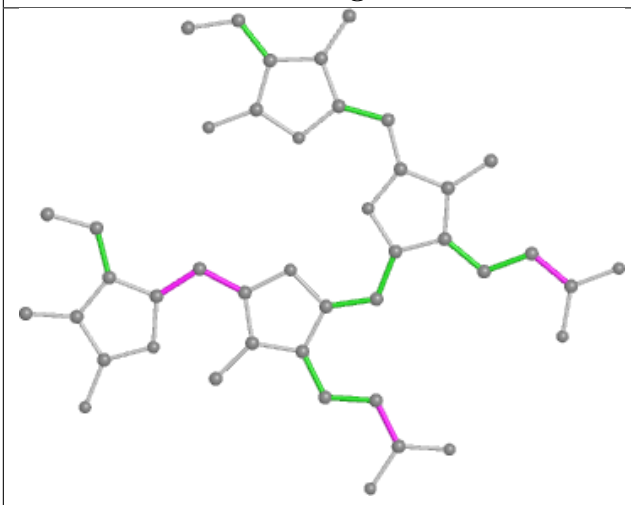
Ligand PEB dI 1002



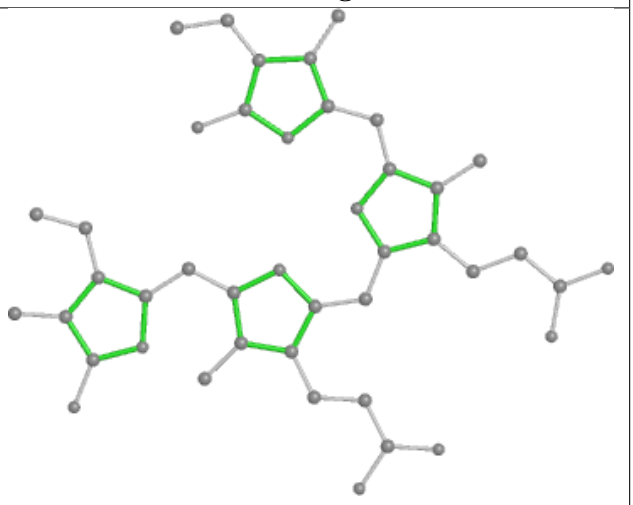
Bond lengths



Bond angles

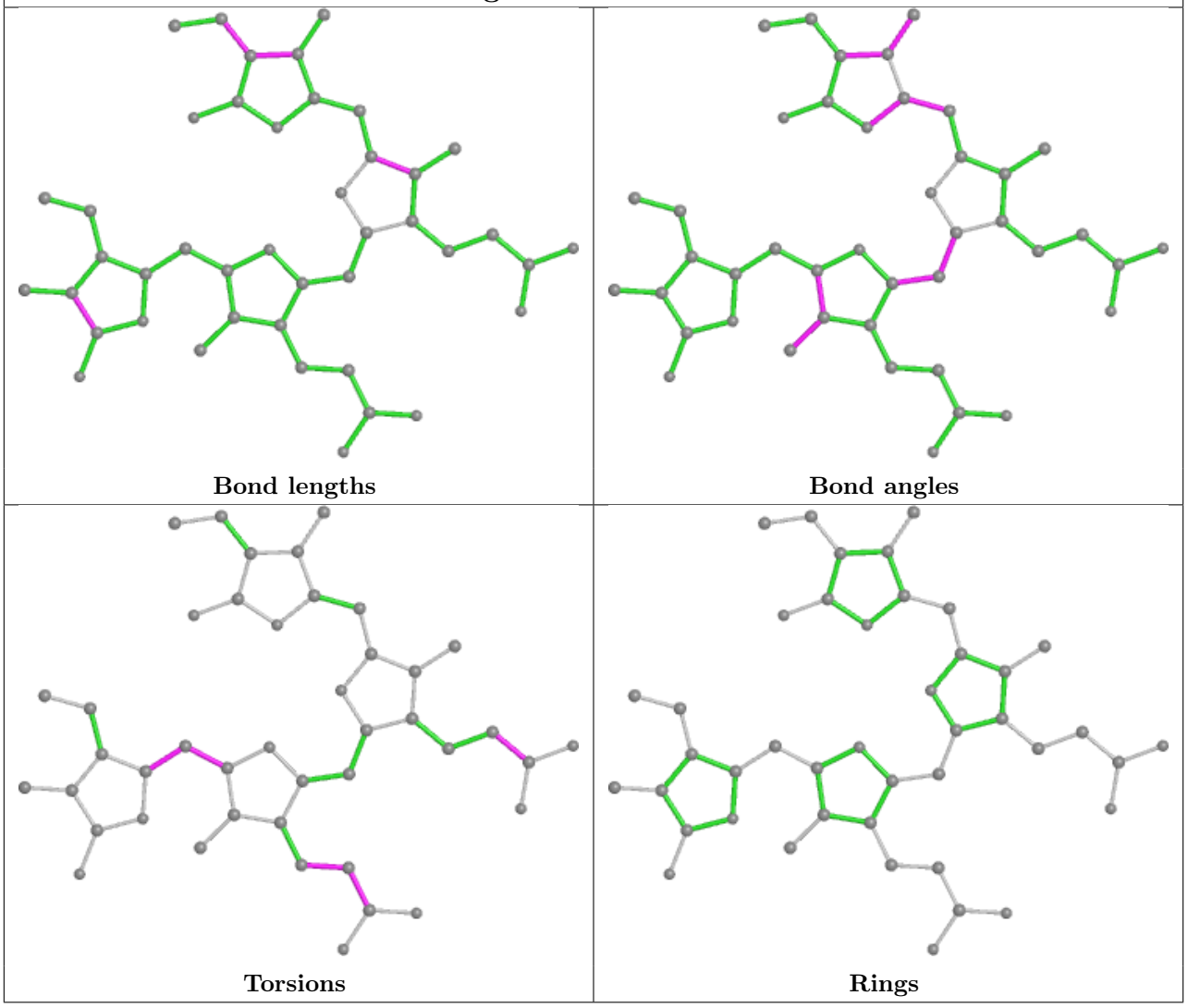


Torsions



Rings

Ligand PEB as 202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

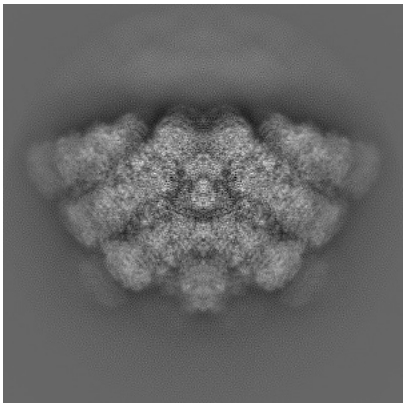
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-6769. These allow visual inspection of the internal detail of the map and identification of artifacts.

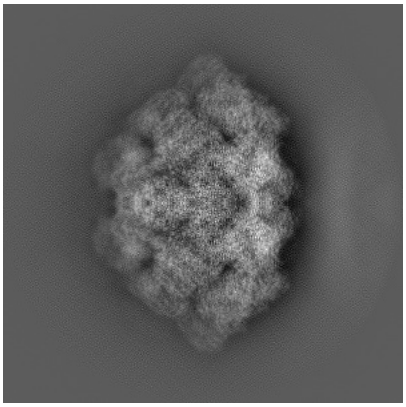
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

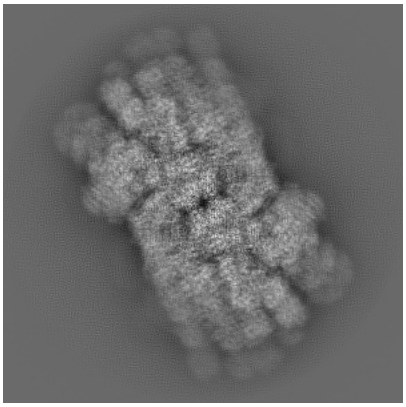
6.1.1 Primary map



X



Y

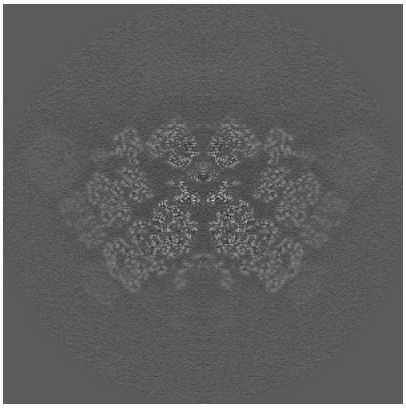


Z

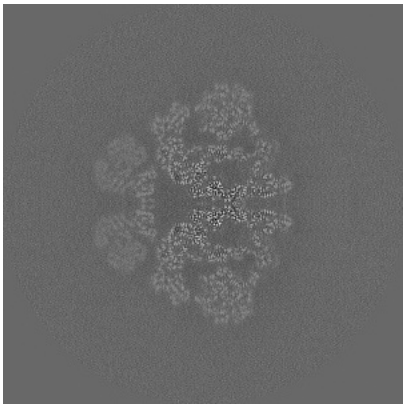
The images above show the map projected in three orthogonal directions.

6.2 Central slices

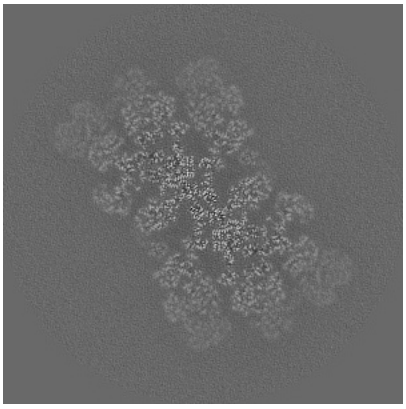
6.2.1 Primary map



X Index: 280



Y Index: 280

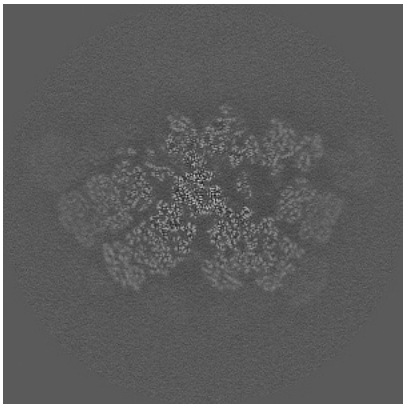


Z Index: 280

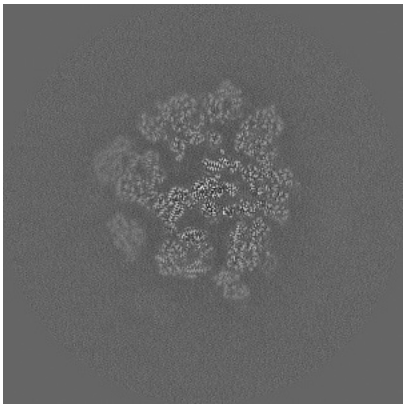
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

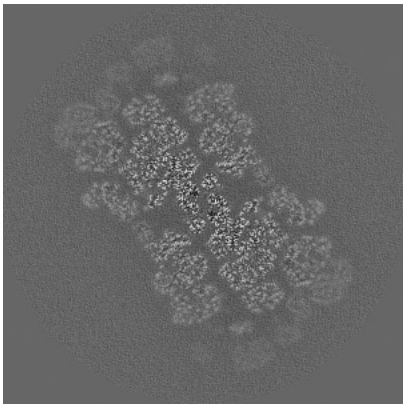
6.3.1 Primary map



X Index: 270



Y Index: 258

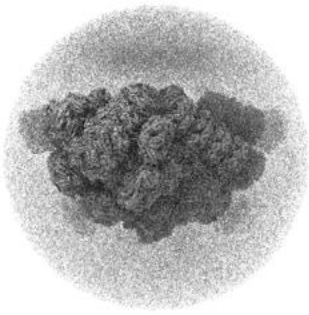


Z Index: 299

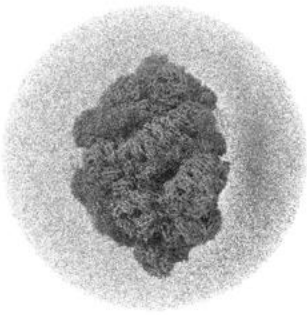
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

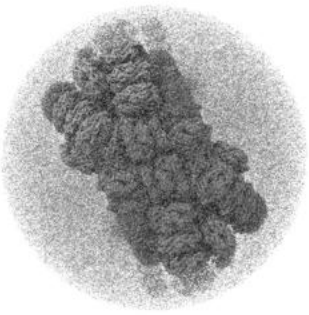
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

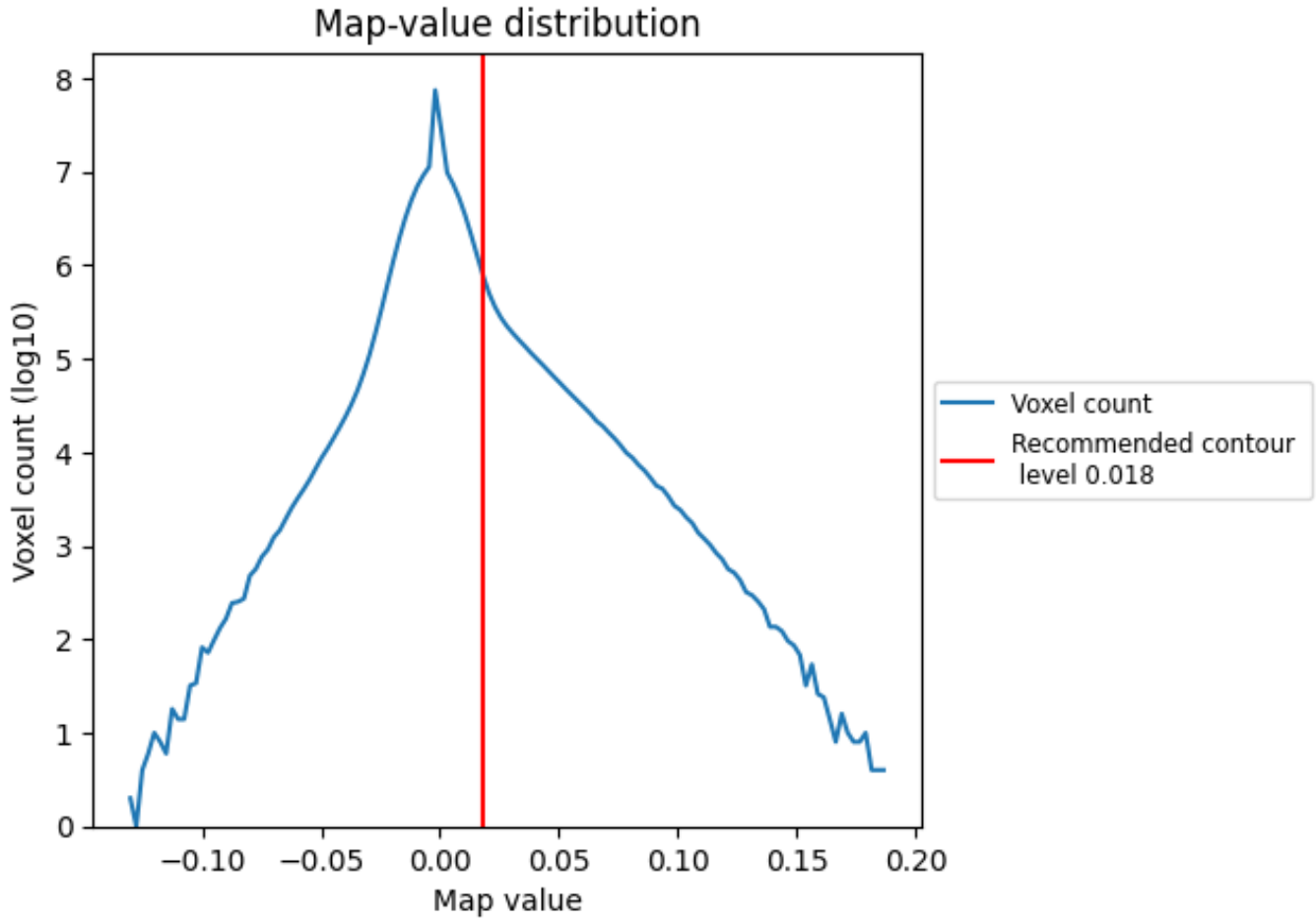
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

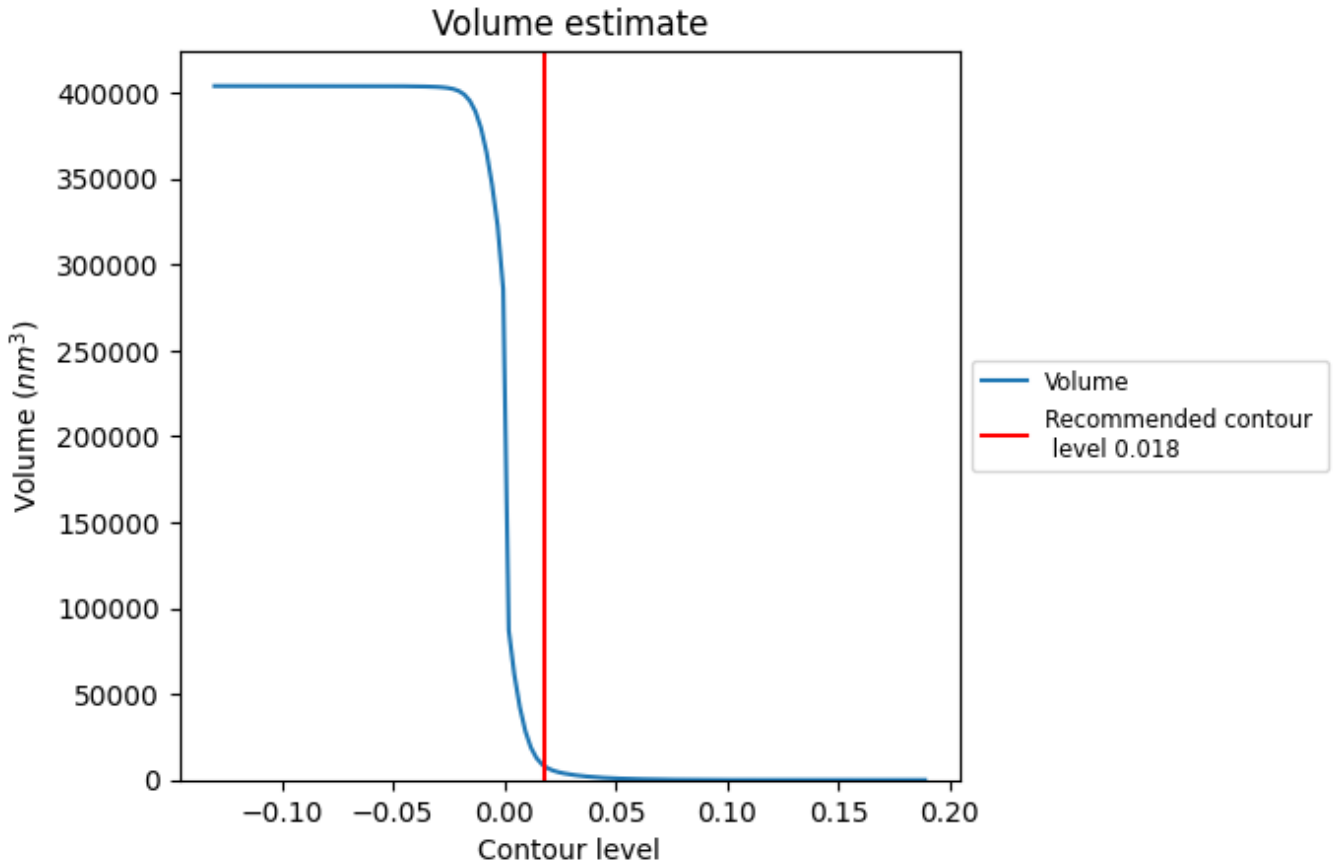
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

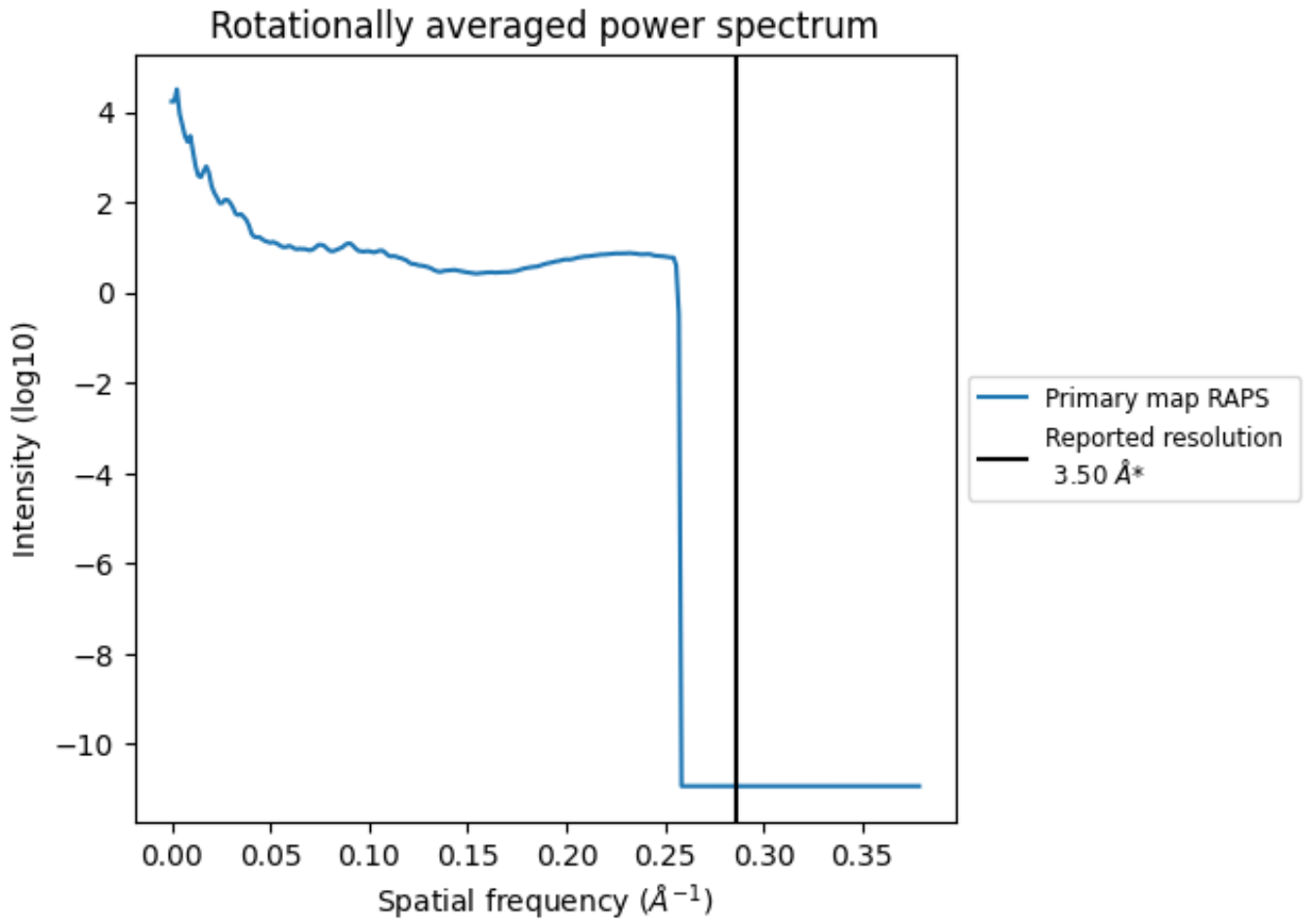
7.2 Volume estimate



The volume at the recommended contour level is 8132 nm^3; this corresponds to an approximate mass of 7346 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

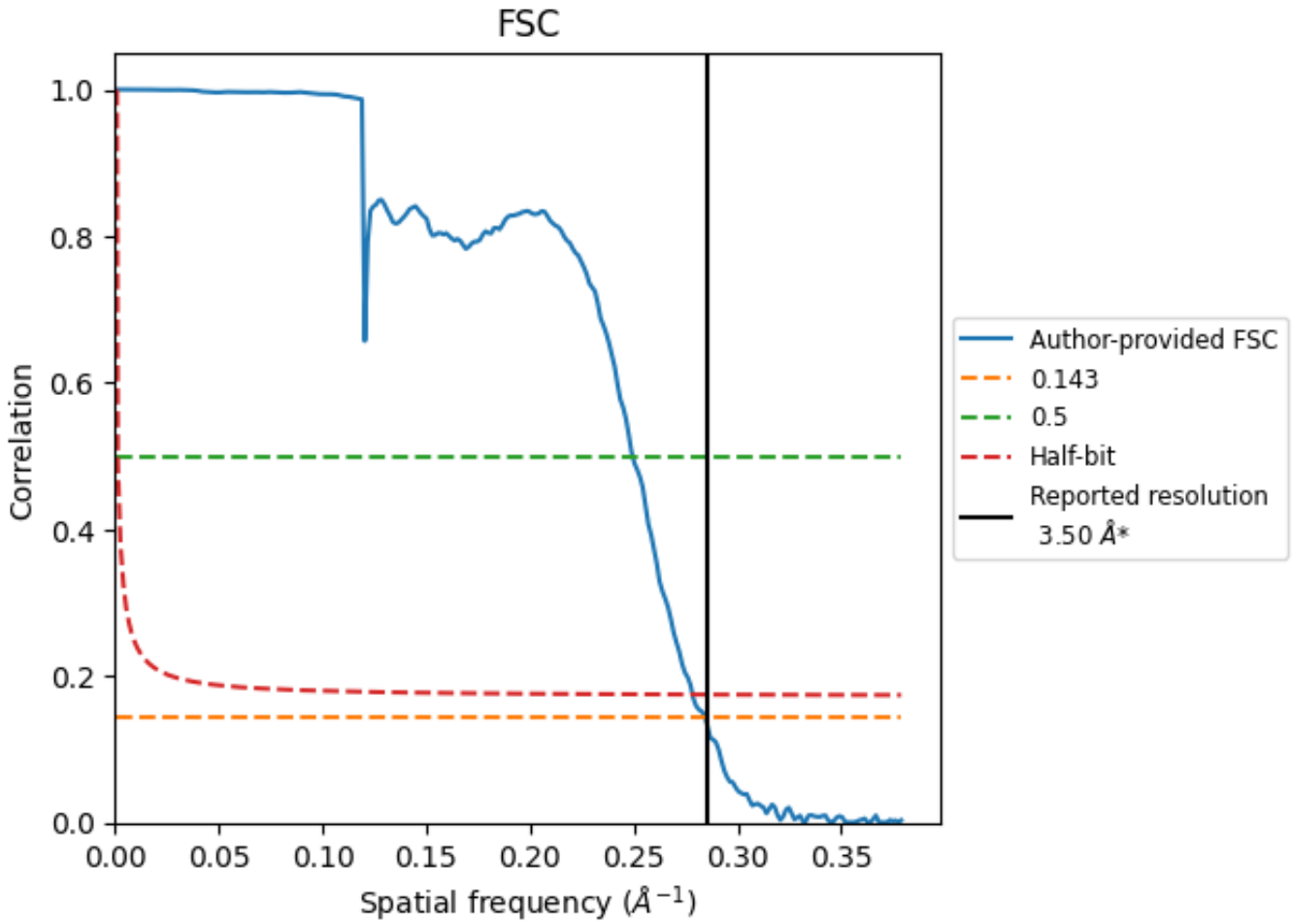


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

8.2 Resolution estimates (i)

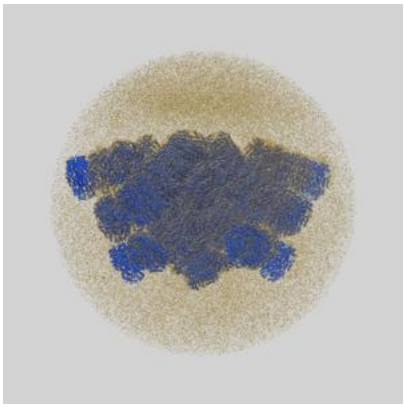
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.01	3.59
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

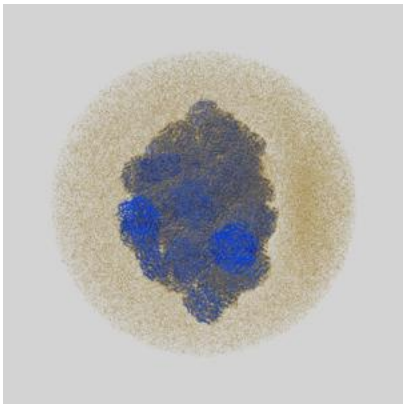
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-6769 and PDB model 5Y6P. Per-residue inclusion information can be found in section 3 on page 183.

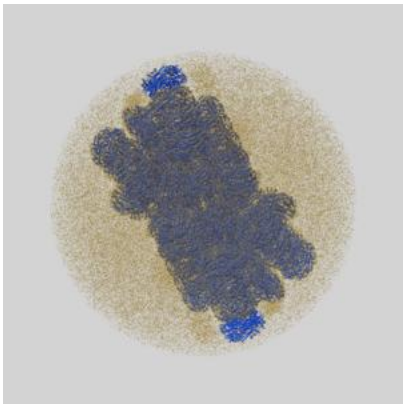
9.1 Map-model overlay



X



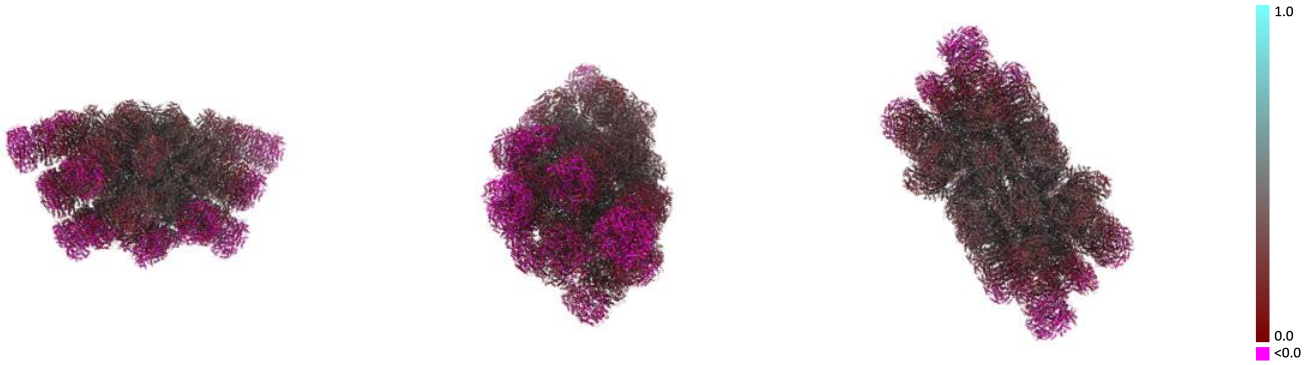
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

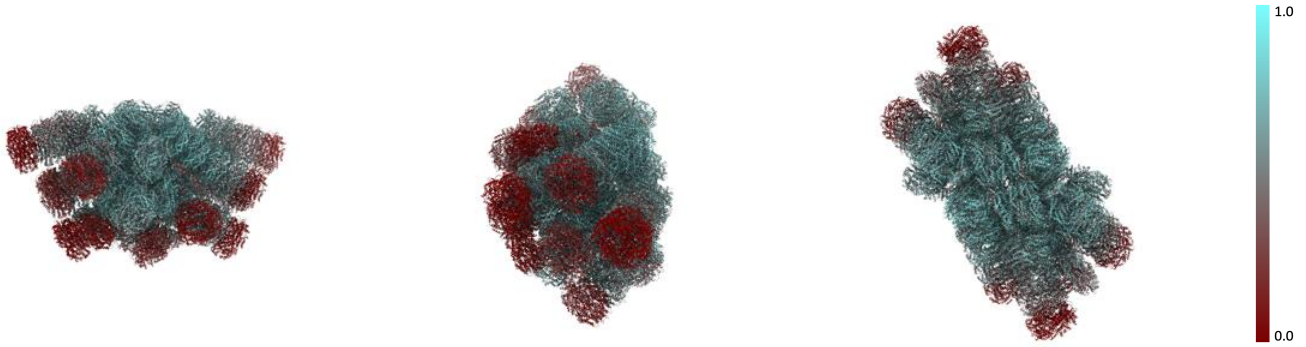
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

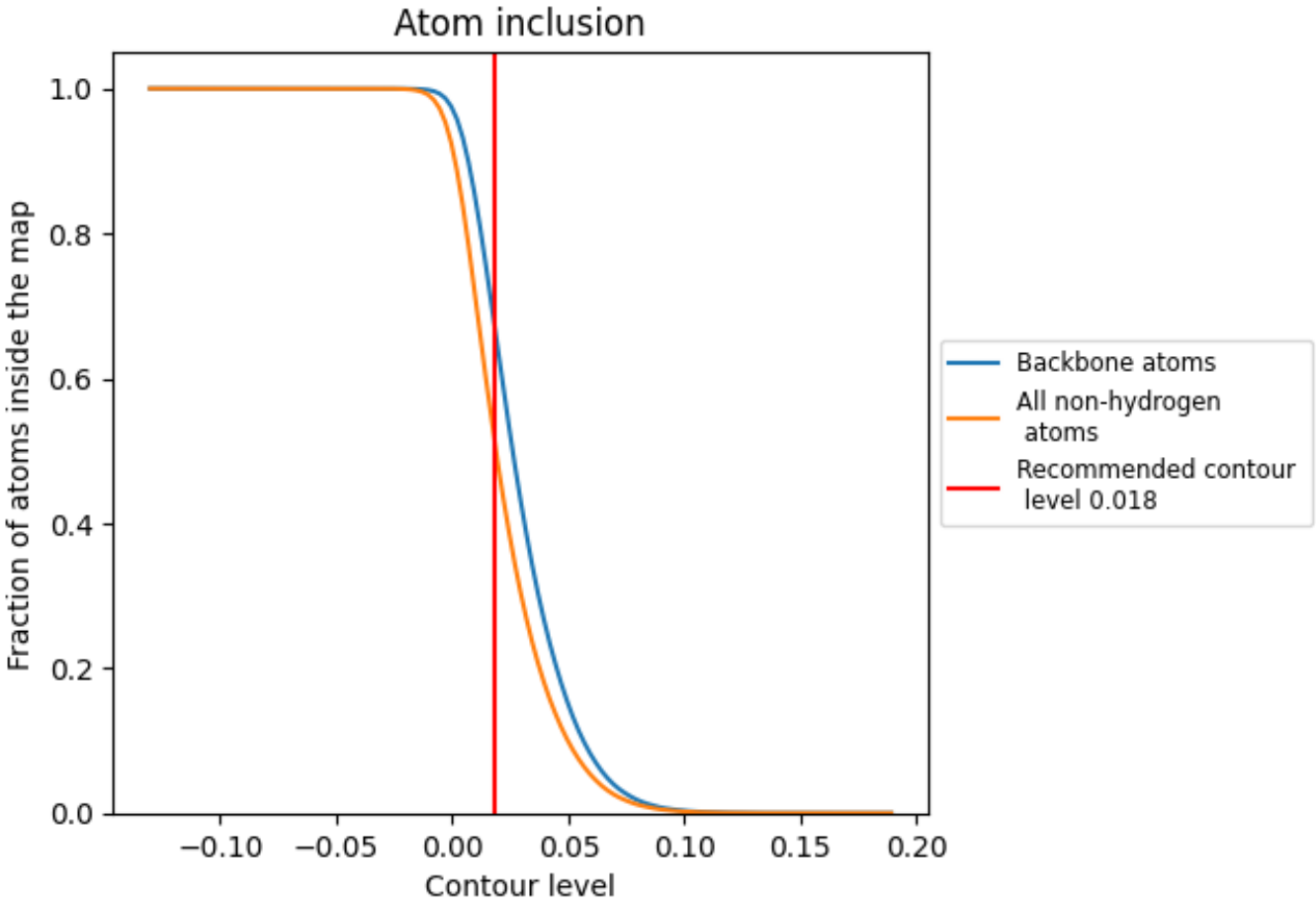
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5172	0.2670
14	0.6492	0.3640
24	0.5769	0.3090
34	0.4103	0.1680
44	0.0093	0.0240
A1	0.7171	0.4280
A2	0.6806	0.3670
A3	0.6677	0.2900
A4	0.6662	0.2890
A5	0.4203	0.0860
A6	0.7533	0.4070
A7	0.7287	0.3570
A8	0.5579	0.2010
A9	0.5944	0.2150
B1	0.7156	0.4240
B2	0.6824	0.3640
B3	0.6896	0.3570
B4	0.6903	0.3600
B5	0.3987	0.0980
B6	0.7533	0.4070
B7	0.7399	0.4250
B8	0.6029	0.2390
B9	0.6346	0.3150
C1	0.7213	0.4110
C2	0.5294	0.2810
C3	0.5798	0.2950
C4	0.5759	0.2930
C5	0.4009	0.1240
C6	0.7278	0.3480
C7	0.7749	0.4210
C8	0.5224	0.1490
C9	0.6207	0.2980
D1	0.7253	0.4310
D2	0.1330	0.0990
D3	0.5434	0.2960

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Chain	Atom inclusion	Q-score
D4	0.5463	0.2950
D5	0.5014	0.1990
D6	0.6915	0.3380
D7	0.7460	0.4110
D8	0.5197	0.1230
D9	0.5796	0.2680
E1	0.7851	0.4420
E2	0.7217	0.3580
E3	0.4888	0.2190
E4	0.4210	0.0850
E5	0.4695	0.1380
E6	0.7286	0.3590
E7	0.7286	0.3480
E8	0.4899	0.1260
E9	0.5497	0.1760
F1	0.7826	0.4410
F2	0.6606	0.3110
F3	0.5130	0.2550
F4	0.4001	0.1010
F5	0.3777	0.0910
F6	0.7344	0.4110
F7	0.6945	0.3420
F8	0.0085	0.0440
F9	0.5535	0.2020
G1	0.7534	0.4290
G2	0.6106	0.2480
G3	0.5243	0.2860
G4	0.4017	0.1230
G5	0.3886	0.0840
G6	0.7348	0.4030
G7	0.6969	0.3130
G8	0.0094	0.0380
G9	0.6099	0.2460
H1	0.7342	0.4300
H2	0.7101	0.3480
H3	0.5789	0.3530
H4	0.5014	0.1960
H5	0.3592	0.0720
H6	0.7301	0.3680
H7	0.7012	0.3580
H8	0.0093	-0.0140
H9	0.5224	0.1490

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Chain	Atom inclusion	Q-score
I1	0.6902	0.3680
I2	0.7255	0.3870
I3	0.5459	0.3070
I4	0.4672	0.1380
I5	0.4356	0.1130
I6	0.6961	0.3100
I7	0.7556	0.3730
I8	0.0072	0.0330
I9	0.5197	0.1240
J1	0.7075	0.3670
J2	0.7206	0.3980
J3	0.5145	0.2580
J4	0.3763	0.0900
J5	0.4378	0.1200
J6	0.6961	0.3480
J7	0.7258	0.3840
J8	0.0077	0.0450
J9	0.4863	0.1260
K1	0.6796	0.3340
K2	0.7186	0.3960
K3	0.4896	0.2020
K4	0.3855	0.0810
K5	0.0216	0.0450
K6	0.7409	0.3590
K7	0.7402	0.4000
K8	0.0029	0.0270
K9	0.0085	0.0420
L1	0.7415	0.4220
L2	0.7012	0.4000
L3	0.4877	0.2240
L4	0.3596	0.0680
L5	0.0116	0.0250
L6	0.7489	0.4140
L7	0.7355	0.3640
L8	0.0100	0.0280
L9	0.0087	0.0400
M1	0.6953	0.3640
M2	0.6800	0.3340
M3	0.5204	0.2100
M4	0.4341	0.1090
M5	0.0154	0.0160
M6	0.7687	0.3950

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Chain	Atom inclusion	Q-score
M7	0.7360	0.3880
M8	0.0130	0.0300
M9	0.0100	-0.0150
N1	0.7113	0.4150
N2	0.6317	0.3200
N3	0.5456	0.2700
N4	0.4378	0.1150
N5	0.0072	-0.0030
N6	0.7402	0.3880
N7	0.7395	0.4240
N8	0.0123	0.0060
N9	0.0094	0.0340
O1	0.7528	0.4350
O2	0.6315	0.2770
O3	0.1365	0.0600
O4	0.0193	0.0430
O5	0.0093	0.0340
O6	0.7317	0.3280
O7	0.7687	0.4010
O8	0.0080	0.0020
O9	0.0069	0.0470
P1	0.7242	0.4120
P2	0.6541	0.3440
P3	0.1216	0.0440
P4	0.0130	0.0230
P5	0.0194	0.0340
P6	0.6910	0.3480
P7	0.7417	0.3900
P8	0.0069	-0.0030
P9	0.0043	0.0250
Q1	0.7238	0.3980
Q2	0.7239	0.3630
Q3	0.1496	0.0870
Q4	0.0142	0.0200
Q5	0.0185	0.0260
Q6	0.7340	0.3780
Q7	0.7340	0.3290
Q8	0.0058	0.0020
Q9	0.0116	0.0260
R1	0.7372	0.4180
R2	0.6693	0.3520
R3	0.1679	0.1200

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Chain	Atom inclusion	Q-score
R4	0.0087	-0.0030
R5	0.0152	0.0220
R6	0.7402	0.4230
R7	0.6997	0.3590
R8	0.7697	0.4470
R9	0.0123	0.0330
S1	0.7159	0.4160
S2	0.6554	0.2820
S3	0.1758	0.1390
S4	0.0093	0.0380
S5	0.0097	0.0300
S6	0.7602	0.4040
S7	0.7008	0.3460
S8	0.7499	0.4250
S9	0.0116	0.0050
T1	0.6815	0.3590
T2	0.6802	0.3410
T3	0.1570	0.0960
T4	0.0194	0.0330
T5	0.0134	-0.0140
T6	0.7337	0.3930
T7	0.7207	0.3620
T8	0.0093	0.0260
T9	0.0101	0.0000
U1	0.6945	0.3500
U2	0.6808	0.3760
U3	0.1403	0.1200
U4	0.0170	0.0300
U5	0.0208	0.0420
U6	0.6901	0.3360
U7	0.7487	0.3580
U8	0.5582	0.2740
U9	0.0093	-0.0050
V1	0.6547	0.3570
V2	0.7171	0.4180
V3	0.1823	0.1960
V4	0.0123	0.0220
V5	0.0145	0.0380
V6	0.7243	0.3620
V7	0.7605	0.4250
V8	0.8034	0.4480
V9	0.0058	0.0000

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Chain	Atom inclusion	Q-score
W1	0.7366	0.4150
W2	0.7340	0.3960
W3	0.1750	0.1450
W4	0.0100	0.0290
W5	0.6450	0.3620
W6	0.7463	0.3590
W7	0.7618	0.4100
W8	0.7754	0.4410
W9	0.7741	0.4470
X1	0.6837	0.3660
X2	0.6729	0.3670
X3	0.1364	0.1230
X4	0.0116	-0.0150
X5	0.5787	0.3100
X6	0.7533	0.4240
X7	0.7453	0.4010
X8	0.7784	0.4350
X9	0.7507	0.4240
Y1	0.7050	0.3620
Y2	0.6800	0.3130
Y3	0.1349	0.1050
Y4	0.0185	0.0380
Y5	0.4105	0.1670
Y6	0.6993	0.3490
Y7	0.6821	0.3530
Y8	0.7672	0.4360
Y9	0.0088	0.0270
Z1	0.6764	0.3340
Z2	0.6368	0.3050
Z3	0.1360	0.1250
Z4	0.0152	0.0430
Z5	0.0087	0.0240
Z6	0.6454	0.3130
Z7	0.6469	0.3170
Z8	0.7816	0.4440
Z9	0.5636	0.2730
a1	0.7472	0.4240
a2	0.7041	0.4070
a3	0.6824	0.3610
a4	0.5931	0.2500
a5	0.6011	0.2510
a6	0.6505	0.3190

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Chain	Atom inclusion	Q-score
a7	0.6954	0.3900
a8	0.7119	0.3930
a9	0.7104	0.3960
aA	0.6554	0.3280
aB	0.7004	0.3730
aC	0.6931	0.3420
aD	0.7004	0.3790
aE	0.6754	0.3240
aF	0.6371	0.2940
aG	0.6627	0.2850
aH	0.6368	0.2920
aI	0.6546	0.2890
aJ	0.6541	0.2950
aK	0.2336	0.1630
aL	0.2265	0.1960
aM	0.1958	0.1390
aN	0.1772	0.1400
aO	0.1957	0.1160
aP	0.2135	0.1840
aQ	0.2028	0.0970
aR	0.2084	0.0830
aS	0.1843	0.1000
aT	0.1968	0.0750
aU	0.2051	0.1120
aV	0.2156	0.0990
aW	0.7855	0.4440
aX	0.7803	0.4530
aY	0.6941	0.3780
aZ	0.1786	0.1570
aa	0.8026	0.4500
ab	0.7710	0.4430
ac	0.7768	0.4310
ad	0.7740	0.4360
ae	0.7768	0.4430
af	0.7844	0.4560
ag	0.7752	0.4310
ah	0.7455	0.4100
ai	0.7575	0.4160
aj	0.7350	0.4020
ak	0.8163	0.4520
al	0.7530	0.4360
am	0.6858	0.3410

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Chain	Atom inclusion	Q-score
an	0.7064	0.3760
ao	0.7101	0.3760
ap	0.7417	0.4240
aq	0.7309	0.3980
ar	0.7236	0.4000
as	0.6870	0.3410
at	0.6946	0.3770
au	0.7294	0.3900
av	0.6932	0.3710
aw	0.6638	0.3100
ax	0.6423	0.3010
ay	0.5258	0.1540
az	0.5810	0.2390
b1	0.7518	0.4280
b2	0.7056	0.4090
b3	0.6797	0.3610
b4	0.7236	0.3970
b5	0.7276	0.3970
b6	0.7019	0.3780
b7	0.6900	0.3960
b8	0.7434	0.4150
b9	0.7422	0.4170
bA	0.6646	0.3320
bB	0.6997	0.3830
bC	0.6985	0.3440
bD	0.7012	0.3820
bE	0.6800	0.3260
bF	0.6425	0.2940
bG	0.6677	0.2970
bH	0.6454	0.2940
bI	0.6530	0.2930
bJ	0.6520	0.2980
bK	0.2344	0.1630
bL	0.2301	0.1990
bM	0.2035	0.1480
bN	0.1831	0.1420
bO	0.1966	0.1230
bP	0.2149	0.1830
bQ	0.2004	0.1000
bR	0.2101	0.0800
bS	0.1858	0.0950
bT	0.2042	0.0770

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Chain	Atom inclusion	Q-score
bU	0.2066	0.1120
bV	0.2149	0.0990
bW	0.7842	0.4460
bX	0.7845	0.4570
bY	0.6871	0.3770
bZ	0.1761	0.1540
ba	0.7736	0.4430
bb	0.7508	0.3980
bc	0.7752	0.4330
bd	0.7852	0.4410
be	0.8058	0.4550
bf	0.7770	0.4430
bg	0.7840	0.4350
bh	0.7635	0.4330
bi	0.7687	0.4290
bj	0.7493	0.4300
bk	0.7905	0.4420
bl	0.7687	0.4400
bm	0.7471	0.4110
bn	0.7459	0.4180
bo	0.7511	0.4150
bp	0.7385	0.4110
bq	0.7540	0.4370
br	0.7344	0.4070
bs	0.7215	0.3800
bt	0.7371	0.3960
bu	0.7386	0.4030
bv	0.7448	0.4090
bw	0.7355	0.3910
bx	0.7409	0.3970
by	0.6916	0.3470
bz	0.6737	0.3560
c1	0.7318	0.4290
c2	0.7461	0.4560
c3	0.5285	0.2800
c4	0.6617	0.3130
c5	0.6602	0.3160
c6	0.6906	0.3880
c7	0.6440	0.3130
c8	0.6776	0.3860
c9	0.6727	0.3870
cA	0.5644	0.2890

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Chain	Atom inclusion	Q-score
cB	0.4370	0.1770
cC	0.4353	0.1460
cD	0.3678	0.1130
cE	0.4479	0.2060
cF	0.4113	0.1600
cG	0.4626	0.1880
cH	0.6192	0.3500
cI	0.5852	0.3280
cJ	0.5391	0.2860
cK	0.4888	0.2260
cL	0.5203	0.2740
cM	0.5333	0.2750
cN	0.6177	0.3430
cO	0.4399	0.1750
cP	0.4378	0.1980
cQ	0.4121	0.1570
cR	0.5224	0.2720
cS	0.4873	0.2190
cT	0.4641	0.1840
cU	0.5921	0.3260
cV	0.4271	0.1370
cW	0.5628	0.2840
cX	0.3670	0.1130
cY	0.1664	0.0850
cZ	0.2352	0.1050
ca	0.7776	0.4460
cb	0.7478	0.4030
cc	0.7824	0.4410
cd	0.7792	0.4410
ce	0.8066	0.4590
cf	0.7724	0.4420
cg	0.7824	0.4370
ch	0.7650	0.4360
ci	0.7728	0.4290
cj	0.7485	0.4330
ck	0.7824	0.4480
cl	0.7665	0.4450
cm	0.7448	0.4180
cn	0.7526	0.4290
co	0.7459	0.4090
cp	0.7395	0.4100
cq	0.7525	0.4400

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Chain	Atom inclusion	Q-score
cr	0.7352	0.4040
cs	0.7214	0.3860
ct	0.7371	0.3990
cu	0.7463	0.4090
cv	0.7402	0.4110
cw	0.7348	0.3880
cx	0.7456	0.3990
cy	0.6931	0.3480
cz	0.6773	0.3610
d1	0.7145	0.4170
d2	0.7463	0.4530
d3	0.1342	0.0960
d4	0.5818	0.2310
d5	0.5802	0.2320
d6	0.6795	0.3730
d7	0.6599	0.3290
d8	0.5538	0.2950
d9	0.5527	0.3010
dA	0.7240	0.3860
dB	0.7161	0.3850
dC	0.6800	0.3030
dD	0.7149	0.3750
dE	0.6969	0.3370
dF	0.6556	0.3090
dG	0.7001	0.3180
dH	0.7048	0.3750
dI	0.7348	0.3930
dJ	0.7540	0.4090
dK	0.7475	0.4190
dL	0.7091	0.3880
dM	0.7317	0.3920
dN	0.7446	0.4170
dO	0.7278	0.3830
dP	0.7171	0.3710
dQ	0.6816	0.3060
dR	0.7113	0.3750
dS	0.6961	0.3320
dT	0.6563	0.3080
dU	0.6993	0.3210
dV	0.7084	0.3780
dW	0.7533	0.4080
dX	0.7200	0.3880

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Chain	Atom inclusion	Q-score
dY	0.5601	0.1930
dZ	0.6554	0.3000
da	0.1773	0.0330
db	0.1742	0.0670
dc	0.2184	0.0660
dd	0.1990	0.0690
de	0.1689	0.0570
df	0.1606	0.0720
dg	0.1850	0.0350
dh	0.1896	0.0870
di	0.2026	0.0810
dj	0.2511	0.1360
dk	0.1689	0.0540
dl	0.2004	0.0740
dm	0.2244	0.0690
dn	0.1997	0.0830
do	0.1781	0.0320
dp	0.1650	0.0700
dq	0.1719	0.0560
dr	0.1838	0.0850
ds	0.1796	0.0390
dt	0.2496	0.1360
du	0.2259	0.0970
dv	0.1706	0.0880
dw	0.1817	0.1010
dx	0.1816	0.0950
dy	0.5195	0.2940
dz	0.5212	0.2920
e1	0.7579	0.4370
e2	0.4904	0.2200
e3	0.7201	0.3580
e4	0.5928	0.2740
e5	0.5887	0.2670
e6	0.6469	0.3190
e7	0.7192	0.3940
e8	0.1175	0.0980
e9	0.1181	0.0960
eA	0.5914	0.2610
eB	0.6512	0.3270
eC	0.6476	0.3500
eD	0.6360	0.3740
eE	0.6153	0.3030

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Chain	Atom inclusion	Q-score
eF	0.6064	0.3050
eG	0.5906	0.2400
eH	0.6064	0.2720
eI	0.6345	0.3250
eJ	0.6454	0.3150
eK	0.6145	0.2730
eL	0.5854	0.2240
eM	0.6191	0.3030
eN	0.6129	0.3020
eO	0.5937	0.2650
eP	0.6491	0.3250
eQ	0.6500	0.3500
eR	0.6389	0.3690
eS	0.6307	0.3220
eT	0.6425	0.3100
eU	0.6060	0.2720
eV	0.5825	0.2210
eW	0.5944	0.2400
eX	0.6118	0.2720
eY	0.6379	0.3270
eZ	0.6377	0.3290
ea	0.5744	0.1940
eb	0.6185	0.3000
ec	0.6158	0.2430
ed	0.5798	0.2190
ee	0.5861	0.2820
ef	0.6284	0.3070
eg	0.6447	0.3590
eh	0.6315	0.2910
ei	0.6093	0.2480
ej	0.5528	0.1890
ek	0.6484	0.2970
el	0.6165	0.2920
em	0.5883	0.2190
en	0.5832	0.2810
eo	0.6222	0.3020
ep	0.6418	0.3580
eq	0.6307	0.2890
er	0.6122	0.2520
es	0.5551	0.1920
et	0.5637	0.1930
eu	0.5713	0.1910

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Chain	Atom inclusion	Q-score
ev	0.6093	0.2440
ew	0.7325	0.4120
ex	0.7355	0.4070
ey	0.6074	0.3050
ez	0.6095	0.3040
f1	0.7226	0.4140
f2	0.5101	0.2550
f3	0.6599	0.3120
f4	0.6575	0.3570
f5	0.6583	0.3570
f6	0.6376	0.2700
f7	0.7001	0.3520
f8	0.1548	0.0930
f9	0.7844	0.4540
fa	0.1371	0.1770
fb	0.1010	0.1440
fc	0.0912	0.1070
fd	0.1185	0.1060
fe	0.0486	0.0490
ff	0.0612	0.0840
fg	0.0748	0.0840
fh	0.0887	0.0620
fi	0.0738	0.0470
fj	0.0847	0.1040
fk	0.0686	0.0440
fl	0.1018	0.0720
fm	0.0507	0.0590
fn	0.0486	0.0470
fo	0.0637	0.0880
fp	0.0802	0.0870
fq	0.0716	0.0530
fr	0.0655	0.0410
fs	0.0499	0.0530
ft	0.0856	0.0650
fu	0.0849	0.0940
fv	0.1010	0.0640
fw	0.1339	0.1760
fx	0.1033	0.1450
fy	0.0902	0.1000
fz	0.1227	0.0990
g1	0.7224	0.3980
g2	0.5251	0.2870

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Chain	Atom inclusion	Q-score
g3	0.6122	0.2430
g4	0.6961	0.4030
g5	0.6909	0.4070
g6	0.6800	0.3510
g7	0.6407	0.2720
g8	0.1692	0.1900
g9	0.7792	0.4310
ga	0.7475	0.4310
gb	0.7664	0.4030
gc	0.7656	0.4340
gd	0.7742	0.4400
ge	0.7590	0.4110
gf	0.7618	0.4260
gg	0.7315	0.3990
gh	0.7186	0.3450
gi	0.7482	0.3810
gj	0.7263	0.3570
gk	0.7033	0.3680
gl	0.7024	0.3660
gm	0.7679	0.4350
gn	0.7359	0.3970
go	0.7170	0.3470
gp	0.7489	0.3750
gq	0.7502	0.3950
gr	0.7750	0.4390
gs	0.7648	0.4360
gt	0.7554	0.4130
gu	0.7286	0.3590
gv	0.7012	0.3650
gw	0.7039	0.3660
gx	0.7417	0.4290
gy	0.7243	0.4100
gz	0.7216	0.4080
h1	0.6888	0.3650
h2	0.5803	0.3550
h3	0.7094	0.3450
h4	0.5719	0.2440
h5	0.5778	0.2400
h6	0.7093	0.3620
h7	0.6608	0.3340
h8	0.1078	0.0660
h9	0.7403	0.4110

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Chain	Atom inclusion	Q-score
hA	0.0879	0.1000
hB	0.1049	0.1400
hC	0.0840	0.0930
hD	0.0962	0.1240
hE	0.0786	0.0790
hF	0.0925	0.0780
hG	0.0969	0.0630
hH	0.0883	0.1300
hI	0.0717	0.0650
hJ	0.0716	0.0650
hK	0.0763	0.0800
hL	0.0847	0.0470
hM	0.0694	0.0820
hN	0.0810	0.0460
hO	0.0810	0.0830
hP	0.0883	0.0580
hQ	0.0740	0.0620
hR	0.0731	0.0640
hS	0.0794	0.0880
hT	0.0942	0.1220
hU	0.0915	0.0810
hV	0.0861	0.1280
hW	0.0879	0.0980
hX	0.1071	0.1350
hY	0.0812	0.0850
hZ	0.0829	0.0820
i1	0.7372	0.4190
i2	0.5459	0.3090
i3	0.7270	0.3890
i4	0.5939	0.2610
i5	0.5898	0.2600
i6	0.6600	0.3250
i7	0.6877	0.3140
i8	0.1114	0.0480
i9	0.7647	0.4120
iA	0.7687	0.4400
iB	0.7741	0.4370
iC	0.7185	0.4050
iD	0.7352	0.4170
iE	0.7251	0.3940
iF	0.6878	0.3560
iG	0.6113	0.3350

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Chain	Atom inclusion	Q-score
iH	0.6166	0.3340
j1	0.7147	0.4200
j2	0.5051	0.2590
j3	0.7258	0.4060
j4	0.6512	0.3510
j5	0.6512	0.3490
j6	0.6831	0.3150
j7	0.7047	0.3850
j8	0.1318	0.1010
j9	0.7343	0.3990
jI	0.5241	0.3390
jJ	0.5180	0.3390
jK	0.5745	0.3070
jL	0.5737	0.3070
jM	0.5144	0.2330
jN	0.5161	0.2360
jO	0.5824	0.2590
jP	0.5745	0.2550
k1	0.6853	0.3560
k2	0.4865	0.2050
k3	0.7178	0.4010
k4	0.7228	0.4160
k5	0.7236	0.4200
k6	0.5505	0.2420
k7	0.5628	0.2700
k8	0.1518	0.1270
k9	0.8155	0.4530
kQ	0.3205	0.2690
kR	0.3169	0.2710
kS	0.3299	0.2830
kT	0.3356	0.2930
kU	0.3398	0.2970
kV	0.3380	0.2950
kW	0.3566	0.3170
kX	0.3609	0.3210
ka	0.7698	0.4330
kb	0.7678	0.4290
l1	0.6985	0.3510
l2	0.4870	0.2240
l3	0.7027	0.4010
l4	0.6183	0.3480
l5	0.6205	0.3450

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Chain	Atom inclusion	Q-score
l6	0.5282	0.2200
l7	0.5499	0.2820
l8	0.1411	0.1200
l9	0.7507	0.4310
la	0.5829	0.2910
lb	0.5224	0.2240
lc	0.4148	0.0800
ld	0.4153	0.1040
le	0.4611	0.1330
lf	0.5449	0.2420
lg	0.5181	0.2180
lh	0.4812	0.1680
li	0.4114	0.0810
lj	0.4158	0.1000
lk	0.4896	0.1710
ll	0.5188	0.2270
lm	0.4102	0.0830
ln	0.4132	0.1080
lo	0.4570	0.1330
lp	0.5478	0.2420
lq	0.5789	0.2880
lr	0.5275	0.2160
ls	0.4888	0.1660
lt	0.5188	0.2230
lu	0.5120	0.2130
lv	0.4717	0.1700
lw	0.4166	0.0790
lx	0.4194	0.0950
ly	0.4601	0.1860
lz	0.4723	0.1910
m1	0.6515	0.3540
m2	0.5204	0.2150
m3	0.6723	0.3350
m4	0.6420	0.3350
m5	0.6380	0.3370
m6	0.5312	0.1920
m7	0.5528	0.2500
m8	0.1087	0.0390
m9	0.6858	0.3430
n1	0.7415	0.4160
n2	0.5478	0.2660
n3	0.6346	0.3230

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Chain	Atom inclusion	Q-score
n4	0.5977	0.2870
n5	0.6027	0.2850
n6	0.4978	0.2130
n7	0.5326	0.2220
n8	0.1334	0.0860
n9	0.7146	0.3730
o1	0.7843	0.4340
o2	0.1380	0.0610
o3	0.6392	0.2750
o4	0.5073	0.1740
o5	0.5096	0.1780
o6	0.5621	0.2700
o7	0.5328	0.1950
o8	0.1266	0.0810
o9	0.7120	0.3700
p1	0.7885	0.4450
p2	0.1201	0.0450
p3	0.6541	0.3510
p4	0.5528	0.2190
p5	0.5514	0.2130
p6	0.5557	0.2810
p7	0.5015	0.2110
p8	0.1491	0.1430
p9	0.7301	0.4140
q1	0.8062	0.4510
q2	0.1527	0.0870
q3	0.7144	0.3640
q4	0.5636	0.2540
q5	0.5628	0.2540
q6	0.5436	0.2750
q7	0.5389	0.2550
q8	0.1303	0.0800
q9	0.7255	0.3970
r1	0.8015	0.4530
r2	0.1737	0.1250
r3	0.6722	0.3510
r4	0.6431	0.3540
r5	0.6425	0.3560
r6	0.6179	0.3440
r7	0.5514	0.2560
r8	0.1180	0.0610
r9	0.7200	0.4020

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Chain	Atom inclusion	Q-score
s1	0.7899	0.4480
s2	0.1850	0.1450
s3	0.6592	0.2830
s4	0.6237	0.3130
s5	0.6230	0.3180
s6	0.5389	0.2560
s7	0.5453	0.2100
s8	0.1396	0.1260
s9	0.6870	0.3370
t1	0.7869	0.4540
t2	0.1563	0.0950
t3	0.6802	0.3420
t4	0.5007	0.2200
t5	0.5022	0.2200
t6	0.5507	0.2550
t7	0.6027	0.3030
t8	0.1180	0.0460
t9	0.6903	0.3760
u1	0.7851	0.4330
u2	0.1388	0.1190
u3	0.6816	0.3740
u4	0.4765	0.1470
u5	0.4742	0.1450
u6	0.5438	0.2090
u7	0.6006	0.3090
u8	0.1550	0.1410
u9	0.7294	0.3890
v1	0.7917	0.4500
v2	0.1758	0.1980
v3	0.7156	0.4140
v4	0.4920	0.1890
v5	0.4913	0.1880
v6	0.5738	0.2910
v7	0.6187	0.3440
v8	0.5952	0.2140
v9	0.6896	0.3660
w1	0.8037	0.4430
w2	0.1818	0.1450
w3	0.7363	0.3980
w4	0.5335	0.2030
w5	0.5359	0.2050
w6	0.1326	0.0830

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Chain	Atom inclusion	Q-score
w7	0.1419	0.1030
w8	0.6245	0.3060
w9	0.6631	0.3030
x1	0.8023	0.4540
x2	0.1364	0.1220
x3	0.6802	0.3710
x4	0.5693	0.2840
x5	0.5730	0.2870
x6	0.1389	0.0810
x7	0.1274	0.0520
x8	0.6191	0.2980
x9	0.6440	0.3050
y1	0.7859	0.4460
y2	0.1442	0.1060
y3	0.6762	0.3140
y4	0.5120	0.2170
y5	0.5158	0.2160
y6	0.1195	0.0500
y7	0.1599	0.1110
y8	0.5803	0.2750
y9	0.5220	0.1520
z1	0.7853	0.4540
z2	0.1462	0.1260
z3	0.6454	0.3050
z4	0.4682	0.1890
z5	0.4776	0.1910
z6	0.1534	0.1380
z7	0.1635	0.1880
z8	0.5428	0.1720
z9	0.5767	0.2430